Structures of Tetrasilylmethane Derivatives $(XMe_2Si)_2C(SiMe_3)_2$ (X = H, Cl, Br) in the Gas Phase, and their Dynamic Structures in Solution

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⊥ Deceased

Table S1. Experimental parameters from the GED analyses of **1**, **2**, and **3**

	1		**2**		**3**	
Nozzle-to-film distance / mm	259.42	94.93	258.2	96.6	259.19	95.16
T_{nozzle} / K	426	460	494	497	486	503
T_{sample} / K	403	435	469	478	462	492
Δs / nm^{-1}	1	2	1	2	1	2
s_{min} / nm^{-1}	25	82	26	82	26	84
sw_1 / nm^{-1}	40	100	40	100	40	100
sw_2 / nm^{-1}	129	292	129	276	103.2	276
s_{max} / nm^{-1}	150	340	150	320	120	320
Correlation parameter	0.496	0.471	0.499	0.484	0.498	0.437
Scale factor (k)	4.91(4)	5.29(6)	3.12(3)	3.40(7)	3.47(5)	3.53(10)
Electron wavelength / pm	6.02	6.02	6.13	6.13	6.02	6.02

Table S2. Least-squares correlation matrix (×100) for the GED refinement of **1**[a]

	p_3	p_4	p_{10}	u_{850}	u_{1411}	u_{1950}	u_{2587}	u_{3057}	k_2
p_2	–73	84							
p_3	100	–79							
p_9			–95						
p_{14}				96	88	70	64	62	
u_{326}									76
u_{850}				100	89	73	64	60	
u_{1411}					100	81	55	58	
u_{1950}						100		53	

[a] Only values ≥ 50% are included. k_2 is a scale factor.

Table S3. Least-squares correlation matrix (×100) for the GED refinement of **2**[a]

	p_4	p_{11}	u_{897}	u_{1752}	u_{2304}	k_2
p_3	–73					
p_9		–77		60	57	
p_{11}		100		–59	–54	
p_{14}			–68			
u_{195}						71
u_{519}			52			56
u_{1322}					53	

[a] Only values ≥ 50% are included. k_2 is a scale factor.

Table S4. Least-squares correlation matrix (×100) for the GED refinement of **3**[a]

	p_3	p_4	p_{10}	p_{11}	u_{513}	u_{1425}	u_{1914}	u_{2567}	k_2
p_2	–58	63			54				
p_3	100	–92		78					
p_4		100		–82					
p_9			–57	–50					
p_{11}				100		–50			
p_{13}					–63				
p_{14}								–55	
u_{189}									70
u_{239}									55
u_{1656}							61		

[a] Only values ≥ 50% are included. k_2 is a scale factor.

Table S5. Calculated Cartesian coordinates [MP2/aug-cc-pVDZ; in Å] for all six conformers of **1**[a]

	1a				**1b**		
	x	*y*	*z*		*x*	*y*	*z*
C(1)	–0.0140	0.1370	0.0025	C(48)	0.0002	0.1355	0.0019
Si(2)	–0.1494	1.8526	–0.8414	Si(49)	0.8913	1.4002	–1.1285
Si(3)	–0.6485	0.2964	1.7969	Si(50)	0.6404	0.3297	1.7913
Si(4)	1.8346	–0.3893	0.0241	Si(51)	0.2992	–1.6374	–0.6646
Si(5)	–1.0581	–1.1141	–1.0081	Si(52)	–1.8783	0.5558	–0.0261
C(6)	–2.7205	–0.3802	–1.5682	C(53)	–2.2083	2.4247	0.0681
C(7)	–1.4569	–2.6930	–0.0248	C(54)	–2.8159	–0.1928	1.4485
C(8)	–2.5416	0.3600	1.9537	C(55)	0.2140	–1.1235	2.9394
C(9)	–0.0859	–1.1044	2.9517	C(56)	2.5253	0.5473	1.9242
C(10)	2.7048	–0.0410	–1.6350	C(57)	0.1528	–1.7255	–2.5604
C(11)	2.0677	–2.2484	0.3528	C(58)	–0.9416	–2.9017	0.0274
C(12)	–1.7439	2.7994	–0.4291	C(59)	1.1235	3.1140	–0.3389
C(13)	1.2501	3.0555	–0.3913	C(60)	2.6211	0.8530	–1.6975
H(14)	–0.1178	1.6344	–2.3276	H(61)	0.0476	1.5823	–2.3584
H(15)	–0.1142	1.5888	2.3495	H(62)	–0.0013	1.5611	2.3666
C(16)	2.8153	0.5277	1.3738	C(63)	2.0221	–2.3006	–0.2000
C(17)	–0.1808	–1.6452	–2.6079	C(64)	–2.7303	–0.0327	–1.6195
H(18)	–2.5859	0.4552	–2.2747	H(65)	–1.8772	2.9610	–0.8356
H(19)	–3.2807	–1.1717	–2.0968	H(66)	–3.3003	2.5650	0.1555
H(20)	–3.3428	–0.0322	–0.7297	H(67)	–1.7388	2.8900	0.9492
H(21)	–1.9861	–3.3931	–0.6953	H(68)	–3.8887	0.0347	1.3174
H(22)	–0.5526	–3.2005	0.3443	H(69)	–2.7104	–1.2855	1.5242
H(23)	–2.1177	–2.4997	0.8352	H(70)	–2.4987	0.2571	2.4038
H(24)	–3.0086	–0.5901	1.6488	H(71)	0.7517	–2.0404	2.6489
H(25)	–2.7928	0.5256	3.0158	H(72)	0.5379	–0.8607	3.9614
H(26)	–2.9974	1.1714	1.3691	H(73)	–0.8611	–1.3493	2.9730
H(27)	–0.5190	–0.9240	3.9508	H(74)	2.7879	0.6458	2.9918
H(28)	–0.4538	–2.0811	2.5986	H(75)	3.0573	–0.3324	1.5291
H(29)	1.0058	–1.1697	3.0678	H(76)	2.9065	1.4392	1.4057
H(30)	3.7944	–0.0063	–1.4574	H(77)	0.5275	–2.7097	–2.8933
H(31)	2.5114	–0.8412	–2.3656	H(78)	–0.8931	–1.6379	–2.8907
H(32)	2.4131	0.9126	–2.1015	H(79)	0.7337	–0.9525	–3.0867
H(33)	1.6473	–2.8738	–0.4503	H(80)	–1.9797	–2.6925	–0.2741
H(34)	3.1530	–2.4500	0.3923	H(81)	–0.6754	–3.8958	–0.3737
H(35)	1.6308	–2.5752	1.3086	H(82)	–0.9078	–2.9644	1.1262
H(36)	–2.6624	2.2451	–0.6677	H(83)	0.1738	3.6048	–0.0873
H(37)	–1.7708	3.0844	0.6359	H(84)	1.7347	3.0714	0.5762
H(38)	–1.7466	3.7317	–1.0200	H(85)	1.6555	3.7554	–1.0630
H(39)	1.2757	3.2325	0.6968	H(86)	3.3015	0.7204	–0.8412
H(40)	2.2478	2.7252	–0.7141	H(87)	2.6205	–0.0780	–2.2830
H(41)	1.0395	4.0212	–0.8827	H(88)	3.0391	1.6503	–2.3364
H(42)	2.3604	0.4553	2.3737	H(89)	2.1344	–2.4498	0.8858

H(43)	3.8211	0.0746	1.4317	H(90)	2.1494	–3.2867	–0.6808
H(44)	2.9437	1.5952	1.1419	H(91)	2.8416	–1.6517	–0.5434
H(45)	0.6997	–2.2809	–2.4288	H(92)	–2.7964	–1.1283	–1.7012
H(46)	–0.8953	–2.2303	–3.2133	H(93)	–3.7613	0.3632	–1.6172
H(47)	0.1349	–0.7757	–3.2067	H(94)	–2.2239	0.3541	–2.5185

	1c				**1d**		
	x	*y*	*z*		*x*	*y*	*z*
C(95)	–0.0013	0.0005	–0.2074	C(142)	0.0000	0.0000	0.0202
Si(96)	–0.8423	–1.2802	–1.3596	Si(143)	1.5490	0.2934	1.0989
Si(97)	–0.2181	1.7183	–1.0242	Si(144)	–1.5490	–0.2934	1.0989
Si(98)	1.8761	–0.4187	–0.2011	Si(145)	0.2764	–1.5460	–1.0907
Si(99)	–0.7573	–0.0349	1.5480	Si(146)	–0.2764	1.5460	–1.0907
C(100)	–2.6569	–0.1441	1.5084	C(147)	0.0000	3.1737	–0.1457
C(101)	–0.3363	1.5256	2.5513	C(148)	–2.0298	1.5980	–1.8291
C(102)	–1.9338	2.4971	–0.7714	C(149)	–1.2539	–1.4311	2.5936
C(103)	1.0232	3.0319	–0.4350	C(150)	–2.3062	1.2950	1.8188
C(104)	2.2051	–2.2837	–0.0315	C(151)	2.0298	–1.5980	–1.8291
C(105)	2.8139	0.4296	1.2196	C(152)	–0.9439	–1.6249	–2.5456
C(106)	–1.2118	–2.9534	–0.5367	C(153)	1.2539	1.4311	2.5936
C(107)	–2.4691	–0.6804	–2.1341	C(154)	2.3062	–1.2950	1.8188
H(108)	0.1062	–1.5472	–2.4923	H(155)	2.5887	0.9473	0.2331
H(109)	–0.0218	1.5321	–2.5024	H(156)	–2.5887	–0.9473	0.2331
C(110)	2.6996	0.0896	–1.8378	C(157)	0.0000	–3.1737	–0.1457
C(111)	–0.1517	–1.5162	2.5750	C(158)	0.9439	1.6249	–2.5456
H(112)	–3.0238	–1.0733	1.0448	H(159)	1.0526	3.2925	0.1600
H(113)	–3.0270	–0.1270	2.5487	H(160)	–0.2384	4.0049	–0.8329
H(114)	–3.1130	0.7056	0.9777	H(161)	–0.6365	3.2814	0.7451
H(115)	–0.7428	1.4008	3.5705	H(162)	–2.1804	2.5874	–2.2964
H(116)	0.7486	1.6893	2.6406	H(163)	–2.1651	0.8358	–2.6110
H(117)	–0.7881	2.4366	2.1275	H(164)	–2.8280	1.4564	–1.0843
H(118)	–2.0998	2.7812	0.2802	H(165)	–0.5922	–0.9589	3.3376
H(119)	–1.9813	3.4209	–1.3739	H(166)	–2.2252	–1.6112	3.0863
H(120)	–2.7598	1.8447	–1.0877	H(167)	–0.8273	–2.4067	2.3222
H(121)	0.7899	3.9788	–0.9525	H(168)	–3.1942	1.0171	2.4126
H(122)	0.9321	3.2119	0.6478	H(169)	–1.5969	1.7987	2.4951
H(123)	2.0710	2.7818	–0.6551	H(170)	–2.6271	2.0194	1.0562
H(124)	3.2981	–2.4302	0.0298	H(171)	2.1804	–2.5874	–2.2964
H(125)	1.7569	–2.7207	0.8737	H(172)	2.1651	–0.8358	–2.6110
H(126)	1.8471	–2.8482	–0.9078	H(173)	2.8280	–1.4564	–1.0843
H(127)	2.4994	0.0604	2.2087	H(174)	–0.7741	–0.8411	–3.2993
H(128)	3.8880	0.1983	1.1073	H(175)	–0.8112	–2.6003	–3.0462
H(129)	2.7036	1.5245	1.2113	H(176)	–1.9903	–1.5619	–2.2055
H(130)	–0.3161	–3.4252	–0.1075	H(177)	0.8273	2.4067	2.3222
H(131)	–1.9718	–2.8689	0.2559	H(178)	0.5922	0.9589	3.3376
H(132)	–1.6136	–3.6316	–1.3096	H(179)	2.2252	1.6112	3.0863
H(133)	–3.2302	–0.4564	–1.3697	H(180)	1.5969	–1.7987	2.4951

H(134)	–2.3336	0.2104	–2.7669	H(181)	2.6271	–2.0194	1.0562
H(135)	–2.8637	–1.4878	–2.7748	H(182)	3.1942	–1.0171	2.4126
H(136)	2.6775	1.1724	–2.0333	H(183)	–1.0526	–3.2925	0.1600
H(137)	3.7582	–0.2233	–1.8049	H(184)	0.2384	–4.0049	–0.8329
H(138)	2.2254	–0.4175	–2.6933	H(185)	0.6365	–3.2814	0.7451
H(139)	0.9314	–1.4820	2.7720	H(186)	0.7741	0.8411	–3.2993
H(140)	–0.6666	–1.4917	3.5517	H(187)	0.8112	2.6003	–3.0462
H(141)	–0.3838	–2.4806	2.0978	H(188)	1.9903	1.5619	–2.2055

	1e				**1f**		
	x	*y*	*z*		*x*	*y*	*z*
C(189)	0.0000	0.0000	0.1407	C(236)	0.0000	0.0000	–0.2100
Si(190)	0.9843	1.1854	1.2782	Si(237)	–0.8711	1.2574	–1.3649
Si(191)	–0.9843	–1.1854	1.2782	Si(238)	0.8711	–1.2574	–1.3649
Si(192)	1.2423	–0.9913	–0.9312	Si(239)	–1.2837	–0.9364	0.8637
Si(193)	–1.2423	0.9913	–0.9312	Si(240)	1.2837	0.9364	0.8637
C(194)	–2.1185	2.3499	0.0701	C(241)	2.2117	2.2669	–0.1311
C(195)	–2.6400	–0.0969	–1.6208	C(242)	2.6235	–0.2121	1.5738
C(196)	–1.6260	–2.7567	0.4240	C(243)	2.4044	–0.5595	–2.2403
C(197)	0.0000	–1.7873	2.7913	C(244)	1.4160	–2.8665	–0.5121
C(198)	2.6400	0.0969	–1.6208	C(245)	–2.6235	0.2121	1.5738
C(199)	0.4080	–1.8439	–2.4121	C(246)	–0.4831	–1.8184	2.3471
C(200)	1.6260	2.7567	0.4240	C(247)	–2.4045	0.5595	–2.2403
C(201)	0.0000	1.7873	2.7913	C(248)	–1.4159	2.8665	–0.5121
H(202)	2.1851	0.4303	1.7744	H(249)	0.1083	1.6322	–2.4406
H(203)	–2.1851	–0.4303	1.7744	H(250)	–0.1083	–1.6322	–2.4406
C(204)	2.1185	–2.3499	0.0701	C(251)	–2.2117	–2.2670	–0.1311
C(205)	–0.4080	1.8439	–2.4121	C(252)	0.4831	1.8184	2.3471
H(206)	–1.4496	3.1744	0.3617	H(253)	1.5502	3.0271	–0.5743
H(207)	–2.9169	2.7795	–0.5604	H(254)	2.9038	2.7871	0.5550
H(208)	–2.5902	1.9462	0.9805	H(255)	2.8116	1.8304	–0.9437
H(209)	–3.2626	0.5286	–2.2847	H(256)	3.2702	0.3864	2.2397
H(210)	–2.2738	–0.9517	–2.2092	H(257)	2.2049	–1.0393	2.1670
H(211)	–3.2939	–0.4775	–0.8190	H(258)	3.2687	–0.6406	0.7901
H(212)	–0.8010	–3.4163	0.1116	H(259)	3.2375	–0.3862	–1.5407
H(213)	–2.2361	–3.3158	1.1548	H(260)	2.7439	–1.3001	–2.9847
H(214)	–2.2553	–2.5492	–0.4530	H(261)	2.1915	0.3814	–2.7704
H(215)	–0.7049	–2.2303	3.5162	H(262)	1.9181	–3.4987	–1.2651
H(216)	0.7159	–2.5719	2.5010	H(263)	2.1365	–2.6734	0.2978
H(217)	0.5616	–0.9956	3.3086	H(264)	0.5784	–3.4460	–0.0967
H(218)	3.2626	–0.5286	–2.2847	H(265)	–3.2702	–0.3864	2.2397
H(219)	2.2738	0.9517	–2.2092	H(266)	–2.2049	1.0393	2.1670
H(220)	3.2939	0.4775	–0.8190	H(267)	–3.2687	0.6405	0.7902
H(221)	–0.0206	–1.1285	–3.1314	H(268)	–0.0427	–1.1169	3.0727
H(222)	1.1736	–2.4333	–2.9469	H(269)	–1.2705	–2.3869	2.8729
H(223)	–0.3896	–2.5356	–2.0995	H(270)	0.2984	–2.5313	2.0425
H(224)	2.2553	2.5492	–0.4530	H(271)	–2.1915	–0.3814	–2.7704

H(225)	0.8010	3.4163	0.1116	H(272)	–3.2376	0.3862	–1.5407
H(226)	2.2361	3.3158	1.1548	H(273)	–2.7440	1.3001	–2.9847
H(227)	–0.7159	2.5719	2.5010	H(274)	–2.1365	2.6734	0.2978
H(228)	–0.5616	0.9956	3.3086	H(275)	–0.5784	3.4460	–0.0967
H(229)	0.7049	2.2303	3.5162	H(276)	–1.9180	3.4987	–1.2650
H(230)	1.4496	–3.1744	0.3617	H(277)	–1.5502	–3.0272	–0.5742
H(231)	2.9169	–2.7795	–0.5604	H(278)	–2.9038	–2.7871	0.5550
H(232)	2.5902	–1.9462	0.9805	H(279)	–2.8115	–1.8304	–0.9438
H(233)	0.0206	1.1285	–3.1314	H(280)	0.0427	1.1169	3.0727
H(234)	–1.1736	2.4333	–2.9469	H(281)	1.2705	2.3869	2.8729
H(235)	0.3896	2.5356	–2.0995	H(282)	–0.2983	2.5313	2.0425

[a] Calculated sums of electronic and thermal free energies (ZPE corrected) using B3LYP/aug-cc-pVDZ = –1596.307994 (**1a**), –1596.308554 (**1b**), –1596.308437 (**1c**), –1596.306982 (**1d**), –1596.307722 (**1e**), and –1596.307462 (**1f**) Hartrees.

Table S6. Calculated Cartesian coordinates [MP2/aug-cc-pVDZ; in Å] for all four conformers of **2**[a]

	2a				**2b**		
	x	*y*	*z*		*x*	*y*	*z*
C(1)	–0.0038	0.1484	0.0091	C(48)	0.0026	0.1472	0.0033
Si(2)	–0.6122	–1.6551	–0.1248	Si(49)	0.9799	–1.0556	–1.1014
Si(3)	1.7546	0.2561	–0.7025	Si(50)	–1.7774	0.2207	–0.6594
Si(4)	–0.0059	0.6933	1.8687	Si(51)	0.7580	1.9273	–0.1154
Si(5)	–1.1252	1.3444	–1.0333	Si(52)	0.0301	–0.4445	1.8596
C(6)	–1.6514	0.5850	–2.6911	C(53)	–0.0365	–2.3297	2.0461
C(7)	–0.2098	2.9656	–1.4412	C(54)	–1.4386	0.2595	2.8379
C(8)	1.8877	0.1615	–2.5838	C(55)	–2.8364	1.6548	–0.0420
C(9)	2.8049	1.7076	–0.1124	C(56)	–1.9384	0.1683	–2.5422
C(10)	–1.6244	0.2317	2.7445	C(57)	2.6509	1.9253	–0.0124
C(11)	0.1853	2.5749	2.0721	C(58)	0.1197	3.0789	1.2555
C(12)	–0.2204	–2.5235	–1.7520	C(59)	0.1463	–2.7161	–1.4168
C(13)	–0.1397	–2.8185	1.2814	C(60)	1.5494	–0.3539	–2.7607
Cl(14)	–2.7483	–1.6476	–0.0487	Cl(61)	2.8084	–1.5633	–0.1321
Cl(15)	2.8582	–1.4575	–0.0569	Cl(62)	–2.8442	–1.5143	–0.0291
C(16)	1.4154	–0.0959	2.8504	C(63)	0.3032	2.7944	–1.7495
C(17)	–2.7153	1.8802	–0.1493	C(64)	1.5996	0.0983	2.7831
H(18)	–2.3134	–0.2837	–2.5547	H(65)	0.8562	–2.8229	1.6321
H(19)	–2.2197	1.3554	–3.2421	H(66)	–0.0602	–2.5414	3.1303
H(20)	–0.7989	0.2878	–3.3204	H(67)	–0.9396	–2.7672	1.5966
H(21)	–0.9271	3.6114	–1.9786	H(68)	–1.3212	–0.0799	3.8826
H(22)	0.1107	3.5075	–0.5385	H(69)	–1.4603	1.3600	2.8484
H(23)	0.6645	2.8379	–2.0976	H(70)	–2.4077	–0.1158	2.4753
H(24)	1.4556	1.0456	–3.0771	H(71)	–2.4868	2.6208	–0.4386
H(25)	2.9613	0.1196	–2.8343	H(72)	–3.8605	1.4832	–0.4144
H(26)	1.4083	–0.7389	–2.9927	H(73)	–2.8758	1.7132	1.0542
H(27)	3.7951	1.6073	–0.5883	H(74)	–3.0152	0.2029	–2.7800
H(28)	2.3722	2.6739	–0.4129	H(75)	–1.4515	1.0332	–3.0184
H(29)	2.9538	1.7081	0.9767	H(76)	–1.5320	–0.7538	–2.9829
H(30)	–1.5326	0.5557	3.7968	H(77)	2.9826	2.9787	–0.0442
H(31)	–2.4944	0.7426	2.3071	H(78)	3.0218	1.4772	0.9201
H(32)	–1.8389	–0.8467	2.7419	H(79)	3.1307	1.3957	–0.8486
H(33)	–0.6692	3.1408	1.6714	H(80)	0.4161	2.7632	2.2664
H(34)	0.2342	2.7789	3.1568	H(81)	0.5627	4.0750	1.0768
H(35)	1.1059	2.9708	1.6187	H(82)	–0.9743	3.1940	1.2384
H(36)	–0.5783	–1.9665	–2.6294	H(83)	–0.0889	–3.2455	–0.4837
H(37)	0.8610	–2.7082	–1.8503	H(84)	–0.7870	–2.6102	–1.9907
H(38)	–0.7357	–3.4987	–1.7337	H(85)	0.8487	–3.3338	–2.0019
H(39)	0.9497	–2.9657	1.3242	H(86)	0.7013	–0.0697	–3.4023
H(40)	–0.4979	–2.4793	2.2634	H(87)	2.2145	0.5145	–2.6491
H(41)	–0.6190	–3.7887	1.0654	H(88)	2.1181	–1.1485	–3.2730
H(42)	2.4119	0.1961	2.4866	H(89)	–0.7726	3.0121	–1.8407

H(43)	1.3245	0.2487	3.8962	H(90)	0.8324	3.7640	–1.7625
H(44)	1.3743	–1.1945	2.8511	H(91)	0.6186	2.2328	–2.6412
H(45)	–2.5299	2.4948	0.7443	H(92)	1.7228	1.1876	2.8702
H(46)	–3.2797	2.5032	–0.8665	H(93)	1.5108	–0.3054	3.8080
H(47)	–3.3467	1.0253	0.1300	H(94)	2.5079	–0.3266	2.3315
	2c				**2d**		
	x	*y*	*z*		*x*	*y*	*z*
C(95)	0.0000	0.0046	0.0000	C(142)	0.0001	0.1641	0.0000
Si(96)	–1.4870	–1.1441	0.3000	Si(143)	–1.0161	–0.9308	–1.1775
Si(97)	1.4870	–1.1437	–0.3015	Si(144)	1.0157	–0.9316	1.1772
Si(98)	0.2757	1.1282	1.5615	Si(145)	–1.1443	1.2852	1.0978
Si(99)	–0.2757	1.1301	–1.5601	Si(146)	1.1449	1.2854	–1.0973
C(100)	–1.1181	0.1935	–2.9823	C(147)	1.8556	0.3785	–2.6090
C(101)	1.3668	1.8209	–2.2180	C(148)	2.6410	1.9561	–0.1442
C(102)	1.6349	–2.5964	0.8991	C(149)	1.8261	–0.0327	2.6261
C(103)	1.6407	–1.8419	–2.0489	C(150)	0.1148	–2.4430	1.8519
C(104)	–1.3668	1.8180	2.2204	C(151)	–2.6403	1.9568	0.1450
C(105)	1.3768	2.6364	1.2222	C(152)	–0.2006	2.7748	1.8126
C(106)	–1.6348	–2.5953	–0.9023	C(153)	–1.8258	–0.0308	–2.6262
C(107)	–1.6405	–1.8444	2.0466	C(154)	–0.1158	–2.4423	–1.8528
Cl(108)	–3.3019	–0.0734	0.0080	Cl(155)	–2.6843	–1.7423	–0.1184
Cl(109)	3.3018	–0.0733	–0.0080	Cl(156)	2.6835	–1.7436	0.1177
C(110)	1.1181	0.1899	2.9825	C(157)	–1.8554	0.3780	2.6091
C(111)	–1.3770	2.6378	–1.2191	C(158)	0.2016	2.7755	–1.8115
H(112)	–2.1501	–0.0952	–2.7277	H(159)	1.0932	0.0687	–3.3399
H(113)	–1.1701	0.8834	–3.8435	H(160)	2.5251	1.0928	–3.1213
H(114)	–0.5674	–0.7016	–3.3078	H(161)	2.4519	–0.5001	–2.3237
H(115)	1.1232	2.4678	–3.0801	H(162)	3.1887	2.6297	–0.8272
H(116)	1.8862	2.4365	–1.4690	H(163)	2.3653	2.5368	0.7483
H(117)	2.0751	1.0543	–2.5641	H(164)	3.3302	1.1496	0.1504
H(118)	0.8256	–3.3317	0.7654	H(165)	1.0851	0.3406	3.3495
H(119)	2.5904	–3.1034	0.6829	H(166)	2.4669	–0.7670	3.1431
H(120)	1.6505	–2.2743	1.9498	H(167)	2.4600	0.8044	2.3027
H(121)	2.5549	–2.4586	–2.0777	H(168)	0.8375	–3.0176	2.4559
H(122)	0.7834	–2.4840	–2.3043	H(169)	–0.7269	–2.1475	2.4965
H(123)	1.7355	–1.0619	–2.8172	H(170)	–0.2787	–3.1015	1.0653
H(124)	–1.1231	2.4642	3.0830	H(171)	–3.1878	2.6301	0.8283
H(125)	–1.8866	2.4342	1.4721	H(172)	–2.3644	2.5378	–0.7473
H(126)	–2.0748	1.0510	2.5660	H(173)	–3.3297	1.1505	–0.1500
H(127)	0.9403	3.3501	0.5084	H(174)	0.1794	3.4736	1.0532
H(128)	1.4913	3.1644	2.1862	H(175)	–0.9117	3.3320	2.4485
H(129)	2.3785	2.3506	0.8711	H(176)	0.6426	2.4684	2.4502
H(130)	–1.6502	–2.2720	–1.9526	H(177)	–2.4591	0.8066	–2.3026
H(131)	–0.8255	–3.3308	–0.7692	H(178)	–1.0844	0.3421	–3.3494
H(132)	–2.5904	–3.1026	–0.6868	H(179)	–2.4670	–0.7646	–3.1434
H(133)	–0.7832	–2.4868	2.3011	H(180)	0.7258	–2.1470	–2.4975

H(134)	–1.7352	–1.0654	2.8159	H(181)	0.2775	–3.1013	–1.0664
H(135)	–2.5547	–2.4612	2.0747	H(182)	–0.8389	–3.0165	–2.4569
H(136)	2.1500	–0.0989	2.7275	H(183)	–1.0931	0.0676	3.3400
H(137)	1.1703	0.8788	3.8444	H(184)	–2.5246	1.0923	3.1218
H(138)	0.5672	–0.7055	3.3070	H(185)	–2.4519	–0.5003	2.3236
H(139)	–0.9406	3.3506	–0.5042	H(186)	–0.1781	3.4742	–1.0519
H(140)	–1.4912	3.1670	–2.1824	H(187)	0.9128	3.3326	–2.4474
H(141)	–2.3787	2.3515	–0.8685	H(188)	–0.6418	2.4696	–2.4491

[a] Calculated sums of electronic and thermal free energies (ZPE corrected) using B3LYP/aug-cc-pVDZ = –2515.681364 (**2a**), –2515.678486 (**2b**), –2515.679005 (**2c**) and –2515.679432 (**2d**) Hartrees.

Table S7. Calculated Cartesian coordinates [MP2/aug-cc-pVDZ-pp; in Å] for all four conformers of **3**[a]

	3a				**3b**		
	x	*y*	*z*		*x*	*y*	*z*
C(1)	–0.0041	0.4191	0.0110	C(48)	0.0031	0.4153	0.0053
Si(2)	–0.6238	–1.3820	–0.0906	Si(49)	0.9795	–0.8056	–1.0797
Si(3)	1.7499	0.5047	–0.7163	Si(50)	–1.7668	0.4973	–0.6853
Si(4)	0.0102	0.9972	1.8607	Si(51)	0.7656	2.1917	–0.1342
Si(5)	–1.1103	1.6145	–1.0492	Si(52)	0.0071	–0.1434	1.8715
C(6)	–1.6522	0.8336	–2.6914	C(53)	–0.0482	–2.0253	2.0902
C(7)	–0.1684	3.2124	–1.4887	C(54)	–1.4752	0.5786	2.8151
C(8)	1.8718	0.3781	–2.5973	C(55)	–2.8273	1.9475	–0.1070
C(9)	2.8239	1.9485	–0.1482	C(56)	–1.9038	0.4084	–2.5694
C(10)	–1.6146	0.5900	2.7510	C(57)	2.6565	2.1926	–0.0096
C(11)	0.2413	2.8772	2.0312	C(58)	0.1110	3.3673	1.2082
C(12)	–0.2449	–2.2832	–1.7038	C(59)	0.1537	–2.4745	–1.3738
C(13)	–0.1872	–2.5208	1.3486	C(60)	1.5635	–0.1292	–2.7453
Br(14)	–2.9138	–1.3828	–0.0206	Br(61)	2.9405	–1.3519	–0.0471
Br(15)	2.9429	–1.3232	–0.0231	Br(62)	–2.9573	–1.3308	–0.0096
C(16)	1.4158	0.1983	2.8559	C(63)	0.3331	3.0318	–1.7880
C(17)	–2.6807	2.2065	–0.1657	C(64)	1.5578	0.4255	2.8116
H(18)	–2.3282	–0.0207	–2.5367	H(65)	0.8577	–2.5138	1.7004
H(19)	–2.2075	1.6035	–3.2564	H(66)	–0.0892	–2.2179	3.1775
H(20)	–0.8055	0.5096	–3.3150	H(67)	–0.9377	–2.4800	1.6318
H(21)	–0.8780	3.8570	–2.0378	H(68)	–1.3753	0.2545	3.8665
H(22)	0.1580	3.7667	–0.5956	H(69)	–1.4903	1.6793	2.8086
H(23)	0.7045	3.0628	–2.1421	H(70)	–2.4400	0.2028	2.4426
H(24)	1.4258	1.2453	–3.1077	H(71)	–2.4547	2.9103	–0.4903
H(25)	2.9450	0.3434	–2.8502	H(72)	–3.8392	1.7840	–0.5146
H(26)	1.4027	–0.5383	–2.9822	H(73)	–2.9035	2.0025	0.9875
H(27)	3.8040	1.8321	–0.6411	H(74)	–2.9777	0.4552	–2.8178
H(28)	2.3986	2.9201	–0.4417	H(75)	–1.3964	1.2534	–3.0599
H(29)	2.9911	1.9443	0.9384	H(76)	–1.5094	–0.5321	–2.9815
H(30)	–1.4875	0.8798	3.8097	H(77)	2.9841	3.2473	–0.0441
H(31)	–2.4634	1.1592	2.3444	H(78)	3.0193	1.7505	0.9288
H(32)	–1.8871	–0.4745	2.7216	H(79)	3.1460	1.6595	–0.8380
H(33)	–0.5996	3.4538	1.6174	H(80)	0.4009	3.0742	2.2275
H(34)	0.2884	3.0970	3.1129	H(81)	0.5521	4.3609	1.0116
H(35)	1.1722	3.2471	1.5773	H(82)	–0.9830	3.4783	1.1806
H(36)	–0.6291	–1.7469	–2.5834	H(83)	–0.0395	–3.0082	–0.4332
H(37)	0.8362	–2.4572	–1.8192	H(84)	–0.7999	–2.3829	–1.9156
H(38)	–0.7505	–3.2623	–1.6536	H(85)	0.8494	–3.0789	–1.9807
H(39)	0.8991	–2.6726	1.4270	H(86)	0.7246	0.1595	–3.3969
H(40)	–0.5761	–2.1585	2.3107	H(87)	2.2409	0.7302	–2.6360
H(41)	–0.6680	–3.4909	1.1357	H(88)	2.1257	–0.9383	–3.2418
H(42)	2.4177	0.4335	2.4670	H(89)	–0.7415	3.2440	–1.9017

H(43)	1.3513	0.5937	3.8857	H(90)	0.8591	4.0030	–1.8060
H(44)	1.3325	–0.8968	2.9088	H(91)	0.6665	2.4584	–2.6656
H(45)	–2.4698	2.8584	0.6953	H(92)	1.6771	1.5167	2.8770
H(46)	–3.2470	2.8056	–0.9016	H(93)	1.4470	0.0449	3.8433
H(47)	–3.3197	1.3756	0.1622	H(94)	2.4759	–0.0075	2.3895

	3c				**3d**		
	x	*y*	*z*		*x*	*y*	*z*
C(95)	0.0000	0.0000	0.0138	C(142)	0.0000	0.4667	0.0001
Si(96)	–0.3039	1.4804	–1.1467	Si(143)	–1.0241	–0.6251	–1.1725
Si(97)	0.3039	–1.4804	–1.1467	Si(144)	1.0241	–0.6254	1.1725
Si(98)	–1.5625	–0.2716	1.1374	Si(145)	–1.1268	1.5913	1.1140
Si(99)	1.5625	0.2716	1.1374	Si(146)	1.1268	1.5916	–1.1138
C(100)	2.9849	1.1113	0.1993	C(147)	1.8062	0.6971	–2.6474
C(101)	2.2218	–1.3709	1.8266	C(148)	2.6387	2.2574	–0.1836
C(102)	–0.8986	–1.6237	–2.6001	C(149)	1.8574	0.2776	2.6070
C(103)	2.0538	–1.6284	–1.8432	C(150)	0.1359	–2.1382	1.8619
C(104)	–2.2218	1.3709	1.8266	C(151)	–2.6387	2.2572	0.1839
C(105)	–1.2277	–1.3638	2.6535	C(152)	–0.1699	3.0829	1.8072
C(106)	0.8986	1.6237	–2.6001	C(153)	–1.8574	0.2780	–2.6069
C(107)	–2.0538	1.6284	–1.8432	C(154)	–0.1359	–2.1379	–1.8622
Br(108)	0.0000	3.4560	–0.0461	Br(155)	–2.8051	–1.5140	–0.0444
Br(109)	0.0000	–3.4560	–0.0461	Br(156)	2.8051	–1.5139	0.0441
C(110)	–2.9849	–1.1113	0.1993	C(157)	–1.8063	0.6965	2.6474
C(111)	1.2277	1.3638	2.6535	C(158)	0.1698	3.0832	–1.8067
H(112)	2.7321	2.1427	–0.0923	H(159)	1.0294	0.3866	–3.3626
H(113)	3.8459	1.1633	0.8895	H(160)	2.4570	1.4216	–3.1696
H(114)	3.3095	0.5571	–0.6940	H(161)	2.4164	–0.1779	–2.3833
H(115)	3.0741	–1.1218	2.4845	H(162)	3.1778	2.9300	–0.8744
H(116)	1.4702	–1.8992	2.4314	H(163)	2.3775	2.8377	0.7134
H(117)	2.5834	–2.0729	1.0614	H(164)	3.3284	1.4473	0.0992
H(118)	–0.7884	–0.7994	–3.3224	H(165)	1.1297	0.6784	3.3291
H(119)	–0.6629	–2.5663	–3.1224	H(166)	2.4844	–0.4651	3.1289
H(120)	–1.9463	–1.6701	–2.2705	H(167)	2.5094	1.0935	2.2657
H(121)	2.0750	–2.5281	–2.4813	H(168)	0.8641	–2.6887	2.4820
H(122)	2.3223	–0.7580	–2.4618	H(169)	–0.7201	–1.8497	2.4905
H(123)	2.8148	–1.7520	–1.0600	H(170)	–0.2319	–2.8148	1.0781
H(124)	–3.0741	1.1218	2.4845	H(171)	–3.1779	2.9297	0.8747
H(125)	–1.4702	1.8992	2.4314	H(172)	–2.3776	2.8377	–0.7130
H(126)	–2.5834	2.0729	1.0614	H(173)	–3.3285	1.4472	–0.0991
H(127)	–0.5167	–0.9217	3.3666	H(174)	0.1973	3.7812	1.0415
H(128)	–2.1946	–1.4714	3.1777	H(175)	–0.8711	3.6399	2.4542
H(129)	–0.8773	–2.3685	2.3793	H(176)	0.6837	2.7779	2.4316
H(130)	1.9463	1.6701	–2.2705	H(177)	–2.5094	1.0939	–2.2655
H(131)	0.7884	0.7994	–3.3224	H(178)	–1.1297	0.6790	–3.3289
H(132)	0.6629	2.5663	–3.1224	H(179)	–2.4843	–0.4646	–3.1289
H(133)	–2.3223	0.7580	–2.4618	H(180)	0.7201	–1.8492	–2.4908

H(134)	–2.8148	1.7520	–1.0600	H(181)	0.2320	–2.8146	–1.0786
H(135)	–2.0750	2.5281	–2.4813	H(182)	–0.8640	–2.6882	–2.4823
H(136)	–2.7321	–2.1427	–0.0923	H(183)	–1.0295	0.3861	3.3626
H(137)	–3.8459	–1.1633	0.8895	H(184)	–2.4573	1.4209	3.1697
H(138)	–3.3095	–0.5571	–0.6940	H(185)	–2.4163	–0.1786	2.3832
H(139)	0.5167	0.9217	3.3666	H(186)	–0.1975	3.7814	–1.0408
H(140)	2.1946	1.4714	3.1777	H(187)	0.8710	3.6404	–2.4535
H(141)	0.8773	2.3685	2.3793	H(188)	–0.6838	2.7783	–2.4311

[a] Calculated sums of electronic and thermal free energies (ZPE corrected) using B3LYP/aug-cc-pVDZ-PP = –2429.038327 (**3a**), –2429.034989 (**3b**), –2429.035041 (**3c**), and –2429.036017 (**3d**) Hartrees.

Model descriptions for use in GED refinements

It should be noted that for ease of reading only atoms for the first conformer (**a**) have been numbered in each case. The numbering of subsequent conformers can be obtained by adding multiples of 47. For compounds **1**, **2**, and **3**, each silyl branch is independently defined in the model, with the two trimethylsilyl branches described first, followed by the two $SiMe_2X$ branches. Once defined, the four branches are then arranged relative to one another using dihedral angles obtained from the geometry calculations. In the case of molecules with C_2 symmetry, only one $SiMe_3$ and one $SiMe_2X$ branch need be explicitly described. These two branches are then positioned relative to each other with the use of a dihedral angle, before being cloned. The cloned branches are rotated about the origin in order to create a molecule with C_2 symmetry. For **1**, **2**, and **3**, thirty-two, twenty-six and twenty-six parameters are used to describe six, four and four conformers, respectively.

The parameters used to describe the bond lengths and angles in each molecule are based on the average values observed between similar types of bonds in the most abundant conformer. Fixed differences are used to adjust for slight deviations in bond lengths and angles between different conformers. In each model parameters p_1–p_6, are used to describe distances between pairs of atoms. Parameters p_1–p_5 have slightly different purposes in each of **1**–**3**, but in all three models p_6 is used to describe the average C–H atomic distance. For all three species, there are four unique *r*CSi distances, defined below:

- *r*CSi1 – the average distance between the central carbon and a silicon on an $SiMe_3$ group [i.e. C(1) to Si(4/5)]

- *r*CSi2 – the average distance between central carbon and a silicon on an $SiMe_2X$ group [i.e. C(1) to Si(2/3)]
- *r*SiMe1 – the average distance between a silicon and a methyl carbon on an $SiMe_3$ group [i.e. between Si(4) and C(10/11/16) or Si(5) and C(6/7/17)]
- *r*SiMe2 – the average distance between a silicon and a methyl carbon on an $SiMe_2X$ group [i.e. between Si(2) and C(12/13) or Si(3) and C(8/9)]

As all of these C–Si distances lie under a single peak in the radial distribution curve, it was decided to describe these with the use of a weighted average and refinable differences. In the models for **1** and **3**, parameters p_2–p_5 are used for this purpose, and are described in full below. For **2**, as the *r*SiCl distance falls under the same peak in the radial distribution curve as the multiple *r*CSi distances it must be taken into account in both the weighted average and refinable differences. Parameters p_1–p_5 are used to describe these distances and a full description of how these are defined can be found below. As the *r*SiH and *r*SiBr distances in **1** and **3**, respectively, do not fall under the same curve as the *r*CSi distances they may be refined independently, and are described by p_1.

Therefore, for **1**:

$$p_2 = \frac{1}{14}(2[rCSi1] + 2[rCSi2] + 6[rSiMe1] + 4[rSiMe2])$$

$$p_3 = [rCSi1] - \frac{1}{12}(2[rCSi2] + 6[rSiMe1] + 4[rSiMe2])$$

$$p_4 = [rCSi2] - \frac{1}{10}(6[rSiMe1] + 4[rSiMe2])$$

$$p_5 = [rSiMe1] - [rSiMe2]$$

The bond lengths observed in **1** can then be defined in the model with these refinable parameters with the use of the following equations:

$$rCSi1 = p_2 + \frac{6}{7}p_3$$

$$rCSi2 = p_2 - \frac{1}{7}p_3 + \frac{5}{6}p_4$$

$$rSiMe1 = p_2 - \frac{1}{7}p_3 - \frac{1}{6}p_4 + \frac{2}{5}p_5$$

$$rSiMe2 = p_2 - \frac{1}{7}p_3 - \frac{1}{6}p_4 - \frac{3}{5}p_5$$

For **2**:

$$p_1 = \frac{1}{16}(2[rSiCl] + 2[rCSi1] + 2[rCSi2] + 6[rSiMe1] + 4[rSiMe2])$$

$$p_2 = [rSiCl] - \frac{1}{14}(2[rCSi1] + 2[rCSi2] + 6[rSiMe1] + 4[rSiMe2])$$

$$p_3 = [rSiMe2] - \frac{1}{10}(2[rCSi1] + 2[rCSi2] + 6[rSiMe1])$$

$$p_4 = [rSiMe1] - \frac{1}{4}(2[rCSi1] + 2[rCSi2])$$

$$p_5 = [rCSi1] - [rCSi2]$$

The bond lengths observed in **2** can then be defined in the model with these refinable parameters with the use of the following equations:

$$rSiCl = p_1 + \frac{7}{8}p_2$$

$$rSiMe2 = p_1 - \frac{1}{8}p_2 + \frac{5}{7}p_3$$

$$rSiMe1 = p_1 - \frac{1}{8}p_2 - \frac{2}{7}p_3 + \frac{2}{5}p_4$$

$$rCSi1 = p_1 - \frac{1}{8}p_2 - \frac{2}{7}p_3 - \frac{3}{5}p_4 + \frac{1}{2}p_5$$

$$rCSi2 = p_1 - \frac{1}{8}p_2 - \frac{2}{7}p_3 - \frac{3}{5}p_4 - \frac{1}{2}p_5$$

For **3**:

$$p_2 = \frac{1}{14}(2[rCSi1] + 2[rCSi2] + 6[rSiMe1] + 4[rSiMe2])$$

$$p_3 = [rCSi1] - \frac{1}{12}(2[rCSi2] + 6[rSiMe1] + 4[rSiMe2])$$

$$p_4 = [rCSi2] - \frac{1}{10}(6[rSiMe1] + 4[rSiMe2])$$

$$p_5 = [rSiMe1] - [rSiMe2]$$

The bond lengths observed in **3** can then be defined in the model with these refinable parameters with the use of the following equations:

$$rCSi1 = p_2 + \frac{6}{7}p_3$$

$$rCSi2 = p_2 - \frac{1}{7}p_3 + \frac{5}{6}p_4$$

$$rSiMe1 = p_2 - \frac{1}{7}p_3 - \frac{1}{6}p_4 + \frac{2}{5}p_5$$

$$rSiMe2 = p_2 - \frac{1}{7}p_3 - \frac{1}{6}p_4 - \frac{3}{5}p_5$$

Parameters p_7–p_{14} are the bond angles used to position atoms relative to one another, and are defined as below:

p_7 = ∠HCH, the average H–C–H angle that is observed between hydrogens on a methyl group, via the methyl carbon.

p_8 = ∠SiCH, the average Si–C–H angle that is observed between the hydrogen on a methyl group and one of the silicon atoms via the methyl carbon

p_9 = ∠CSiMe, the average angle between the central carbon and a methyl carbon on an $SiMe_3$ group via the silicon atom [i.e. C(1)–Si(4)–C(10/11/16) and C(1)–Si(5)–C(6/7/17)]

p_{10} = ∠CSiMe (X), the average angle between the central carbon and a methyl carbon on an $SiMe_2X$ group via the silicon atom [i.e. C(1)–Si(2)–C(12/13) and C(1)–Si(3)–C(8/9)]

p_{11} = ∠CSiX, the average angle between the central carbon and atom X on an $SiMe_2X$ group via the silicon atom [i.e. C(1)–Si(2)–X(14) and C(1)–Si(3)–X(15)]

p_{12} = ∠MeSiMe the average angle between two methyl groups on an $SiMe_3$ group [i.e C(10/6)–Si(4/5)–C(11/7), C(10/6)–Si(4/5)–C(16/17) and C(11/7)–Si(4/5)–C(16/17)]

p_{13} = ∠MeSiX, the average angle between a methyl group and atom X via the silicon atom on an $SiMe_2X$ group [i.e. C(12/8)–Si(2/3)–X(14/15) and C(13/9)–Si(2/3)–X(14/15)]

p_{14} = ∠SiCSi, the average angle between silicon atoms surrounding the central carbon [i.e. Si(2)–C(1)–Si(3), Si(2)–C(1)–Si(4), Si(2)–C(1)–Si(5), Si(3)–C(1)–Si(4), Si(3)–C(1)–Si(5) and Si(4)–C(1)–Si(5)]

Table S8. Refined (r_{h1}) and calculated (r_e) parameters values and their SARACEN restraints used in the six-conformer least-squares refinement of **1**[a]

parameter		r_{h1} value	r_e value	restraint
p_1	*r*Si–H	153.3(21)	150.3[b]	—
p_2	*r*Si–C average	189.5(1)	190.6[b]	—
p_3	*r*Si–C difference 1	1.7(8)	1.6[b]	1.6(10)
p_4	*r*Si–C difference 2	1.0(6)	1.2[b]	1.2(10)
p_5	*r*Si–C difference 3	0.2(2)	0.3[b]	0.3(2)
p_6	*r*C–H	109.2(2)	110.2[b]	—
p_7	∠H–C–H	107.8(4)	107.8[b]	107.8(4)
p_8	∠Si–C–H	111.7(3)	111.1[b]	—
p_9	∠C–Si–Me	113.1(5)	112.3[b]	112.3(8)
p_{10}	∠C–Si–Me_H[c]	115.2(8)	114.2[b]	114.2(17)
p_{11}	∠C–Si–H	108.4(6)	107.5[b]	107.5(7)
p_{12}	∠Me–Si–Me	107.2(8)	106.5[b]	106.5(9)
p_{13}	∠Me–Si–H	107.9(7)	107.7[b]	107.7(3)
p_{14}	∠Si–C–Si	108.6(4)	109.5[b]	—
p_{15}	ϕC(10)Si(4)C(1)Si(2)	–43.6(7)	–43.6[b]	–43.6(7)
p_{16}	ϕH(14)Si(2)C(1)Si(4)	81.9(33)	80.7[b]	80.7(36)
p_{17}	ϕ H(15)Si(3)C(1)Si(4)	76.7(12)	76.5[b]	76.5(13)
p_{18}	ϕC(7)Si(5)C(1)Si(4)	79.0(5)	78.9[b]	78.9(6)
p_{19}	ϕC(57)Si(51)C(48)Si(49)	–42.1(10)	–42.2[b]	42.2(11)
p_{20}	ϕ H(61)Si(49)C(48)Si(51)	78.2(7)	78.1[b]	78.1(8)
p_{21}	ϕ H(52)Si(50)C(48)Si(51)	–162.8(30)	–162.7[b]	–162.7(35)
p_{22}	ϕC(54)Si(52)C(48)Si(51)	80.8(18)	79.9[b]	79.9(21)
p_{23}	ϕC(104)Si(98)C(95)Si(96)	–44.1(13)	–44.2[b]	–44.2(15)
p_{24}	ϕ H(108)Si(96)C(95)Si(98)	–36.2(12)	–36.4[b]	–36.4(13)
p_{25}	ϕH(109)Si(97)C(95)Si(98)	74.6(9)	74.6[b]	74.6(9)
p_{26}	ϕC(101)Si(99)C(95)Si(98)	77.6(5)	77.6[b]	77.6(6)
p_{27}	ϕC(151)Si(145)C(142)Si(143)	–41.9(5)	–41.9[b]	–41.9(5)
p_{28}	ϕ H(155)Si(143)C(142)Si(145)	78.3(7)	78.2[b]	78.2(8)
p_{29}	ϕC(198)Si(192)C(189)Si(190)	–43.0(9)	–43.1[b]	–43.1(10)
p_{30}	ϕH(202)Si(190)C(189)Si(192)	–40.5(8)	–40.6[b]	–40.6(9)
p_{31}	ϕC(245)Si(239)C(236)Si(237)	–43.3(11)	–43.4[b]	–43.4(12)
p_{32}	ϕH(249)Si(237)C(236)Si(239)	–162.9(13)	–163.0[b]	–163.0(14)
f_1	proportion of conformer **a**	(fixed)	0.204[d]	—
f_2	proportion of conformer **b**	(fixed)	0.311[d]	—
f_3	proportion of conformer **c**	(fixed)	0.285[d]	—
f_4	proportion of conformer **d**	(fixed)	0.048[d]	—
f_5	proportion of conformer **e**	(fixed)	0.083[d]	—

[a] Distances (r) are in pm, angles (∠) and dihedral angles (ϕ) are in degrees. See Figure 1 for atom numbering. [b] Calculated using MP2/aug-cc-pVDZ. [c] H denotes an $SiMe_2H$ branch. [d] Calculated using B3LYP/aug-cc-pVDZ and Equation 1.

Table S9. Refined (r_{h1}) and calculated (r_e) parameters values and their SARACEN restraints used in the four-conformer least-squares refinement of **2**[a]

parameter		r_{h1} value	r_e value	restraint
p_1	*r*Si–C/*r*Si–Cl average	191.7(1)	193.2[b]	—
p_2	*r*Si–C/*r*Si–Cl difference 1	19.0(2)	23.5[b]	23.5(30)
p_3	*r*Si–C/*r*Si–Cl difference 2	–2.3(10)	–2.2[b]	–2.2(10)
p_4	*r*Si–C/*r*Si–Cl difference 3	–3.2(5)	–2.2[b]	—
p_5	*r*Si–C/*r*Si–Cl difference 4	3.7(5)	3.6[b]	3.6(5)
p_6	*r*C–H	109.8(3)	110.1[b]	110.1(10)
p_7	∠H–C–H	108.1(4)	108.1[b]	108.1(4)
p_8	∠Si–C–H	111.3(3)	110.8[b]	110.8(4)
p_9	∠C–Si–Me	111.8(3)	112.4[b]	112.4(4)
p_{10}	∠C–Si–Me_{Cl}[c]	116.1(2)	116.1[b]	116.1(2)
p_{11}	∠C–Si–Cl	109.6(6)	108.4[b]	—
p_{12}	∠Me–Si–Me	105.9(7)	106.4[b]	106.4(8)
p_{13}	∠Me–Si–Cl	102.7(5)	103.4[b]	103.4(6)
p_{14}	∠Si–C–Si	110.4(2)	109.5[b]	—
p_{15}	ϕC(10)Si(4)C(1)Si(2)	–46.7(9)	–47.1[b]	–47.1(10)
p_{16}	ϕCl(14)Si(2)C(1)Si(4)	81.0(8)	81.0[b]	81.0(9)
p_{17}	ϕ Cl(15)Si(3)C(1)Si(4)	79.0(6)	78.7[b]	78.7(6)
p_{18}	ϕC(7)Si(5)C(1)Si(4)	79.9(5)	79.7[b]	79.7(5)
p_{19}	ϕC(57)Si(51)C(48)Si(49)	–44.8(7)	–44.8[b]	–44.8(7)
p_{20}	ϕ Cl(61)Si(49)C(48)Si(51)	76.9(2)	76.9[b]	76.9(2)
p_{21}	ϕ Cl(52)Si(50)C(48)Si(51)	–163.1(6)	–163.1[b]	–163.1(6)
p_{22}	ϕC(54)Si(52)C(48)Si(51)	81.6(10)	81.5[b]	81.5(10)
p_{23}	ϕC(104)Si(98)C(95)Si(96)	–43.6(10)	–43.8[b]	–43.8(10)
p_{24}	ϕ Cl(108)Si(96)C(95)Si(98)	78.8(6)	78.7[b]	78.7(6)
p_{25}	ϕC(151)Si(145)C(142)Si(143)	–38.5(7)	–38.7[b]	–38.7(7)
p_{26}	ϕ Cl(155)Si(143)C(142)Si(145)	–42.8(4)	–43.0[b]	–43(4)
f_1	proportion of conformer **a**	0.721(140)[d]	0.720[e]	—
f_2	proportion of conformer **b**	0.105(140)[d]	0.106[e]	—
f_3	proportion of conformer **c**	(fixed)	0.075[e]	—

[a] Distances (*r*) are in pm, angles (∠) and dihedral angles (ϕ) are in degrees. See Figure 1 for atom numbering. [b] Calculated using MP2/aug-cc-pVDZ. [c] Cl denotes an $SiMe_2Cl$ branch. [d] Uncertainties in conformer amounts obtained from Figure 3(a), and are approximately equal to 2σ. [e] Calculated using B3LYP/aug-cc-pVDZ and Equation 1.

Table S10. Refined (r_{h1}) and calculated (r_e) parameters values and their SARACEN restraints used in the four-conformer least-squares refinement of **3**[a]

parameter		r_{h1} value	r_e value	restraint
p_1	*r*Si–Br	227.7(2)	229.1[b]	—
p_2	*r*Si–C average	189.5(1)	190.3[b]	—
p_3	*r*Si–C difference 1	6.5(16)	4.4[b]	4.4(24)
p_4	*r*Si–C difference 2	1.2(12)	0.9[b]	0.9(29)
p_5	*r*Si–C difference 3	1.2(2)	1.2[b]	1.2(2)
p_6	*r*C–H	108.2(4)	110.1[b]	—
p_7	∠H–C–H	108.1(4)	108.1[b]	108.1(4)
p_8	∠Si–C–H	110.9(3)	110.8[b]	110.8(4)
p_9	∠C–Si–Me	112.1(6)	112.4[b]	—
p_{10}	∠C–Si–Me_{Br}[c]	116.2(7)	116.2[b]	116.2(7)
p_{11}	∠C–Si–Br	110.4(7)	109.0[b]	—
p_{12}	∠Me–Si–Me	106.1(7)	106.3[b]	106.3(7)
p_{13}	∠Me–Si–Br	102.5(6)	102.6[b]	102.6(10)
p_{14}	∠Si–C–Si	110.0(2)	109.5[b]	—
p_{15}	ϕC(10)Si(4)C(1)Si(2)	–48.3(11)	–48.1[b]	–48.1(13)
p_{16}	ϕBr(14)Si(2)C(1)Si(4)	80.1(12)	81.6[b]	81.6(15)
p_{17}	ϕBr(15)Si(3)C(1)Si(4)	79.3(13)	79.1[b]	79.1(17)
p_{18}	ϕC(7)Si(5)C(1)Si(4)	79.8(11)	79.7[b]	79.7(11)
p_{19}	ϕC(57)Si(51)C(48)Si(49)	–45.3(4)	–45.3[b]	–45.3(4)
p_{20}	ϕBr(61)Si(49)C(48)Si(51)	75.7(10)	75.8[b]	75.8(10)
p_{21}	ϕBr(52)Si(50)C(48)Si(51)	–163.1(10)	–163.0[b]	–163.0(10)
p_{22}	ϕC(54)Si(52)C(48)Si(51)	81.9(25)	81.7[b]	81.7(25)
p_{23}	ϕC(104)Si(98)C(95)Si(96)	–44.1(14)	–44.2[b]	–44.2(14)
p_{24}	ϕBr(108)Si(96)C(95)Si(98)	78.8(13)	78.9[b]	78.9(13)
p_{25}	ϕC(151)Si(145)C(142)Si(143)	–38.1(12)	–38.1[b]	–38.1(12)
p_{26}	ϕBr(155)Si(143)C(142)Si(145)	–43.3(8)	–43.3[b]	–43.3(8)
f_1	proportion of conformer **a**	0.764(180)[d]	0.785[e]	—
f_2	proportion of conformer **b**	0.106(180)[d]	0.086[e]	—
f_3	proportion of conformer **c**	(fixed)	0.044[e]	—

[a] Distances (r) are in pm, angles (∠) and dihedral angles (ϕ) are in degrees. See Figure 1 for atom numbering. [b] Calculated using MP2/aug-cc-pVDZ-PP. [c] Br denotes an $SiMe_2Br$ branch. [d] Uncertainties in conformer amounts obtained from Figure 3(b), and are approximately equal to 2σ. [e] Calculated using B3LYP/aug-cc-pVDZ-PP and Equation 1.

Table S11. Interatomic distances (r_a / pm), refined and calculated amplitudes of vibration (u_{hl} / pm) and perpendicular corrections (k_{hl} / pm) for the SARACEN-restrained GED structure of **1**

	Atom pair	r_a	u_{hl} (GED)	Restraint	k_{hl}	u_{hl} (calc.)
*u*71	C(59)–H(84)	108.8(2)	9.3(tied to *u*128)	—	0.4	8.1
*u*1	C(59)–H(83)	108.8(2)	9.2(tied to *u*128)	—	0.4	8.0
*u*17	C(16)–H(44)	108.8(2)	9.2(tied to *u*128)	—	0.4	8.0
*u*45	C(16)–H(42)	108.8(2)	9.2(tied to *u*128)	—	0.4	8.0
*u*112	C(59)–H(85)	108.8(2)	9.2(tied to *u*128)	—	0.4	8.0
*u*130	C(16)–H(43)	108.8(2)	9.1(tied to *u*128)	—	0.4	8.0
*u*44	C(110)–H(136)	108.8(2)	9.0(tied to *u*128)	—	0.4	7.9
*u*47	C(197)–H(216)	108.8(2)	9.0(tied to *u*128)	—	0.4	7.9
*u*15	C(197)–H(217)	108.8(2)	9.0(tied to *u*128)	—	0.4	7.8
*u*60	C(110)–H(138)	108.8(2)	9.0(tied to *u*128)	—	0.4	7.8
*u*118	C(197)–H(215)	108.8(2)	9.0(tied to *u*128)	—	0.4	7.9
*u*133	C(110)–H(137)	108.8(2)	9.0(tied to *u*128)	—	0.4	7.8
*u*41	C(57)–H(79)	108.8(2)	8.9(tied to *u*128)	—	0.4	7.7
*u*19	C(57)–H(78)	108.8(2)	8.9(tied to *u*128)	—	0.4	7.7
*u*51	C(241)–H(253)	108.8(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*131	C(57)–H(77)	108.8(2)	8.9(tied to *u*128)	—	0.4	7.8
*u*55	C(56)–H(75)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*48	C(148)–H(164)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*74	C(7)–H(23)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*28	C(241)–H(255)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*134	C(241)–H(254)	108.9(2)	8.9(tied to *u*128)	—	0.4	7.7
*u*12	C(148)–H(163)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*84	C(54)–H(70)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*77	C(101)–H(117)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*78	C(106)–H(131)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*34	C(10)–H(32)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*66	C(105)–H(127)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*80	C(243)–H(259)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*65	C(100)–H(112)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*52	C(244)–H(263)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*56	C(111)–H(139)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*46	C(64)–H(92)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*59	C(103)–H(122)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*61	C(199)–H(221)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*63	C(9)–H(28)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*64	C(64)–H(94)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*67	C(107)–H(133)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*49	C(246)–H(268)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*50	C(58)–H(80)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*57	C(11)–H(33)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*35	C(152)–H(174)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*72	C(60)–H(86)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7

*u*18	C(56)–H(76)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*40	C(17)–H(45)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*68	C(194)–H(208)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*135	C(10)–H(30)	108.9(2)	8.9(tied to *u*128)	—	0.4	7.7
*u*132	C(148)–H(162)	108.9(2)	8.9(tied to *u*128)	—	0.4	7.7
*u*96	C(56)–H(74)	108.9(2)	8.9(tied to *u*128)	—	0.4	7.7
*u*27	C(195)–H(210)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*38	C(199)–H(223)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*42	C(58)–H(82)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*21	C(147)–H(161)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*37	C(111)–H(141)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*53	C(53)–H(67)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*16	C(10)–H(31)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*33	C(104)–H(125)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*31	C(6)–H(20)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*25	C(105)–H(129)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*36	C(107)–H(134)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*39	C(246)–H(270)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*24	C(7)–H(22)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*29	C(242)–H(257)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*111	C(7)–H(21)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*127	C(6)–H(19)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*125	C(100)–H(113)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*121	C(11)–H(34)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*126	C(195)–H(209)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*129	C(104)–H(124)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*128	C(53)–H(66)	108.9(2)	8.8(2)	—	0.4	7.7
*u*30	C(243)–H(261)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*10	C(60)–H(87)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*20	C(244)–H(264)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*22	C(54)–H(69)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*23	C(63)–H(91)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*11	C(9)–H(29)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*13	C(150)–H(170)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*26	C(101)–H(116)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*14	C(103)–H(123)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*99	C(153)–H(179)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*113	C(63)–H(90)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*110	C(246)–H(269)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*123	C(58)–H(81)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*91	C(9)–H(27)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*119	C(199)–H(222)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*94	C(8)–H(25)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*105	C(244)–H(262)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*93	C(243)–H(260)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*124	C(147)–H(160)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7

*u*95	C(13)–H(41)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*108	C(101)–H(115)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*106	C(12)–H(38)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*98	C(149)–H(166)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*101	C(103)–H(121)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*104	C(196)–H(213)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*122	C(54)–H(68)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*117	C(194)–H(207)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*102	C(106)–H(132)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*107	C(17)–H(46)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*109	C(111)–H(140)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*114	C(64)–H(93)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*92	C(55)–H(72)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*120	C(242)–H(256)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*103	C(107)–H(135)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*116	C(105)–H(128)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*115	C(152)–H(175)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*97	C(60)–H(88)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*100	C(102)–H(119)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*8	C(13)–H(40)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*6	C(102)–H(120)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*5	C(55)–H(73)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*9	C(106)–H(130)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*4	C(196)–H(214)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*89	C(12)–H(37)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*86	C(8)–H(24)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*90	C(149)–H(165)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*3	C(149)–H(167)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*2	C(12)–H(36)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*7	C(8)–H(26)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.6
*u*85	C(55)–H(71)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*73	C(63)–H(89)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*88	C(13)–H(39)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*82	C(195)–H(211)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*76	C(157)–H(183)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*87	C(102)–H(118)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*83	C(198)–H(220)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*79	C(242)–H(258)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*75	C(147)–H(159)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*81	C(150)–H(169)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*69	C(6)–H(18)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*58	C(53)–H(65)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*54	C(194)–H(206)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*70	C(17)–H(47)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*62	C(104)–H(126)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*32	C(11)–H(35)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7

*u*43	C(100)–H(114)	108.9(2)	8.8(tied to *u*128)	—	0.4	7.7
*u*144	Si(3)–H(15)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*141	Si(143)–H(155)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*143	Si(50)–H(62)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*140	Si(97)–H(109)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*142	Si(2)–H(14)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*139	Si(49)–H(61)	153.2(21)	8.5(8)	9.0(9)	0.4	9.0
*u*138	Si(190)–H(202)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*136	Si(96)–H(108)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*137	Si(237)–H(249)	153.2(21)	8.5(tied to *u*139)	—	0.4	9.0
*u*170	H(42)...H(44)	172.0(16)	13.0(fixed)	—	–0.5	13.0
*u*188	H(163)...H(164)	172.3(15)	12.6(fixed)	—	–0.4	12.6
*u*192	H(31)...H(32)	172.3(16)	12.6(fixed)	—	–0.3	12.6
*u*251	H(22)...H(23)	172.3(16)	12.6(fixed)	—	–0.3	12.6
*u*183	H(78)...H(79)	172.3(15)	12.7(fixed)	—	–0.5	12.7
*u*252	H(33)...H(35)	172.4(16)	12.6(fixed)	—	–0.2	12.6
*u*266	H(45)...H(47)	172.4(16)	12.6(fixed)	—	–0.2	12.6
*u*274	H(18)...H(20)	172.4(16)	12.6(fixed)	—	–0.2	12.6
*u*247	H(221)...H(223)	172.4(16)	12.6(fixed)	—	–0.2	12.6
*u*267	H(174)...H(176)	172.5(15)	12.6(fixed)	—	–0.2	12.6
*u*271	H(210)...H(211)	172.5(16)	12.6(fixed)	—	–0.2	12.6
*u*273	H(159)...H(161)	172.5(15)	12.6(fixed)	—	–0.2	12.6
*u*268	H(206)...H(208)	172.5(16)	12.6(fixed)	—	–0.2	12.6
*u*223	H(136)...H(138)	172.5(15)	12.9(fixed)	—	–0.5	12.9
*u*253	H(80)...H(82)	172.6(15)	12.6(fixed)	—	–0.2	12.6
*u*248	H(89)...H(91)	172.6(15)	12.6(fixed)	—	–0.2	12.6
*u*272	H(69)...H(70)	172.6(15)	12.6(fixed)	—	–0.2	12.6
*u*270	H(92)...H(94)	172.6(15)	12.6(fixed)	—	–0.2	12.6
*u*279	H(65)...H(67)	172.6(15)	12.6(fixed)	—	–0.2	12.6
*u*193	H(253)...H(255)	172.7(15)	12.7(fixed)	—	–0.3	12.7
*u*243	H(112)...H(114)	172.8(15)	12.6(fixed)	—	–0.3	12.6
*u*244	H(127)...H(129)	172.8(15)	12.6(fixed)	—	–0.2	12.6
*u*249	H(116)...H(117)	172.8(15)	12.6(fixed)	—	–0.2	12.6
*u*254	H(139)...H(141)	172.8(15)	12.6(fixed)	—	–0.2	12.6
*u*275	H(125)...H(126)	172.8(15)	12.6(fixed)	—	–0.2	12.6
*u*245	H(268)...H(270)	172.8(15)	12.6(fixed)	—	–0.2	12.6
*u*259	H(257)...H(258)	172.8(15)	12.6(fixed)	—	–0.2	12.6
*u*208	H(83)...H(84)	173.2(15)	13.1(fixed)	—	–0.6	13.1
*u*258	H(263)...H(264)	173.4(15)	12.6(fixed)	—	–0.2	12.6
*u*277	H(259)...H(261)	173.4(15)	12.6(fixed)	—	–0.2	12.6
*u*263	H(130)...H(131)	173.5(15)	12.6(fixed)	—	–0.2	12.6
*u*265	H(118)...H(120)	173.5(15)	12.6(fixed)	—	–0.2	12.6
*u*257	H(122)...H(123)	173.5(15)	12.6(fixed)	—	–0.2	12.6
*u*278	H(133)...H(134)	173.5(15)	12.6(fixed)	—	–0.2	12.6
*u*246	H(75)...H(76)	173.6(15)	12.6(fixed)	—	–0.3	12.6
*u*255	H(86)...H(87)	173.7(15)	12.6(fixed)	—	–0.2	12.6

*u*262	H(71)...H(73)	173.7(15)	12.6(fixed)	—	–0.2	12.6
*u*187	H(216)...H(217)	173.8(15)	12.9(fixed)	—	–0.4	12.9
*u*261	H(165)...H(167)	174.0(15)	12.6(fixed)	—	–0.2	12.6
*u*256	H(169)...H(170)	174.0(15)	12.6(fixed)	—	–0.2	12.6
*u*264	H(212)...H(214)	174.0(15)	12.6(fixed)	—	–0.2	12.6
*u*260	H(24)...H(26)	174.1(15)	12.6(fixed)	—	–0.2	12.6
*u*250	H(28)...H(29)	174.1(15)	12.6(fixed)	—	–0.2	12.6
*u*269	H(39)...H(40)	174.1(15)	12.6(fixed)	—	–0.2	12.6
*u*276	H(36)...H(37)	174.1(15)	12.6(fixed)	—	–0.2	12.6
*u*180	H(84)...H(85)	174.7(5)	13.1(fixed)	—	–0.8	13.1
*u*234	H(83)...H(85)	174.8(5)	13.0(fixed)	—	–0.7	13.0
*u*179	H(42)...H(43)	174.9(5)	13.0(fixed)	—	–0.6	13.0
*u*182	H(77)...H(79)	174.9(5)	12.7(fixed)	—	–0.6	12.7
*u*198	H(43)...H(44)	174.9(5)	13.0(fixed)	—	–0.5	13.0
*u*241	H(137)...H(138)	174.9(5)	12.8(fixed)	—	–0.6	12.8
*u*194	H(136)...H(137)	174.9(5)	12.9(fixed)	—	–0.5	12.9
*u*219	H(77)...H(78)	175.0(5)	12.7(fixed)	—	–0.5	12.7
*u*225	H(215)...H(216)	175.0(5)	12.9(fixed)	—	–0.5	12.9
*u*210	H(215)...H(217)	175.0(5)	12.9(fixed)	—	–0.5	12.9
*u*177	H(162)...H(164)	175.1(5)	12.7(fixed)	—	–0.4	12.7
*u*215	H(162)...H(163)	175.1(5)	12.7(fixed)	—	–0.4	12.7
*u*168	H(30)...H(32)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*197	H(30)...H(31)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*181	H(253)...H(254)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*217	H(254)...H(255)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*154	H(74)...H(76)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*149	H(21)...H(23)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*145	H(112)...H(113)	175.2(5)	12.6(fixed)	—	–0.3	12.6
*u*189	H(113)...H(114)	175.2(5)	12.6(fixed)	—	–0.3	12.6
*u*228	H(74)...H(75)	175.2(5)	12.7(fixed)	—	–0.3	12.7
*u*211	H(21)...H(22)	175.3(5)	12.6(fixed)	—	–0.3	12.6
*u*157	H(165)...H(166)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*158	H(127)...H(128)	175.3(5)	12.7(fixed)	—	–0.3	12.7
*u*161	H(80)...H(81)	175.3(5)	12.6(fixed)	—	–0.3	12.6
*u*171	H(262)...H(264)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*173	H(87)...H(88)	175.3(5)	12.6(fixed)	—	–0.3	12.6
*u*222	H(130)...H(132)	175.3(5)	12.6(fixed)	—	–0.3	12.6
*u*238	H(166)...H(167)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*209	H(175)...H(176)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*156	H(159)...H(160)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*196	H(259)...H(260)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*146	H(89)...H(90)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*152	H(68)...H(70)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*185	H(131)...H(132)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*242	H(260)...H(261)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*239	H(262)...H(263)	175.3(5)	12.6(fixed)	—	–0.2	12.6

*u*231	H(168)...H(169)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*190	H(71)...H(72)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*202	H(140)...H(141)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*207	H(269)...H(270)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*163	H(268)...H(269)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*184	H(168)...H(170)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*148	H(256)...H(258)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*204	H(81)...H(82)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*199	H(90)...H(91)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*166	H(139)...H(140)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*164	H(174)...H(175)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*174	H(121)...H(123)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*206	H(128)...H(129)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*233	H(39)...H(41)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*237	H(27)...H(28)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*229	H(93)...H(94)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*169	H(24)...H(25)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*230	H(121)...H(122)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*205	H(86)...H(88)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*165	H(118)...H(119)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*178	H(212)...H(213)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*147	H(33)...H(34)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*226	H(46)...H(47)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*162	H(221)...H(222)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*213	H(66)...H(67)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*195	H(34)...H(35)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*160	H(65)...H(66)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*155	H(115)...H(117)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*167	H(92)...H(93)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*186	H(134)...H(135)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*236	H(256)...H(257)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*224	H(222)...H(223)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*201	H(25)...H(26)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*175	H(27)...H(29)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*221	H(115)...H(116)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*176	H(45)...H(46)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*216	H(119)...H(120)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*220	H(160)...H(161)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*191	H(40)...H(41)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*227	H(72)...H(73)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*172	H(37)...H(38)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*153	H(209)...H(211)	175.3(5)	12.7(fixed)	—	–0.2	12.7
*u*159	H(18)...H(19)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*240	H(133)...H(135)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*150	H(124)...H(126)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*232	H(207)...H(208)	175.3(5)	12.6(fixed)	—	–0.2	12.6

*u*200	H(209)...H(210)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*151	H(206)...H(207)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*214	H(68)...H(69)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*235	H(213)...H(214)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*212	H(36)...H(38)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*203	H(19)...H(20)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*218	H(124)...H(125)	175.3(5)	12.6(fixed)	—	–0.2	12.6
*u*281	Si(96)–C(107)	188.7(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*302	Si(190)–C(201)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*292	Si(50)–C(56)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*300	Si(143)–C(154)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*293	Si(3)–C(8)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*289	Si(96)–C(106)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*298	Si(49)–C(60)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*286	Si(237)–C(248)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*283	Si(2)–C(13)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*288	Si(97)–C(103)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*295	Si(143)–C(153)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*285	Si(190)–C(200)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*297	Si(49)–C(59)	188.7(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*284	Si(50)–C(55)	188.7(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*290	Si(3)–C(9)	188.7(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*287	Si(97)–C(102)	188.7(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*282	Si(2)–C(12)	188.7(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*280	Si(237)–C(247)	188.7(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*313	Si(4)–C(10)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*321	Si(239)–C(251)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*307	Si(145)–C(152)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*318	Si(145)–C(157)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*316	Si(98)–C(105)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*312	Si(98)–C(110)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*317	Si(99)–C(101)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*305	Si(52)–C(54)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*320	Si(4)–C(11)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*322	Si(51)–C(63)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*323	Si(4)–C(16)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*324	Si(99)–C(100)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*319	Si(5)–C(7)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*306	Si(145)–C(151)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*314	Si(239)–C(245)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*309	Si(51)–C(58)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*304	Si(51)–C(57)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*299	Si(52)–C(64)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*296	Si(192)–C(198)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*311	Si(192)–C(199)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*303	Si(5)–C(6)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8

*u*291	Si(5)–C(17)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*301	Si(99)–C(111)	189.0(1)	6.4(tied to *u*326)	—	0.2	5.8
*u*308	Si(239)–C(246)	189.0(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*294	Si(52)–C(53)	189.0(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*310	Si(98)–C(104)	189.0(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*315	Si(192)–C(204)	189.0(1)	6.3(tied to *u*326)	—	0.2	5.7
*u*333	C(95)–Si(96)	190.1(6)	6.8(tied to *u*326)	—	0.2	6.2
*u*328	C(95)–Si(97)	190.1(6)	6.8(tied to *u*326)	—	0.2	6.1
*u*326	C(48)–Si(50)	190.1(6)	6.7(1)	—	0.2	6.1
*u*330	C(189)–Si(190)	190.1(6)	6.8(tied to *u*326)	—	0.2	6.2
*u*334	C(1)–Si(2)	190.1(6)	6.8(tied to *u*326)	—	0.2	6.2
*u*331	C(48)–Si(49)	190.1(6)	6.8(tied to *u*326)	—	0.2	6.2
*u*332	C(236)–Si(237)	190.1(6)	6.8(tied to *u*326)	—	0.2	6.1
*u*325	C(1)–Si(3)	190.1(6)	6.7(tied to *u*326)	—	0.2	6.1
*u*327	C(142)–Si(143)	190.1(6)	6.7(tied to *u*326)	—	0.2	6.1
*u*339	C(1)–Si(4)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.3
*u*338	C(48)–Si(51)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.2
*u*335	C(189)–Si(192)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.2
*u*337	C(1)–Si(5)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.2
*u*336	C(236)–Si(239)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.2
*u*342	C(48)–Si(52)	191.0(6)	7.0(tied to *u*326)	—	0.2	6.3
*u*340	C(142)–Si(145)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.3
*u*341	C(95)–Si(98)	191.0(6)	6.9(tied to *u*326)	—	0.2	6.3
*u*329	C(95)–Si(99)	191.0(6)	6.8(tied to *u*326)	—	0.2	6.1
*u*352	H(112)...H(131)	202.4(72)	41.0(fixed)	—	22.9	41.0
*u*396	H(125)...H(139)	203.7(81)	41.8(fixed)	—	10.0	41.8
*u*368	H(71)...H(89)	211.6(141)	40.7(fixed)	—	18.0	40.7
*u*435	H(116)...H(127)	212.4(47)	46.3(fixed)	—	11.1	46.3
*u*360	H(31)...H(45)	218.7(68)	45.2(fixed)	—	22.2	45.2
*u*372	H(206)...H(225)	219.7(66)	41.8(fixed)	—	17.0	41.8
*u*380	H(165)...H(178)	220.4(70)	43.8(fixed)	—	18.7	43.8
*u*398	H(257)...H(268)	220.8(67)	45.4(fixed)	—	10.7	45.4
*u*374	H(123)...H(129)	221.3(85)	42.5(fixed)	—	13.4	42.5
*u*461	H(210)...H(221)	221.8(59)	47.4(fixed)	—	11.4	47.4
*u*397	H(22)...H(33)	222.0(45)	47.5(fixed)	—	15.1	47.5
*u*401	H(130)...H(141)	223.0(79)	46.6(fixed)	—	13.3	46.6
*u*371	H(264)...H(270)	225.0(81)	41.1(fixed)	—	13.3	41.1
*u*382	H(258)...H(263)	225.3(69)	41.4(fixed)	—	14.1	41.4
*u*377	H(29)...H(35)	225.3(73)	42.7(fixed)	—	13.5	42.7
*u*400	H(76)...H(86)	228.7(90)	46.3(fixed)	—	16.4	46.3
*u*393	H(69)...H(80)	230.4(85)	45.0(fixed)	—	11.8	45.0
*u*559	H(131)...H(141)	231.5(110)	51.1(fixed)	—	11.7	51.1
*u*456	H(212)...H(223)	231.5(94)	45.0(fixed)	—	13.5	45.0
*u*460	H(258)...H(259)	232.2(76)	43.6(fixed)	—	15.0	43.6
*u*348	H(32)...H(40)	234.3(134)	41.8(fixed)	—	28.6	41.8
*u*365	H(78)...H(92)	234.7(84)	47.4(fixed)	—	28.7	47.4

*u*459	H(71)...H(82)	234.8(112)	44.8(fixed)	—	12.8	44.8
*u*449	H(75)...H(89)	235.8(134)	47.1(fixed)	—	18.9	47.1
*u*361	H(211)...H(214)	236.5(46)	41.7(fixed)	—	12.5	41.7
*u*564	H(75)...H(91)	236.8(95)	56.6(fixed)	—	17.1	56.6
*u*530	H(125)...H(141)	239.3(84)	48.5(fixed)	—	9.7	48.5
*u*582	H(75)...H(86)	239.4(126)	71.9(fixed)	—	13.1	71.9
*u*399	H(161)...H(170)	239.5(55)	44.7(fixed)	—	10.5	44.7
*u*562	H(165)...H(180)	239.6(58)	50.2(fixed)	—	12.2	50.2
*u*402	H(117)...H(122)	239.7(112)	43.8(fixed)	—	13.7	43.8
*u*388	H(87)...H(91)	240.4(67)	48.5(fixed)	—	13.2	48.5
*u*387	H(120)...H(134)	240.7(72)	41.1(fixed)	—	11.9	41.1
*u*362	H(80)...H(92)	240.7(161)	41.2(fixed)	—	18.0	41.2
*u*351	H(253)...H(275)	241.8(104)	39.8(fixed)	—	24.1	39.8
*u*347	H(164)...H(170)	242.4(50)	42.1(fixed)	—	29.6	42.1
*u*518	H(214)...H(223)	242.5(37)	53.8(fixed)	—	13.1	53.8
*u*355	H(163)...H(174)	242.6(40)	46.1(fixed)	—	24.8	46.1
*u*369	H(255)...H(259)	243.2(63)	44.1(fixed)	—	19.6	44.1
*u*373	H(174)...H(186)	243.6(125)	41.6(fixed)	—	17.6	41.6
*u*364	H(159)...H(177)	243.6(40)	39.5(fixed)	—	12.0	39.5
*u*454	H(23)...H(28)	243.9(117)	50.2(fixed)	—	14.2	50.2
*u*375	H(23)...H(24)	244.5(97)	46.4(fixed)	—	22.0	46.4
*u*410	Si(49)...H(88)	245.0(4)	13.3(tied to *u*446)	—	–0.4	13.2
*u*427	Si(50)...H(72)	245.0(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*430	Si(50)...H(74)	245.1(4)	13.4(tied to *u*446)	—	–0.4	13.3
*u*406	Si(2)...H(41)	245.1(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*429	Si(143)...H(179)	245.1(4)	13.3(tied to *u*446)	—	–0.4	13.2
*u*423	Si(143)...H(182)	245.1(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*405	Si(2)...H(38)	245.1(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*426	Si(3)...H(27)	245.1(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*420	Si(3)...H(25)	245.1(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*408	Si(237)...H(276)	245.1(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*419	Si(237)...H(273)	245.1(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*411	Si(97)...H(121)	245.2(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*407	Si(96)...H(135)	245.2(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*415	Si(96)...H(132)	245.2(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*413	Si(97)...H(119)	245.2(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*418	Si(190)...H(226)	245.2(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*444	Si(51)...H(90)	245.3(4)	13.4(tied to *u*446)	—	–0.4	13.2
*u*421	Si(52)...H(93)	245.3(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*416	Si(52)...H(68)	245.3(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*434	Si(51)...H(81)	245.3(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*404	Si(52)...H(66)	245.3(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*412	Si(145)...H(175)	245.3(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*409	Si(145)...H(184)	245.3(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*428	Si(5)...H(46)	245.4(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*414	Si(5)...H(19)	245.4(4)	13.2(tied to *u*446)	—	–0.4	13.1

*u*422	Si(49)...H(85)	245.4(4)	13.8(tied to *u*446)	—	0.0	13.6
*u*424	Si(4)...H(34)	245.4(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*445	Si(5)...H(21)	245.4(4)	13.4(tied to *u*446)	—	–0.4	13.2
*u*441	Si(239)...H(269)	245.4(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*432	Si(190)...H(229)	245.4(4)	13.5(tied to *u*446)	—	–0.2	13.3
*u*446	Si(239)...H(265)	245.4(4)	13.3(3)	—	–0.4	13.1
*u*438	Si(99)...H(140)	245.4(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*431	Si(4)...H(30)	245.4(4)	13.4(tied to *u*446)	—	–0.3	13.3
*u*433	Si(98)...H(128)	245.4(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*451	Si(99)...H(115)	245.4(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*417	Si(98)...H(124)	245.4(4)	13.2(tied to *u*446)	—	–0.4	13.1
*u*439	Si(239)...H(278)	245.5(4)	13.3(tied to *u*446)	—	–0.3	13.2
*u*448	Si(99)...H(113)	245.5(4)	13.2(tied to *u*446)	—	–0.3	13.1
*u*447	Si(192)...H(222)	245.5(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*425	Si(192)...H(218)	245.5(4)	13.3(tied to *u*446)	—	–0.4	13.1
*u*440	Si(192)...H(231)	245.5(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*443	Si(51)...H(77)	245.5(4)	13.6(tied to *u*446)	—	–0.1	13.4
*u*437	Si(145)...H(171)	245.5(4)	13.5(tied to *u*446)	—	–0.2	13.4
*u*436	Si(4)...H(43)	245.6(4)	13.7(tied to *u*446)	—	–0.1	13.5
*u*442	Si(98)...H(137)	245.6(4)	13.6(tied to *u*446)	—	–0.2	13.5
*u*346	H(217)...H(228)	245.7(106)	45.4(fixed)	—	37.8	45.4
*u*345	H(29)...H(42)	246.0(116)	48.9(fixed)	—	39.4	48.9
*u*343	H(79)...H(87)	247.3(61)	46.1(fixed)	—	35.9	46.1
*u*386	H(31)...H(47)	247.6(82)	47.3(fixed)	—	20.8	47.3
*u*567	H(257)...H(263)	248.9(47)	52.6(fixed)	—	12.0	52.6
*u*577	H(263)...H(270)	249.0(61)	53.8(fixed)	—	11.2	53.8
*u*384	H(78)...H(94)	249.1(97)	53.4(fixed)	—	26.5	53.4
*u*383	H(126)...H(130)	249.2(61)	41.3(fixed)	—	10.8	41.3
*u*366	H(206)...H(227)	249.3(69)	47.4(fixed)	—	26.8	47.4
*u*510	H(73)...H(82)	249.8(86)	49.5(fixed)	—	12.8	49.5
*u*462	Si(2)...H(39)	250.2(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*487	Si(3)...H(24)	250.2(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*467	Si(3)...H(28)	250.2(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*464	Si(2)...H(37)	250.2(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*475	Si(190)...H(225)	250.2(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*466	Si(143)...H(180)	250.4(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*476	Si(143)...H(178)	250.4(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*465	Si(190)...H(227)	250.6(4)	13.4(tied to *u*446)	—	0.0	13.2
*u*477	Si(50)...H(71)	250.8(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*474	Si(49)...H(86)	250.8(4)	13.2(tied to *u*446)	—	–0.3	13.1
*u*472	Si(50)...H(75)	250.9(4)	13.5(tied to *u*446)	—	–0.3	13.3
*u*479	Si(97)...H(118)	251.1(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*473	Si(97)...H(122)	251.1(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*497	Si(96)...H(131)	251.1(4)	13.2(tied to *u*446)	—	–0.3	13.1
*u*490	Si(96)...H(133)	251.1(4)	13.1(tied to *u*446)	—	–0.3	12.9
*u*482	Si(237)...H(274)	251.2(4)	13.2(tied to *u*446)	—	–0.4	13.0

*u*492	Si(237)...H(272)	251.2(4)	13.0(tied to *u*446)	—	–0.3	12.9
*u*390	H(120)...H(133)	251.4(97)	44.0(fixed)	—	15.1	44.0
*u*481	Si(49)...H(84)	251.4(4)	13.8(tied to *u*446)	—	0.3	13.7
*u*515	Si(96)...H(130)	251.8(4)	13.0(tied to *u*446)	—	–0.4	12.9
*u*503	Si(96)...H(134)	251.8(4)	13.0(tied to *u*446)	—	–0.4	12.8
*u*549	Si(97)...H(123)	251.9(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*533	Si(237)...H(275)	251.9(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*489	Si(237)...H(271)	251.9(4)	12.9(tied to *u*446)	—	–0.4	12.8
*u*537	Si(97)...H(120)	251.9(4)	12.9(tied to *u*446)	—	–0.3	12.8
*u*529	Si(190)...H(224)	252.0(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*547	Si(50)...H(76)	252.0(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*524	Si(50)...H(73)	252.0(4)	13.0(tied to *u*446)	—	–0.3	12.9
*u*557	Si(49)...H(87)	252.0(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*522	Si(99)...H(139)	252.1(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*509	Si(98)...H(127)	252.1(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*513	Si(99)...H(117)	252.1(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*504	Si(239)...H(267)	252.1(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*495	Si(99)...H(141)	252.1(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*527	Si(98)...H(129)	252.1(4)	13.2(tied to *u*446)	—	–0.3	13.0
*u*514	Si(239)...H(268)	252.1(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*511	Si(239)...H(270)	252.1(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*496	Si(98)...H(126)	252.1(4)	12.9(tied to *u*446)	—	–0.4	12.8
*u*508	Si(99)...H(116)	252.1(4)	13.0(tied to *u*446)	—	–0.3	12.9
*u*558	Si(143)...H(181)	252.1(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*536	Si(143)...H(177)	252.1(4)	12.9(tied to *u*446)	—	–0.3	12.8
*u*539	Si(98)...H(125)	252.1(4)	12.9(tied to *u*446)	—	–0.3	12.8
*u*519	Si(239)...H(266)	252.1(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*560	Si(2)...H(40)	252.1(4)	12.9(tied to *u*446)	—	–0.4	12.8
*u*550	Si(3)...H(29)	252.1(4)	12.9(tied to *u*446)	—	–0.4	12.8
*u*498	Si(239)...H(279)	252.1(4)	13.4(tied to *u*446)	—	–0.3	13.2
*u*531	Si(3)...H(26)	252.1(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*535	Si(99)...H(112)	252.1(4)	13.2(tied to *u*446)	—	–0.3	13.0
*u*521	Si(99)...H(114)	252.1(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*555	Si(2)...H(36)	252.1(4)	12.8(tied to *u*446)	—	–0.3	12.6
*u*483	Si(192)...H(220)	252.2(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*502	Si(192)...H(223)	252.2(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*552	Si(239)...H(277)	252.2(4)	13.1(tied to *u*446)	—	–0.3	12.9
*u*480	Si(52)...H(70)	252.2(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*505	Si(51)...H(89)	252.2(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*538	Si(192)...H(219)	252.2(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*491	Si(192)...H(232)	252.2(4)	13.0(tied to *u*446)	—	–0.4	12.9
*u*516	Si(192)...H(221)	252.2(4)	13.1(tied to *u*446)	—	–0.3	12.9
*u*542	Si(192)...H(230)	252.2(4)	13.0(tied to *u*446)	—	–0.4	12.8
*u*486	Si(52)...H(94)	252.2(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*543	Si(52)...H(92)	252.2(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*526	Si(51)...H(80)	252.2(4)	13.1(tied to *u*446)	—	–0.4	13.0

*u*534	Si(51)...H(91)	252.2(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*499	Si(51)...H(82)	252.2(4)	13.1(tied to *u*446)	—	–0.3	13.0
*u*551	Si(52)...H(69)	252.3(4)	13.0(tied to *u*446)	—	–0.3	12.9
*u*520	Si(52)...H(65)	252.3(4)	12.9(tied to *u*446)	—	–0.3	12.7
*u*506	Si(52)...H(67)	252.3(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*553	Si(145)...H(174)	252.3(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*484	Si(145)...H(183)	252.3(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*488	Si(145)...H(176)	252.3(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*507	Si(5)...H(23)	252.3(4)	13.4(tied to *u*446)	—	–0.4	13.2
*u*478	Si(5)...H(47)	252.3(4)	13.1(tied to *u*446)	—	–0.4	12.9
*u*471	Si(98)...H(138)	252.3(4)	13.8(tied to *u*446)	—	0.0	13.7
*u*544	Si(5)...H(45)	252.3(4)	13.2(tied to *u*446)	—	–0.4	13.0
*u*493	Si(5)...H(18)	252.3(4)	13.0(tied to *u*446)	—	–0.4	12.9
*u*561	Si(190)...H(228)	252.3(4)	13.2(tied to *u*446)	—	0.0	13.0
*u*554	Si(145)...H(185)	252.3(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*528	Si(4)...H(33)	252.3(4)	13.1(tied to *u*446)	—	–0.4	13.0
*u*523	Si(4)...H(35)	252.3(4)	13.0(tied to *u*446)	—	–0.3	12.8
*u*525	Si(5)...H(22)	252.4(4)	13.1(tied to *u*446)	—	–0.3	13.0
*u*541	Si(5)...H(20)	252.4(4)	12.9(tied to *u*446)	—	–0.3	12.7
*u*501	Si(4)...H(31)	252.4(4)	13.2(tied to *u*446)	—	–0.3	13.1
*u*548	Si(4)...H(32)	252.4(4)	13.3(tied to *u*446)	—	–0.2	13.1
*u*532	Si(145)...H(173)	252.4(4)	13.3(tied to *u*446)	—	–0.2	13.1
*u*556	Si(98)...H(136)	252.5(4)	13.7(tied to *u*446)	—	0.1	13.5
*u*500	Si(145)...H(172)	252.5(4)	13.4(tied to *u*446)	—	–0.1	13.3
*u*540	Si(49)...H(83)	252.6(4)	13.8(tied to *u*446)	—	0.3	13.7
*u*546	Si(51)...H(79)	252.6(4)	13.4(tied to *u*446)	—	0.0	13.2
*u*545	Si(4)...H(42)	252.6(4)	13.9(tied to *u*446)	—	0.0	13.8
*u*485	Si(51)...H(78)	252.6(4)	13.6(tied to *u*446)	—	0.1	13.4
*u*512	Si(4)...H(44)	252.7(4)	13.9(tied to *u*446)	—	0.1	13.7
*u*569	H(28)...H(35)	253.3(60)	51.7(fixed)	—	12.7	51.7
*u*358	H(33)...H(45)	253.8(135)	40.9(fixed)	—	17.5	40.9
*u*349	H(123)...H(136)	254.0(118)	50.6(fixed)	—	40.9	50.6
*u*376	H(26)...H(37)	254.1(123)	40.8(fixed)	—	14.1	40.8
*u*574	H(112)...H(133)	254.2(79)	52.6(fixed)	—	11.8	52.6
*u*565	H(161)...H(169)	254.2(35)	50.5(fixed)	—	10.5	50.5
*u*469	H(210)...H(223)	254.2(82)	47.7(fixed)	—	12.1	47.7
*u*571	H(122)...H(129)	254.3(58)	54.3(fixed)	—	12.6	54.3
*u*566	H(167)...H(180)	255.1(49)	50.4(fixed)	—	12.1	50.4
*u*450	H(257)...H(270)	255.3(83)	45.5(fixed)	—	11.4	45.5
*u*354	H(221)...H(233)	255.4(140)	39.2(fixed)	—	19.7	39.2
*u*357	H(268)...H(280)	255.8(148)	37.4(fixed)	—	17.7	37.4
*u*359	H(161)...H(177)	255.9(54)	41.2(fixed)	—	14.0	41.2
*u*385	H(26)...H(36)	256.5(102)	44.3(fixed)	—	14.3	44.3
*u*457	H(114)...H(118)	256.8(95)	46.9(fixed)	—	14.4	46.9
*u*379	H(117)...H(118)	257.3(87)	41.1(fixed)	—	16.9	41.1
*u*458	H(255)...H(261)	257.4(58)	48.8(fixed)	—	16.8	48.8

*u*470	H(86)...H(91)	257.6(41)	49.6(fixed)	—	14.3	49.6
*u*394	H(210)...H(214)	257.7(42)	45.8(fixed)	—	13.5	45.8
*u*494	H(208)...H(227)	257.8(45)	56.6(fixed)	—	20.4	56.6
*u*455	H(116)...H(129)	258.5(95)	48.1(fixed)	—	11.7	48.1
*u*468	H(69)...H(82)	258.8(93)	50.9(fixed)	—	11.9	50.9
*u*367	H(18)...H(36)	259.1(135)	40.1(fixed)	—	10.7	40.1
*u*604	H(114)...H(133)	259.1(47)	60.5(fixed)	—	10.3	60.5
*u*344	H(76)...H(84)	259.3(125)	53.7(fixed)	—	50.4	53.7
*u*370	H(70)...H(73)	259.7(148)	42.3(fixed)	—	12.3	42.3
*u*363	H(127)...H(139)	261.6(143)	40.1(fixed)	—	18.5	40.1
*u*356	H(40)...H(44)	261.7(93)	51.7(fixed)	—	35.1	51.7
*u*453	H(22)...H(35)	263.2(86)	48.3(fixed)	—	15.8	48.3
*u*517	H(20)...H(24)	263.8(95)	47.0(fixed)	—	10.3	47.0
*u*381	H(163)...H(176)	263.8(80)	50.8(fixed)	—	23.7	50.8
*u*658	C(111)...H(125)	264.0(65)	29.7(fixed)	—	7.2	29.7
*u*395	H(39)...H(44)	264.0(81)	57.1(fixed)	—	35.3	57.1
*u*575	H(22)...H(28)	264.0(110)	60.3(fixed)	—	12.2	60.3
*u*378	H(20)...H(36)	264.3(98)	41.9(fixed)	—	12.4	41.9
*u*576	H(14)...H(47)	265.2(60)	38.6(fixed)	—	9.8	38.6
*u*669	H(14)...H(18)	265.6(85)	44.2(fixed)	—	5.6	44.2
*u*350	H(65)...H(83)	267.9(57)	49.7(fixed)	—	35.0	49.7
*u*677	H(61)...H(65)	268.9(61)	45.6(fixed)	—	5.5	45.6
*u*654	C(106)...H(141)	269.2(77)	33.0(tied to *u*446)	—	9.5	32.6
*u*452	H(125)...H(130)	269.3(52)	43.4(fixed)	—	12.6	43.4
*u*572	H(116)...H(122)	269.5(107)	50.8(fixed)	—	12.1	50.8
*u*391	H(69)...H(73)	271.4(130)	44.7(fixed)	—	13.1	44.7
*u*463	H(20)...H(26)	272.0(84)	48.8(fixed)	—	10.9	48.8
*u*570	H(61)...H(94)	272.3(80)	37.8(fixed)	—	11.2	37.8
*u*633	H(25)...H(27)	273.1(67)	36.0(fixed)	—	7.3	36.0
*u*642	H(166)...H(168)	273.2(67)	36.4(fixed)	—	6.7	36.4
*u*626	H(109)...H(136)	273.7(43)	70.6(fixed)	—	10.1	70.6
*u*621	H(38)...H(41)	274.0(67)	34.3(fixed)	—	7.7	34.3
*u*353	H(67)...H(83)	274.4(68)	51.6(fixed)	—	39.3	51.6
*u*714	H(15)...H(37)	274.5(94)	49.0(fixed)	—	5.6	49.0
*u*643	H(132)...H(135)	274.6(67)	34.2(fixed)	—	6.6	34.2
*u*635	H(119)...H(121)	274.9(67)	37.4(fixed)	—	7.7	37.4
*u*573	H(155)...H(188)	275.2(37)	40.4(fixed)	—	11.4	40.4
*u*584	C(244)...H(250)	275.3(17)	13.9(fixed)	—	–0.1	13.9
*u*583	C(243)...H(250)	275.4(17)	13.8(fixed)	—	–0.1	13.8
*u*601	H(108)...H(126)	275.6(52)	40.3(fixed)	—	5.8	40.3
*u*613	C(17)...H(31)	275.7(58)	33.8(fixed)	—	19.0	33.8
*u*585	C(106)...H(108)	275.8(17)	14.0(fixed)	—	–0.1	14.0
*u*581	C(107)...H(108)	275.8(17)	13.9(fixed)	—	–0.1	13.9
*u*593	C(103)...H(109)	275.8(17)	13.9(fixed)	—	–0.1	13.9
*u*591	C(102)...H(109)	275.8(17)	13.8(fixed)	—	–0.1	13.8
*u*590	C(56)...H(62)	276.2(17)	13.9(fixed)	—	–0.2	13.9

*u*656	H(260)...H(262)	276.2(67)	36.1(fixed)	—	6.8	36.1
*u*589	C(55)...H(62)	276.2(17)	13.8(fixed)	—	–0.1	13.8
*u*592	C(60)...H(61)	276.2(17)	13.9(fixed)	—	–0.1	13.9
*u*594	C(59)...H(61)	276.2(17)	13.9(fixed)	—	–0.1	13.9
*u*588	C(196)...H(203)	276.3(17)	13.8(fixed)	—	–0.1	13.8
*u*600	C(197)...H(203)	276.3(17)	13.8(fixed)	—	–0.1	13.8
*u*597	C(150)...H(156)	276.5(17)	13.8(fixed)	—	–0.1	13.8
*u*595	C(149)...H(156)	276.5(17)	13.9(fixed)	—	–0.1	13.9
*u*598	C(12)...H(14)	276.5(17)	13.9(fixed)	—	–0.1	13.9
*u*602	C(13)...H(14)	276.5(17)	13.9(fixed)	—	–0.1	13.9
*u*647	H(72)...H(74)	276.5(67)	37.5(fixed)	—	9.9	37.5
*u*596	C(9)...H(15)	276.5(17)	13.9(fixed)	—	–0.1	13.9
*u*586	C(8)...H(15)	276.6(17)	13.8(fixed)	—	–0.1	13.8
*u*694	H(213)...H(215)	276.9(68)	42.8(fixed)	—	11.4	42.8
*u*605	C(95)...H(109)	277.9(20)	13.6(tied to *u*446)	—	0.0	13.4
*u*609	C(95)...H(108)	278.0(20)	13.6(tied to *u*446)	—	0.0	13.5
*u*644	C(105)...H(116)	278.0(47)	29.9(fixed)	—	8.5	29.9
*u*607	C(189)...H(202)	278.1(20)	13.6(tied to *u*446)	—	0.0	13.5
*u*707	C(56)...H(86)	278.4(75)	38.6(tied to *u*446)	—	10.5	38.1
*u*612	C(236)...H(249)	278.4(20)	13.7(tied to *u*446)	—	0.0	13.5
*u*659	C(244)...H(270)	278.4(56)	31.5(tied to *u*446)	—	9.2	31.2
*u*615	C(48)...H(61)	278.5(20)	13.7(tied to *u*446)	—	0.0	13.6
*u*608	C(48)...H(62)	278.5(20)	13.6(tied to *u*446)	—	0.0	13.5
*u*563	H(202)...H(232)	278.6(56)	34.8(fixed)	—	10.9	34.8
*u*901	C(100)...H(131)	278.6(59)	33.4(tied to *u*446)	—	8.1	33.0
*u*617	C(1)...H(14)	278.7(20)	13.7(tied to *u*446)	—	0.0	13.5
*u*606	C(1)...H(15)	278.7(20)	13.6(tied to *u*446)	—	0.0	13.4
*u*660	C(196)...H(223)	278.8(53)	34.2(tied to *u*446)	—	10.4	33.8
*u*614	C(142)...H(155)	278.8(20)	13.6(tied to *u*446)	—	0.0	13.4
*u*648	C(103)...H(129)	279.1(62)	32.1(tied to *u*446)	—	10.1	31.7
*u*667	C(242)...H(263)	279.5(46)	34.3(tied to *u*446)	—	10.1	33.9
*u*684	C(63)...H(75)	279.7(95)	38.5(tied to *u*446)	—	14.7	38.0
*u*403	H(114)...H(120)	280.2(80)	49.0(fixed)	—	15.1	49.0
*u*652	C(9)...H(35)	280.3(53)	32.1(tied to *u*446)	—	10.3	31.7
*u*579	H(15)...H(39)	280.3(106)	43.5(fixed)	—	11.5	43.5
*u*639	H(66)...H(93)	280.5(72)	35.5(fixed)	—	6.3	35.5
*u*636	C(246)...H(257)	280.5(53)	29.7(fixed)	—	8.4	29.7
*u*629	H(85)...H(88)	280.8(68)	49.1(fixed)	—	18.0	49.1
*u*628	H(19)...H(46)	281.0(72)	34.6(fixed)	—	5.5	34.6
*u*661	H(81)...H(90)	281.0(72)	37.5(fixed)	—	7.3	37.5
*u*676	C(199)...H(210)	281.1(51)	31.4(fixed)	—	9.0	31.4
*u*698	H(207)...H(234)	281.6(72)	36.2(fixed)	—	6.4	36.2
*u*848	C(106)...H(112)	281.9(51)	33.5(tied to *u*446)	—	10.6	33.1
*u*625	H(160)...H(187)	281.9(72)	34.7(fixed)	—	6.9	34.7
*u*675	H(202)...H(220)	282.8(38)	44.9(fixed)	—	6.7	44.9
*u*672	H(155)...H(159)	282.9(39)	42.6(fixed)	—	5.7	42.6

*u*653	H(113)...H(140)	283.1(72)	37.4(fixed)	—	8.1	37.4
*u*646	H(254)...H(281)	283.7(72)	38.8(fixed)	—	9.7	38.8
*u*665	C(55)...H(82)	283.7(58)	32.5(tied to *u*446)	—	10.1	32.1
*u*580	H(109)...H(134)	284.0(59)	38.5(fixed)	—	6.8	38.5
*u*611	C(64)...H(78)	284.8(62)	38.0(fixed)	—	24.8	38.0
*u*1026	C(104)...H(139)	285.0(62)	36.8(fixed)	—	4.2	36.8
*u*634	C(11)...H(22)	285.5(45)	31.9(fixed)	—	12.7	31.9
*u*392	H(249)...H(261)	286.1(59)	33.7(fixed)	—	11.6	33.7
*u*680	H(61)...H(79)	286.4(35)	62.6(fixed)	—	10.7	62.6
*u*649	H(15)...H(42)	287.1(48)	61.4(fixed)	—	13.1	61.4
*u*623	C(107)...H(120)	287.3(76)	29.8(tied to *u*446)	—	11.1	29.4
*u*691	H(128)...H(137)	287.3(73)	46.5(fixed)	—	15.0	46.5
*u*645	C(58)...H(69)	287.4(66)	31.7(fixed)	—	9.0	31.7
*u*904	C(10)...H(45)	287.5(53)	34.7(fixed)	—	4.0	34.7
*u*701	H(155)...H(173)	287.6(34)	55.4(fixed)	—	8.8	55.4
*u*936	C(55)...H(89)	287.8(101)	34.8(fixed)	—	8.1	34.8
*u*662	C(150)...H(161)	288.1(36)	31.9(fixed)	—	7.6	31.9
*u*632	H(34)...H(43)	288.3(73)	48.4(fixed)	—	16.9	48.4
*u*1017	C(63)...H(71)	289.2(110)	33.8(fixed)	—	6.8	33.8
*u*678	H(68)...H(93)	289.2(25)	37.9(fixed)	—	6.4	37.9
*u*704	C(149)...H(180)	289.3(45)	34.6(tied to *u*446)	—	9.1	34.2
*u*630	H(66)...H(68)	289.6(25)	35.3(fixed)	—	6.1	35.3
*u*619	C(195)...H(214)	290.0(39)	29.5(fixed)	—	10.4	29.5
*u*788	H(62)...H(84)	290.2(92)	73.8(fixed)	—	10.1	73.8
*u*668	H(256)...H(281)	290.2(25)	35.3(fixed)	—	6.1	35.3
*u*620	H(249)...H(253)	290.3(49)	50.7(fixed)	—	7.5	50.7
*u*664	H(115)...H(140)	290.5(25)	37.0(fixed)	—	6.1	37.0
*u*657	H(124)...H(128)	290.9(25)	35.3(fixed)	—	6.0	35.3
*u*631	C(60)...H(91)	291.0(46)	31.1(fixed)	—	10.8	31.1
*u*637	H(207)...H(209)	291.0(25)	35.9(fixed)	—	6.5	35.9
*u*655	H(19)...H(21)	291.0(25)	38.6(fixed)	—	7.3	38.6
*u*666	H(209)...H(234)	291.0(25)	37.4(fixed)	—	6.9	37.4
*u*695	H(21)...H(46)	291.3(25)	38.6(fixed)	—	7.5	38.6
*u*389	H(108)...H(138)	291.4(63)	44.3(fixed)	—	30.0	44.3
*u*689	H(254)...H(256)	291.5(25)	39.3(fixed)	—	8.3	39.3
*u*624	C(243)...H(255)	291.7(48)	32.5(fixed)	—	15.7	32.5
*u*731	C(8)...C(9)	291.8(41)	13.0(tied to *u*850)	—	–0.2	11.2
*u*683	H(113)...H(115)	291.8(25)	36.2(fixed)	—	7.2	36.2
*u*713	C(12)...C(13)	291.9(41)	12.8(tied to *u*850)	—	–0.2	11.1
*u*846	H(15)...H(44)	292.1(51)	84.3(fixed)	—	4.2	84.3
*u*587	C(147)...H(177)	292.2(36)	27.8(fixed)	—	10.7	27.8
*u*723	C(149)...C(150)	292.3(41)	13.1(tied to *u*850)	—	–0.2	11.3
*u*1076	C(101)...H(127)	292.4(38)	40.8(fixed)	—	4.3	40.8
*u*641	H(160)...H(162)	292.7(26)	43.9(fixed)	—	10.9	43.9
*u*727	C(59)...C(60)	292.9(41)	13.0(tied to *u*850)	—	–0.2	11.3
*u*735	C(55)...C(56)	293.0(41)	13.2(tied to *u*850)	—	–0.2	11.4

*u*732	C(196)...C(197)	293.1(40)	13.3(tied to *u*850)	—	–0.2	11.5
*u*736	C(58)...C(63)	293.5(54)	13.2(tied to *u*850)	—	–0.2	11.5
*u*730	C(53)...C(64)	293.5(54)	13.2(tied to *u*850)	—	–0.2	11.4
*u*751	C(241)...C(252)	293.6(54)	13.3(tied to *u*850)	—	–0.2	11.5
*u*681	H(30)...H(34)	293.7(25)	42.6(fixed)	—	11.1	42.6
*u*716	C(147)...C(158)	293.7(54)	13.1(tied to *u*850)	—	–0.2	11.4
*u*758	C(194)...C(205)	293.8(54)	13.3(tied to *u*850)	—	–0.2	11.5
*u*721	C(6)...C(17)	293.9(54)	13.1(tied to *u*850)	—	–0.2	11.4
*u*773	C(105)...C(110)	293.9(53)	13.6(tied to *u*850)	—	–0.2	11.8
*u*745	C(11)...C(16)	293.9(54)	13.2(tied to *u*850)	—	–0.1	11.4
*u*740	C(100)...C(111)	293.9(53)	13.1(tied to *u*850)	—	–0.2	11.3
*u*743	C(106)...C(107)	294.0(40)	11.5(fixed)	—	–0.2	11.5
*u*726	C(102)...C(103)	294.0(40)	11.3(fixed)	—	–0.2	11.3
*u*702	H(162)...H(187)	294.1(25)	42.5(fixed)	—	11.9	42.5
*u*950	C(57)...H(92)	294.5(60)	35.4(fixed)	—	4.4	35.4
*u*650	H(77)...H(90)	294.8(26)	45.8(fixed)	—	14.2	45.8
*u*671	H(14)...H(32)	294.9(88)	56.5(fixed)	—	9.0	56.5
*u*686	H(77)...H(81)	295.0(26)	43.6(fixed)	—	13.8	43.6
*u*744	C(243)...C(244)	295.1(40)	13.2(tied to *u*850)	—	–0.2	11.4
*u*599	C(152)...H(163)	295.4(47)	36.4(fixed)	—	21.4	36.4
*u*616	C(12)...H(26)	296.2(81)	29.0(tied to *u*446)	—	11.6	28.7
*u*1016	C(7)...H(33)	296.3(38)	41.0(fixed)	—	4.4	41.0
*u*705	H(249)...H(276)	296.4(16)	26.7(fixed)	—	0.4	26.7
*u*651	H(124)...H(137)	296.7(26)	46.5(fixed)	—	15.0	46.5
*u*1007	C(194)...H(225)	296.7(50)	35.5(fixed)	—	7.0	35.5
*u*696	C(101)...H(122)	296.8(104)	34.2(fixed)	—	10.0	34.2
*u*946	C(196)...H(230)	296.8(48)	34.8(fixed)	—	7.1	34.8
*u*640	C(194)...H(227)	296.8(31)	39.1(fixed)	—	20.5	39.1
*u*708	H(61)...H(88)	296.9(16)	27.4(fixed)	—	0.4	27.4
*u*706	H(62)...H(74)	296.9(16)	30.1(fixed)	—	1.1	30.1
*u*715	H(14)...H(41)	297.0(16)	27.5(fixed)	—	0.3	27.5
*u*703	H(108)...H(135)	297.0(16)	25.6(fixed)	—	0.2	25.6
*u*673	H(249)...H(273)	297.0(16)	25.2(fixed)	—	0.8	25.2
*u*710	H(109)...H(121)	297.0(16)	26.8(fixed)	—	0.5	26.8
*u*712	H(15)...H(27)	297.2(16)	26.6(fixed)	—	0.4	26.6
*u*687	H(108)...H(132)	297.4(16)	25.8(fixed)	—	0.7	25.8
*u*674	H(62)...H(70)	297.5(123)	44.2(fixed)	—	6.8	44.2
*u*709	H(155)...H(182)	297.5(16)	25.1(fixed)	—	0.5	25.1
*u*693	H(62)...H(72)	297.7(16)	24.8(fixed)	—	0.8	24.8
*u*690	H(14)...H(38)	297.7(16)	25.5(fixed)	—	0.6	25.5
*u*1058	C(149)...H(178)	297.8(52)	37.9(tied to *u*446)	—	7.3	37.5
*u*711	H(109)...H(138)	297.8(53)	71.1(fixed)	—	6.3	71.1
*u*692	H(155)...H(179)	297.9(16)	25.5(fixed)	—	1.0	25.5
*u*679	H(109)...H(119)	298.0(16)	25.4(fixed)	—	1.2	25.4
*u*1004	C(244)...H(258)	298.0(53)	34.4(fixed)	—	4.2	34.4
*u*682	H(15)...H(25)	298.1(16)	25.1(fixed)	—	1.0	25.1

*u*688	H(202)...H(226)	298.2(16)	25.2(fixed)	—	0.8	25.2
*u*700	C(7)...H(28)	298.4(105)	35.4(fixed)	—	9.6	35.4
*u*1027	C(242)...H(268)	298.6(50)	39.7(fixed)	—	3.9	39.7
*u*1093	C(195)...H(221)	298.8(46)	41.6(fixed)	—	4.2	41.6
*u*697	H(61)...H(85)	299.2(16)	35.8(fixed)	—	4.5	35.8
*u*685	H(202)...H(229)	299.5(16)	31.0(fixed)	—	3.2	31.0
*u*871	C(105)...H(123)	299.8(69)	36.9(fixed)	—	5.6	36.9
*u*770	C(10)...H(40)	299.9(105)	30.6(fixed)	—	9.0	30.6
*u*875	C(9)...H(25)	300.2(50)	26.0(fixed)	—	0.6	26.0
*u*838	C(13)...H(38)	300.4(50)	24.6(fixed)	—	0.5	24.6
*u*1081	C(56)...H(89)	300.5(94)	39.2(fixed)	—	4.1	39.2
*u*880	C(150)...H(166)	300.9(50)	25.6(fixed)	—	0.6	25.6
*u*792	C(100)...H(133)	301.0(46)	38.0(fixed)	—	7.3	38.0
*u*804	C(8)...H(27)	301.1(50)	24.8(fixed)	—	1.3	24.8
*u*800	C(149)...H(168)	301.2(50)	25.6(fixed)	—	0.9	25.6
*u*908	C(11)...H(29)	301.4(60)	36.6(fixed)	—	5.2	36.6
*u*889	C(56)...H(72)	301.4(50)	25.6(fixed)	—	0.6	25.6
*u*818	H(24)...H(28)	301.4(66)	39.2(fixed)	—	5.3	39.2
*u*750	C(12)...H(41)	301.5(50)	24.7(fixed)	—	1.6	24.7
*u*627	C(104)...H(130)	301.6(49)	29.7(fixed)	—	9.4	29.7
*u*877	C(197)...H(213)	301.6(50)	25.7(fixed)	—	0.5	25.7
*u*757	H(37)...H(39)	301.7(66)	38.7(fixed)	—	5.5	38.7
*u*896	C(103)...H(119)	301.8(50)	26.7(fixed)	—	0.5	26.7
*u*925	C(196)...H(215)	301.9(50)	33.7(fixed)	—	2.4	33.7
*u*1169	C(111)...H(131)	302.0(86)	44.2(fixed)	—	3.8	44.2
*u*797	C(59)...H(88)	302.2(50)	25.5(fixed)	—	1.4	25.5
*u*777	H(165)...H(169)	302.5(65)	39.5(fixed)	—	5.2	39.5
*u*893	C(107)...H(132)	302.5(50)	24.3(fixed)	—	0.8	24.3
*u*826	C(106)...H(135)	302.5(50)	24.2(fixed)	—	0.9	24.2
*u*865	C(60)...H(85)	302.7(51)	38.8(fixed)	—	4.8	38.8
*u*853	H(65)...H(94)	302.8(106)	38.4(fixed)	—	4.5	38.4
*u*794	C(102)...H(121)	302.8(50)	25.7(fixed)	—	1.4	25.7
*u*828	C(55)...H(74)	302.9(50)	27.6(fixed)	—	2.4	27.6
*u*888	H(206)...H(235)	303.0(105)	40.8(fixed)	—	5.0	40.8
*u*766	C(54)...C(64)	303.1(14)	13.6(tied to *u*850)	—	–0.2	11.7
*u*763	C(57)...C(63)	303.1(14)	13.4(tied to *u*850)	—	–0.2	11.6
*u*746	C(57)...C(58)	303.1(14)	13.3(tied to *u*850)	—	–0.2	11.5
*u*722	C(53)...C(54)	303.1(14)	13.0(tied to *u*850)	—	–0.1	11.3
*u*907	C(246)...H(264)	303.2(65)	35.4(fixed)	—	5.8	35.4
*u*1012	H(253)...H(282)	303.2(106)	44.5(fixed)	—	6.9	44.5
*u*663	H(30)...H(43)	303.2(26)	48.3(fixed)	—	22.4	48.3
*u*748	C(242)...C(252)	303.3(14)	13.3(tied to *u*850)	—	–0.2	11.5
*u*760	C(147)...C(148)	303.3(14)	13.5(tied to *u*850)	—	–0.2	11.6
*u*762	C(148)...C(158)	303.3(14)	13.4(tied to *u*850)	—	–0.2	11.6
*u*737	C(241)...C(242)	303.3(14)	13.2(tied to *u*850)	—	–0.1	11.5
*u*755	C(195)...C(205)	303.3(14)	13.4(tied to *u*850)	—	–0.2	11.6

*u*725	C(194)...C(195)	303.4(14)	13.2(tied to *u*850)	—	–0.2	11.4
*u*951	C(244)...H(260)	303.4(50)	25.2(fixed)	—	0.5	25.2
*u*815	H(18)...H(47)	303.4(105)	36.5(fixed)	—	4.0	36.5
*u*765	C(7)...C(17)	303.4(14)	13.7(tied to *u*850)	—	–0.2	11.9
*u*752	C(10)...C(16)	303.5(14)	13.5(tied to *u*850)	—	–0.2	11.7
*u*738	C(10)...C(11)	303.5(14)	13.3(tied to *u*850)	—	–0.2	11.5
*u*739	C(6)...C(7)	303.5(14)	13.2(tied to *u*850)	—	–0.2	11.4
*u*729	C(104)...C(110)	303.5(14)	13.3(tied to *u*850)	—	–0.2	11.5
*u*749	C(101)...C(111)	303.5(14)	13.2(tied to *u*850)	—	–0.2	11.5
*u*742	C(104)...C(105)	303.5(14)	13.2(tied to *u*850)	—	–0.1	11.4
*u*741	C(100)...C(101)	303.5(14)	13.1(tied to *u*850)	—	–0.1	11.3
*u*819	H(82)...H(89)	303.6(106)	40.6(fixed)	—	5.8	40.6
*u*791	H(159)...H(188)	303.6(105)	38.7(fixed)	—	4.9	38.7
*u*895	H(112)...H(141)	303.8(105)	40.8(fixed)	—	6.2	40.8
*u*771	C(16)...H(29)	303.9(93)	29.3(fixed)	—	8.0	29.3
*u*1104	C(243)...H(258)	303.9(58)	36.7(fixed)	—	6.0	36.7
*u*610	C(6)...H(36)	304.0(109)	28.2(fixed)	—	9.2	28.2
*u*1013	C(60)...H(76)	304.1(69)	40.6(tied to *u*446)	—	7.7	40.1
*u*969	C(54)...H(80)	304.1(61)	39.3(fixed)	—	4.8	39.3
*u*820	C(243)...H(262)	304.2(50)	24.9(fixed)	—	1.3	24.9
*u*603	C(13)...H(44)	304.3(41)	43.2(fixed)	—	32.5	43.2
*u*776	H(249)...H(271)	304.4(18)	25.8(fixed)	—	0.0	25.8
*u*927	C(64)...H(66)	304.6(59)	25.1(fixed)	—	0.2	25.1
*u*928	C(58)...H(90)	304.8(59)	26.8(fixed)	—	0.7	26.8
*u*568	H(62)...H(67)	304.8(99)	35.3(fixed)	—	8.9	35.3
*u*775	H(108)...H(130)	304.8(18)	26.8(fixed)	—	0.0	26.8
*u*1115	C(199)...H(212)	304.8(71)	38.6(fixed)	—	4.4	38.6
*u*801	H(109)...H(120)	305.0(18)	26.4(fixed)	—	0.1	26.4
*u*733	H(249)...H(275)	305.0(18)	26.1(fixed)	—	0.6	26.1
*u*870	C(148)...H(174)	305.1(37)	35.7(fixed)	—	4.7	35.7
*u*874	C(152)...H(184)	305.2(58)	24.7(fixed)	—	0.3	24.7
*u*879	C(17)...H(19)	305.5(58)	24.6(fixed)	—	0.3	24.6
*u*1035	C(199)...H(231)	305.5(58)	25.1(fixed)	—	0.3	25.1
*u*718	H(108)...H(134)	305.5(18)	25.1(fixed)	—	0.4	25.1
*u*827	C(63)...H(81)	305.6(59)	25.4(fixed)	—	1.2	25.4
*u*1153	C(242)...H(259)	305.6(57)	37.2(fixed)	—	6.4	37.2
*u*842	H(202)...H(228)	305.7(18)	33.4(fixed)	—	1.1	33.4
*u*779	C(148)...H(170)	305.7(46)	30.2(fixed)	—	8.4	30.2
*u*795	H(61)...H(83)	305.7(19)	39.4(fixed)	—	2.5	39.4
*u*747	H(109)...H(123)	305.7(18)	26.2(fixed)	—	0.8	26.2
*u*844	C(241)...H(281)	305.8(58)	25.2(fixed)	—	1.0	25.2
*u*783	C(53)...H(93)	305.9(59)	24.6(fixed)	—	1.4	24.6
*u*1041	H(61)...H(78)	305.9(39)	72.4(fixed)	—	3.3	72.4
*u*1134	C(58)...H(71)	306.1(79)	37.7(fixed)	—	3.9	37.7
*u*789	H(202)...H(224)	306.1(18)	25.9(fixed)	—	0.1	25.9
*u*790	H(62)...H(73)	306.1(18)	25.8(fixed)	—	0.1	25.8

*u*814	C(196)...H(211)	306.1(32)	35.7(fixed)	—	4.7	35.7
*u*911	C(111)...H(113)	306.2(58)	26.8(fixed)	—	1.2	26.8
*u*782	C(6)...H(46)	306.2(58)	24.0(fixed)	—	1.0	24.0
*u*841	C(100)...H(140)	306.3(58)	25.2(fixed)	—	1.1	25.2
*u*866	C(110)...H(128)	306.4(58)	25.8(fixed)	—	1.2	25.8
*u*823	C(16)...H(34)	306.4(58)	25.6(fixed)	—	1.3	25.6
*u*899	C(246)...H(278)	306.4(59)	28.2(fixed)	—	2.1	28.2
*u*852	C(194)...H(234)	306.4(58)	25.1(fixed)	—	1.3	25.1
*u*761	C(147)...H(187)	306.5(58)	24.6(fixed)	—	1.6	24.6
*u*1002	H(35)...H(42)	306.5(107)	54.4(fixed)	—	12.5	54.4
*u*813	H(71)...H(75)	306.6(65)	43.5(fixed)	—	7.1	43.5
*u*754	H(61)...H(87)	306.6(18)	26.5(fixed)	—	0.7	26.5
*u*756	H(62)...H(76)	306.6(18)	28.7(fixed)	—	1.2	28.7
*u*805	H(155)...H(177)	306.7(18)	26.1(fixed)	—	0.1	26.1
*u*724	C(13)...H(32)	306.7(91)	34.6(fixed)	—	17.3	34.6
*u*1045	H(129)...H(136)	306.7(107)	53.4(fixed)	—	13.0	53.4
*u*787	H(15)...H(26)	306.8(18)	26.3(fixed)	—	0.2	26.3
*u*812	H(14)...H(36)	306.9(18)	25.1(fixed)	—	0.0	25.1
*u*1019	H(155)...H(172)	307.0(33)	68.6(fixed)	—	3.1	68.6
*u*876	C(11)...H(43)	307.0(59)	38.1(fixed)	—	4.6	38.1
*u*769	H(155)...H(181)	307.0(18)	25.9(fixed)	—	0.5	25.9
*u*1021	C(105)...H(137)	307.1(59)	35.2(fixed)	—	3.9	35.2
*u*753	C(57)...H(87)	307.2(51)	29.3(fixed)	—	9.6	29.3
*u*920	C(58)...H(92)	307.3(124)	34.4(fixed)	—	7.3	34.4
*u*759	H(15)...H(29)	307.4(18)	25.6(fixed)	—	0.6	25.6
*u*764	H(14)...H(40)	307.5(18)	25.9(fixed)	—	0.8	25.9
*u*622	C(54)...H(73)	307.8(129)	29.0(fixed)	—	10.1	29.0
*u*1036	C(241)...H(259)	307.9(46)	37.2(fixed)	—	4.2	37.2
*u*858	Si(49)...Si(50)	308.2(12)	11.5(tied to *u*850)	—	–0.1	10.0
*u*836	Si(2)...Si(3)	308.2(12)	11.5(tied to *u*850)	—	–0.1	9.9
*u*798	Si(96)...Si(97)	308.3(12)	11.5(tied to *u*850)	—	0.0	9.9
*u*720	H(212)...H(216)	308.5(65)	46.8(fixed)	—	11.4	46.8
*u*670	C(8)...H(20)	308.6(83)	32.2(fixed)	—	7.7	32.2
*u*903	H(131)...H(133)	308.7(64)	39.3(fixed)	—	4.7	39.3
*u*924	C(197)...H(230)	308.9(50)	35.8(fixed)	—	4.2	35.8
*u*1176	C(111)...H(130)	308.9(75)	39.7(fixed)	—	3.9	39.7
*u*872	Si(49)...Si(51)	308.9(6)	11.7(tied to *u*850)	—	–0.1	10.1
*u*878	Si(143)...Si(145)	309.0(6)	11.6(tied to *u*850)	—	–0.1	10.0
*u*864	Si(3)...Si(4)	309.0(6)	11.4(tied to *u*850)	—	0.0	9.8
*u*854	Si(2)...Si(5)	309.0(6)	11.5(tied to *u*850)	—	0.0	9.9
*u*831	Si(49)...Si(52)	309.0(6)	11.3(tied to *u*850)	—	0.0	9.8
*u*855	Si(2)...Si(4)	309.0(6)	11.3(tied to *u*850)	—	0.0	9.8
*u*850	Si(190)...Si(192)	309.0(6)	11.3(4)	—	0.0	9.7
*u*961	Si(50)...Si(51)	309.0(6)	11.0(tied to *u*850)	—	0.0	9.5
*u*930	Si(237)...Si(239)	309.0(6)	10.9(tied to *u*850)	—	0.0	9.4
*u*963	Si(96)...Si(99)	309.0(6)	11.2(tied to *u*850)	—	0.0	9.7

*u*802	Si(96)...Si(98)	309.1(6)	11.1(tied to *u*850)	—	0.0	9.6
*u*840	Si(97)...Si(98)	309.1(6)	11.1(tied to *u*850)	—	0.0	9.6
*u*799	H(118)...H(122)	309.6(64)	40.4(fixed)	—	5.9	40.4
*u*638	C(102)...H(114)	309.7(83)	31.1(fixed)	—	12.0	31.1
*u*954	Si(51)...Si(52)	309.7(11)	10.9(tied to *u*850)	—	0.0	9.4
*u*942	Si(4)...Si(5)	309.8(11)	10.8(tied to *u*850)	—	0.0	9.4
*u*1005	Si(98)...Si(99)	309.8(11)	11.1(tied to *u*850)	—	0.0	9.6
*u*811	H(84)...H(86)	310.2(66)	55.6(fixed)	—	14.9	55.6
*u*780	C(110)...H(123)	310.2(92)	31.2(fixed)	—	8.8	31.2
*u*830	C(241)...H(275)	310.2(83)	31.0(fixed)	—	8.1	31.0
*u*886	C(64)...H(80)	310.5(124)	34.5(fixed)	—	8.1	34.5
*u*803	Si(190)...Si(191)	310.8(12)	11.7(tied to *u*850)	—	–0.1	10.1
*u*917	Si(143)...Si(144)	310.8(12)	11.1(tied to *u*850)	—	–0.1	9.6
*u*806	C(102)...H(134)	310.8(63)	33.7(fixed)	—	4.6	33.7
*u*781	Si(237)...Si(238)	310.9(12)	11.2(tied to *u*850)	—	0.0	9.7
*u*768	C(59)...H(76)	311.5(99)	34.2(fixed)	—	13.5	34.2
*u*847	Si(143)...Si(146)	311.5(7)	11.4(tied to *u*850)	—	0.0	9.9
*u*873	H(259)...H(263)	311.5(64)	39.6(fixed)	—	5.1	39.6
*u*816	C(149)...H(183)	311.6(30)	33.4(fixed)	—	4.1	33.4
*u*860	Si(237)...Si(240)	311.6(7)	11.2(tied to *u*850)	—	0.0	9.7
*u*906	Si(190)...Si(193)	311.6(7)	10.9(tied to *u*850)	—	0.0	9.4
*u*919	C(63)...H(87)	311.6(46)	41.1(fixed)	—	5.3	41.1
*u*734	C(150)...H(164)	311.8(32)	34.5(fixed)	—	18.1	34.5
*u*618	H(202)...H(217)	311.9(44)	50.5(fixed)	—	14.3	50.5
*u*959	C(147)...H(170)	312.0(37)	39.3(fixed)	—	5.0	39.3
*u*1006	Si(192)...Si(193)	312.3(12)	10.8(tied to *u*850)	—	0.0	9.4
*u*910	Si(145)...Si(146)	312.3(12)	10.7(tied to *u*850)	—	0.0	9.3
*u*996	Si(239)...Si(240)	312.3(12)	10.9(tied to *u*850)	—	0.0	9.5
*u*784	H(249)...H(255)	312.4(42)	58.6(fixed)	—	3.4	58.6
*u*849	C(16)...H(40)	312.5(55)	35.2(fixed)	—	5.6	35.2
*u*1187	C(150)...H(178)	312.7(47)	43.2(fixed)	—	3.9	43.2
*u*767	C(244)...H(277)	312.8(73)	33.0(fixed)	—	14.0	33.0
*u*933	C(152)...H(186)	312.8(101)	35.0(fixed)	—	7.8	35.0
*u*1146	Si(50)...H(89)	313.3(26)	32.4(fixed)	—	4.3	32.4
*u*1029	C(54)...H(93)	313.3(15)	26.8(fixed)	—	0.4	26.8
*u*1064	Si(49)...H(65)	313.4(23)	31.5(fixed)	—	3.2	31.5
*u*1022	C(148)...H(187)	313.4(15)	28.2(fixed)	—	0.3	28.2
*u*898	C(53)...H(68)	313.7(15)	25.6(fixed)	—	0.5	25.6
*u*774	C(59)...H(65)	313.7(35)	30.9(fixed)	—	4.5	30.9
*u*944	C(57)...H(81)	313.7(15)	26.3(fixed)	—	0.7	26.3
*u*968	C(241)...H(256)	313.9(15)	25.2(fixed)	—	0.3	25.2
*u*1065	C(12)...H(39)	313.9(49)	27.8(fixed)	—	0.1	27.8
*u*1031	C(7)...H(46)	314.0(15)	25.7(fixed)	—	0.2	25.7
*u*1101	C(8)...H(28)	314.1(49)	26.7(fixed)	—	0.1	26.7
*u*981	C(242)...H(281)	314.1(15)	25.5(fixed)	—	0.6	25.5
*u*578	C(53)...H(83)	314.3(39)	41.8(fixed)	—	35.3	41.8

*u*833	C(64)...H(68)	314.3(15)	25.6(fixed)	—	1.1	25.6
*u*778	C(54)...H(66)	314.3(15)	24.2(fixed)	—	0.9	24.2
*u*915	C(194)...H(209)	314.3(15)	25.8(fixed)	—	0.5	25.8
*u*943	C(10)...H(34)	314.4(15)	26.6(fixed)	—	0.7	26.6
*u*956	C(101)...H(140)	314.4(15)	26.5(fixed)	—	0.6	26.5
*u*1028	C(9)...H(24)	314.4(49)	27.1(fixed)	—	0.4	27.1
*u*918	C(110)...H(124)	314.4(15)	24.4(fixed)	—	0.3	24.4
*u*829	C(148)...H(160)	314.5(15)	24.6(fixed)	—	0.7	24.6
*u*984	C(195)...H(234)	314.5(15)	26.1(fixed)	—	0.7	26.1
*u*1194	H(202)...H(216)	314.5(50)	73.9(fixed)	—	0.6	73.9
*u*975	C(100)...H(115)	314.5(15)	24.7(fixed)	—	0.4	24.7
*u*938	C(6)...H(21)	314.5(15)	28.3(fixed)	—	1.1	28.3
*u*856	C(57)...H(90)	314.5(15)	25.6(fixed)	—	1.4	25.6
*u*1057	Si(2)...H(18)	314.6(17)	30.4(fixed)	—	3.2	30.4
*u*902	C(13)...H(37)	314.6(49)	25.7(fixed)	—	0.4	25.7
*u*868	C(242)...H(254)	314.7(15)	29.6(fixed)	—	1.9	29.6
*u*948	C(104)...H(128)	314.7(15)	25.5(fixed)	—	0.7	25.5
*u*822	C(7)...H(19)	314.8(15)	24.3(fixed)	—	0.7	24.3
*u*1072	C(149)...H(169)	314.8(49)	27.0(fixed)	—	0.0	27.0
*u*912	C(63)...H(77)	314.8(15)	35.3(fixed)	—	3.5	35.3
*u*909	C(147)...H(162)	314.8(15)	33.7(fixed)	—	2.8	33.7
*u*835	C(246)...H(265)	314.9(15)	23.7(fixed)	—	1.0	23.7
*u*1062	C(103)...H(117)	314.9(107)	36.8(fixed)	—	3.9	36.8
*u*837	C(199)...H(218)	314.9(15)	25.8(fixed)	—	1.1	25.8
*u*821	C(105)...H(124)	315.0(15)	23.8(fixed)	—	0.8	23.8
*u*1110	C(11)...H(42)	315.1(74)	43.5(fixed)	—	2.5	43.5
*u*843	C(111)...H(115)	315.1(15)	24.4(fixed)	—	0.9	24.4
*u*869	C(11)...H(30)	315.1(15)	32.2(fixed)	—	2.4	32.2
*u*882	C(58)...H(77)	315.2(15)	34.1(fixed)	—	3.7	34.1
*u*978	C(150)...H(165)	315.3(49)	27.3(fixed)	—	0.5	27.3
*u*786	C(195)...H(207)	315.3(15)	24.1(fixed)	—	1.2	24.1
*u*859	C(101)...H(113)	315.3(15)	26.5(fixed)	—	1.5	26.5
*u*857	C(17)...H(21)	315.4(15)	27.6(fixed)	—	1.9	27.6
*u*1123	C(246)...H(277)	315.4(74)	32.8(fixed)	—	0.9	32.8
*u*891	C(16)...H(30)	315.6(15)	31.0(fixed)	—	2.7	31.0
*u*1138	C(53)...H(94)	315.7(74)	26.9(fixed)	—	–0.1	26.9
*u*1191	C(110)...H(129)	315.7(73)	27.9(fixed)	—	0.0	27.9
*u*699	C(197)...H(228)	315.8(86)	35.9(fixed)	—	20.8	35.9
*u*1106	C(63)...H(82)	315.8(74)	27.5(fixed)	—	0.2	27.5
*u*884	C(152)...H(171)	315.8(15)	31.4(fixed)	—	3.2	31.4
*u*1157	C(241)...H(282)	315.8(74)	26.3(fixed)	—	0.0	26.3
*u*1160	C(194)...H(235)	316.0(74)	27.7(fixed)	—	0.0	27.7
*u*1105	C(147)...H(188)	316.0(74)	27.3(fixed)	—	0.1	27.3
*u*1118	C(105)...H(136)	316.1(74)	41.6(fixed)	—	3.3	41.6
*u*1024	C(60)...H(84)	316.1(49)	44.5(fixed)	—	3.6	44.5
*u*717	C(60)...H(79)	316.1(42)	35.4(fixed)	—	22.2	35.4

*u*1089	C(111)...H(112)	316.1(73)	29.5(fixed)	—	0.7	29.5
*u*817	Si(98)...H(108)	316.1(20)	21.0(fixed)	—	0.6	21.0
*u*1071	Si(190)...H(220)	316.2(25)	34.3(fixed)	—	3.8	34.3
*u*1151	C(16)...H(35)	316.2(73)	27.5(fixed)	—	0.1	27.5
*u*885	C(11)...H(45)	316.2(104)	33.5(fixed)	—	6.3	33.5
*u*834	C(106)...H(126)	316.3(41)	33.1(fixed)	—	3.9	33.1
*u*1192	Si(51)...H(92)	316.3(37)	30.5(fixed)	—	4.1	30.5
*u*1126	C(100)...H(141)	316.3(73)	26.0(fixed)	—	0.2	26.0
*u*1015	C(58)...H(89)	316.3(74)	27.5(fixed)	—	0.7	27.5
*u*1111	C(6)...H(47)	316.4(73)	25.2(fixed)	—	–0.1	25.2
*u*1245	Si(99)...H(131)	316.4(38)	33.0(fixed)	—	4.0	33.0
*u*929	C(95)...C(110)	316.4(12)	12.4(tied to *u*850)	—	–0.1	10.7
*u*934	C(95)...C(101)	316.4(12)	12.2(tied to *u*850)	—	–0.1	10.5
*u*994	C(95)...C(105)	316.5(12)	12.2(tied to *u*850)	—	–0.1	10.5
*u*993	C(1)...C(11)	316.5(12)	12.4(tied to *u*850)	—	–0.1	10.7
*u*937	C(95)...C(100)	316.5(12)	12.1(tied to *u*850)	—	–0.1	10.4
*u*965	C(95)...C(111)	316.5(12)	12.1(tied to *u*850)	—	0.0	10.5
*u*1099	C(55)...H(75)	316.5(48)	31.6(fixed)	—	0.7	31.6
*u*953	C(1)...C(16)	316.5(12)	12.3(tied to *u*850)	—	–0.1	10.6
*u*992	C(95)...C(104)	316.5(12)	11.9(tied to *u*850)	—	0.0	10.3
*u*1001	C(64)...H(65)	316.5(74)	25.1(fixed)	—	0.5	25.1
*u*971	C(1)...C(17)	316.5(12)	12.2(tied to *u*850)	—	–0.1	10.5
*u*962	C(1)...C(7)	316.5(12)	12.2(tied to *u*850)	—	–0.1	10.5
*u*979	C(1)...C(10)	316.5(12)	12.1(tied to *u*850)	—	0.0	10.5
*u*985	C(1)...C(6)	316.5(12)	12.1(tied to *u*850)	—	0.0	10.4
*u*987	C(189)...C(195)	316.5(12)	12.4(tied to *u*850)	—	–0.1	10.7
*u*719	C(9)...H(42)	316.5(84)	40.4(fixed)	—	27.8	40.4
*u*807	C(104)...H(137)	316.5(15)	37.8(fixed)	—	5.0	37.8
*u*995	C(142)...C(152)	316.6(12)	12.7(tied to *u*850)	—	–0.1	11.0
*u*964	C(189)...C(199)	316.6(12)	12.1(tied to *u*850)	—	–0.1	10.4
*u*1096	C(59)...H(86)	316.6(48)	27.6(fixed)	—	0.2	27.6
*u*940	C(189)...C(194)	316.6(12)	12.0(tied to *u*850)	—	0.0	10.4
*u*997	C(142)...C(147)	316.6(12)	12.3(tied to *u*850)	—	–0.1	10.6
*u*966	C(142)...C(148)	316.6(12)	12.4(tied to *u*850)	—	–0.1	10.7
*u*1014	C(197)...H(212)	316.6(48)	26.5(fixed)	—	0.4	26.5
*u*972	C(236)...C(242)	316.6(12)	12.2(tied to *u*850)	—	–0.1	10.5
*u*967	C(236)...C(246)	316.7(12)	12.1(tied to *u*850)	—	–0.1	10.5
*u*947	C(236)...C(241)	316.7(12)	11.9(tied to *u*850)	—	0.0	10.3
*u*1046	Si(5)...H(14)	316.7(34)	22.0(fixed)	—	0.6	22.0
*u*1063	C(199)...H(230)	316.7(73)	26.3(fixed)	—	0.6	26.3
*u*955	C(48)...C(63)	316.7(12)	12.5(tied to *u*850)	—	–0.1	10.8
*u*914	C(152)...H(183)	316.7(73)	25.0(fixed)	—	0.4	25.0
*u*990	C(48)...C(64)	316.8(12)	12.4(tied to *u*850)	—	–0.1	10.7
*u*991	C(48)...C(54)	316.8(12)	12.3(tied to *u*850)	—	–0.1	10.7
*u*977	C(48)...C(58)	316.8(12)	12.3(tied to *u*850)	—	–0.1	10.6
*u*960	C(48)...C(57)	316.8(12)	12.2(tied to *u*850)	—	–0.1	10.6

*u*998	C(48)...C(53)	316.8(12)	12.0(tied to *u*850)	—	0.0	10.4
*u*958	C(196)...H(216)	316.8(48)	36.6(fixed)	—	2.6	36.6
*u*974	C(17)...H(18)	316.9(73)	24.9(fixed)	—	0.3	24.9
*u*1216	C(56)...H(91)	316.9(82)	46.0(fixed)	—	3.0	46.0
*u*1051	C(7)...H(24)	317.1(87)	37.3(fixed)	—	7.4	37.3
*u*1039	C(56)...H(71)	317.1(48)	26.6(fixed)	—	0.3	26.6
*u*1173	Si(4)...H(45)	317.1(33)	29.5(fixed)	—	3.5	29.5
*u*887	C(10)...H(43)	317.1(15)	35.5(fixed)	—	5.2	35.5
*u*1162	Si(237)...H(267)	317.2(26)	29.9(fixed)	—	3.5	29.9
*u*1172	Si(3)...H(37)	317.4(38)	35.8(fixed)	—	3.2	35.8
*u*973	Si(96)...H(126)	317.5(27)	29.4(fixed)	—	3.2	29.4
*u*1059	H(14)...H(31)	317.6(68)	65.4(fixed)	—	2.9	65.4
*u*1137	Si(96)...H(112)	317.8(17)	33.3(fixed)	—	6.0	33.3
*u*905	C(8)...H(37)	317.9(87)	35.3(fixed)	—	4.9	35.3
*u*1070	Si(143)...H(159)	317.9(20)	31.6(fixed)	—	3.1	31.6
*u*862	H(62)...H(83)	318.0(66)	79.9(fixed)	—	7.9	79.9
*u*1183	Si(98)...H(139)	318.6(33)	30.8(fixed)	—	4.1	30.8
*u*1102	C(102)...H(122)	318.6(48)	27.7(fixed)	—	0.1	27.7
*u*932	Si(97)...Si(99)	318.6(39)	10.9(tied to *u*850)	—	0.0	9.4
*u*922	Si(97)...H(136)	318.6(28)	51.8(fixed)	—	14.0	51.8
*u*851	Si(50)...Si(52)	318.8(39)	11.3(tied to *u*850)	—	0.0	9.8
*u*1084	C(107)...H(131)	318.8(48)	27.9(fixed)	—	0.3	27.9
*u*957	Si(3)...Si(5)	318.8(39)	11.1(tied to *u*850)	—	–0.1	9.6
*u*1135	C(106)...H(133)	318.9(48)	25.3(fixed)	—	–0.1	25.3
*u*1011	C(142)...C(149)	319.2(16)	12.2(tied to *u*850)	—	–0.1	10.5
*u*1023	C(48)...C(56)	319.2(16)	12.7(tied to *u*850)	—	–0.1	10.9
*u*1042	C(142)...C(150)	319.2(16)	12.2(tied to *u*850)	—	–0.1	10.5
*u*1055	C(236)...C(244)	319.2(16)	12.4(tied to *u*850)	—	–0.1	10.7
*u*1049	C(48)...C(60)	319.2(16)	12.6(tied to *u*850)	—	–0.1	10.9
*u*1032	C(48)...C(55)	319.2(16)	12.2(tied to *u*850)	—	–0.1	10.6
*u*1079	C(57)...H(94)	319.2(80)	43.3(fixed)	—	3.5	43.3
*u*1018	C(236)...C(243)	319.2(16)	12.0(tied to *u*850)	—	–0.1	10.4
*u*989	C(103)...H(118)	319.2(48)	27.3(fixed)	—	0.7	27.3
*u*1033	C(48)...C(59)	319.3(16)	12.2(tied to *u*850)	—	–0.1	10.5
*u*1050	C(1)...C(13)	319.3(16)	12.6(tied to *u*850)	—	–0.1	10.9
*u*1044	C(1)...C(12)	319.3(16)	12.4(tied to *u*850)	—	–0.1	10.7
*u*1047	C(189)...C(196)	319.3(16)	12.1(tied to *u*850)	—	–0.1	10.5
*u*1038	C(189)...C(197)	319.3(16)	12.1(tied to *u*850)	—	–0.1	10.5
*u*1030	C(1)...C(8)	319.3(16)	12.2(tied to *u*850)	—	–0.1	10.5
*u*1040	C(1)...C(9)	319.3(16)	12.3(tied to *u*850)	—	–0.1	10.7
*u*1097	C(9)...H(23)	319.5(109)	44.4(fixed)	—	5.5	44.4
*u*1048	C(95)...C(103)	319.5(16)	12.4(tied to *u*850)	—	–0.1	10.7
*u*1037	C(95)...C(102)	319.5(16)	12.1(tied to *u*850)	—	–0.1	10.5
*u*1043	C(95)...C(106)	319.6(16)	12.0(tied to *u*850)	—	–0.1	10.4
*u*1054	C(95)...C(107)	319.6(16)	12.1(tied to *u*850)	—	–0.1	10.5
*u*1003	Si(52)...H(61)	319.7(22)	22.2(fixed)	—	0.4	22.2

*u*976	C(8)...H(23)	319.7(93)	39.4(fixed)	—	10.7	39.4
*u*1122	Si(190)...H(206)	319.7(21)	30.3(fixed)	—	3.9	30.3
*u*1000	Si(192)...H(202)	320.1(18)	20.8(fixed)	—	0.5	20.8
*u*728	C(103)...H(136)	320.2(86)	42.5(fixed)	—	26.7	42.5
*u*1080	C(10)...H(47)	320.3(69)	38.9(fixed)	—	3.2	38.9
*u*883	C(199)...H(233)	320.3(111)	32.9(fixed)	—	8.2	32.9
*u*1186	C(107)...H(112)	320.3(56)	45.5(fixed)	—	5.4	45.5
*u*881	C(17)...H(33)	320.3(107)	35.0(fixed)	—	8.4	35.0
*u*1140	C(243)...H(263)	320.3(47)	27.3(fixed)	—	0.0	27.3
*u*916	Si(97)...H(134)	320.5(38)	29.4(fixed)	—	4.0	29.4
*u*1222	C(104)...H(141)	320.6(72)	44.0(fixed)	—	2.7	44.0
*u*1008	Si(2)...H(15)	320.8(26)	21.6(fixed)	—	0.4	21.6
*u*785	H(108)...H(109)	320.9(48)	31.5(fixed)	—	1.7	31.5
*u*1061	C(244)...H(259)	321.0(47)	25.9(fixed)	—	0.5	25.9
*u*1009	Si(143)...H(173)	321.0(24)	38.8(fixed)	—	10.5	38.8
*u*890	C(246)...H(280)	321.4(117)	31.3(fixed)	—	7.3	31.3
*u*1147	Si(52)...H(80)	321.5(36)	31.9(fixed)	—	4.6	31.9
*u*809	C(12)...H(18)	321.7(92)	33.1(fixed)	—	4.4	33.1
*u*913	C(110)...H(109)	321.7(29)	28.7(fixed)	—	1.4	28.7
*u*1264	Si(51)...H(71)	321.8(39)	30.1(fixed)	—	3.6	30.1
*u*1277	Si(239)...H(272)	322.1(34)	32.2(fixed)	—	3.5	32.2
*u*863	Si(96)...H(109)	322.1(24)	21.0(fixed)	—	0.4	21.0
*u*949	Si(2)...H(32)	322.1(24)	38.6(fixed)	—	10.2	38.6
*u*1119	Si(4)...H(40)	322.2(45)	29.6(fixed)	—	5.4	29.6
*u*1178	Si(5)...H(33)	322.2(35)	33.4(fixed)	—	4.5	33.4
*u*1207	Si(99)...H(127)	322.5(38)	32.8(fixed)	—	4.3	32.8
*u*926	C(105)...H(139)	322.6(109)	33.1(fixed)	—	7.3	33.1
*u*1197	H(84)...H(88)	322.7(56)	67.1(fixed)	—	–1.8	67.1
*u*1174	Si(145)...H(186)	322.9(35)	30.3(fixed)	—	4.4	30.3
*u*1397	C(60)...H(75)	322.9(102)	63.4(fixed)	—	2.6	63.4
*u*900	Si(237)...H(253)	323.1(22)	36.1(fixed)	—	8.2	36.1
*u*1189	Si(192)...H(233)	323.2(37)	32.5(fixed)	—	4.3	32.5
*u*980	Si(49)...H(79)	323.2(26)	41.9(fixed)	—	13.0	41.9
*u*1180	Si(239)...H(280)	323.3(37)	31.9(fixed)	—	3.8	31.9
*u*921	Si(3)...H(42)	323.4(26)	44.0(fixed)	—	16.7	44.0
*u*1231	Si(143)...H(165)	323.6(29)	33.7(fixed)	—	3.7	33.7
*u*923	H(257)...H(280)	323.8(40)	38.8(fixed)	—	4.5	38.8
*u*1250	Si(192)...H(212)	324.0(29)	31.8(fixed)	—	3.8	31.8
*u*1127	Si(145)...H(181)	324.1(41)	30.9(fixed)	—	4.8	30.9
*u*772	C(56)...H(84)	324.1(88)	44.3(fixed)	—	29.4	44.3
*u*897	H(125)...H(127)	324.2(40)	38.4(fixed)	—	4.7	38.4
*u*945	H(116)...H(139)	324.3(40)	37.8(fixed)	—	4.6	37.8
*u*1025	H(69)...H(92)	324.4(40)	38.7(fixed)	—	4.8	38.7
*u*839	H(114)...H(117)	324.5(40)	40.9(fixed)	—	5.6	40.9
*u*825	H(208)...H(211)	324.5(40)	39.4(fixed)	—	4.8	39.4
*u*796	H(126)...H(138)	324.7(41)	54.3(fixed)	—	9.7	54.3

*u*982	H(22)...H(45)	324.8(40)	41.7(fixed)	—	5.3	41.7
*u*1117	Si(51)...H(87)	324.9(41)	30.4(fixed)	—	5.6	30.4
*u*1247	C(199)...H(214)	324.9(40)	46.0(fixed)	—	3.0	46.0
*u*983	H(210)...H(233)	324.9(40)	39.5(fixed)	—	5.2	39.5
*u*1343	H(85)...H(86)	325.0(56)	60.4(fixed)	—	–2.0	60.4
*u*810	H(67)...H(70)	325.0(40)	36.6(fixed)	—	4.9	36.6
*u*793	H(255)...H(258)	325.0(40)	43.6(fixed)	—	7.0	43.6
*u*939	C(111)...H(127)	325.3(114)	33.6(fixed)	—	8.2	33.6
*u*1078	C(16)...H(15)	325.5(34)	31.4(fixed)	—	1.1	31.4
*u*935	Si(237)...H(250)	325.5(24)	21.5(fixed)	—	0.5	21.5
*u*1034	Si(145)...H(156)	325.8(22)	21.6(fixed)	—	0.4	21.6
*u*1083	Si(49)...H(76)	325.9(48)	33.0(fixed)	—	8.3	33.0
*u*894	H(20)...H(23)	326.1(40)	39.7(fixed)	—	6.1	39.7
*u*1260	H(34)...H(42)	326.2(76)	64.3(fixed)	—	–2.5	64.3
*u*1125	Si(4)...H(29)	326.2(42)	29.8(fixed)	—	4.9	29.8
*u*1236	H(213)...H(216)	326.5(55)	56.7(fixed)	—	–1.7	56.7
*u*1068	H(161)...H(164)	326.5(40)	44.9(fixed)	—	8.1	44.9
*u*1163	C(17)...H(14)	326.7(50)	29.2(fixed)	—	2.2	29.2
*u*1066	H(79)...H(91)	326.7(41)	50.3(fixed)	—	10.2	50.3
*u*988	C(102)...H(117)	327.3(88)	34.5(fixed)	—	6.3	34.5
*u*1300	H(212)...H(215)	327.3(55)	53.4(fixed)	—	–1.9	53.4
*u*1148	C(16)...H(39)	327.3(67)	45.9(fixed)	—	3.7	45.9
*u*808	H(31)...H(33)	327.6(40)	46.4(fixed)	—	9.4	46.4
*u*1341	H(38)...H(39)	327.7(55)	43.0(fixed)	—	–2.4	43.0
*u*1136	C(100)...H(118)	327.8(87)	40.7(fixed)	—	3.5	40.7
*u*1161	Si(50)...H(84)	327.8(30)	53.0(fixed)	—	14.7	53.0
*u*1108	Si(98)...H(123)	327.9(41)	31.4(fixed)	—	5.3	31.4
*u*1256	H(128)...H(136)	328.0(76)	63.0(fixed)	—	–1.0	63.0
*u*1141	H(249)...H(250)	328.0(57)	36.2(fixed)	—	0.2	36.2
*u*1361	H(25)...H(28)	328.1(55)	42.6(fixed)	—	–2.2	42.6
*u*867	H(163)...H(186)	328.2(40)	44.9(fixed)	—	9.8	44.9
*u*832	H(78)...H(80)	328.4(41)	48.9(fixed)	—	11.5	48.9
*u*1353	H(72)...H(75)	328.5(55)	48.5(fixed)	—	–2.5	48.5
*u*1103	C(104)...H(138)	328.5(23)	42.4(fixed)	—	1.5	42.4
*u*845	C(55)...H(70)	328.6(122)	36.9(fixed)	—	4.6	36.9
*u*1380	H(35)...H(43)	328.7(76)	59.2(fixed)	—	–1.8	59.2
*u*1312	C(6)...H(14)	328.8(71)	34.0(fixed)	—	0.4	34.0
*u*1177	C(102)...H(133)	329.1(85)	38.8(fixed)	—	3.1	38.8
*u*1154	Si(239)...H(264)	329.2(38)	29.6(fixed)	—	5.2	29.6
*u*1350	H(166)...H(169)	329.3(55)	41.6(fixed)	—	–2.0	41.6
*u*1232	C(244)...H(257)	329.3(42)	43.8(fixed)	—	2.7	43.8
*u*1195	H(24)...H(27)	329.4(55)	43.3(fixed)	—	–0.6	43.3
*u*1112	C(10)...H(44)	329.4(23)	44.1(fixed)	—	2.5	44.1
*u*1166	C(57)...H(61)	329.5(27)	33.1(fixed)	—	1.0	33.1
*u*1476	H(129)...H(137)	329.6(75)	54.8(fixed)	—	–2.2	54.8
*u*1360	C(246)...H(263)	329.6(61)	48.3(fixed)	—	2.2	48.3

*u*1144	C(63)...H(79)	329.8(23)	38.7(fixed)	—	1.9	38.7
*u*1100	H(37)...H(41)	329.8(55)	43.3(fixed)	—	–0.3	43.3
*u*1182	H(165)...H(168)	329.9(55)	43.9(fixed)	—	–0.9	43.9
*u*1092	C(242)...H(255)	329.9(23)	32.6(fixed)	—	0.9	32.6
*u*1175	C(148)...H(156)	330.0(27)	31.8(fixed)	—	1.1	31.8
*u*1170	C(246)...H(266)	330.1(23)	26.0(fixed)	—	–0.1	26.0
*u*1067	C(101)...H(118)	330.1(80)	35.0(fixed)	—	7.3	35.0
*u*1181	C(57)...H(91)	330.1(23)	27.5(fixed)	—	0.1	27.5
*u*1204	C(64)...H(69)	330.2(23)	26.1(fixed)	—	–0.1	26.1
*u*1130	C(195)...H(208)	330.3(23)	26.8(fixed)	—	–0.2	26.8
*u*1116	C(101)...H(114)	330.3(23)	29.3(fixed)	—	0.4	29.3
*u*1098	C(58)...H(78)	330.4(23)	37.7(fixed)	—	2.3	37.7
*u*1184	C(17)...H(22)	330.4(23)	29.6(fixed)	—	0.2	29.6
*u*1121	C(54)...H(67)	330.4(23)	24.7(fixed)	—	–0.1	24.7
*u*1164	C(111)...H(116)	330.4(23)	25.5(fixed)	—	0.0	25.5
*u*1158	C(105)...H(125)	330.6(23)	24.5(fixed)	—	–0.1	24.5
*u*1129	C(147)...H(164)	330.6(23)	34.9(fixed)	—	1.7	34.9
*u*1128	C(16)...H(32)	330.6(23)	34.6(fixed)	—	1.4	34.6
*u*1179	C(199)...H(219)	330.6(23)	26.0(fixed)	—	0.1	26.0
*u*1133	C(152)...H(172)	330.7(23)	34.2(fixed)	—	1.6	34.2
*u*1095	C(11)...H(31)	330.7(23)	34.2(fixed)	—	1.4	34.2
*u*1020	C(241)...H(258)	330.7(23)	25.7(fixed)	—	0.4	25.7
*u*1075	C(57)...H(80)	330.7(23)	27.1(fixed)	—	0.6	27.1
*u*1069	C(242)...H(280)	330.7(23)	26.3(fixed)	—	0.5	26.3
*u*1190	C(148)...H(161)	330.8(23)	24.2(fixed)	—	–0.1	24.2
*u*1082	Si(50)...H(70)	330.8(78)	34.6(fixed)	—	3.8	34.6
*u*1056	C(104)...H(127)	330.8(23)	27.6(fixed)	—	0.6	27.6
*u*1087	C(54)...H(92)	330.8(23)	26.5(fixed)	—	0.6	26.5
*u*1052	C(100)...H(117)	330.9(23)	25.6(fixed)	—	0.4	25.6
*u*1085	C(195)...H(233)	330.9(23)	27.5(fixed)	—	0.6	27.5
*u*986	C(110)...H(126)	330.9(23)	24.8(fixed)	—	0.3	24.8
*u*1088	C(101)...H(139)	331.0(23)	25.9(fixed)	—	0.5	25.9
*u*941	C(53)...H(70)	331.0(23)	26.2(fixed)	—	0.7	26.2
*u*1152	C(7)...H(20)	331.0(23)	24.3(fixed)	—	0.0	24.3
*u*1215	H(71)...H(74)	331.1(55)	46.8(fixed)	—	–0.4	46.8
*u*1227	C(58)...H(73)	331.2(74)	43.7(fixed)	—	3.0	43.7
*u*970	C(194)...H(211)	331.2(23)	26.2(fixed)	—	0.7	26.2
*u*931	H(32)...H(44)	331.2(41)	59.0(fixed)	—	17.1	59.0
*u*1053	C(10)...H(33)	331.2(23)	27.4(fixed)	—	0.7	27.4
*u*1090	C(7)...H(45)	331.3(23)	25.4(fixed)	—	0.4	25.4
*u*1060	C(6)...H(23)	331.3(23)	29.5(fixed)	—	1.1	29.5
*u*1387	H(119)...H(122)	331.3(55)	44.1(fixed)	—	–2.6	44.1
*u*1073	C(148)...H(186)	331.4(23)	26.0(fixed)	—	0.8	26.0
*u*1010	C(59)...H(67)	331.5(54)	36.7(fixed)	—	3.6	36.7
*u*1278	H(253)...H(281)	331.6(75)	49.4(fixed)	—	–1.4	49.4
*u*1124	C(64)...H(61)	331.8(65)	28.0(fixed)	—	2.1	28.0

*u*952	C(241)...H(249)	332.0(35)	30.3(fixed)	—	1.3	30.3
*u*1298	C(53)...H(61)	332.2(49)	34.9(fixed)	—	0.2	34.9
*u*1402	H(82)...H(90)	332.3(75)	43.6(fixed)	—	–2.1	43.6
*u*1305	C(11)...H(28)	332.5(60)	46.4(fixed)	—	2.4	46.4
*u*1143	Si(97)...H(117)	332.7(75)	30.7(fixed)	—	3.6	30.7
*u*1453	H(66)...H(94)	332.9(75)	40.0(fixed)	—	–2.4	40.0
*u*1393	H(254)...H(282)	333.1(75)	44.7(fixed)	—	–1.3	44.7
*u*1074	C(197)...H(232)	333.1(32)	44.1(fixed)	—	3.4	44.1
*u*1077	C(149)...H(185)	333.1(40)	36.8(fixed)	—	3.2	36.8
*u*1091	C(148)...H(176)	333.1(67)	45.0(fixed)	—	3.4	45.0
*u*861	C(110)...H(108)	333.1(48)	25.8(fixed)	—	2.2	25.8
*u*1408	H(160)...H(188)	333.2(75)	41.0(fixed)	—	–2.3	41.0
*u*1165	H(118)...H(121)	333.3(55)	44.9(fixed)	—	–0.3	44.9
*u*1230	H(131)...H(135)	333.3(55)	42.6(fixed)	—	–0.9	42.6
*u*1248	H(112)...H(140)	333.4(75)	46.1(fixed)	—	–1.0	46.1
*u*1159	Si(3)...H(23)	333.5(75)	36.0(fixed)	—	5.8	36.0
*u*1318	C(105)...H(122)	333.5(61)	48.5(fixed)	—	2.3	48.5
*u*1377	H(132)...H(133)	333.6(54)	39.0(fixed)	—	–1.5	39.0
*u*1477	H(207)...H(235)	333.6(74)	40.6(fixed)	—	–2.3	40.6
*u*1379	H(113)...H(141)	333.6(74)	43.0(fixed)	—	–1.6	43.0
*u*1214	C(195)...H(223)	333.7(68)	42.5(fixed)	—	3.3	42.5
*u*1199	H(81)...H(89)	333.8(75)	43.9(fixed)	—	–0.6	43.9
*u*1420	H(260)...H(263)	334.2(54)	41.3(fixed)	—	–2.1	41.3
*u*1193	C(242)...H(270)	334.4(68)	40.4(fixed)	—	2.9	40.4
*u*1665	H(113)...H(131)	334.5(53)	44.3(fixed)	—	4.4	44.3
*u*1406	H(19)...H(47)	334.6(74)	38.1(fixed)	—	–2.0	38.1
*u*1167	C(241)...H(261)	334.8(48)	41.8(fixed)	—	3.1	41.8
*u*1149	C(6)...H(24)	334.9(88)	40.9(fixed)	—	4.3	40.9
*u*1390	H(32)...H(47)	334.9(73)	71.0(fixed)	—	0.7	71.0
*u*1388	H(79)...H(94)	335.0(80)	81.2(fixed)	—	0.3	81.2
*u*1142	C(152)...H(156)	335.2(31)	29.3(fixed)	—	1.8	29.3
*u*1326	H(30)...H(44)	335.2(20)	72.5(fixed)	—	–3.5	72.5
*u*1156	C(196)...H(210)	335.3(33)	41.2(fixed)	—	3.1	41.2
*u*1114	H(65)...H(93)	335.3(75)	40.9(fixed)	—	0.2	40.9
*u*1206	H(206)...H(234)	335.6(75)	41.5(fixed)	—	–0.1	41.5
*u*1086	H(159)...H(187)	335.6(75)	41.4(fixed)	—	0.2	41.4
*u*999	Si(52)...H(62)	335.6(64)	21.0(fixed)	—	0.4	21.0
*u*1139	C(8)...H(36)	335.7(88)	38.2(fixed)	—	3.7	38.2
*u*1185	C(104)...H(108)	335.8(41)	31.6(fixed)	—	0.5	31.6
*u*824	Si(190)...H(217)	335.8(37)	35.0(fixed)	—	14.8	35.0
*u*1205	H(259)...H(262)	336.0(54)	41.5(fixed)	—	–0.3	41.5
*u*1132	H(18)...H(46)	336.0(74)	39.1(fixed)	—	–0.3	39.1
*u*1240	C(150)...H(177)	336.3(42)	44.8(fixed)	—	3.4	44.8
*u*1094	C(194)...H(203)	336.6(43)	25.8(fixed)	—	2.1	25.8
*u*1242	C(63)...H(86)	336.7(38)	45.0(fixed)	—	3.2	45.0
*u*1201	C(101)...H(129)	337.2(78)	43.1(fixed)	—	3.3	43.1

*u*1290	C(147)...H(169)	337.3(32)	43.9(fixed)	—	2.9	43.9
*u*1150	C(10)...H(14)	337.4(72)	34.0(fixed)	—	1.0	34.0
*u*1271	Si(5)...H(24)	337.4(63)	31.9(fixed)	—	4.0	31.9
*u*1468	C(104)...C(111)	337.7(56)	24.7(tied to *u*1411)	—	0.9	22.1
*u*1188	C(59)...H(62)	338.0(70)	32.9(fixed)	—	1.2	32.9
*u*1392	C(12)...H(15)	338.1(73)	36.6(fixed)	—	0.0	36.6
*u*1196	C(7)...H(35)	338.3(72)	43.0(fixed)	—	3.1	43.0
*u*1363	C(10)...C(17)	338.7(50)	22.8(tied to *u*1411)	—	1.4	20.3
*u*1220	C(54)...H(82)	338.9(79)	45.6(fixed)	—	3.0	45.6
*u*1333	H(32)...H(43)	339.0(20)	67.3(fixed)	—	–1.7	67.3
*u*1616	H(30)...H(45)	339.3(54)	53.2(fixed)	—	–1.0	53.2
*u*1203	C(13)...H(15)	339.5(84)	30.7(fixed)	—	1.8	30.7
*u*1285	Si(99)...H(118)	339.7(61)	32.9(fixed)	—	3.6	32.9
*u*1404	H(124)...H(138)	339.8(20)	57.0(fixed)	—	–4.4	57.0
*u*1482	C(106)...C(111)	339.8(67)	26.7(tied to *u*850)	—	1.1	23.1
*u*1631	H(77)...H(92)	340.3(56)	60.8(fixed)	—	–2.1	60.8
*u*1355	H(78)...H(81)	340.6(20)	57.9(fixed)	—	–2.7	57.9
*u*1296	H(79)...H(90)	341.5(20)	57.8(fixed)	—	–1.8	57.8
*u*1436	H(163)...H(187)	341.7(20)	54.3(fixed)	—	–3.2	54.3
*u*1372	C(57)...C(64)	341.9(53)	23.4(tied to *u*1411)	—	1.4	20.9
*u*1308	C(195)...H(203)	342.1(30)	33.2(fixed)	—	0.3	33.2
*u*1330	C(95)...H(127)	342.1(14)	24.2(fixed)	—	0.5	24.2
*u*1297	C(95)...H(117)	342.2(14)	22.7(fixed)	—	0.4	22.7
*u*1320	C(95)...H(126)	342.2(14)	21.5(fixed)	—	0.2	21.5
*u*1319	C(189)...H(211)	342.2(14)	24.0(fixed)	—	0.4	24.0
*u*1244	C(95)...H(141)	342.3(14)	24.5(fixed)	—	0.8	24.5
*u*1302	C(95)...H(139)	342.3(14)	23.1(fixed)	—	0.6	23.1
*u*1310	C(236)...H(268)	342.4(14)	23.7(fixed)	—	0.4	23.7
*u*1403	C(107)...H(114)	342.4(39)	52.2(fixed)	—	3.0	52.2
*u*1331	C(142)...H(159)	342.4(14)	22.5(fixed)	—	0.2	22.5
*u*1315	C(1)...H(18)	342.4(14)	21.8(fixed)	—	0.2	21.8
*u*1306	C(189)...H(221)	342.4(14)	23.8(fixed)	—	0.6	23.8
*u*1223	C(95)...H(116)	342.4(14)	22.9(fixed)	—	0.7	22.9
*u*1303	C(95)...H(136)	342.4(15)	36.5(fixed)	—	3.0	36.5
*u*1405	H(77)...H(91)	342.5(20)	55.1(fixed)	—	–1.7	55.1
*u*1332	C(189)...H(206)	342.5(14)	22.3(fixed)	—	0.4	22.3
*u*1267	C(95)...H(125)	342.5(14)	21.8(fixed)	—	0.5	21.8
*u*1337	C(1)...H(33)	342.5(14)	24.0(fixed)	—	0.6	24.0
*u*1301	C(1)...H(23)	342.5(14)	26.2(fixed)	—	0.9	26.2
*u*1342	C(1)...H(45)	342.5(14)	21.9(fixed)	—	0.3	21.9
*u*1325	C(48)...H(70)	342.5(14)	24.1(fixed)	—	0.3	24.1
*u*1224	C(142)...H(176)	342.5(14)	26.6(fixed)	—	0.9	26.6
*u*1218	C(1)...H(47)	342.5(14)	23.6(fixed)	—	0.6	23.6
*u*1317	C(236)...H(258)	342.6(14)	21.9(fixed)	—	0.4	21.9
*u*1292	C(95)...H(112)	342.7(14)	24.5(fixed)	—	1.1	24.5
*u*1258	C(1)...H(20)	342.7(14)	22.2(fixed)	—	0.6	22.2

*u*1263	C(142)...H(163)	342.7(15)	33.2(fixed)	—	2.2	33.2
*u*1239	C(236)...H(257)	342.7(14)	22.8(fixed)	—	0.7	22.8
*u*1261	C(189)...H(210)	342.8(14)	23.5(fixed)	—	0.9	23.5
*u*1131	C(197)...H(202)	342.8(37)	31.2(fixed)	—	1.3	31.2
*u*1351	C(48)...H(65)	342.8(14)	21.5(fixed)	—	0.3	21.5
*u*1262	C(142)...H(161)	342.8(14)	22.6(fixed)	—	0.6	22.6
*u*1299	C(48)...H(89)	342.8(14)	23.8(fixed)	—	0.6	23.8
*u*1253	C(95)...H(129)	342.9(14)	23.2(fixed)	—	1.1	23.2
*u*1210	C(189)...H(208)	342.9(14)	23.2(fixed)	—	0.9	23.2
*u*1251	C(95)...H(114)	342.9(14)	24.4(fixed)	—	1.3	24.4
*u*1235	C(236)...H(270)	342.9(14)	23.2(fixed)	—	0.9	23.2
*u*1229	C(189)...H(223)	342.9(14)	24.0(fixed)	—	1.1	24.0
*u*1354	C(48)...H(92)	342.9(14)	22.4(fixed)	—	0.5	22.4
*u*1314	C(48)...H(80)	342.9(14)	23.5(fixed)	—	0.6	23.5
*u*1358	C(142)...H(174)	342.9(14)	22.3(fixed)	—	0.6	22.3
*u*1171	C(107)...H(109)	342.9(47)	29.1(fixed)	—	0.8	29.1
*u*1113	C(12)...H(20)	343.0(82)	36.9(fixed)	—	3.6	36.9
*u*1221	C(48)...H(94)	343.0(14)	24.8(fixed)	—	0.9	24.8
*u*1238	C(48)...H(67)	343.1(14)	22.8(fixed)	—	0.7	22.8
*u*1281	H(77)...H(80)	343.1(20)	56.4(fixed)	—	–0.7	56.4
*u*1252	C(1)...H(35)	343.1(14)	23.5(fixed)	—	1.1	23.5
*u*1249	C(48)...H(82)	343.1(14)	24.2(fixed)	—	0.9	24.2
*u*1237	C(48)...H(91)	343.2(14)	24.4(fixed)	—	1.0	24.4
*u*892	C(243)...H(249)	343.2(46)	25.1(fixed)	—	2.6	25.1
*u*1241	C(1)...H(22)	343.2(14)	25.5(fixed)	—	1.5	25.5
*u*1257	C(48)...H(69)	343.3(14)	23.3(fixed)	—	1.0	23.3
*u*1362	H(31)...H(34)	343.3(20)	52.1(fixed)	—	–2.6	52.1
*u*1270	C(9)...H(22)	343.3(96)	52.3(fixed)	—	3.5	52.3
*u*1283	C(1)...H(31)	343.3(14)	28.9(fixed)	—	2.2	28.9
*u*1282	C(236)...H(253)	343.4(14)	26.5(fixed)	—	1.8	26.5
*u*1259	C(236)...H(255)	343.4(14)	26.2(fixed)	—	1.8	26.2
*u*1701	H(112)...H(132)	343.4(47)	40.4(fixed)	—	7.5	40.4
*u*1526	H(39)...H(42)	343.4(56)	92.2(fixed)	—	–1.9	92.2
*u*1272	C(48)...H(78)	343.6(15)	34.2(fixed)	—	3.1	34.2
*u*1288	C(1)...H(32)	343.7(14)	28.4(fixed)	—	2.5	28.4
*u*1627	H(126)...H(141)	343.9(82)	51.9(fixed)	—	2.8	51.9
*u*1265	C(1)...H(44)	343.9(15)	36.7(fixed)	—	4.2	36.7
*u*1375	H(255)...H(256)	344.1(20)	47.7(fixed)	—	–2.4	47.7
*u*1389	C(189)...H(216)	344.1(20)	32.2(fixed)	—	1.1	32.2
*u*1287	C(142)...H(164)	344.1(14)	28.4(fixed)	—	2.7	28.4
*u*1309	C(147)...H(155)	344.1(33)	32.2(fixed)	—	0.4	32.2
*u*1577	H(130)...H(139)	344.2(97)	49.8(fixed)	—	3.5	49.8
*u*1268	H(160)...H(164)	344.3(20)	51.4(fixed)	—	–1.4	51.4
*u*1374	C(1)...H(37)	344.4(20)	23.6(fixed)	—	0.0	23.6
*u*1487	C(56)...C(63)	344.5(75)	26.3(tied to *u*1411)	—	0.8	23.4
*u*1293	C(1)...H(39)	344.5(20)	26.8(fixed)	—	0.6	26.8

*u*1386	C(189)...H(212)	344.6(20)	23.1(fixed)	—	0.2	23.1
*u*1365	C(142)...H(165)	344.6(20)	23.4(fixed)	—	0.2	23.4
*u*1168	H(126)...H(137)	344.6(20)	57.4(fixed)	—	0.6	57.4
*u*1307	C(1)...H(28)	344.7(20)	25.3(fixed)	—	0.5	25.3
*u*1246	H(30)...H(33)	344.8(20)	52.5(fixed)	—	–1.0	52.5
*u*1316	C(48)...H(75)	344.8(20)	30.2(fixed)	—	1.1	30.2
*u*1381	C(1)...H(24)	344.8(20)	22.4(fixed)	—	0.3	22.4
*u*1276	C(48)...H(79)	344.9(14)	30.1(fixed)	—	3.6	30.1
*u*1753	H(72)...H(89)	344.9(87)	42.2(fixed)	—	5.4	42.2
*u*1439	Si(50)...C(63)	345.0(25)	18.6(tied to *u*1411)	—	0.1	16.6
*u*1733	H(114)...H(131)	345.0(66)	45.5(fixed)	—	1.8	45.5
*u*1322	C(48)...H(86)	345.0(20)	26.3(fixed)	—	0.6	26.3
*u*1254	C(103)...H(116)	345.1(94)	42.8(fixed)	—	2.5	42.8
*u*1311	C(142)...H(169)	345.1(20)	22.4(fixed)	—	0.6	22.4
*u*1394	C(236)...H(259)	345.2(20)	23.0(fixed)	—	0.1	23.0
*u*1413	H(161)...H(162)	345.2(20)	48.6(fixed)	—	–1.3	48.6
*u*1369	C(48)...H(71)	345.3(20)	22.0(fixed)	—	0.3	22.0
*u*1329	C(236)...H(263)	345.3(20)	25.1(fixed)	—	0.5	25.1
*u*1280	C(1)...H(42)	345.4(15)	31.9(fixed)	—	4.8	31.9
*u*1626	H(124)...H(139)	345.5(59)	44.1(fixed)	—	3.6	44.1
*u*1383	C(95)...H(131)	345.6(20)	23.7(fixed)	—	0.3	23.7
*u*1243	H(162)...H(186)	345.6(20)	52.2(fixed)	—	0.1	52.2
*u*1399	C(95)...H(118)	345.6(20)	23.1(fixed)	—	0.2	23.1
*u*1335	C(95)...H(133)	345.6(20)	23.6(fixed)	—	0.3	23.6
*u*1368	C(48)...H(84)	345.7(20)	36.4(fixed)	—	3.2	36.4
*u*1485	H(22)...H(46)	345.7(20)	43.1(fixed)	—	–2.5	43.1
*u*1211	C(95)...H(138)	345.7(14)	31.2(fixed)	—	5.3	31.2
*u*1522	H(69)...H(93)	345.7(20)	40.8(fixed)	—	–2.3	40.8
*u*1321	C(95)...H(122)	345.8(20)	25.0(fixed)	—	0.7	25.0
*u*1338	Si(3)...C(16)	345.9(24)	20.0(tied to *u*1411)	—	0.1	17.9
*u*1407	H(114)...H(115)	345.9(20)	43.6(fixed)	—	–2.1	43.6
*u*1228	H(254)...H(258)	345.9(20)	46.8(fixed)	—	–0.8	46.8
*u*1202	C(106)...H(125)	346.0(43)	38.2(fixed)	—	2.5	38.2
*u*1347	Si(49)...C(53)	346.3(21)	19.7(tied to *u*1411)	—	0.3	17.6
*u*1339	C(142)...H(170)	346.3(20)	23.4(fixed)	—	0.6	23.4
*u*1636	H(112)...H(130)	346.4(64)	44.2(fixed)	—	5.1	44.2
*u*1416	H(67)...H(68)	346.4(20)	39.3(fixed)	—	–2.0	39.3
*u*1274	C(48)...H(73)	346.5(20)	23.7(fixed)	—	0.8	23.7
*u*1346	C(236)...H(264)	346.5(20)	22.9(fixed)	—	0.9	22.9
*u*1426	H(208)...H(209)	346.6(20)	40.5(fixed)	—	–2.2	40.5
*u*1764	H(71)...H(90)	346.6(102)	44.5(fixed)	—	3.7	44.5
*u*1450	H(257)...H(281)	346.6(20)	39.7(fixed)	—	–1.9	39.7
*u*1234	C(236)...H(261)	346.6(20)	22.5(fixed)	—	1.0	22.5
*u*1497	Si(99)...C(106)	346.7(32)	18.2(tied to *u*1411)	—	0.2	16.3
*u*1284	C(189)...H(214)	346.7(20)	23.0(fixed)	—	0.9	23.0
*u*1327	C(95)...H(134)	346.7(20)	21.7(fixed)	—	0.5	21.7

*u*1349	C(95)...H(123)	346.7(20)	23.9(fixed)	—	0.8	23.9
*u*1294	Si(97)...C(110)	346.8(27)	19.1(tied to *u*1411)	—	0.3	17.0
*u*1554	H(76)...H(91)	346.8(119)	65.5(fixed)	—	1.6	65.5
*u*1422	H(20)...H(21)	346.8(20)	41.8(fixed)	—	–1.8	41.8
*u*1427	H(116)...H(140)	346.8(20)	40.5(fixed)	—	–1.9	40.5
*u*1348	C(48)...H(87)	346.9(20)	22.6(fixed)	—	1.0	22.6
*u*1255	C(142)...H(167)	346.9(20)	23.0(fixed)	—	1.1	23.0
*u*1336	C(1)...H(29)	346.9(20)	22.4(fixed)	—	0.8	22.4
*u*1456	H(210)...H(234)	346.9(20)	40.5(fixed)	—	–1.9	40.5
*u*1273	C(1)...H(26)	347.0(20)	23.6(fixed)	—	1.1	23.6
*u*1289	C(1)...H(36)	347.0(20)	21.6(fixed)	—	0.9	21.6
*u*1373	C(1)...H(40)	347.0(20)	22.1(fixed)	—	0.9	22.1
*u*1266	C(95)...H(120)	347.2(20)	23.8(fixed)	—	1.3	23.8
*u*1275	C(95)...H(130)	347.2(20)	21.7(fixed)	—	1.1	21.7
*u*1209	H(19)...H(23)	347.2(20)	44.7(fixed)	—	–0.6	44.7
*u*1313	C(48)...H(76)	347.4(20)	25.0(fixed)	—	1.9	25.0
*u*1145	C(55)...H(69)	347.4(115)	39.8(fixed)	—	3.2	39.8
*u*1198	H(68)...H(92)	347.4(20)	42.6(fixed)	—	–0.2	42.6
*u*1219	H(209)...H(233)	347.5(20)	43.8(fixed)	—	–0.5	43.8
*u*1433	H(125)...H(128)	347.5(20)	38.5(fixed)	—	–1.7	38.5
*u*1225	H(113)...H(117)	347.5(20)	43.2(fixed)	—	–0.6	43.2
*u*1107	H(66)...H(70)	347.6(20)	41.9(fixed)	—	–0.2	41.9
*u*1504	H(29)...H(43)	347.7(85)	60.8(fixed)	—	–1.3	60.8
*u*1366	Si(2)...C(6)	347.8(13)	19.3(tied to *u*1411)	—	0.3	17.3
*u*1200	H(124)...H(127)	347.8(20)	41.8(fixed)	—	–0.6	41.8
*u*1660	C(100)...C(106)	348.1(44)	26.2(tied to *u*1411)	—	0.4	23.4
*u*1212	H(256)...H(280)	348.2(20)	40.0(fixed)	—	–0.3	40.0
*u*1470	C(242)...C(244)	348.2(39)	26.0(tied to *u*1411)	—	1.0	23.2
*u*1542	C(56)...C(60)	348.2(65)	30.7(tied to *u*850)	—	1.0	26.6
*u*1226	H(115)...H(139)	348.3(20)	40.2(fixed)	—	–0.5	40.2
*u*1217	H(21)...H(45)	348.4(20)	43.3(fixed)	—	0.2	43.3
*u*1391	H(65)...H(85)	348.5(23)	74.3(fixed)	—	–3.6	74.3
*u*1496	C(196)...C(199)	348.5(46)	27.6(tied to *u*1411)	—	1.1	24.6
*u*1378	Si(143)...C(151)	348.6(18)	20.4(tied to *u*1411)	—	0.1	18.3
*u*1120	H(207)...H(211)	348.7(20)	40.9(fixed)	—	0.0	40.9
*u*1465	C(101)...C(105)	348.8(42)	24.3(tied to *u*1411)	—	1.0	21.7
*u*1370	Si(49)...C(57)	349.0(20)	20.5(tied to *u*1411)	—	0.1	18.3
*u*1445	Si(51)...C(64)	349.0(35)	18.1(tied to *u*1411)	—	0.3	16.2
*u*1459	Si(96)...C(100)	349.1(13)	18.9(tied to *u*1411)	—	0.1	16.8
*u*1474	H(30)...H(40)	349.2(99)	52.5(fixed)	—	4.0	52.5
*u*1483	H(67)...H(84)	349.3(55)	87.6(fixed)	—	–4.9	87.6
*u*1269	C(189)...H(217)	349.4(20)	27.4(fixed)	—	4.3	27.4
*u*1457	C(103)...C(105)	349.4(55)	25.6(tied to *u*1411)	—	1.0	22.9
*u*1481	C(244)...C(246)	349.6(51)	25.6(tied to *u*1411)	—	1.2	22.8
*u*1384	Si(190)...C(198)	349.7(20)	20.6(tied to *u*1411)	—	0.1	18.4
*u*1464	C(9)...C(11)	349.7(49)	25.9(tied to *u*1411)	—	1.2	23.1

*u*1359	Si(2)...C(10)	350.1(19)	20.4(tied to *u*1411)	—	0.1	18.2
*u*1428	Si(3)...C(12)	350.2(37)	22.9(tied to *u*1411)	—	0.2	20.4
*u*1743	H(74)...H(89)	350.2(74)	54.9(fixed)	—	0.4	54.9
*u*1452	Si(237)...C(245)	350.2(21)	19.2(tied to *u*1411)	—	0.1	17.2
*u*1279	C(48)...H(83)	350.3(20)	32.8(fixed)	—	6.0	32.8
*u*1431	Si(4)...C(17)	350.5(29)	17.9(tied to *u*1411)	—	0.3	16.0
*u*1367	Si(143)...C(147)	350.6(15)	19.6(tied to *u*1411)	—	0.2	17.5
*u*1328	Si(97)...C(107)	350.7(32)	18.3(tied to *u*1411)	—	0.4	16.3
*u*1446	C(242)...C(246)	350.8(46)	24.1(tied to *u*1411)	—	0.9	21.6
*u*1541	H(40)...H(43)	350.9(40)	69.9(fixed)	—	–2.1	69.9
*u*1486	C(195)...C(199)	350.9(45)	24.7(tied to *u*1411)	—	1.0	22.1
*u*1334	Si(96)...C(104)	350.9(23)	19.1(tied to *u*1411)	—	0.1	17.1
*u*1441	C(7)...C(11)	351.3(41)	24.5(tied to *u*1411)	—	1.0	21.9
*u*1414	H(164)...H(176)	351.6(61)	79.2(fixed)	—	0.7	79.2
*u*1410	Si(4)...C(13)	351.6(43)	17.2(tied to *u*1411)	—	0.6	15.4
*u*1480	Si(98)...C(111)	351.8(29)	18.2(tied to *u*1411)	—	0.2	16.2
*u*1503	C(55)...C(58)	351.9(50)	25.9(tied to *u*1411)	—	1.0	23.1
*u*1395	Si(190)...C(194)	351.9(17)	18.1(tied to *u*1411)	—	0.3	16.1
*u*1789	H(32)...H(45)	352.1(63)	50.1(fixed)	—	–5.6	50.1
*u*1323	Si(237)...C(241)	352.1(18)	19.2(tied to *u*1411)	—	0.2	17.1
*u*1794	H(75)...H(87)	352.3(92)	71.8(fixed)	—	3.1	71.8
*u*1423	Si(49)...C(56)	352.9(45)	18.3(tied to *u*1411)	—	0.3	16.4
*u*1213	C(6)...H(26)	352.9(69)	44.2(fixed)	—	3.7	44.2
*u*1603	H(21)...H(33)	352.9(43)	55.3(fixed)	—	2.5	55.3
*u*1652	H(214)...H(221)	353.0(70)	55.3(fixed)	—	2.4	55.3
*u*1356	C(13)...C(16)	353.3(31)	23.0(tied to *u*1411)	—	1.9	20.5
*u*1643	H(115)...H(127)	353.4(44)	48.7(fixed)	—	3.7	48.7
*u*1357	C(102)...C(107)	353.5(64)	22.6(tied to *u*1411)	—	1.5	20.2
*u*1352	C(148)...C(152)	353.6(42)	23.6(tied to *u*1411)	—	1.4	21.0
*u*1473	H(77)...H(87)	353.6(48)	55.3(fixed)	—	2.3	55.3
*u*1540	Si(51)...C(55)	353.7(37)	19.3(tied to *u*1411)	—	0.1	17.2
*u*1795	H(263)...H(268)	353.7(81)	58.5(fixed)	—	1.8	58.5
*u*1411	Si(50)...C(59)	354.2(22)	21.7(8)	—	0.1	19.4
*u*1458	Si(52)...C(58)	354.2(32)	18.8(tied to *u*1411)	—	0.2	16.8
*u*1592	H(76)...H(85)	354.2(100)	58.4(fixed)	—	2.0	58.4
*u*1578	H(162)...H(174)	354.2(44)	60.1(fixed)	—	–0.4	60.1
*u*1535	Si(239)...C(247)	354.5(27)	19.2(tied to *u*1411)	—	0.1	17.1
*u*1417	C(241)...C(243)	354.5(37)	24.4(tied to *u*1411)	—	1.2	21.8
*u*1699	H(125)...H(140)	354.5(71)	32.4(fixed)	—	2.7	32.4
*u*1747	H(131)...H(140)	354.5(75)	53.0(fixed)	—	2.7	53.0
*u*1672	H(258)...H(262)	354.6(42)	44.0(fixed)	—	2.0	44.0
*u*1520	H(162)...H(170)	354.6(45)	51.9(fixed)	—	2.5	51.9
*u*1449	Si(145)...C(154)	354.7(33)	17.8(tied to *u*1411)	—	0.4	15.9
*u*1437	Si(51)...C(60)	354.7(33)	17.4(tied to *u*1411)	—	0.5	15.6
*u*1233	H(208)...H(228)	354.9(43)	81.2(fixed)	—	2.3	81.2
*u*1425	Si(145)...C(158)	354.9(31)	18.3(tied to *u*1411)	—	0.3	16.3

*u*1559	H(123)...H(137)	355.0(82)	57.7(fixed)	—	–0.7	57.7
*u*1490	Si(143)...C(149)	355.2(22)	20.3(tied to *u*1411)	—	0.1	18.1
*u*1773	H(207)...H(225)	355.3(42)	43.8(fixed)	—	4.6	43.8
*u*1364	C(195)...C(196)	355.4(28)	23.2(tied to *u*1411)	—	1.5	20.7
*u*1448	C(54)...C(58)	355.4(55)	25.7(tied to *u*1411)	—	1.1	22.9
*u*1461	Si(5)...C(11)	355.4(31)	18.5(tied to *u*1411)	—	0.1	16.5
*u*1731	H(206)...H(226)	355.6(45)	42.8(fixed)	—	4.3	42.8
*u*1155	C(100)...H(120)	355.6(65)	43.7(fixed)	—	3.5	43.7
*u*1931	H(126)...H(139)	355.6(76)	41.2(fixed)	—	–0.6	41.2
*u*1532	Si(192)...C(196)	355.6(21)	19.8(tied to *u*1411)	—	0.2	17.6
*u*1724	C(55)...C(63)	355.9(84)	27.9(tied to *u*1411)	—	0.2	24.9
*u*1376	C(194)...C(201)	355.9(25)	25.0(tied to *u*1411)	—	1.2	22.4
*u*1475	Si(192)...C(205)	356.0(32)	18.0(tied to *u*1411)	—	0.2	16.1
*u*1488	Si(99)...C(105)	356.1(34)	18.3(tied to *u*1411)	—	0.2	16.3
*u*1344	Si(190)...C(197)	356.1(31)	19.4(tied to *u*1411)	—	0.3	17.4
*u*1467	Si(239)...C(252)	356.4(33)	17.7(tied to *u*1411)	—	0.2	15.8
*u*1455	Si(4)...C(9)	356.5(34)	18.1(tied to *u*1411)	—	0.3	16.2
*u*1304	C(54)...H(62)	356.9(107)	32.6(fixed)	—	0.3	32.6
*u*1324	C(147)...C(153)	356.9(26)	21.7(tied to *u*1411)	—	1.5	19.4
*u*1807	H(165)...H(179)	357.0(47)	45.6(fixed)	—	4.0	45.6
*u*1785	H(122)...H(127)	357.0(86)	60.5(fixed)	—	1.4	60.5
*u*1286	C(53)...C(59)	357.1(27)	20.5(tied to *u*1411)	—	2.0	18.3
*u*1466	C(147)...C(150)	357.3(26)	26.1(tied to *u*1411)	—	1.2	23.3
*u*1432	C(60)...C(63)	357.3(35)	24.6(tied to *u*1411)	—	1.3	22.0
*u*1599	Si(3)...H(44)	357.5(37)	66.3(fixed)	—	–1.6	66.3
*u*1762	H(71)...H(91)	357.5(127)	42.0(fixed)	—	1.8	42.0
*u*1570	H(257)...H(264)	357.7(61)	55.5(fixed)	—	2.3	55.5
*u*1653	H(209)...H(221)	357.7(47)	51.7(fixed)	—	3.3	51.7
*u*1759	H(206)...H(229)	357.7(34)	51.3(fixed)	—	–3.1	51.3
*u*1396	Si(98)...H(109)	358.0(19)	20.0(fixed)	—	–0.1	20.0
*u*1545	C(149)...C(154)	358.1(38)	28.7(tied to *u*1411)	—	0.9	25.7
*u*1774	H(28)...H(33)	358.1(75)	58.6(fixed)	—	1.5	58.6
*u*1440	Si(98)...C(103)	358.2(33)	18.1(tied to *u*1411)	—	0.2	16.2
*u*1536	H(29)...H(34)	358.4(52)	48.1(fixed)	—	4.0	48.1
*u*1498	H(123)...H(128)	358.6(59)	47.7(fixed)	—	4.8	47.7
*u*1478	Si(239)...C(244)	358.8(32)	18.2(tied to *u*1411)	—	0.3	16.3
*u*1610	H(256)...H(268)	358.9(49)	46.8(fixed)	—	3.2	46.8
*u*1697	H(254)...H(259)	359.2(39)	51.8(fixed)	—	0.4	51.8
*u*1802	H(79)...H(92)	359.5(77)	52.8(fixed)	—	–7.3	52.8
*u*1837	H(258)...H(260)	359.5(50)	44.6(fixed)	—	3.4	44.6
*u*1675	H(81)...H(92)	359.7(114)	44.2(fixed)	—	4.6	44.2
*u*1382	C(8)...C(12)	359.9(65)	22.6(tied to *u*1411)	—	1.9	20.2
*u*1723	H(73)...H(89)	360.0(126)	42.9(fixed)	—	3.7	42.9
*u*1637	H(211)...H(223)	360.4(63)	52.4(fixed)	—	3.1	52.4
*u*1563	Si(96)...H(141)	360.5(35)	29.8(fixed)	—	4.1	29.8
*u*1596	H(258)...H(270)	360.5(65)	50.8(fixed)	—	2.7	50.8

*u*1735	H(71)...H(81)	360.7(59)	47.9(fixed)	—	2.3	47.9
*u*1606	Si(99)...H(125)	360.8(37)	26.3(fixed)	—	3.0	26.3
*u*1669	H(29)...H(44)	360.9(107)	55.7(fixed)	—	–6.2	55.7
*u*1571	H(68)...H(80)	361.0(56)	49.8(fixed)	—	4.1	49.8
*u*1841	H(256)...H(259)	361.0(54)	45.4(fixed)	—	4.2	45.4
*u*1442	Si(4)...H(15)	361.1(22)	20.8(fixed)	—	–0.2	20.8
*u*1524	H(61)...H(84)	361.1(19)	17.7(fixed)	—	–9.4	17.7
*u*1609	H(23)...H(35)	361.3(63)	61.4(fixed)	—	1.6	61.4
*u*1686	H(212)...H(222)	361.4(55)	49.1(fixed)	—	3.1	49.1
*u*1632	H(76)...H(88)	361.6(69)	49.5(fixed)	—	6.7	49.5
*u*1385	Si(50)...C(54)	361.6(69)	20.5(tied to *u*1411)	—	0.2	18.3
*u*1109	C(53)...H(62)	361.6(87)	26.7(fixed)	—	1.9	26.7
*u*1438	H(211)...H(213)	361.7(29)	47.1(fixed)	—	3.9	47.1
*u*1421	H(253)...H(261)	361.8(62)	67.7(fixed)	—	2.0	67.7
*u*1602	H(117)...H(129)	362.0(65)	52.8(fixed)	—	3.4	52.8
*u*1716	H(132)...H(141)	362.0(87)	34.7(fixed)	—	4.5	34.7
*u*1443	Si(2)...H(47)	362.0(35)	31.1(fixed)	—	3.4	31.1
*u*1956	H(117)...H(127)	362.1(47)	45.4(fixed)	—	–1.2	45.4
*u*1754	H(118)...H(133)	362.1(92)	50.9(fixed)	—	1.0	50.9
*u*1544	H(264)...H(269)	362.5(54)	45.3(fixed)	—	4.9	45.3
*u*1479	Si(51)...H(61)	362.6(19)	21.5(fixed)	—	–0.3	21.5
*u*1613	H(73)...H(80)	362.7(78)	55.6(fixed)	—	2.5	55.6
*u*1454	Si(3)...C(7)	363.0(65)	19.5(tied to *u*1411)	—	0.2	17.4
*u*1491	Si(145)...H(155)	363.1(18)	20.8(fixed)	—	–0.3	20.8
*u*1558	C(10)...C(13)	363.3(77)	23.7(tied to *u*1411)	—	0.8	21.2
*u*1447	Si(49)...H(62)	363.5(43)	21.2(fixed)	—	–0.3	21.2
*u*1508	H(202)...H(227)	363.7(19)	16.8(fixed)	—	–6.6	16.8
*u*1703	C(194)...C(200)	363.9(38)	28.6(tied to *u*1411)	—	0.2	25.5
*u*1484	H(32)...H(41)	363.9(72)	47.0(fixed)	—	15.3	47.0
*u*1444	Si(97)...C(101)	363.9(65)	19.0(tied to *u*1411)	—	0.1	17.0
*u*1501	C(101)...C(103)	363.9(93)	26.5(tied to *u*1411)	—	0.8	23.6
*u*1493	Si(97)...H(138)	363.9(42)	57.1(fixed)	—	0.7	57.1
*u*1401	Si(239)...H(250)	364.0(24)	20.9(fixed)	—	–0.1	20.9
*u*1568	H(254)...H(275)	364.2(74)	48.4(fixed)	—	4.3	48.4
*u*1340	H(119)...H(134)	364.3(65)	49.2(fixed)	—	4.0	49.2
*u*1941	H(23)...H(33)	364.8(44)	47.0(fixed)	—	–3.4	47.0
*u*1400	C(104)...C(106)	364.8(35)	23.2(tied to *u*1411)	—	1.1	20.7
*u*1635	Si(50)...H(91)	365.2(38)	36.2(fixed)	—	0.0	36.2
*u*1656	Si(99)...H(130)	365.2(42)	32.8(fixed)	—	0.6	32.8
*u*1757	C(149)...C(153)	365.3(42)	31.1(tied to *u*1411)	—	–0.1	27.8
*u*1565	C(9)...C(16)	365.3(70)	23.1(tied to *u*1411)	—	0.5	20.6
*u*1714	H(80)...H(93)	365.5(114)	43.9(fixed)	—	5.7	43.9
*u*1516	H(62)...H(75)	365.5(19)	15.6(fixed)	—	–5.2	15.6
*u*1550	Si(97)...H(129)	365.6(30)	27.4(fixed)	—	4.7	27.4
*u*1546	Si(237)...H(282)	365.9(25)	27.5(fixed)	—	4.0	27.5
*u*1748	H(165)...H(177)	365.9(66)	46.4(fixed)	—	2.6	46.4

*u*1537	H(87)...H(90)	366.1(39)	51.4(fixed)	—	4.5	51.4
*u*1615	C(100)...C(107)	366.1(35)	30.5(tied to *u*1411)	—	0.7	27.2
*u*1644	Si(49)...H(78)	366.1(28)	57.5(fixed)	—	–1.5	57.5
*u*1418	Si(97)...H(108)	366.1(29)	20.7(fixed)	—	–0.2	20.7
*u*1412	H(159)...H(179)	366.2(24)	46.8(fixed)	—	3.1	46.8
*u*1752	H(208)...H(225)	366.3(60)	42.7(fixed)	—	2.4	42.7
*u*1345	C(6)...C(12)	366.4(79)	22.2(tied to *u*1411)	—	1.9	19.8
*u*1531	C(7)...C(9)	366.4(94)	27.8(tied to *u*1411)	—	1.0	24.8
*u*1409	Si(190)...H(203)	366.4(24)	20.9(fixed)	—	–0.3	20.9
*u*1633	Si(143)...H(172)	366.6(22)	54.3(fixed)	—	–1.3	54.3
*u*1548	Si(190)...H(235)	366.7(23)	29.0(fixed)	—	4.7	29.0
*u*1511	H(249)...H(274)	366.7(19)	15.2(fixed)	—	–3.6	15.2
*u*1678	H(34)...H(45)	366.7(96)	44.8(fixed)	—	3.3	44.8
*u*1529	H(14)...H(39)	366.8(19)	15.2(fixed)	—	–3.8	15.2
*u*1695	H(31)...H(40)	366.8(118)	44.6(fixed)	—	–0.4	44.6
*u*1419	Si(49)...H(94)	366.8(48)	31.1(fixed)	—	4.5	31.1
*u*1525	H(109)...H(122)	366.8(19)	15.2(fixed)	—	–3.7	15.2
*u*1518	H(61)...H(86)	366.9(19)	15.2(fixed)	—	–3.8	15.2
*u*1556	Si(3)...H(35)	367.0(22)	27.6(fixed)	—	4.8	27.6
*u*1513	H(109)...H(118)	367.0(19)	15.4(fixed)	—	–3.5	15.4
*u*1569	H(161)...H(178)	367.0(43)	50.9(fixed)	—	1.8	50.9
*u*1755	H(206)...H(224)	367.0(55)	42.9(fixed)	—	2.5	42.9
*u*1514	H(108)...H(131)	367.0(19)	15.2(fixed)	—	–3.5	15.2
*u*1499	H(249)...H(272)	367.1(19)	15.2(fixed)	—	–3.2	15.2
*u*1523	H(15)...H(28)	367.1(19)	15.1(fixed)	—	–3.5	15.1
*u*1604	H(116)...H(123)	367.1(92)	55.5(fixed)	—	1.8	55.5
*u*1517	H(155)...H(178)	367.2(19)	15.4(fixed)	—	–3.5	15.4
*u*1507	H(202)...H(225)	367.2(19)	15.2(fixed)	—	–3.3	15.2
*u*1509	H(15)...H(24)	367.2(19)	15.3(fixed)	—	–3.4	15.3
*u*1471	Si(4)...H(14)	367.3(44)	22.1(fixed)	—	–0.3	22.1
*u*1574	C(148)...C(150)	367.3(31)	23.7(tied to *u*1411)	—	0.6	21.2
*u*1519	H(155)...H(180)	367.4(19)	15.1(fixed)	—	–3.3	15.1
*u*1534	Si(5)...C(8)	367.4(52)	19.7(tied to *u*1411)	—	0.2	17.6
*u*1512	H(14)...H(37)	367.5(19)	15.2(fixed)	—	–3.1	15.2
*u*1469	H(164)...H(168)	367.5(31)	45.2(fixed)	—	16.1	45.2
*u*1502	H(108)...H(133)	367.5(19)	15.0(fixed)	—	–3.1	15.0
*u*1515	H(62)...H(71)	367.5(19)	15.2(fixed)	—	–3.2	15.2
*u*1208	H(215)...H(228)	367.5(86)	65.7(fixed)	—	17.4	65.7
*u*1590	H(76)...H(83)	367.6(109)	67.7(fixed)	—	–0.7	67.7
*u*1648	Si(50)...H(86)	367.6(39)	33.0(fixed)	—	4.5	33.0
*u*1720	H(174)...H(187)	367.6(97)	45.4(fixed)	—	5.2	45.4
*u*1555	Si(5)...H(31)	367.8(32)	30.8(fixed)	—	9.6	30.8
*u*1547	H(160)...H(170)	367.8(32)	47.0(fixed)	—	4.9	47.0
*u*1560	C(57)...C(60)	367.9(36)	22.6(tied to *u*1411)	—	0.7	20.2
*u*1576	Si(98)...H(116)	368.1(21)	27.2(fixed)	—	3.6	27.2
*u*1793	H(74)...H(86)	368.1(80)	39.8(fixed)	—	2.3	39.8

*u*1430	Si(143)...H(188)	368.1(19)	33.3(fixed)	—	4.7	33.3
*u*1580	H(31)...H(46)	368.3(62)	35.7(fixed)	—	15.9	35.7
*u*1585	H(167)...H(181)	368.4(49)	57.1(fixed)	—	3.3	57.1
*u*1689	H(116)...H(128)	368.7(48)	32.6(fixed)	—	3.6	32.6
*u*1611	H(210)...H(212)	368.7(43)	54.3(fixed)	—	2.1	54.3
*u*1564	Si(49)...H(67)	368.7(38)	30.5(fixed)	—	0.1	30.5
*u*1868	H(123)...H(127)	368.8(82)	42.3(fixed)	—	–0.9	42.3
*u*1664	H(78)...H(87)	368.9(55)	52.5(fixed)	—	–2.8	52.5
*u*1463	C(197)...C(201)	369.2(72)	22.3(tied to *u*1411)	—	0.7	19.9
*u*1642	H(123)...H(138)	369.2(107)	58.1(fixed)	—	–4.1	58.1
*u*1809	H(165)...H(182)	369.4(46)	50.2(fixed)	—	2.4	50.2
*u*1787	C(242)...C(243)	369.5(45)	30.4(tied to *u*1411)	—	0.0	27.2
*u*1567	Si(50)...H(82)	369.6(26)	28.7(fixed)	—	4.5	28.7
*u*1472	H(253)...H(276)	369.6(66)	44.6(fixed)	—	12.1	44.6
*u*1940	H(258)...H(268)	369.7(64)	44.8(fixed)	—	–1.3	44.8
*u*1552	C(103)...C(110)	369.9(71)	24.0(tied to *u*1411)	—	0.5	21.5
*u*1822	H(258)...H(264)	369.9(68)	43.2(fixed)	—	–1.7	43.2
*u*1586	C(56)...C(59)	370.0(75)	26.0(tied to *u*1411)	—	0.5	23.2
*u*1717	H(86)...H(89)	370.0(56)	58.0(fixed)	—	2.4	58.0
*u*1530	Si(99)...C(102)	370.1(51)	18.7(tied to *u*1411)	—	0.0	16.7
*u*1977	H(211)...H(221)	370.1(55)	45.2(fixed)	—	–1.5	45.2
*u*1510	H(25)...H(37)	370.2(73)	48.2(fixed)	—	3.8	48.2
*u*1415	H(126)...H(132)	370.2(35)	44.7(fixed)	—	2.9	44.7
*u*1581	Si(239)...H(257)	370.5(29)	26.8(fixed)	—	3.6	26.8
*u*1659	H(70)...H(82)	370.7(85)	54.2(fixed)	—	2.6	54.2
*u*1671	H(163)...H(170)	370.8(47)	48.2(fixed)	—	–1.7	48.2
*u*1721	H(262)...H(270)	370.9(66)	33.3(fixed)	—	4.1	33.3
*u*1451	H(79)...H(88)	371.0(40)	47.7(fixed)	—	19.6	47.7
*u*1649	Si(2)...H(31)	371.0(24)	49.2(fixed)	—	–1.2	49.2
*u*1666	C(58)...C(64)	371.0(99)	27.9(tied to *u*1950)	—	0.4	24.5
*u*1398	Si(190)...H(232)	371.0(40)	28.3(fixed)	—	4.3	28.3
*u*1776	Si(190)...H(216)	371.1(41)	54.2(fixed)	—	–3.5	54.2
*u*1623	Si(192)...H(210)	371.1(27)	28.4(fixed)	—	4.1	28.4
*u*1698	H(121)...H(129)	371.3(72)	34.2(fixed)	—	4.8	34.2
*u*1786	H(164)...H(174)	371.3(38)	47.7(fixed)	—	–6.0	47.7
*u*1618	H(22)...H(29)	371.4(97)	59.7(fixed)	—	4.1	59.7
*u*1598	Si(2)...H(20)	371.4(21)	31.1(fixed)	—	0.0	31.1
*u*1641	Si(239)...H(274)	371.6(33)	30.4(fixed)	—	4.2	30.4
*u*1670	Si(51)...H(75)	371.8(60)	35.5(fixed)	—	6.7	35.5
*u*1711	H(256)...H(263)	371.8(52)	35.5(fixed)	—	6.1	35.5
*u*1736	H(213)...H(223)	371.9(62)	36.1(fixed)	—	5.4	36.1
*u*1371	C(54)...C(55)	371.9(109)	22.9(tied to *u*1411)	—	1.4	20.4
*u*1706	Si(96)...H(114)	371.9(22)	39.3(fixed)	—	–0.3	39.3
*u*1601	C(241)...C(248)	371.9(61)	24.2(tied to *u*1411)	—	0.4	21.7
*u*1435	H(27)...H(42)	372.0(80)	51.0(fixed)	—	26.1	51.0
*u*1614	Si(51)...H(94)	372.1(54)	35.3(fixed)	—	0.2	35.3

*u*1910	H(29)...H(33)	372.2(71)	42.2(fixed)	—	–1.0	42.2
*u*1572	Si(143)...H(185)	372.3(38)	28.1(fixed)	—	3.1	28.1
*u*1744	H(75)...H(90)	372.3(103)	39.4(fixed)	—	10.2	39.4
*u*1587	Si(237)...H(255)	372.4(27)	44.4(fixed)	—	–0.5	44.4
*u*1654	H(257)...H(269)	372.4(57)	32.4(fixed)	—	3.9	32.4
*u*1617	Si(97)...H(133)	372.4(44)	32.0(fixed)	—	–0.2	32.0
*u*1865	H(264)...H(268)	372.6(80)	41.0(fixed)	—	0.1	41.0
*u*1538	Si(3)...H(39)	372.6(72)	35.8(fixed)	—	4.5	35.8
*u*1730	H(210)...H(222)	372.8(54)	33.9(fixed)	—	4.2	33.9
*u*1658	Si(4)...H(39)	372.8(68)	36.8(fixed)	—	–0.1	36.8
*u*1591	Si(143)...H(161)	373.0(20)	31.2(fixed)	—	0.1	31.2
*u*1772	H(159)...H(169)	373.0(44)	50.2(fixed)	—	2.6	50.2
*u*1549	Si(52)...H(78)	373.0(35)	36.0(fixed)	—	12.7	36.0
*u*1573	Si(4)...H(22)	373.2(21)	28.6(fixed)	—	6.3	28.6
*u*1710	H(27)...H(35)	373.2(62)	34.2(fixed)	—	5.5	34.2
*u*1750	Si(49)...H(75)	373.3(68)	45.9(fixed)	—	–1.2	45.9
*u*1521	Si(96)...H(120)	373.5(40)	27.1(fixed)	—	5.0	27.1
*u*1639	Si(3)...H(36)	373.5(62)	32.6(fixed)	—	0.2	32.6
*u*1718	H(128)...H(139)	373.6(100)	41.7(fixed)	—	4.3	41.7
*u*1424	H(18)...H(38)	373.6(73)	43.4(fixed)	—	3.9	43.4
*u*1539	Si(49)...H(91)	373.6(41)	28.2(fixed)	—	4.7	28.2
*u*1597	Si(50)...H(83)	373.6(26)	64.3(fixed)	—	1.0	64.3
*u*1800	H(112)...H(135)	373.7(39)	51.7(fixed)	—	4.9	51.7
*u*1460	C(100)...C(102)	373.8(72)	25.1(tied to *u*1411)	—	0.9	22.4
*u*1925	H(76)...H(89)	373.8(120)	48.7(fixed)	—	–4.2	48.7
*u*1527	Si(237)...H(279)	374.0(42)	29.3(fixed)	—	7.9	29.3
*u*1434	H(121)...H(136)	374.0(83)	54.2(fixed)	—	24.5	54.2
*u*1696	H(206)...H(228)	374.1(70)	59.8(fixed)	—	–6.0	59.8
*u*1693	H(221)...H(234)	374.2(106)	42.4(fixed)	—	5.1	42.4
*u*1640	Si(143)...H(169)	374.4(24)	28.4(fixed)	—	3.9	28.4
*u*1619	Si(190)...H(219)	374.5(26)	33.8(fixed)	—	–0.1	33.8
*u*1562	Si(190)...H(208)	374.5(25)	34.4(fixed)	—	0.2	34.4
*u*1588	H(24)...H(36)	374.6(92)	49.6(fixed)	—	2.8	49.6
*u*1923	H(76)...H(87)	374.8(83)	47.4(fixed)	—	0.3	47.4
*u*1662	C(152)...C(158)	374.9(83)	28.1(tied to *u*1950)	—	0.4	24.7
*u*1594	Si(51)...H(69)	374.9(38)	28.3(fixed)	—	4.1	28.3
*u*1702	H(33)...H(46)	375.1(102)	42.5(fixed)	—	6.5	42.5
*u*1663	Si(237)...H(266)	375.1(29)	33.9(fixed)	—	–0.2	33.9
*u*1612	Si(4)...H(47)	375.5(42)	32.4(fixed)	—	0.1	32.4
*u*1690	H(268)...H(281)	375.7(111)	39.9(fixed)	—	4.6	39.9
*u*1495	C(6)...C(8)	375.8(72)	27.5(tied to *u*1950)	—	1.3	24.1
*u*1769	H(21)...H(24)	375.9(102)	49.9(fixed)	—	3.2	49.9
*u*1625	H(108)...H(136)	376.2(64)	61.7(fixed)	—	–8.3	61.7
*u*1291	Si(237)...H(261)	376.3(43)	28.2(fixed)	—	4.4	28.2
*u*2009	H(212)...H(221)	376.7(90)	44.9(fixed)	—	–1.8	44.9
*u*1704	H(117)...H(121)	376.8(119)	47.1(fixed)	—	1.7	47.1

*u*1605	Si(96)...H(125)	376.8(32)	30.9(fixed)	—	–0.3	30.9
*u*1661	H(22)...H(34)	377.0(47)	34.6(fixed)	—	8.1	34.6
*u*1707	Si(98)...H(141)	377.1(42)	35.3(fixed)	—	–0.2	35.3
*u*1751	H(255)...H(275)	377.3(95)	43.2(fixed)	—	0.2	43.2
*u*1500	H(74)...H(84)	377.3(75)	60.8(fixed)	—	25.3	60.8
*u*1742	H(72)...H(82)	377.4(68)	34.4(fixed)	—	5.5	34.4
*u*1628	H(32)...H(39)	377.5(119)	39.8(fixed)	—	10.2	39.8
*u*1792	H(40)...H(42)	377.7(80)	52.2(fixed)	—	–9.3	52.2
*u*1930	H(70)...H(80)	378.0(77)	43.0(fixed)	—	–1.1	43.0
*u*1694	H(216)...H(228)	378.0(93)	43.2(fixed)	—	8.0	43.2
*u*1745	Si(192)...H(214)	378.1(25)	35.3(fixed)	—	0.0	35.3
*u*1505	Si(2)...H(26)	378.2(43)	27.5(fixed)	—	4.7	27.5
*u*1584	H(78)...H(93)	378.3(67)	39.2(fixed)	—	21.3	39.2
*u*1553	Si(192)...H(224)	378.3(40)	27.2(fixed)	—	4.3	27.2
*u*1650	C(11)...C(17)	378.4(85)	27.7(tied to *u*1950)	—	0.4	24.3
*u*1655	Si(143)...H(167)	378.4(25)	35.7(fixed)	—	0.2	35.7
*u*1732	Si(51)...H(73)	378.4(58)	35.6(fixed)	—	0.0	35.6
*u*1708	H(127)...H(140)	378.4(109)	42.7(fixed)	—	5.6	42.7
*u*1622	Si(145)...H(188)	378.7(43)	37.6(fixed)	—	–0.1	37.6
*u*1727	Si(51)...H(86)	378.7(41)	36.7(fixed)	—	–0.3	36.7
*u*1533	Si(145)...H(163)	378.8(23)	34.7(fixed)	—	10.5	34.7
*u*1810	H(253)...H(259)	378.8(60)	49.1(fixed)	—	–3.9	49.1
*u*1779	H(65)...H(84)	379.3(51)	47.5(fixed)	—	–12.6	47.5
*u*1813	H(258)...H(261)	379.5(68)	43.0(fixed)	—	1.7	43.0
*u*1685	H(69)...H(81)	379.6(72)	34.4(fixed)	—	4.2	34.4
*u*1749	Si(145)...H(180)	379.8(41)	32.7(fixed)	—	–0.1	32.7
*u*1607	H(69)...H(71)	379.8(134)	51.3(fixed)	—	2.4	51.3
*u*2075	H(131)...H(139)	379.9(99)	49.4(fixed)	—	–2.1	49.4
*u*1528	Si(145)...H(167)	380.1(38)	26.1(fixed)	—	4.7	26.1
*u*1998	H(71)...H(80)	380.2(104)	44.5(fixed)	—	–2.1	44.5
*u*1673	C(199)...C(205)	380.3(90)	26.4(tied to *u*1950)	—	0.3	23.2
*u*1705	Si(239)...H(271)	380.4(34)	33.0(fixed)	—	0.2	33.0
*u*1295	Si(96)...H(138)	380.5(44)	34.9(fixed)	—	17.1	34.9
*u*1924	H(257)...H(259)	380.6(65)	42.6(fixed)	—	2.2	42.6
*u*1918	H(117)...H(123)	380.8(97)	44.6(fixed)	—	–2.1	44.6
*u*1691	Si(52)...H(82)	381.0(50)	36.4(fixed)	—	–0.2	36.4
*u*1506	H(112)...H(120)	381.1(66)	61.9(fixed)	—	2.9	61.9
*u*1778	H(22)...H(24)	381.2(76)	47.9(fixed)	—	1.1	47.9
*u*1814	H(14)...H(45)	381.2(63)	37.1(fixed)	—	–0.8	37.1
*u*1489	Si(2)...H(44)	381.2(39)	37.9(fixed)	—	17.2	37.9
*u*1668	Si(192)...H(235)	381.3(46)	35.1(fixed)	—	0.1	35.1
*u*1955	C(17)...H(32)	381.3(56)	52.4(fixed)	—	–4.7	52.4
*u*1651	Si(192)...H(216)	381.3(24)	35.4(fixed)	—	9.9	35.4
*u*1768	H(23)...H(25)	381.4(108)	47.0(fixed)	—	7.7	47.0
*u*1734	C(7)...C(8)	381.5(80)	31.4(tied to *u*1950)	—	0.1	27.6
*u*1741	H(23)...H(27)	381.6(121)	52.1(fixed)	—	4.5	52.1

*u*1621	H(120)...H(135)	381.6(82)	31.8(fixed)	—	7.5	31.8
*u*1674	C(246)...C(252)	381.8(95)	24.9(tied to *u*1950)	—	0.3	21.9
*u*1679	Si(99)...H(122)	381.8(59)	30.3(fixed)	—	4.4	30.3
*u*1816	H(211)...H(212)	381.9(42)	40.1(fixed)	—	–1.5	40.1
*u*1726	H(161)...H(168)	382.0(37)	34.3(fixed)	—	2.8	34.3
*u*1763	Si(4)...H(28)	382.1(45)	35.8(fixed)	—	–0.5	35.8
*u*1608	Si(50)...H(69)	382.3(72)	33.3(fixed)	—	0.0	33.3
*u*1667	Si(239)...H(282)	382.3(47)	33.0(fixed)	—	0.0	33.0
*u*1842	C(60)...H(83)	382.4(34)	16.0(fixed)	—	–10.5	16.0
*u*1797	Si(239)...H(263)	382.5(44)	36.5(fixed)	—	–0.6	36.5
*u*1683	Si(5)...H(28)	382.5(60)	31.2(fixed)	—	3.9	31.2
*u*1700	C(105)...C(111)	382.6(89)	26.9(tied to *u*1950)	—	0.3	23.6
*u*1788	H(166)...H(180)	382.7(49)	37.3(fixed)	—	4.1	37.3
*u*1589	H(209)...H(214)	382.8(38)	32.0(fixed)	—	6.6	32.0
*u*1725	H(125)...H(131)	383.1(54)	50.7(fixed)	—	0.7	50.7
*u*1657	Si(3)...H(22)	383.5(62)	40.6(fixed)	—	–0.1	40.6
*u*1878	C(11)...H(44)	383.5(45)	16.1(fixed)	—	–10.5	16.1
*u*1681	Si(5)...H(35)	383.8(47)	34.6(fixed)	—	0.0	34.6
*u*1543	Si(97)...H(114)	383.8(61)	27.6(fixed)	—	5.8	27.6
*u*1575	Si(3)...H(20)	384.0(61)	27.8(fixed)	—	3.1	27.8
*u*1766	H(82)...H(92)	384.0(140)	42.5(fixed)	—	2.2	42.5
*u*1676	H(88)...H(91)	384.2(49)	34.1(fixed)	—	5.4	34.1
*u*1915	C(105)...H(138)	384.4(45)	15.9(fixed)	—	–9.5	15.9
*u*1765	Si(98)...H(122)	384.7(41)	36.1(fixed)	—	–0.6	36.1
*u*1692	Si(99)...H(129)	384.8(52)	34.9(fixed)	—	0.2	34.9
*u*1958	C(64)...H(79)	384.9(62)	58.4(fixed)	—	–6.0	58.4
*u*1715	H(80)...H(94)	385.0(141)	40.9(fixed)	—	3.1	40.9
*u*1805	H(61)...H(92)	385.0(83)	36.9(fixed)	—	–1.3	36.9
*u*1729	H(253)...H(274)	385.1(87)	38.1(fixed)	—	7.8	38.1
*u*1806	H(155)...H(186)	385.2(42)	37.2(fixed)	—	–1.6	37.2
*u*1647	H(164)...H(169)	385.5(39)	40.1(fixed)	—	11.7	40.1
*u*1866	C(196)...H(217)	385.8(34)	14.0(fixed)	—	–7.4	14.0
*u*1780	Si(99)...H(133)	385.8(29)	31.4(fixed)	—	2.9	31.4
*u*1551	H(160)...H(177)	386.0(34)	30.1(fixed)	—	7.6	30.1
*u*1945	H(14)...H(20)	386.1(78)	39.6(fixed)	—	–2.1	39.6
*u*1582	Si(98)...H(130)	386.1(44)	26.0(fixed)	—	4.3	26.0
*u*1783	H(117)...H(119)	386.2(105)	43.1(fixed)	—	2.9	43.1
*u*1629	H(255)...H(260)	386.3(50)	34.5(fixed)	—	11.8	34.5
*u*2023	H(165)...H(181)	386.5(53)	50.4(fixed)	—	–2.0	50.4
*u*1728	H(23)...H(26)	386.5(81)	47.3(fixed)	—	5.4	47.3
*u*1646	Si(97)...H(116)	386.5(62)	33.7(fixed)	—	–0.2	33.7
*u*1928	H(87)...H(89)	386.6(60)	46.6(fixed)	—	–1.2	46.6
*u*2102	H(130)...H(140)	386.7(72)	46.1(fixed)	—	–1.4	46.1
*u*1630	H(79)...H(86)	386.9(49)	42.9(fixed)	—	13.6	42.9
*u*1756	H(113)...H(118)	387.0(101)	51.5(fixed)	—	1.3	51.5
*u*2139	C(111)...H(126)	387.1(67)	32.0(fixed)	—	–1.5	32.0

*u*1922	H(118)...H(134)	387.2(65)	36.9(fixed)	—	–1.8	36.9
*u*1593	H(20)...H(37)	387.2(123)	46.3(fixed)	—	2.8	46.3
*u*1561	Si(5)...H(36)	387.3(71)	26.0(fixed)	—	3.8	26.0
*u*1761	H(174)...H(188)	387.3(111)	41.3(fixed)	—	2.7	41.3
*u*1799	H(114)...H(134)	387.4(58)	56.1(fixed)	—	3.4	56.1
*u*1917	Si(96)...C(111)	387.5(27)	18.6(tied to *u*1950)	—	–0.2	16.4
*u*1620	H(18)...H(26)	387.5(67)	51.4(fixed)	—	4.1	51.4
*u*1462	H(70)...H(72)	387.5(127)	48.3(fixed)	—	3.9	48.3
*u*1937	H(23)...H(29)	387.5(101)	50.6(fixed)	—	–1.1	50.6
*u*1857	C(55)...H(76)	387.7(34)	13.9(fixed)	—	–5.5	13.9
*u*1429	Si(50)...H(67)	387.8(65)	29.2(fixed)	—	3.5	29.2
*u*1831	H(159)...H(178)	388.0(41)	37.6(fixed)	—	–1.9	37.6
*u*1892	C(246)...H(279)	388.2(45)	13.9(fixed)	—	–5.6	13.9
*u*1817	C(12)...H(40)	388.4(34)	13.3(fixed)	—	–3.9	13.3
*u*1851	C(9)...H(26)	388.5(34)	13.0(fixed)	—	–3.8	13.0
*u*1846	C(8)...H(29)	388.6(34)	13.2(fixed)	—	–3.7	13.2
*u*1943	Si(99)...C(104)	388.6(29)	17.3(tied to *u*1950)	—	–0.2	15.2
*u*1557	Si(52)...H(73)	388.7(80)	27.3(fixed)	—	4.1	27.3
*u*1796	Si(2)...C(17)	388.9(27)	20.6(tied to *u*1950)	—	–0.3	18.1
*u*1944	H(159)...H(170)	388.9(50)	42.8(fixed)	—	0.0	42.8
*u*1835	C(150)...H(167)	388.9(34)	13.0(fixed)	—	–3.7	13.0
*u*1836	C(149)...H(170)	389.0(34)	13.2(fixed)	—	–3.7	13.2
*u*1821	C(13)...H(36)	389.0(34)	12.8(fixed)	—	–3.3	12.8
*u*1929	H(61)...H(67)	389.0(64)	37.7(fixed)	—	–2.3	37.7
*u*1840	C(59)...H(87)	389.1(34)	13.4(fixed)	—	–4.0	13.4
*u*1858	Si(5)...C(10)	389.3(25)	16.7(tied to *u*1950)	—	–0.1	14.6
*u*1713	Si(5)...H(26)	389.4(46)	35.8(fixed)	—	0.2	35.8
*u*1566	H(163)...H(175)	389.5(50)	38.1(fixed)	—	18.1	38.1
*u*1767	H(21)...H(28)	389.5(114)	37.9(fixed)	—	3.0	37.9
*u*1860	C(56)...H(73)	389.7(34)	13.0(fixed)	—	–3.6	13.0
*u*1881	C(111)...H(114)	389.7(45)	13.3(fixed)	—	–4.4	13.3
*u*1833	C(102)...H(123)	389.7(33)	13.4(fixed)	—	–4.1	13.4
*u*1853	C(197)...H(214)	389.7(34)	13.1(fixed)	—	–3.6	13.1
*u*1844	C(103)...H(120)	389.8(33)	13.2(fixed)	—	–4.0	13.2
*u*1988	H(83)...H(88)	389.8(48)	30.6(fixed)	—	–12.1	30.6
*u*1863	C(58)...H(91)	389.8(45)	13.3(fixed)	—	–4.0	13.3
*u*1758	H(115)...H(122)	389.9(112)	36.2(fixed)	—	6.1	36.2
*u*1852	C(63)...H(80)	390.0(45)	13.3(fixed)	—	–3.8	13.3
*u*1914	C(110)...H(127)	390.1(45)	13.7(fixed)	—	–4.0	13.7
*u*1883	C(107)...H(130)	390.2(33)	13.0(fixed)	—	–3.6	13.0
*u*1896	C(194)...H(233)	390.2(45)	13.5(fixed)	—	–3.9	13.5
*u*1830	C(53)...H(92)	390.2(45)	13.5(fixed)	—	–3.6	13.5
*u*1645	H(28)...H(42)	390.2(95)	43.6(fixed)	—	20.0	43.6
*u*1819	C(147)...H(186)	390.2(45)	13.5(fixed)	—	–3.8	13.5
*u*1874	C(16)...H(33)	390.2(45)	13.6(fixed)	—	–3.9	13.6
*u*1886	C(241)...H(280)	390.3(45)	13.4(fixed)	—	–3.6	13.4

*u*1777	H(115)...H(118)	390.5(96)	43.3(fixed)	—	5.0	43.3
*u*1872	C(100)...H(139)	390.5(45)	13.3(fixed)	—	–3.6	13.3
*u*1862	C(106)...H(134)	390.6(33)	13.2(fixed)	—	–3.2	13.2
*u*1901	C(199)...H(232)	390.6(45)	13.0(fixed)	—	–3.5	13.0
*u*1843	C(64)...H(67)	390.7(45)	12.9(fixed)	—	–3.2	12.9
*u*1848	Si(97)...C(105)	390.7(22)	17.9(tied to *u*1950)	—	–0.2	15.7
*u*1738	C(101)...C(102)	390.8(75)	28.4(tied to *u*1950)	—	0.0	25.0
*u*1771	H(202)...H(230)	390.8(57)	37.3(fixed)	—	–1.3	37.3
*u*1828	C(152)...H(185)	391.0(45)	12.9(fixed)	—	–3.1	12.9
*u*1873	C(243)...H(264)	391.0(33)	13.3(fixed)	—	–3.8	13.3
*u*1826	C(6)...H(45)	391.0(45)	13.1(fixed)	—	–3.2	13.1
*u*1600	H(26)...H(38)	391.1(87)	30.7(fixed)	—	8.0	30.7
*u*1634	H(207)...H(227)	391.1(36)	40.0(fixed)	—	17.2	40.0
*u*1834	C(17)...H(20)	391.2(45)	12.9(fixed)	—	–3.0	12.9
*u*1875	C(244)...H(261)	391.4(33)	13.0(fixed)	—	–3.4	13.0
*u*1887	Si(3)...C(11)	391.5(16)	17.9(tied to *u*1950)	—	–0.3	15.7
*u*1908	C(10)...H(42)	391.5(10)	16.1(fixed)	—	–10.2	16.1
*u*1850	C(104)...H(136)	391.5(10)	16.8(fixed)	—	–10.0	16.8
*u*1859	Si(52)...C(57)	391.6(27)	17.2(tied to *u*1950)	—	–0.1	15.1
*u*1782	Si(49)...C(64)	391.9(37)	20.0(tied to *u*1950)	—	–0.2	17.6
*u*1861	Si(237)...C(252)	391.9(19)	17.7(tied to *u*1950)	—	–0.2	15.6
*u*1897	Si(190)...C(205)	392.0(17)	18.5(tied to *u*1950)	—	–0.2	16.3
*u*1680	H(75)...H(84)	392.3(111)	49.2(fixed)	—	19.5	49.2
*u*1939	H(113)...H(133)	392.9(52)	40.8(fixed)	—	0.8	40.8
*u*1950	Si(50)...C(60)	393.0(31)	20.4(7)	17.9(18)	–0.4	17.9
*u*1904	C(63)...H(78)	393.1(10)	15.2(fixed)	—	–8.3	15.2
*u*1790	Si(143)...C(158)	393.3(14)	20.9(tied to *u*1950)	—	–0.3	18.3
*u*1900	C(58)...H(79)	393.4(10)	15.2(fixed)	—	–8.0	15.2
*u*1688	Si(96)...C(110)	393.5(32)	18.7(tied to *u*1950)	—	–0.2	16.5
*u*1909	H(126)...H(131)	393.6(53)	38.5(fixed)	—	–2.1	38.5
*u*1811	H(15)...H(40)	393.7(110)	39.9(fixed)	—	–1.6	39.9
*u*2068	H(77)...H(94)	393.7(91)	47.5(fixed)	—	–9.5	47.5
*u*1933	Si(98)...C(101)	393.7(17)	17.5(tied to *u*1950)	—	–0.2	15.3
*u*1920	Si(50)...C(58)	393.8(19)	18.2(tied to *u*1950)	—	–0.2	16.0
*u*1494	Si(52)...H(83)	393.9(38)	33.8(fixed)	—	19.3	33.8
*u*2094	H(213)...H(217)	393.9(48)	27.3(fixed)	—	–8.8	27.3
*u*2194	H(74)...H(91)	393.9(83)	52.2(fixed)	—	–5.9	52.2
*u*1624	H(249)...H(259)	394.1(64)	37.0(fixed)	—	–0.8	37.0
*u*1739	H(19)...H(24)	394.2(101)	49.2(fixed)	—	3.9	49.2
*u*1902	C(147)...H(163)	394.4(10)	14.7(fixed)	—	–7.2	14.7
*u*1684	Si(99)...H(120)	394.5(42)	35.6(fixed)	—	0.4	35.6
*u*1737	H(35)...H(45)	394.5(116)	41.2(fixed)	—	1.3	41.2
*u*1798	Si(2)...C(16)	394.5(29)	16.8(tied to *u*1950)	—	–0.1	14.7
*u*1682	H(122)...H(136)	394.6(95)	44.3(fixed)	—	18.6	44.3
*u*1984	H(15)...H(36)	394.6(101)	41.9(fixed)	—	–2.3	41.9
*u*1912	C(152)...H(173)	394.7(10)	14.4(fixed)	—	–6.9	14.4

*u*1890	C(11)...H(32)	394.9(10)	14.8(fixed)	—	–6.8	14.8
*u*1820	Si(237)...C(251)	395.0(31)	17.2(tied to *u*1950)	—	–0.2	15.1
*u*1709	H(221)...H(235)	395.1(123)	42.3(fixed)	—	3.0	42.3
*u*1770	Si(190)...C(204)	395.1(30)	18.5(tied to *u*1950)	—	–0.1	16.3
*u*1894	C(16)...H(31)	395.1(10)	14.8(fixed)	—	–6.7	14.8
*u*2010	H(34)...H(44)	395.1(53)	31.4(fixed)	—	–12.0	31.4
*u*1971	H(112)...H(118)	395.3(79)	49.1(fixed)	—	–3.4	49.1
*u*1960	Si(51)...C(56)	395.3(45)	19.1(tied to *u*1950)	—	–0.3	16.8
*u*1926	Si(4)...C(7)	395.5(16)	17.4(tied to *u*1950)	—	–0.2	15.3
*u*1638	H(124)...H(130)	395.7(50)	32.0(fixed)	—	5.9	32.0
*u*1804	H(108)...H(125)	395.7(49)	37.9(fixed)	—	–2.1	37.9
*u*1885	C(242)...H(253)	395.9(10)	13.8(fixed)	—	–5.7	13.8
*u*2148	C(106)...H(139)	396.0(83)	35.6(fixed)	—	–2.0	35.6
*u*1818	Si(96)...C(102)	396.0(30)	17.2(tied to *u*1950)	—	–0.2	15.1
*u*1935	Si(239)...C(242)	396.0(23)	17.3(tied to *u*1950)	—	–0.2	15.2
*u*2092	H(39)...H(43)	396.2(84)	49.6(fixed)	—	–12.4	49.6
*u*1952	Si(192)...C(195)	396.2(21)	17.6(tied to *u*1950)	—	–0.2	15.4
*u*2082	H(128)...H(138)	396.2(53)	29.9(fixed)	—	–11.1	29.9
*u*1949	Si(239)...C(248)	396.2(25)	18.4(tied to *u*1950)	—	–0.2	16.2
*u*2028	C(13)...H(42)	396.3(47)	63.1(fixed)	—	–8.4	63.1
*u*1919	H(24)...H(37)	396.4(106)	39.4(fixed)	—	–1.4	39.4
*u*1832	Si(49)...C(63)	396.6(30)	17.8(tied to *u*1950)	—	–0.3	15.6
*u*1906	Si(143)...C(157)	396.7(28)	18.3(tied to *u*1950)	—	–0.2	16.1
*u*2062	H(72)...H(76)	396.7(48)	27.3(fixed)	—	–5.8	27.3
*u*1905	C(17)...H(23)	397.0(10)	14.1(fixed)	—	–4.9	14.1
*u*1719	H(268)...H(282)	397.0(130)	40.0(fixed)	—	2.6	40.0
*u*1888	C(6)...H(22)	397.2(10)	13.4(fixed)	—	–4.7	13.4
*u*1882	C(101)...H(112)	397.3(10)	13.5(fixed)	—	–4.5	13.5
*u*1932	H(67)...H(85)	397.3(65)	46.7(fixed)	—	–13.8	46.7
*u*2113	C(63)...H(76)	397.4(104)	44.4(fixed)	—	–3.9	44.4
*u*1838	Si(3)...C(13)	397.5(55)	22.4(tied to *u*1950)	—	–0.4	19.7
*u*1712	H(33)...H(47)	397.5(118)	40.5(fixed)	—	4.0	40.5
*u*1898	C(57)...H(89)	397.6(10)	13.7(fixed)	—	–3.9	13.7
*u*1722	H(117)...H(120)	397.6(72)	43.6(fixed)	—	1.7	43.6
*u*1884	C(57)...H(82)	397.7(10)	13.1(fixed)	—	–3.9	13.1
*u*1907	C(148)...H(188)	397.8(10)	13.3(fixed)	—	–4.0	13.3
*u*1913	C(54)...H(94)	397.8(10)	13.2(fixed)	—	–3.7	13.2
*u*1903	C(195)...H(235)	397.8(10)	13.2(fixed)	—	–3.9	13.2
*u*1889	C(64)...H(70)	397.9(10)	13.7(fixed)	—	–3.6	13.7
*u*1825	Si(145)...C(148)	397.9(19)	17.2(tied to *u*1950)	—	–0.1	15.1
*u*1961	H(38)...H(40)	397.9(48)	25.7(fixed)	—	–3.9	25.7
*u*1877	C(10)...H(35)	398.0(10)	13.3(fixed)	—	–3.9	13.3
*u*1891	C(104)...H(129)	398.0(10)	13.1(fixed)	—	–3.8	13.1
*u*1839	C(53)...H(69)	398.0(10)	13.0(fixed)	—	–3.5	13.0
*u*1899	C(242)...H(282)	398.1(10)	13.1(fixed)	—	–3.5	13.1
*u*1867	C(199)...H(220)	398.1(10)	13.6(fixed)	—	–3.6	13.6

*u*1895	C(101)...H(141)	398.1(10)	13.1(fixed)	—	–3.6	13.1
*u*1847	C(194)...H(210)	398.2(10)	13.1(fixed)	—	–3.6	13.1
*u*2044	H(25)...H(29)	398.2(48)	26.6(fixed)	—	–3.4	26.6
*u*1829	C(195)...H(206)	398.3(10)	13.3(fixed)	—	–3.4	13.3
*u*2181	C(103)...H(127)	398.3(72)	36.3(fixed)	—	–2.8	36.3
*u*2007	H(26)...H(27)	398.4(48)	25.2(fixed)	—	–3.5	25.2
*u*1869	C(241)...H(257)	398.4(10)	13.0(fixed)	—	–3.2	13.0
*u*1959	C(152)...H(164)	398.4(39)	53.3(fixed)	—	–5.4	53.3
*u*1870	C(246)...H(267)	398.4(10)	13.2(fixed)	—	–3.2	13.2
*u*1823	C(54)...H(65)	398.5(10)	13.3(fixed)	—	–3.1	13.3
*u*1876	C(111)...H(117)	398.5(10)	13.2(fixed)	—	–3.3	13.2
*u*1978	C(1)...H(43)	398.6(10)	15.6(fixed)	—	–9.6	15.6
*u*2189	C(244)...H(268)	398.6(67)	34.8(fixed)	—	–2.0	34.8
*u*1803	H(109)...H(133)	398.6(55)	36.3(fixed)	—	–2.2	36.3
*u*1880	C(100)...H(116)	398.6(10)	12.9(fixed)	—	–3.2	12.9
*u*1934	Si(51)...C(54)	398.6(28)	15.6(fixed)	—	–0.1	15.6
*u*2011	H(167)...H(168)	398.6(48)	25.6(fixed)	—	–3.7	25.6
*u*2138	C(105)...H(117)	398.7(38)	33.8(fixed)	—	–1.8	33.8
*u*1911	C(7)...H(47)	398.7(10)	13.1(fixed)	—	–3.2	13.1
*u*1871	C(148)...H(159)	398.7(10)	13.4(fixed)	—	–3.0	13.4
*u*2058	H(166)...H(170)	398.8(48)	26.6(fixed)	—	–3.4	26.6
*u*1579	H(19)...H(36)	398.8(116)	30.5(fixed)	—	6.0	30.5
*u*1855	C(105)...H(126)	398.9(10)	13.2(fixed)	—	–2.9	13.2
*u*1856	C(110)...H(125)	398.9(10)	12.9(fixed)	—	–2.9	12.9
*u*2050	H(119)...H(123)	398.9(47)	27.4(fixed)	—	–3.9	27.4
*u*1854	C(7)...H(18)	398.9(10)	13.2(fixed)	—	–3.0	13.2
*u*1968	C(95)...H(137)	399.0(10)	15.7(fixed)	—	–9.2	15.7
*u*1953	Si(143)...C(150)	399.0(19)	19.1(tied to *u*1950)	—	–0.3	16.8
*u*2073	H(30)...H(47)	399.1(76)	42.5(fixed)	—	–7.0	42.5
*u*1677	Si(237)...C(243)	399.1(33)	18.7(tied to *u*1950)	—	–0.1	16.4
*u*1948	H(36)...H(41)	399.2(48)	24.6(fixed)	—	–2.7	24.6
*u*1995	H(120)...H(121)	399.3(47)	26.0(fixed)	—	–3.7	26.0
*u*2172	C(196)...H(221)	399.5(67)	37.1(fixed)	—	–2.4	37.1
*u*2019	H(130)...H(135)	399.5(47)	24.6(fixed)	—	–3.6	24.6
*u*1815	Si(2)...C(8)	399.6(32)	17.3(tied to *u*1950)	—	–0.2	15.2
*u*2129	C(11)...H(23)	399.7(38)	40.7(fixed)	—	–3.8	40.7
*u*2022	C(48)...H(85)	399.8(13)	15.9(fixed)	—	–10.0	15.9
*u*1791	H(116)...H(118)	399.9(68)	41.3(fixed)	—	3.1	41.3
*u*1936	H(155)...H(161)	400.2(40)	37.9(fixed)	—	–2.0	37.9
*u*2025	C(53)...H(84)	400.2(37)	62.6(fixed)	—	–11.0	62.6
*u*2101	H(214)...H(215)	400.3(48)	31.1(fixed)	—	–1.9	31.1
*u*1775	H(108)...H(137)	400.3(41)	47.1(fixed)	—	–9.2	47.1
*u*2190	C(9)...H(33)	400.3(60)	36.2(fixed)	—	–2.5	36.2
*u*2208	C(56)...H(87)	400.3(68)	38.7(fixed)	—	–2.5	38.7
*u*1879	Si(192)...C(200)	400.4(29)	17.5(tied to *u*1950)	—	–0.1	15.4
*u*1583	H(41)...H(44)	400.4(42)	44.9(fixed)	—	29.2	44.9

*u*2048	H(132)...H(134)	400.4(47)	25.2(fixed)	—	–2.7	25.2
*u*2077	H(112)...H(134)	400.4(72)	50.3(fixed)	—	–0.2	50.3
*u*2039	H(73)...H(74)	400.4(48)	26.7(fixed)	—	–2.1	26.7
*u*2076	H(260)...H(264)	400.5(47)	26.4(fixed)	—	–3.7	26.4
*u*2106	C(242)...H(264)	400.5(53)	37.9(fixed)	—	–2.1	37.9
*u*1985	C(48)...H(77)	400.6(10)	14.6(fixed)	—	–7.8	14.6
*u*1947	H(202)...H(219)	401.0(36)	39.4(fixed)	—	–2.6	39.4
*u*1740	H(129)...H(139)	401.2(123)	42.7(fixed)	—	2.4	42.7
*u*1927	Si(192)...C(197)	401.3(17)	18.0(tied to *u*1950)	—	–0.2	15.8
*u*2033	H(261)...H(262)	401.3(47)	25.2(fixed)	—	–3.0	25.2
*u*2038	H(255)...H(281)	401.4(53)	27.0(fixed)	—	–5.9	27.0
*u*2131	C(246)...H(258)	401.4(52)	33.6(fixed)	—	–1.9	33.6
*u*1990	C(142)...H(162)	401.6(10)	14.3(fixed)	—	–6.7	14.3
*u*1812	C(194)...H(228)	401.7(42)	62.2(fixed)	—	–4.3	62.2
*u*2173	C(199)...H(211)	401.7(47)	33.3(fixed)	—	–2.1	33.3
*u*1808	Si(52)...C(59)	401.8(27)	16.4(tied to *u*1950)	—	0.0	14.4
*u*2027	H(85)...H(87)	401.8(48)	35.1(fixed)	—	0.6	35.1
*u*1827	Si(145)...C(149)	401.8(27)	16.8(tied to *u*1950)	—	–0.1	14.7
*u*1849	H(70)...H(71)	401.9(128)	40.6(fixed)	—	–1.3	40.6
*u*2255	C(100)...H(130)	401.9(56)	37.4(fixed)	—	–2.4	37.4
*u*1997	C(1)...H(30)	402.1(10)	14.1(fixed)	—	–6.2	14.1
*u*1595	H(68)...H(73)	402.4(138)	31.4(fixed)	—	6.3	31.4
*u*2069	H(124)...H(136)	402.4(17)	33.9(fixed)	—	–11.4	33.9
*u*1760	H(127)...H(141)	402.6(124)	41.1(fixed)	—	3.3	41.1
*u*1824	H(18)...H(37)	403.1(113)	37.3(fixed)	—	–0.9	37.3
*u*2021	C(189)...H(215)	403.2(13)	14.1(fixed)	—	–6.9	14.1
*u*2052	H(81)...H(91)	403.3(53)	25.9(fixed)	—	–3.8	25.9
*u*2078	H(80)...H(90)	403.3(53)	27.4(fixed)	—	–3.6	27.4
*u*2042	H(66)...H(92)	403.4(53)	26.7(fixed)	—	–3.6	26.7
*u*2051	H(114)...H(140)	403.4(53)	26.1(fixed)	—	–4.5	26.1
*u*2079	H(30)...H(42)	403.5(17)	32.7(fixed)	—	–10.5	32.7
*u*1973	C(236)...H(254)	403.5(10)	13.2(fixed)	—	–5.0	13.2
*u*2000	H(160)...H(186)	403.7(53)	26.3(fixed)	—	–3.8	26.3
*u*1981	C(1)...H(21)	403.9(10)	13.3(fixed)	—	–4.5	13.3
*u*2104	H(207)...H(233)	403.9(53)	26.7(fixed)	—	–3.8	26.7
*u*1746	H(20)...H(25)	404.0(87)	34.9(fixed)	—	3.0	34.9
*u*1970	C(95)...H(113)	404.3(10)	13.1(fixed)	—	–4.0	13.1
*u*2098	H(79)...H(81)	404.4(17)	30.2(fixed)	—	–9.2	30.2
*u*1687	H(114)...H(119)	404.4(87)	33.9(fixed)	—	7.1	33.9
*u*2049	H(78)...H(90)	404.4(17)	30.2(fixed)	—	–9.2	30.2
*u*1972	H(67)...H(93)	404.5(53)	24.7(fixed)	—	–2.8	24.7
*u*2020	C(48)...H(74)	404.7(13)	13.6(fixed)	—	–5.3	13.6
*u*2002	C(1)...H(34)	404.7(10)	13.2(fixed)	—	–3.6	13.2
*u*1994	C(142)...H(175)	404.8(10)	13.5(fixed)	—	–3.6	13.5
*u*2015	H(19)...H(45)	404.8(53)	25.7(fixed)	—	–3.1	25.7
*u*2085	H(208)...H(234)	404.8(53)	25.2(fixed)	—	–3.1	25.2

*u*1974	C(48)...H(90)	404.9(10)	13.2(fixed)	—	–3.7	13.2
*u*1976	C(243)...H(253)	404.9(51)	48.8(fixed)	—	–3.5	48.8
*u*2006	C(95)...H(128)	404.9(10)	13.0(fixed)	—	–3.5	13.0
*u*1975	C(95)...H(140)	405.0(10)	13.0(fixed)	—	–3.4	13.0
*u*1982	C(189)...H(222)	405.0(10)	13.0(fixed)	—	–3.5	13.0
*u*2066	H(113)...H(139)	405.0(53)	27.1(fixed)	—	–2.8	27.1
*u*1991	C(48)...H(81)	405.0(10)	13.0(fixed)	—	–3.5	13.0
*u*1992	C(48)...H(93)	405.1(10)	13.2(fixed)	—	–3.4	13.2
*u*1993	C(189)...H(209)	405.1(10)	13.0(fixed)	—	–3.4	13.0
*u*1966	H(20)...H(46)	405.2(53)	24.4(fixed)	—	–2.9	24.4
*u*2001	C(48)...H(68)	405.2(10)	13.1(fixed)	—	–3.3	13.1
*u*1983	C(236)...H(269)	405.2(10)	13.0(fixed)	—	–3.3	13.0
*u*2054	H(254)...H(280)	405.3(53)	28.0(fixed)	—	–1.9	28.0
*u*1957	H(161)...H(187)	405.3(53)	24.5(fixed)	—	–2.4	24.5
*u*1965	C(189)...H(207)	405.4(10)	13.0(fixed)	—	–3.1	13.0
*u*1969	C(95)...H(115)	405.4(10)	12.8(fixed)	—	–3.0	12.8
*u*1979	C(1)...H(46)	405.4(10)	13.0(fixed)	—	–2.9	13.0
*u*1845	Si(97)...C(100)	405.5(51)	17.5(tied to *u*1950)	—	–0.2	15.3
*u*1989	C(236)...H(256)	405.6(10)	12.9(fixed)	—	–2.9	12.9
*u*1986	C(1)...H(19)	405.6(10)	12.8(fixed)	—	–2.8	12.8
*u*1999	C(142)...H(160)	405.6(10)	12.9(fixed)	—	–2.8	12.9
*u*2003	C(95)...H(124)	405.7(10)	12.8(fixed)	—	–2.7	12.8
*u*1996	C(48)...H(66)	405.7(10)	12.9(fixed)	—	–2.8	12.9
*u*1964	Si(99)...C(103)	405.8(51)	16.3(fixed)	—	–0.3	16.3
*u*2310	H(75)...H(88)	405.8(116)	68.9(fixed)	—	–3.8	68.9
*u*2149	C(55)...H(80)	405.8(69)	37.7(fixed)	—	–2.4	37.7
*u*2312	C(106)...H(114)	405.9(49)	40.5(fixed)	—	–3.7	40.5
*u*1916	Si(98)...C(106)	406.1(31)	17.2(tied to *u*1950)	—	–0.2	15.1
*u*2005	H(14)...H(46)	406.1(47)	37.3(fixed)	—	–1.0	37.3
*u*2112	H(164)...H(187)	406.1(17)	30.6(fixed)	—	–7.9	30.6
*u*2013	H(160)...H(163)	406.1(17)	28.7(fixed)	—	–8.2	28.7
*u*2041	C(48)...H(88)	406.2(13)	13.2(fixed)	—	–3.8	13.2
*u*2157	H(214)...H(222)	406.2(34)	53.0(fixed)	—	–2.5	53.0
*u*2040	C(1)...H(41)	406.3(13)	13.3(fixed)	—	–3.8	13.3
*u*2047	C(236)...H(262)	406.5(13)	13.1(fixed)	—	–3.6	13.1
*u*2037	C(95)...H(121)	406.5(13)	13.2(fixed)	—	–3.8	13.2
*u*2008	C(142)...H(166)	406.6(13)	13.1(fixed)	—	–3.4	13.1
*u*2030	C(1)...H(27)	406.6(13)	13.0(fixed)	—	–3.5	13.0
*u*2016	C(95)...H(119)	406.8(13)	13.3(fixed)	—	–3.6	13.3
*u*2014	C(1)...H(25)	406.8(13)	13.1(fixed)	—	–3.4	13.1
*u*2029	C(142)...H(168)	406.8(13)	12.9(fixed)	—	–3.3	12.9
*u*2100	H(127)...H(137)	406.8(53)	32.5(fixed)	—	–0.2	32.5
*u*2018	C(48)...H(72)	406.9(13)	13.0(fixed)	—	–3.2	13.0
*u*2153	H(124)...H(141)	406.9(78)	47.5(fixed)	—	–1.4	47.5
*u*2012	C(236)...H(260)	406.9(13)	13.1(fixed)	—	–3.2	13.1
*u*2034	H(33)...H(43)	406.9(53)	34.6(fixed)	—	0.3	34.6

*u*2093	H(32)...H(34)	407.0(17)	29.8(fixed)	—	–7.5	29.8
*u*2032	C(189)...H(213)	407.0(13)	13.1(fixed)	—	–3.2	13.1
*u*2026	C(95)...H(132)	407.1(13)	13.0(fixed)	—	–3.3	13.0
*u*2024	C(1)...H(38)	407.1(13)	13.0(fixed)	—	–3.0	13.0
*u*1864	Si(5)...C(12)	407.2(51)	17.0(tied to *u*1950)	—	0.0	14.9
*u*2241	H(35)...H(44)	407.2(70)	30.9(fixed)	—	–12.9	30.9
*u*1980	Si(5)...C(9)	407.3(51)	19.1(tied to *u*1950)	—	–0.3	16.8
*u*2045	C(95)...H(135)	407.3(13)	12.9(fixed)	—	–3.0	12.9
*u*1921	Si(3)...C(6)	407.4(51)	18.3(tied to *u*1950)	—	–0.2	16.0
*u*2086	Si(99)...C(107)	407.7(20)	19.9(tied to *u*1950)	—	–0.3	17.4
*u*2103	H(253)...H(256)	407.8(17)	27.7(fixed)	—	–6.4	27.7
*u*2242	H(14)...H(19)	407.9(68)	39.4(fixed)	—	–2.5	39.4
*u*2182	H(83)...H(86)	408.1(44)	32.2(fixed)	—	–12.8	32.2
*u*2252	H(129)...H(138)	408.2(70)	31.7(fixed)	—	–11.4	31.7
*u*2123	H(208)...H(229)	408.4(42)	47.1(fixed)	—	–9.3	47.1
*u*2059	H(18)...H(24)	408.9(80)	44.2(fixed)	—	–0.6	44.2
*u*2178	C(107)...H(118)	409.0(69)	31.4(fixed)	—	–2.7	31.4
*u*2258	C(64)...H(77)	409.2(56)	40.9(fixed)	—	–9.2	40.9
*u*2099	H(23)...H(46)	409.4(17)	28.3(fixed)	—	–5.2	28.3
*u*1962	H(119)...H(133)	409.6(89)	45.5(fixed)	—	–2.1	45.5
*u*1942	H(62)...H(69)	409.6(105)	39.3(fixed)	—	–2.4	39.3
*u*2043	H(19)...H(22)	409.8(17)	25.8(fixed)	—	–5.2	25.8
*u*2245	C(9)...H(44)	409.9(83)	59.8(fixed)	—	–10.3	59.8
*u*2151	C(58)...H(70)	410.0(67)	33.1(fixed)	—	–2.2	33.1
*u*1781	Si(50)...C(53)	410.1(53)	19.0(tied to *u*1950)	—	–0.1	16.7
*u*2096	H(112)...H(115)	410.1(17)	26.5(fixed)	—	–4.8	26.5
*u*2128	C(101)...H(123)	410.1(84)	38.5(fixed)	—	–2.5	38.5
*u*1893	Si(52)...C(55)	410.1(64)	17.4(tied to *u*1950)	—	–0.2	15.2
*u*2071	H(31)...H(43)	410.2(17)	33.4(fixed)	—	–3.6	33.4
*u*2064	H(68)...H(94)	410.5(17)	25.9(fixed)	—	–3.7	25.9
*u*1492	H(66)...H(83)	410.5(38)	43.7(fixed)	—	33.5	43.7
*u*2089	H(70)...H(93)	410.5(17)	27.8(fixed)	—	–3.4	27.8
*u*2063	H(162)...H(176)	410.5(76)	46.2(fixed)	—	–8.0	46.2
*u*2253	C(17)...H(30)	410.7(52)	35.5(fixed)	—	–7.0	35.5
*u*1963	H(66)...H(69)	410.7(17)	24.6(fixed)	—	–3.6	24.6
*u*1951	H(61)...H(93)	410.8(56)	38.0(fixed)	—	–1.6	38.0
*u*2056	H(209)...H(235)	411.0(17)	26.1(fixed)	—	–3.9	26.1
*u*2046	H(124)...H(129)	411.2(17)	24.6(fixed)	—	–4.0	24.6
*u*2117	C(195)...H(212)	411.2(37)	34.2(fixed)	—	–2.3	34.2
*u*2061	H(256)...H(282)	411.3(17)	24.4(fixed)	—	–3.4	24.4
*u*2017	H(65)...H(68)	411.4(17)	26.4(fixed)	—	–2.7	26.4
*u*2060	H(115)...H(141)	411.4(17)	25.3(fixed)	—	–3.6	25.3
*u*2080	H(211)...H(234)	411.6(17)	27.3(fixed)	—	–3.2	27.3
*u*2127	H(109)...H(137)	411.6(30)	35.3(fixed)	—	–14.6	35.3
*u*2083	H(258)...H(281)	411.6(17)	26.1(fixed)	—	–2.9	26.1
*u*2035	H(206)...H(209)	411.7(17)	26.8(fixed)	—	–3.1	26.8

*u*1987	H(207)...H(210)	411.7(17)	24.8(fixed)	—	–3.3	24.8
*u*2087	H(30)...H(35)	411.7(17)	30.5(fixed)	—	–2.6	30.5
*u*2244	H(61)...H(66)	411.8(41)	41.8(fixed)	—	–2.7	41.8
*u*2074	H(117)...H(140)	411.8(17)	27.0(fixed)	—	–3.0	27.0
*u*2147	C(149)...H(181)	411.9(43)	40.5(fixed)	—	–2.1	40.5
*u*2095	H(162)...H(188)	411.9(17)	29.5(fixed)	—	–2.3	29.5
*u*2090	H(77)...H(82)	411.9(17)	31.1(fixed)	—	–1.6	31.1
*u*2088	H(254)...H(257)	411.9(17)	28.3(fixed)	—	–2.3	28.3
*u*2159	H(73)...H(81)	412.1(85)	48.3(fixed)	—	–2.4	48.3
*u*2133	H(212)...H(217)	412.2(44)	29.1(fixed)	—	–8.7	29.1
*u*2217	H(257)...H(262)	412.3(42)	49.2(fixed)	—	–3.2	49.2
*u*2057	H(77)...H(89)	412.3(17)	32.8(fixed)	—	–0.9	32.8
*u*2081	H(113)...H(116)	412.4(17)	26.0(fixed)	—	–2.6	26.0
*u*2317	C(55)...H(91)	412.5(95)	37.0(fixed)	—	–3.0	37.0
*u*2084	H(21)...H(47)	412.6(17)	27.0(fixed)	—	–2.2	27.0
*u*2065	H(126)...H(128)	412.6(17)	26.1(fixed)	—	–2.4	26.1
*u*2158	C(60)...H(89)	412.6(50)	36.1(fixed)	—	–2.5	36.1
*u*2105	C(147)...H(178)	412.6(32)	33.3(fixed)	—	–2.3	33.3
*u*2067	H(18)...H(21)	412.7(17)	28.0(fixed)	—	–2.0	28.0
*u*2126	H(254)...H(261)	413.0(52)	44.9(fixed)	—	–5.3	44.9
*u*2304	C(106)...H(140)	413.3(59)	33.9(fixed)	—	–2.9	33.9
*u*2243	H(255)...H(282)	413.3(70)	27.1(fixed)	—	–6.8	27.1
*u*2097	H(108)...H(124)	413.4(37)	36.9(fixed)	—	–2.2	36.9
*u*2036	H(159)...H(162)	413.5(17)	31.6(fixed)	—	–0.3	31.6
*u*2257	H(263)...H(269)	414.1(58)	52.7(fixed)	—	–2.9	52.7
*u*2216	C(13)...H(43)	414.4(34)	47.4(fixed)	—	–11.1	47.4
*u*1946	H(161)...H(179)	414.5(48)	41.4(fixed)	—	–2.0	41.4
*u*2053	H(25)...H(36)	414.5(99)	44.7(fixed)	—	–1.7	44.7
*u*2031	H(125)...H(137)	414.6(17)	34.5(fixed)	—	0.9	34.5
*u*2124	H(37)...H(40)	414.6(45)	25.8(fixed)	—	–4.7	25.8
*u*2202	C(150)...H(159)	414.7(40)	31.1(fixed)	—	–1.5	31.1
*u*2193	H(26)...H(28)	414.9(45)	26.5(fixed)	—	–4.4	26.5
*u*2164	H(24)...H(29)	414.9(45)	26.8(fixed)	—	–4.3	26.8
*u*2219	H(15)...H(43)	414.9(36)	36.2(fixed)	—	–15.9	36.2
*u*2341	C(63)...H(74)	414.9(63)	38.6(fixed)	—	–6.2	38.6
*u*2165	H(71)...H(76)	415.1(44)	27.3(fixed)	—	–6.7	27.3
*u*2227	H(33)...H(42)	415.2(70)	39.9(fixed)	—	–3.4	39.9
*u*1784	H(62)...H(65)	415.2(86)	33.7(fixed)	—	–0.8	33.7
*u*1938	H(202)...H(231)	415.2(37)	34.3(fixed)	—	–1.4	34.3
*u*2110	C(53)...H(85)	415.2(29)	52.5(fixed)	—	–11.8	52.5
*u*2220	H(114)...H(141)	415.3(69)	26.4(fixed)	—	–5.1	26.4
*u*1967	H(155)...H(187)	415.4(28)	40.8(fixed)	—	–2.3	40.8
*u*2155	H(36)...H(39)	415.5(45)	27.1(fixed)	—	–3.7	27.1
*u*2235	H(127)...H(136)	415.5(70)	38.0(fixed)	—	–3.1	38.0
*u*2233	H(253)...H(280)	415.6(70)	31.0(fixed)	—	–4.0	31.0
*u*2198	H(82)...H(91)	415.7(70)	27.5(fixed)	—	–4.5	27.5

*u*2141	C(7)...H(29)	415.7(88)	36.6(fixed)	—	–2.0	36.6
*u*2161	H(167)...H(169)	415.7(45)	27.2(fixed)	—	–4.2	27.2
*u*2212	H(28)...H(34)	415.8(57)	51.1(fixed)	—	–3.1	51.1
*u*2137	H(165)...H(170)	415.8(45)	27.0(fixed)	—	–4.2	27.0
*u*2156	H(80)...H(89)	415.9(70)	27.1(fixed)	—	–4.3	27.1
*u*2188	H(206)...H(233)	416.1(70)	26.3(fixed)	—	–4.5	26.3
*u*2205	H(112)...H(139)	416.1(70)	28.5(fixed)	—	–4.0	28.5
*u*2125	H(159)...H(186)	416.1(70)	25.3(fixed)	—	–4.6	25.3
*u*2152	H(65)...H(92)	416.2(70)	25.2(fixed)	—	–4.3	25.2
*u*2222	H(208)...H(235)	416.5(70)	27.6(fixed)	—	–3.9	27.6
*u*2162	H(84)...H(87)	416.7(44)	40.8(fixed)	—	–2.7	40.8
*u*2214	H(67)...H(94)	416.7(70)	26.5(fixed)	—	–3.6	26.5
*u*2130	H(86)...H(90)	417.1(38)	49.2(fixed)	—	–2.5	49.2
*u*2294	C(111)...H(124)	417.1(55)	30.5(fixed)	—	–2.0	30.5
*u*2183	H(161)...H(188)	417.1(70)	26.9(fixed)	—	–3.4	26.9
*u*2144	H(18)...H(45)	417.2(70)	24.8(fixed)	—	–3.7	24.8
*u*2315	C(63)...H(73)	417.3(107)	37.6(fixed)	—	–2.6	37.6
*u*2111	H(15)...H(41)	417.3(71)	41.1(fixed)	—	–2.8	41.1
*u*2199	H(20)...H(47)	417.3(70)	25.3(fixed)	—	–3.6	25.3
*u*2070	H(210)...H(213)	417.4(37)	45.1(fixed)	—	–2.2	45.1
*u*2215	H(122)...H(128)	417.6(55)	53.1(fixed)	—	–3.1	53.1
*u*2192	C(56)...H(83)	417.6(77)	66.6(fixed)	—	–9.1	66.6
*u*2187	H(73)...H(75)	417.6(44)	29.9(fixed)	—	–3.8	29.9
*u*2308	H(15)...H(38)	417.7(59)	42.1(fixed)	—	–3.4	42.1
*u*2134	H(209)...H(223)	417.8(77)	47.0(fixed)	—	–1.7	47.0
*u*2195	C(103)...H(138)	417.9(85)	57.5(fixed)	—	–8.2	57.5
*u*2121	H(214)...H(216)	418.0(44)	33.6(fixed)	—	–2.3	33.6
*u*2213	H(167)...H(182)	418.5(45)	48.4(fixed)	—	–2.0	48.4
*u*2426	C(106)...H(113)	418.6(43)	34.4(fixed)	—	–4.4	34.4
*u*2118	C(12)...H(24)	418.6(80)	32.8(fixed)	—	–1.7	32.8
*u*2256	C(60)...H(78)	418.7(41)	53.2(fixed)	—	–8.0	53.2
*u*2234	H(202)...H(218)	418.8(29)	40.6(fixed)	—	–3.3	40.6
*u*2174	H(160)...H(169)	418.9(34)	49.7(fixed)	—	–1.2	49.7
*u*2271	C(13)...H(31)	419.0(80)	44.4(fixed)	—	–6.1	44.4
*u*2146	H(118)...H(123)	419.0(43)	27.2(fixed)	—	–4.7	27.2
*u*2186	H(120)...H(122)	419.1(43)	27.6(fixed)	—	–4.5	27.6
*u*2115	H(256)...H(270)	419.3(78)	44.6(fixed)	—	–1.7	44.6
*u*2284	C(197)...H(227)	419.4(78)	43.4(fixed)	—	–9.1	43.4
*u*2223	H(130)...H(133)	419.6(43)	25.5(fixed)	—	–4.3	25.5
*u*2200	H(131)...H(134)	419.9(43)	27.1(fixed)	—	–3.8	27.1
*u*2254	C(150)...H(163)	420.4(31)	49.1(fixed)	—	–6.7	49.1
*u*2116	H(21)...H(35)	420.7(81)	47.3(fixed)	—	–3.8	47.3
*u*2185	H(259)...H(264)	421.0(43)	25.9(fixed)	—	–4.4	25.9
*u*2228	H(32)...H(42)	421.2(23)	35.2(fixed)	—	–12.1	35.2
*u*2145	H(126)...H(136)	421.3(23)	28.7(fixed)	—	–12.6	28.7
*u*2108	C(102)...H(112)	421.4(65)	42.9(fixed)	—	–3.1	42.9

*u*2221	H(261)...H(263)	421.4(43)	26.8(fixed)	—	–3.9	26.8
*u*2325	H(114)...H(135)	421.7(41)	58.2(fixed)	—	–1.8	58.2
*u*2132	H(68)...H(82)	421.8(87)	50.4(fixed)	—	–1.8	50.4
*u*2004	H(20)...H(38)	422.1(73)	42.1(fixed)	—	–0.5	42.1
*u*2276	H(61)...H(77)	422.4(29)	37.9(fixed)	—	–12.5	37.9
*u*2248	C(10)...H(39)	422.5(106)	32.9(fixed)	—	–3.1	32.9
*u*2282	C(196)...H(232)	422.6(47)	36.4(fixed)	—	–2.6	36.4
*u*2321	C(194)...H(224)	422.6(43)	37.4(fixed)	—	–2.8	37.4
*u*2119	H(115)...H(129)	422.8(89)	47.3(fixed)	—	–1.4	47.3
*u*2072	H(109)...H(135)	422.9(45)	36.0(fixed)	—	–2.2	36.0
*u*2169	C(104)...H(131)	423.1(46)	33.8(fixed)	—	–2.9	33.8
*u*2225	C(152)...H(162)	423.3(48)	39.4(fixed)	—	–7.6	39.4
*u*2313	C(149)...H(177)	423.3(51)	40.1(fixed)	—	–2.9	40.1
*u*2259	H(78)...H(91)	423.4(23)	29.5(fixed)	—	–10.4	29.5
*u*2247	H(155)...H(160)	423.9(30)	38.2(fixed)	—	–2.6	38.2
*u*2339	C(56)...H(88)	424.0(71)	38.0(fixed)	—	–3.5	38.0
*u*2328	C(242)...H(262)	424.0(33)	33.4(fixed)	—	–3.5	33.4
*u*1801	H(249)...H(260)	424.1(39)	34.0(fixed)	—	–1.2	34.0
*u*2191	H(79)...H(80)	424.1(23)	28.9(fixed)	—	–9.8	28.9
*u*2466	C(100)...H(132)	424.4(41)	30.6(fixed)	—	–3.6	30.6
*u*2326	C(194)...H(229)	424.4(21)	34.0(fixed)	—	–9.5	34.0
*u*2307	C(196)...H(222)	424.6(34)	36.2(fixed)	—	–3.0	36.2
*u*2120	C(54)...H(71)	425.0(119)	32.5(fixed)	—	–2.0	32.5
*u*2285	H(155)...H(171)	425.1(28)	35.2(fixed)	—	–10.3	35.2
*u*2218	H(31)...H(44)	425.3(23)	40.4(fixed)	—	–7.1	40.4
*u*2267	H(161)...H(163)	425.5(23)	26.9(fixed)	—	–8.9	26.9
*u*2261	C(9)...H(34)	425.8(43)	35.0(fixed)	—	–2.8	35.0
*u*2311	H(62)...H(85)	425.9(73)	38.6(fixed)	—	–17.6	38.6
*u*2197	H(164)...H(186)	426.0(23)	27.4(fixed)	—	–8.3	27.4
*u*2302	C(243)...H(254)	426.0(34)	33.7(fixed)	—	–5.6	33.7
*u*2168	H(32)...H(33)	426.2(23)	28.8(fixed)	—	–8.1	28.8
*u*2265	C(11)...H(21)	426.4(46)	35.7(fixed)	—	–4.3	35.7
*u*2324	C(55)...H(81)	426.5(45)	33.3(fixed)	—	–3.2	33.3
*u*2091	H(125)...H(132)	426.7(46)	43.8(fixed)	—	–2.5	43.8
*u*2249	C(103)...H(128)	426.7(47)	34.3(fixed)	—	–2.8	34.3
*u*2346	C(9)...H(43)	426.8(64)	48.9(fixed)	—	–11.6	48.9
*u*2298	C(59)...H(75)	426.9(98)	39.7(fixed)	—	–5.4	39.7
*u*2277	C(244)...H(279)	427.2(71)	41.7(fixed)	—	–5.0	41.7
*u*2150	H(253)...H(258)	427.2(23)	26.6(fixed)	—	–6.8	26.6
*u*2283	C(105)...H(115)	427.3(49)	31.1(fixed)	—	–2.3	31.1
*u*2109	C(107)...H(119)	427.3(65)	36.0(fixed)	—	–2.0	36.0
*u*2278	C(244)...H(269)	427.7(44)	33.5(fixed)	—	–2.4	33.5
*u*2489	C(63)...H(72)	428.0(74)	31.7(fixed)	—	–3.5	31.7
*u*2230	H(22)...H(27)	428.2(102)	57.8(fixed)	—	–2.4	57.8
*u*2303	C(199)...H(209)	428.3(49)	33.4(fixed)	—	–2.7	33.4
*u*2211	H(23)...H(45)	428.8(23)	25.8(fixed)	—	–5.9	25.8

*u*2280	C(16)...H(28)	428.8(79)	32.0(fixed)	—	–3.1	32.0
*u*2170	H(112)...H(117)	428.8(23)	26.0(fixed)	—	–5.3	26.0
*u*2269	C(100)...H(134)	428.9(51)	34.5(fixed)	—	–1.9	34.5
*u*2403	C(56)...H(85)	428.9(79)	46.6(fixed)	—	–13.4	46.6
*u*2266	C(57)...H(86)	429.0(44)	34.4(fixed)	—	–3.4	34.4
*u*2114	C(6)...H(37)	429.0(106)	30.3(fixed)	—	–1.3	30.3
*u*2251	H(79)...H(89)	429.1(23)	35.7(fixed)	—	–3.7	35.7
*u*2229	H(20)...H(22)	429.1(23)	25.6(fixed)	—	–5.5	25.6
*u*2273	C(246)...H(256)	429.1(49)	30.7(fixed)	—	–2.3	30.7
*u*2479	C(55)...H(90)	429.3(81)	35.1(fixed)	—	–4.1	35.1
*u*2332	C(13)...H(30)	429.3(77)	41.8(fixed)	—	–6.2	41.8
*u*2231	H(125)...H(129)	429.8(23)	25.2(fixed)	—	–4.5	25.2
*u*2279	C(148)...H(169)	429.8(40)	32.1(fixed)	—	–2.8	32.1
*u*2238	H(257)...H(282)	429.9(23)	26.1(fixed)	—	–4.2	26.1
*u*2250	H(210)...H(235)	429.9(23)	26.2(fixed)	—	–4.5	26.2
*u*2263	H(69)...H(94)	429.9(23)	26.0(fixed)	—	–4.3	26.0
*u*2236	H(116)...H(141)	430.0(23)	25.6(fixed)	—	–4.3	25.6
*u*2210	H(70)...H(92)	430.0(23)	26.0(fixed)	—	–4.2	26.0
*u*2207	H(208)...H(210)	430.0(23)	27.0(fixed)	—	–4.2	27.0
*u*2166	C(8)...H(18)	430.1(64)	32.8(fixed)	—	–1.2	32.8
*u*2331	Si(5)...H(32)	430.1(29)	41.6(fixed)	—	–2.6	41.6
*u*2203	H(211)...H(233)	430.1(23)	26.8(fixed)	—	–4.1	26.8
*u*2163	C(195)...H(213)	430.2(27)	32.2(fixed)	—	–2.2	32.2
*u*2184	H(78)...H(82)	430.3(23)	34.3(fixed)	—	–2.8	34.3
*u*2204	H(67)...H(69)	430.3(23)	25.1(fixed)	—	–4.0	25.1
*u*2264	Si(96)...H(136)	430.3(42)	53.4(fixed)	—	–5.7	53.4
*u*2140	H(249)...H(254)	430.4(36)	33.1(fixed)	—	–7.0	33.1
*u*2177	H(31)...H(35)	430.4(23)	32.1(fixed)	—	–3.4	32.1
*u*2209	H(163)...H(188)	430.4(23)	31.2(fixed)	—	–3.3	31.2
*u*2143	H(206)...H(211)	430.5(23)	26.0(fixed)	—	–3.9	26.0
*u*2196	H(258)...H(280)	430.5(23)	25.8(fixed)	—	–3.6	25.8
*u*2201	H(114)...H(116)	430.5(23)	28.2(fixed)	—	–3.4	28.2
*u*2171	H(255)...H(257)	430.5(23)	30.8(fixed)	—	–2.9	30.8
*u*2206	H(117)...H(139)	430.6(23)	25.4(fixed)	—	–3.7	25.4
*u*2180	H(125)...H(138)	430.6(23)	38.8(fixed)	—	–1.7	38.8
*u*2055	H(69)...H(72)	430.6(119)	44.6(fixed)	—	–2.0	44.6
*u*2175	H(126)...H(127)	430.8(23)	26.8(fixed)	—	–3.3	26.8
*u*2136	H(65)...H(70)	430.8(23)	25.7(fixed)	—	–3.4	25.7
*u*2239	H(159)...H(164)	430.9(23)	32.3(fixed)	—	–2.7	32.3
*u*2246	H(22)...H(47)	430.9(23)	28.3(fixed)	—	–3.4	28.3
*u*2362	Si(96)...H(139)	430.9(33)	29.1(fixed)	—	–1.7	29.1
*u*2232	C(60)...H(90)	431.0(30)	33.9(fixed)	—	–2.7	33.9
*u*2224	H(116)...H(121)	431.0(100)	48.0(fixed)	—	–3.5	48.0
*u*2262	C(58)...H(68)	431.0(54)	34.4(fixed)	—	–2.4	34.4
*u*2176	H(18)...H(23)	431.4(23)	28.3(fixed)	—	–3.0	28.3
*u*2122	C(147)...H(179)	431.5(27)	32.3(fixed)	—	–2.2	32.3

*u*2337	C(60)...H(77)	431.6(35)	44.7(fixed)	—	–8.7	44.7
*u*2361	C(103)...H(137)	431.9(63)	47.1(fixed)	—	–11.4	47.1
*u*2364	C(243)...H(257)	431.9(51)	36.4(fixed)	—	–2.7	36.4
*u*2330	Si(52)...H(79)	432.2(32)	45.6(fixed)	—	–2.9	45.6
*u*2275	C(58)...H(94)	432.2(115)	35.4(fixed)	—	–2.6	35.4
*u*2260	C(150)...H(160)	432.4(23)	33.4(fixed)	—	–1.6	33.4
*u*2179	C(12)...H(25)	432.5(62)	33.8(fixed)	—	–1.9	33.8
*u*2350	C(242)...H(261)	432.8(54)	36.5(fixed)	—	–2.6	36.5
*u*2391	Si(99)...H(126)	432.8(36)	25.8(fixed)	—	–1.5	25.8
*u*2327	C(241)...H(274)	432.9(72)	33.3(fixed)	—	–3.4	33.3
*u*2356	C(150)...H(162)	433.1(33)	41.7(fixed)	—	–7.5	41.7
*u*2355	Si(2)...H(45)	433.4(33)	27.3(fixed)	—	–1.8	27.3
*u*2272	H(14)...H(30)	433.5(75)	37.7(fixed)	—	–9.4	37.7
*u*2288	C(110)...H(122)	433.8(76)	32.6(fixed)	—	–3.4	32.6
*u*2359	C(149)...H(182)	434.1(38)	32.8(fixed)	—	–3.1	32.8
*u*2371	Si(3)...H(43)	434.1(21)	26.3(fixed)	—	–14.4	26.3
*u*2316	Si(2)...H(42)	434.1(37)	49.0(fixed)	—	–4.0	49.0
*u*2378	Si(97)...H(127)	434.5(30)	30.0(fixed)	—	–2.2	30.0
*u*2373	Si(190)...H(233)	434.7(23)	30.2(fixed)	—	–2.0	30.2
*u*2376	Si(237)...H(280)	434.7(26)	28.6(fixed)	—	–2.0	28.6
*u*2286	Si(99)...H(108)	434.9(21)	13.7(fixed)	—	–1.1	13.7
*u*2357	Si(97)...H(137)	435.2(23)	27.3(fixed)	—	–13.7	27.3
*u*2160	C(197)...H(229)	435.3(70)	50.7(fixed)	—	–6.8	50.7
*u*2335	C(16)...H(27)	435.3(68)	33.0(fixed)	—	–3.2	33.0
*u*2319	C(64)...H(82)	435.4(112)	37.1(fixed)	—	–3.1	37.1
*u*2384	Si(3)...H(33)	435.7(23)	29.7(fixed)	—	–2.2	29.7
*u*2351	C(10)...H(41)	435.9(61)	34.2(fixed)	—	–3.2	34.2
*u*2472	C(104)...H(140)	436.0(59)	25.0(fixed)	—	–4.2	25.0
*u*2329	C(8)...H(22)	436.0(71)	42.6(fixed)	—	–4.0	42.6
*u*2135	H(19)...H(26)	436.2(78)	48.0(fixed)	—	–0.3	48.0
*u*2291	C(152)...H(188)	436.5(92)	36.1(fixed)	—	–3.0	36.1
*u*2270	Si(3)...H(14)	436.7(25)	13.7(fixed)	—	–1.5	13.7
*u*2354	Si(49)...H(92)	436.9(46)	27.8(fixed)	—	–2.0	27.8
*u*2353	Si(143)...H(186)	437.3(19)	27.8(fixed)	—	–2.0	27.8
*u*2485	C(196)...H(231)	437.3(33)	33.6(fixed)	—	–3.4	33.6
*u*2237	H(202)...H(215)	437.7(39)	34.0(fixed)	—	–11.4	34.0
*u*2240	H(62)...H(68)	437.8(110)	39.6(fixed)	—	–3.3	39.6
*u*2465	C(194)...H(226)	437.8(38)	33.0(fixed)	—	–3.5	33.0
*u*2268	Si(50)...H(61)	437.9(23)	14.0(fixed)	—	–1.3	14.0
*u*2407	C(10)...H(46)	438.1(52)	23.4(fixed)	—	–2.8	23.4
*u*2154	C(104)...H(132)	438.1(32)	32.7(fixed)	—	–2.4	32.7
*u*2314	C(7)...H(26)	438.2(69)	39.7(fixed)	—	–2.9	39.7
*u*2107	H(113)...H(120)	438.3(74)	47.3(fixed)	—	–3.3	47.3
*u*2401	Si(50)...H(87)	438.3(35)	29.9(fixed)	—	–1.8	29.9
*u*2340	C(57)...H(88)	438.3(34)	33.5(fixed)	—	–3.5	33.5
*u*2142	C(6)...H(38)	438.4(63)	31.0(fixed)	—	–1.1	31.0

*u*2404	C(100)...H(135)	438.4(26)	36.4(fixed)	—	–2.6	36.4
*u*2301	Si(239)...H(249)	438.5(20)	13.6(fixed)	—	–1.2	13.6
*u*2320	Si(237)...H(277)	438.5(40)	38.6(fixed)	—	–2.3	38.6
*u*2347	C(148)...H(168)	438.6(29)	32.8(fixed)	—	–2.9	32.8
*u*2306	Si(51)...H(62)	438.6(22)	13.6(fixed)	—	–1.1	13.6
*u*2345	C(59)...H(74)	438.6(63)	42.3(fixed)	—	–5.6	42.3
*u*2322	C(110)...H(121)	438.8(70)	35.2(fixed)	—	–3.4	35.2
*u*2367	Si(50)...H(80)	438.9(26)	30.3(fixed)	—	–1.9	30.3
*u*2516	C(149)...H(179)	439.1(40)	35.1(fixed)	—	–4.2	35.1
*u*2383	Si(98)...H(117)	439.2(19)	27.5(fixed)	—	–1.6	27.5
*u*2292	Si(143)...H(156)	439.3(24)	13.6(fixed)	—	–1.2	13.6
*u*2290	Si(192)...H(203)	439.4(22)	13.5(fixed)	—	–1.2	13.5
*u*2389	Si(49)...H(77)	439.5(19)	26.6(fixed)	—	–11.4	26.6
*u*2334	Si(145)...H(164)	439.5(21)	41.1(fixed)	—	–2.8	41.1
*u*2366	Si(52)...H(84)	439.7(34)	52.3(fixed)	—	–6.5	52.3
*u*2431	Si(50)...H(85)	439.8(22)	27.2(fixed)	—	–15.8	27.2
*u*2381	Si(4)...H(23)	439.8(19)	33.4(fixed)	—	–2.5	33.4
*u*2491	C(111)...H(132)	440.0(72)	26.0(fixed)	—	–4.3	26.0
*u*2430	C(64)...H(81)	440.1(92)	34.1(fixed)	—	–3.5	34.1
*u*2379	Si(51)...H(76)	440.3(57)	34.3(fixed)	—	–1.9	34.3
*u*2417	Si(192)...H(211)	440.5(25)	27.8(fixed)	—	–1.7	27.8
*u*2392	Si(239)...H(258)	440.6(27)	26.6(fixed)	—	–1.5	26.6
*u*2336	Si(190)...H(230)	440.7(38)	28.4(fixed)	—	–1.9	28.4
*u*2405	Si(96)...H(118)	441.1(37)	27.0(fixed)	—	–2.4	27.0
*u*2395	Si(143)...H(171)	441.2(17)	23.8(fixed)	—	–9.7	23.8
*u*2418	C(57)...H(93)	441.2(56)	24.0(fixed)	—	–3.5	24.0
*u*2530	C(242)...H(260)	441.3(40)	34.6(fixed)	—	–3.6	34.6
*u*2520	C(243)...H(256)	441.6(43)	34.7(fixed)	—	–3.3	34.7
*u*2274	C(11)...H(47)	441.6(94)	34.0(fixed)	—	–2.2	34.0
*u*2370	C(244)...H(278)	441.8(56)	38.3(fixed)	—	–5.4	38.3
*u*2382	Si(239)...H(275)	442.3(30)	29.5(fixed)	—	–1.5	29.5
*u*1954	H(62)...H(66)	442.4(93)	35.1(fixed)	—	–1.0	35.1
*u*2363	Si(49)...H(89)	442.5(38)	29.3(fixed)	—	–2.0	29.3
*u*2287	C(199)...H(235)	442.5(100)	36.8(fixed)	—	–2.8	36.8
*u*2460	C(58)...H(93)	443.1(91)	33.5(fixed)	—	–3.4	33.5
*u*2377	Si(2)...H(30)	443.1(18)	24.6(fixed)	—	–8.8	24.6
*u*2338	C(101)...H(121)	443.4(101)	34.3(fixed)	—	–3.9	34.3
*u*2386	Si(143)...H(183)	443.4(35)	25.6(fixed)	—	–1.7	25.6
*u*2483	C(56)...H(90)	443.5(79)	26.5(fixed)	—	–4.8	26.5
*u*2443	Si(50)...H(90)	443.6(21)	19.7(fixed)	—	–4.9	19.7
*u*2349	C(241)...H(276)	443.7(56)	33.7(fixed)	—	–3.2	33.7
*u*2297	Si(237)...H(259)	443.7(40)	28.7(fixed)	—	–2.2	28.7
*u*2380	Si(143)...H(170)	444.1(22)	31.3(fixed)	—	–1.8	31.3
*u*2296	C(17)...H(35)	444.1(97)	35.7(fixed)	—	–2.9	35.7
*u*2281	Si(192)...H(217)	444.3(21)	46.3(fixed)	—	–1.4	46.3
*u*2358	Si(3)...H(40)	444.5(68)	29.3(fixed)	—	–1.8	29.3

*u*2515	C(60)...H(74)	444.6(67)	28.9(fixed)	—	–7.9	28.9
*u*2293	C(246)...H(282)	444.9(106)	34.4(fixed)	—	–2.6	34.4
*u*2410	Si(51)...H(70)	445.0(35)	27.5(fixed)	—	–1.9	27.5
*u*2348	C(7)...H(27)	445.1(102)	35.4(fixed)	—	–3.2	35.4
*u*2299	Si(5)...H(15)	445.2(36)	13.6(fixed)	—	–1.2	13.6
*u*2289	Si(99)...H(109)	445.3(36)	13.4(fixed)	—	–1.1	13.4
*u*2446	Si(96)...H(113)	445.7(12)	20.6(fixed)	—	–5.7	20.6
*u*2374	Si(2)...H(24)	445.8(39)	27.7(fixed)	—	–2.1	27.7
*u*2323	C(105)...H(141)	446.0(97)	35.6(fixed)	—	–2.8	35.6
*u*2385	Si(49)...H(66)	446.1(18)	20.2(fixed)	—	–3.3	20.2
*u*2445	C(152)...H(187)	446.2(79)	34.6(fixed)	—	–3.5	34.6
*u*2432	C(17)...H(34)	446.3(78)	35.4(fixed)	—	–3.8	35.4
*u*2493	Si(99)...H(132)	446.5(29)	19.0(fixed)	—	–4.4	19.0
*u*2476	C(101)...H(128)	446.5(42)	24.9(fixed)	—	–4.5	24.9
*u*2402	Si(192)...H(225)	446.6(35)	28.3(fixed)	—	–2.2	28.3
*u*2390	Si(145)...H(165)	446.7(33)	28.3(fixed)	—	–2.2	28.3
*u*2344	Si(97)...H(112)	446.9(47)	33.7(fixed)	—	–2.0	33.7
*u*2394	Si(2)...H(19)	447.1(12)	19.8(fixed)	—	–3.3	19.8
*u*2455	Si(51)...H(93)	447.2(29)	18.5(fixed)	—	–4.2	18.5
*u*2365	Si(237)...H(254)	447.6(17)	21.9(fixed)	—	–7.1	21.9
*u*2419	Si(49)...H(74)	447.6(38)	21.8(fixed)	—	–7.2	21.8
*u*2411	Si(190)...H(218)	447.6(18)	21.5(fixed)	—	–4.3	21.5
*u*2408	Si(99)...H(123)	447.6(43)	30.5(fixed)	—	–1.8	30.5
*u*2469	C(244)...H(256)	447.7(42)	25.9(fixed)	—	–3.5	25.9
*u*2342	Si(190)...H(215)	447.9(28)	27.3(fixed)	—	–9.9	27.3
*u*2461	C(105)...H(121)	448.1(60)	25.6(fixed)	—	–4.9	25.6
*u*2451	Si(237)...H(265)	448.5(19)	19.3(fixed)	—	–3.9	19.3
*u*2309	C(111)...H(129)	448.6(102)	37.1(fixed)	—	–2.8	37.1
*u*2500	C(199)...H(213)	448.7(52)	27.3(fixed)	—	–4.2	27.3
*u*2477	C(246)...H(262)	448.9(56)	25.3(fixed)	—	–4.4	25.3
*u*2333	C(102)...H(116)	448.9(66)	35.3(fixed)	—	–2.7	35.3
*u*2444	Si(4)...H(46)	449.0(25)	18.2(fixed)	—	–3.5	18.2
*u*2167	C(54)...H(72)	449.0(112)	32.7(fixed)	—	–2.2	32.7
*u*2470	Si(98)...H(140)	449.1(25)	19.1(fixed)	—	–4.4	19.1
*u*2467	C(11)...H(27)	449.2(53)	25.8(fixed)	—	–4.2	25.8
*u*2454	C(7)...H(34)	449.3(41)	25.3(fixed)	—	–4.7	25.3
*u*2436	Si(3)...H(38)	449.4(30)	22.5(fixed)	—	–3.9	22.5
*u*2369	Si(96)...H(124)	449.5(20)	19.6(fixed)	—	–3.4	19.6
*u*2487	C(195)...H(222)	449.5(46)	25.4(fixed)	—	–4.5	25.4
*u*2424	Si(4)...H(41)	449.6(36)	18.9(fixed)	—	–4.4	18.9
*u*2456	C(242)...H(269)	449.8(47)	24.9(fixed)	—	–4.1	24.9
*u*2360	Si(97)...H(135)	450.0(29)	19.5(fixed)	—	–3.5	19.5
*u*2300	C(101)...H(120)	450.2(61)	37.9(fixed)	—	–2.8	37.9
*u*2397	Si(143)...H(160)	450.2(15)	20.0(fixed)	—	–3.5	20.0
*u*2412	Si(5)...H(29)	450.4(44)	28.4(fixed)	—	–1.5	28.4
*u*2448	C(11)...H(46)	450.5(80)	31.6(fixed)	—	–2.7	31.6

*u*2423	Si(190)...H(207)	450.6(16)	18.5(fixed)	—	–4.1	18.5
*u*2449	Si(52)...H(81)	450.7(26)	19.8(fixed)	—	–4.6	19.8
*u*2305	C(102)...H(113)	450.8(81)	32.7(fixed)	—	–4.3	32.7
*u*2468	C(111)...H(128)	450.9(81)	32.5(fixed)	—	–3.8	32.5
*u*2372	Si(3)...H(18)	450.9(46)	25.9(fixed)	—	–1.5	25.9
*u*2452	C(199)...H(234)	451.0(86)	32.6(fixed)	—	–3.8	32.6
*u*2458	Si(5)...H(34)	451.3(25)	20.2(fixed)	—	–4.9	20.2
*u*2429	Si(51)...H(88)	451.4(30)	20.0(fixed)	—	–4.8	20.0
*u*2512	Si(51)...H(72)	451.7(30)	19.0(fixed)	—	–4.3	19.0
*u*2478	Si(99)...H(128)	452.0(27)	19.4(fixed)	—	–4.7	19.4
*u*2434	Si(145)...H(182)	452.1(30)	19.9(fixed)	—	–4.1	19.9
*u*2502	C(58)...H(72)	452.1(55)	25.8(fixed)	—	–4.1	25.8
*u*2510	Si(239)...H(273)	452.3(25)	19.3(fixed)	—	–4.2	19.3
*u*2438	Si(145)...H(187)	452.4(27)	18.7(fixed)	—	–4.6	18.7
*u*2393	C(148)...H(175)	452.9(43)	24.3(fixed)	—	–3.8	24.3
*u*2447	C(246)...H(281)	452.9(90)	30.9(fixed)	—	–3.4	30.9
*u*2416	H(109)...H(129)	452.9(53)	30.9(fixed)	—	2.8	30.9
*u*2473	Si(192)...H(234)	453.0(28)	19.4(fixed)	—	–4.7	19.4
*u*2459	C(105)...H(140)	453.2(86)	32.9(fixed)	—	–3.5	32.9
*u*2486	Si(143)...H(166)	453.3(21)	20.3(fixed)	—	–4.8	20.3
*u*2433	Si(4)...H(27)	453.3(30)	19.7(fixed)	—	–4.4	19.7
*u*2406	Si(52)...H(71)	453.3(68)	26.9(fixed)	—	–2.0	26.9
*u*2409	C(16)...H(41)	453.5(32)	23.6(fixed)	—	–3.5	23.6
*u*2428	Si(98)...H(131)	453.6(37)	28.6(fixed)	—	–2.4	28.6
*u*2318	C(8)...H(19)	453.7(82)	32.5(fixed)	—	–1.6	32.5
*u*2464	Si(239)...H(281)	453.8(28)	19.1(fixed)	—	–4.3	19.1
*u*2425	Si(98)...H(121)	454.1(30)	20.5(fixed)	—	–4.9	20.5
*u*2496	Si(192)...H(213)	454.2(20)	19.7(fixed)	—	–4.4	19.7
*u*2457	C(54)...H(81)	454.3(57)	26.0(fixed)	—	–4.4	26.0
*u*2343	Si(50)...H(65)	454.4(52)	25.4(fixed)	—	–1.6	25.4
*u*2400	C(102)...H(135)	454.6(67)	23.0(fixed)	—	–2.6	23.0
*u*2480	C(8)...H(21)	454.9(89)	39.2(fixed)	—	–5.3	39.2
*u*2439	C(241)...H(260)	454.9(38)	24.7(fixed)	—	–3.6	24.7
*u*2399	C(196)...H(209)	454.9(28)	23.8(fixed)	—	–3.2	23.8
*u*2396	Si(5)...H(37)	455.6(62)	26.0(fixed)	—	–1.8	26.0
*u*2415	C(197)...H(231)	455.7(29)	25.3(fixed)	—	–3.5	25.3
*u*2387	H(249)...H(282)	455.9(49)	31.1(fixed)	—	2.3	31.1
*u*2441	Si(239)...H(262)	456.0(28)	19.6(fixed)	—	–4.4	19.6
*u*2450	C(63)...H(88)	456.7(37)	25.5(fixed)	—	–4.7	25.5
*u*2295	H(202)...H(203)	456.8(44)	25.3(fixed)	—	–1.5	25.3
*u*2501	C(7)...H(25)	457.2(91)	34.8(fixed)	—	–3.9	34.8
*u*2475	C(147)...H(168)	457.5(28)	26.3(fixed)	—	–4.1	26.3
*u*2440	Si(99)...H(134)	457.6(25)	25.9(fixed)	—	–1.5	25.9
*u*2375	C(149)...H(184)	457.7(25)	22.4(fixed)	—	–2.3	22.4
*u*2508	H(108)...H(141)	458.1(44)	36.4(fixed)	—	2.8	36.4
*u*2521	C(150)...H(179)	458.1(41)	28.8(fixed)	—	–4.6	28.8

*u*2352	C(59)...H(66)	458.4(27)	21.1(fixed)	—	–1.6	21.1
*u*2427	H(15)...H(35)	458.8(46)	30.7(fixed)	—	2.9	30.7
*u*2453	Si(3)...H(21)	459.7(66)	21.1(fixed)	—	–6.2	21.1
*u*2759	H(113)...H(130)	459.9(62)	47.6(fixed)	—	–5.9	47.6
*u*2414	Si(50)...H(68)	460.8(68)	21.3(fixed)	—	–4.2	21.3
*u*2484	H(62)...H(86)	461.1(64)	33.8(fixed)	—	2.6	33.8
*u*2421	C(8)...H(38)	461.2(68)	23.2(fixed)	—	–2.3	23.2
*u*2442	Si(97)...H(115)	462.7(66)	19.3(fixed)	—	–3.9	19.3
*u*2543	H(62)...H(89)	463.7(33)	33.8(fixed)	—	2.6	33.8
*u*2494	C(103)...H(115)	464.1(98)	26.5(fixed)	—	–3.7	26.5
*u*2506	C(9)...H(21)	464.2(99)	28.3(fixed)	—	–6.3	28.3
*u*2514	C(101)...H(119)	464.3(89)	33.4(fixed)	—	–4.4	33.4
*u*2571	C(107)...H(113)	464.5(38)	30.5(fixed)	—	–6.2	30.5
*u*2584	H(116)...H(125)	465.2(60)	36.8(fixed)	—	4.0	36.8
*u*2422	C(106)...H(124)	465.6(36)	23.4(fixed)	—	–2.9	23.4
*u*2505	Si(5)...H(25)	465.7(55)	19.7(fixed)	—	–4.6	19.7
*u*2481	C(102)...H(115)	466.1(85)	32.8(fixed)	—	–3.3	32.8
*u*2504	Si(99)...H(119)	467.2(54)	19.3(fixed)	—	–5.0	19.3
*u*2534	H(108)...H(112)	467.5(27)	34.3(fixed)	—	4.0	34.3
*u*2720	H(27)...H(44)	467.5(86)	72.3(fixed)	—	–13.2	72.3
*u*2388	C(12)...H(19)	467.7(83)	22.7(fixed)	—	–1.9	22.7
*u*2552	H(249)...H(267)	467.8(33)	31.3(fixed)	—	1.6	31.3
*u*2463	H(155)...H(185)	469.7(47)	31.2(fixed)	—	1.5	31.2
*u*2462	H(14)...H(15)	469.9(36)	22.3(fixed)	—	–2.0	22.3
*u*2435	H(61)...H(91)	470.2(52)	31.6(fixed)	—	2.7	31.6
*u*2526	H(202)...H(206)	470.6(31)	31.8(fixed)	—	2.2	31.8
*u*2944	H(114)...H(132)	470.8(50)	47.6(fixed)	—	–6.8	47.6
*u*2437	H(108)...H(120)	471.5(49)	31.1(fixed)	—	2.7	31.1
*u*2923	H(72)...H(91)	472.0(91)	45.4(fixed)	—	–5.9	45.4
*u*2611	Si(2)...H(43)	472.2(23)	32.4(fixed)	—	–12.1	32.4
*u*2507	Si(96)...H(137)	472.6(25)	32.7(fixed)	—	–11.2	32.7
*u*2697	H(215)...H(227)	472.7(79)	76.8(fixed)	—	–15.2	76.8
*u*2413	C(55)...H(68)	472.8(114)	23.6(fixed)	—	–3.2	23.6
*u*2688	Si(52)...H(77)	472.9(24)	28.2(fixed)	—	–9.8	28.2
*u*2532	C(105)...H(109)	473.3(36)	22.1(fixed)	—	–1.1	22.1
*u*2686	Si(5)...H(30)	473.5(22)	24.9(fixed)	—	–7.8	24.9
*u*2665	H(83)...H(87)	473.5(24)	18.5(fixed)	—	–12.5	18.5
*u*2471	C(100)...H(119)	474.3(75)	25.6(fixed)	—	–4.7	25.6
*u*2627	H(155)...H(165)	474.3(37)	35.0(fixed)	—	1.7	35.0
*u*2525	H(202)...H(235)	474.4(30)	35.9(fixed)	—	3.4	35.9
*u*2673	H(74)...H(83)	474.9(66)	84.4(fixed)	—	–13.7	84.4
*u*2674	H(121)...H(138)	474.9(91)	70.9(fixed)	—	–11.2	70.9
*u*2653	H(33)...H(44)	475.1(32)	19.0(fixed)	—	–12.3	19.0
*u*2843	H(114)...H(130)	475.3(54)	44.9(fixed)	—	–7.4	44.9
*u*2658	H(127)...H(138)	475.5(31)	18.8(fixed)	—	–11.6	18.8
*u*2602	Si(51)...C(53)	475.6(14)	12.8(tied to *u*2587)	—	–0.9	11.1

*u*2583	H(257)...H(266)	475.8(71)	38.2(fixed)	—	4.0	38.2
*u*2685	Si(96)...H(140)	476.1(23)	22.7(fixed)	—	–4.2	22.7
*u*2590	Si(50)...C(57)	476.2(10)	12.4(tied to *u*2587)	—	–0.8	10.8
*u*2917	H(75)...H(85)	476.2(110)	62.5(fixed)	—	–16.7	62.5
*u*2592	Si(4)...C(6)	476.3(11)	12.8(tied to *u*2587)	—	–0.8	11.2
*u*2545	Si(49)...C(54)	476.4(10)	13.3(tied to *u*2587)	—	–1.0	11.6
*u*2554	Si(3)...C(10)	476.5(10)	12.9(tied to *u*2587)	—	–0.8	11.3
*u*2523	Si(98)...C(107)	476.7(14)	13.7(tied to *u*2587)	—	–1.0	11.9
*u*2546	Si(97)...C(106)	476.7(13)	12.7(tied to *u*2587)	—	–0.9	11.0
*u*2580	Si(5)...C(13)	476.7(20)	13.1(tied to *u*2587)	—	–1.1	11.4
*u*2581	Si(4)...C(12)	476.7(16)	12.9(tied to *u*2587)	—	–1.2	11.2
*u*2539	Si(97)...C(104)	476.8(10)	12.8(tied to *u*2587)	—	–0.8	11.1
*u*2678	H(214)...H(217)	476.9(24)	16.2(fixed)	—	–9.4	16.2
*u*2616	Si(98)...C(100)	476.9(11)	12.6(tied to *u*2587)	—	–0.7	11.0
*u*2556	Si(2)...C(7)	477.0(7)	12.9(tied to *u*2587)	—	–0.9	11.3
*u*2513	H(61)...H(76)	477.0(54)	34.3(fixed)	—	6.7	34.3
*u*2499	C(6)...H(25)	477.1(75)	27.1(fixed)	—	–4.1	27.1
*u*2587	Si(49)...C(55)	477.2(19)	12.6(2)	10.9(11)	–1.0	10.9
*u*2576	Si(143)...C(152)	477.3(10)	12.9(tied to *u*2587)	—	–0.9	11.2
*u*2572	Si(52)...H(85)	477.4(22)	35.4(fixed)	—	–12.1	35.4
*u*2594	Si(96)...C(101)	477.5(7)	12.7(tied to *u*2587)	—	–0.8	11.0
*u*2567	Si(49)...C(58)	477.5(11)	12.9(tied to *u*2587)	—	–0.8	11.3
*u*2560	Si(190)...C(199)	477.7(10)	12.6(tied to *u*2587)	—	–0.9	11.0
*u*2524	C(246)...H(250)	477.7(37)	23.0(fixed)	—	–1.2	23.0
*u*2599	Si(52)...C(63)	477.7(11)	12.6(tied to *u*2587)	—	–0.8	10.9
*u*2566	H(169)...H(180)	477.8(60)	43.1(fixed)	—	5.2	43.1
*u*2569	C(11)...H(15)	477.8(34)	22.6(fixed)	—	–1.3	22.6
*u*2561	Si(2)...C(11)	477.8(10)	12.8(tied to *u*2587)	—	–0.8	11.1
*u*2562	Si(2)...H(46)	477.9(23)	24.2(fixed)	—	–3.5	24.2
*u*2596	Si(237)...C(246)	477.9(10)	12.4(tied to *u*2587)	—	–0.8	10.8
*u*2542	Si(96)...C(105)	478.0(10)	12.6(tied to *u*2587)	—	–0.8	11.0
*u*2591	Si(5)...C(16)	478.1(10)	12.5(tied to *u*2587)	—	–0.8	10.9
*u*2570	Si(2)...C(9)	478.1(18)	13.2(tied to *u*2587)	—	–1.0	11.5
*u*2574	Si(52)...C(60)	478.1(15)	13.0(tied to *u*2587)	—	–1.0	11.4
*u*2699	Si(99)...H(124)	478.2(25)	20.6(fixed)	—	–3.2	20.6
*u*2729	H(30)...H(39)	478.2(117)	53.0(fixed)	—	–8.5	53.0
*u*2603	Si(99)...C(110)	478.2(11)	12.5(tied to *u*2587)	—	–0.8	10.9
*u*2535	H(62)...H(82)	478.3(53)	34.8(fixed)	—	3.3	34.8
*u*2598	Si(145)...C(153)	478.3(10)	12.7(tied to *u*2587)	—	–1.0	11.1
*u*2558	H(75)...H(82)	478.4(100)	41.1(fixed)	—	8.4	41.1
*u*2585	Si(145)...C(147)	478.4(11)	12.9(tied to *u*2587)	—	–0.9	11.2
*u*2746	H(78)...H(88)	478.4(42)	63.4(fixed)	—	–11.3	63.4
*u*2527	H(22)...H(31)	478.4(48)	41.4(fixed)	—	11.6	41.4
*u*2593	Si(51)...C(59)	478.4(10)	12.5(tied to *u*2587)	—	–1.0	10.9
*u*2568	Si(192)...C(201)	478.5(13)	13.0(tied to *u*2587)	—	–0.9	11.3
*u*2666	H(73)...H(76)	478.5(24)	16.3(fixed)	—	–7.8	16.3

*u*2668	H(31)...H(42)	478.6(8)	19.0(fixed)	—	–13.6	19.0
*u*2551	Si(143)...C(148)	478.6(9)	12.7(tied to *u*2587)	—	–0.9	11.1
*u*2614	Si(97)...H(128)	478.7(17)	22.5(fixed)	—	–4.0	22.5
*u*2537	Si(96)...C(103)	478.8(17)	13.1(tied to *u*2587)	—	–0.9	11.4
*u*2577	Si(190)...C(195)	478.9(10)	12.9(tied to *u*2587)	—	–0.9	11.3
*u*2604	Si(4)...C(8)	478.9(10)	12.4(tied to *u*2587)	—	–1.0	10.8
*u*2646	H(255)...H(280)	478.9(32)	17.1(fixed)	—	–8.1	17.1
*u*2612	Si(192)...C(194)	478.9(12)	12.4(tied to *u*2587)	—	–0.8	10.8
*u*2622	Si(3)...H(34)	478.9(13)	23.1(fixed)	—	–4.3	23.1
*u*2557	Si(190)...C(196)	479.0(13)	12.7(tied to *u*2587)	—	–1.0	11.1
*u*2680	H(210)...H(219)	479.0(60)	38.0(fixed)	—	5.3	38.0
*u*2609	Si(239)...C(241)	479.1(12)	12.4(tied to *u*2587)	—	–0.7	10.8
*u*2548	Si(237)...C(242)	479.1(10)	13.0(tied to *u*2587)	—	–0.8	11.3
*u*2226	H(261)...H(271)	479.2(104)	49.8(fixed)	—	4.3	49.8
*u*2661	H(26)...H(29)	479.3(24)	15.8(fixed)	—	–6.5	15.8
*u*2657	H(120)...H(123)	479.4(24)	16.0(fixed)	—	–7.0	16.0
*u*2647	Si(237)...H(278)	479.4(24)	23.3(fixed)	—	–6.4	23.3
*u*2662	H(167)...H(170)	479.5(24)	15.7(fixed)	—	–6.5	15.7
*u*2735	Si(51)...H(74)	479.5(36)	25.4(fixed)	—	–6.7	25.4
*u*2536	Si(49)...H(93)	479.5(30)	25.1(fixed)	—	–4.0	25.1
*u*2918	H(73)...H(90)	479.6(114)	48.5(fixed)	—	–6.1	48.5
*u*2644	H(36)...H(40)	479.6(24)	15.6(fixed)	—	–6.2	15.6
*u*2706	Si(50)...H(88)	479.9(27)	24.1(fixed)	—	–4.8	24.1
*u*2540	Si(237)...C(244)	480.0(16)	12.8(tied to *u*2587)	—	–1.0	11.2
*u*2773	H(31)...H(41)	480.0(67)	57.6(fixed)	—	–9.5	57.6
*u*2588	Si(98)...C(102)	480.1(10)	12.4(tied to *u*2587)	—	–0.9	10.8
*u*2660	H(114)...H(139)	480.2(31)	16.3(fixed)	—	–7.0	16.3
*u*2669	H(125)...H(136)	480.3(8)	18.5(fixed)	—	–11.5	18.5
*u*2663	H(80)...H(91)	480.3(32)	16.0(fixed)	—	–6.9	16.0
*u*2633	Si(145)...H(162)	480.4(17)	27.6(fixed)	—	–8.3	27.6
*u*2650	H(130)...H(134)	480.4(24)	15.9(fixed)	—	–6.0	15.9
*u*2498	H(167)...H(176)	480.4(70)	42.1(fixed)	—	5.2	42.1
*u*2739	H(163)...H(168)	480.4(29)	60.2(fixed)	—	–9.4	60.2
*u*2519	H(216)...H(223)	480.4(55)	41.2(fixed)	—	12.8	41.2
*u*2634	Si(190)...H(234)	480.6(15)	23.0(fixed)	—	–4.2	23.0
*u*2655	H(261)...H(264)	480.7(23)	16.0(fixed)	—	–6.4	16.0
*u*2497	H(61)...H(62)	480.8(49)	26.1(fixed)	—	–1.5	26.1
*u*2664	H(208)...H(233)	480.8(32)	16.1(fixed)	—	–6.6	16.1
*u*2620	Si(237)...H(281)	480.8(16)	22.3(fixed)	—	–3.9	22.3
*u*2684	Si(50)...H(81)	480.9(15)	22.2(fixed)	—	–4.2	22.2
*u*2578	Si(145)...C(150)	480.9(12)	13.1(tied to *u*2587)	—	–0.9	11.4
*u*2600	Si(239)...C(243)	481.0(10)	12.3(tied to *u*2587)	—	–1.0	10.7
*u*2681	Si(4)...H(21)	481.0(15)	24.0(fixed)	—	–5.3	24.0
*u*2849	H(32)...H(46)	481.2(60)	56.8(fixed)	—	–9.7	56.8
*u*2635	H(67)...H(92)	481.2(32)	15.9(fixed)	—	–6.0	15.9
*u*2740	C(101)...H(125)	481.2(54)	28.5(fixed)	—	1.8	28.5

*u*2550	Si(143)...H(187)	481.3(12)	26.6(fixed)	—	–4.4	26.6
*u*2639	H(78)...H(89)	481.4(8)	18.3(fixed)	—	–10.5	18.3
*u*2641	H(161)...H(186)	481.4(32)	15.7(fixed)	—	–6.1	15.7
*u*2528	H(249)...H(279)	481.5(45)	36.8(fixed)	—	6.1	36.8
*u*2623	C(60)...H(62)	481.5(54)	23.5(fixed)	—	–1.6	23.5
*u*2694	Si(98)...H(115)	481.7(15)	21.1(fixed)	—	–3.5	21.1
*u*2671	H(79)...H(82)	481.9(8)	17.3(fixed)	—	–10.0	17.3
*u*2794	H(28)...H(43)	482.0(79)	59.4(fixed)	—	–13.1	59.4
*u*2642	H(20)...H(45)	482.1(32)	15.6(fixed)	—	–5.5	15.6
*u*2533	Si(190)...H(231)	482.5(23)	22.9(fixed)	—	–3.6	22.9
*u*2730	Si(192)...H(215)	482.5(14)	22.6(fixed)	—	–9.5	22.6
*u*2547	Si(96)...H(119)	482.7(25)	24.5(fixed)	—	–3.9	24.5
*u*2715	Si(239)...H(276)	482.8(21)	22.2(fixed)	—	–4.4	22.2
*u*2618	Si(49)...H(90)	482.8(24)	23.0(fixed)	—	–4.4	23.0
*u*2517	H(14)...H(26)	482.9(69)	33.1(fixed)	—	3.3	33.1
*u*2675	H(164)...H(188)	483.0(8)	17.0(fixed)	—	–9.2	17.0
*u*2677	H(32)...H(35)	483.0(8)	17.1(fixed)	—	–9.3	17.1
*u*2632	H(159)...H(163)	483.1(8)	17.7(fixed)	—	–9.0	17.7
*u*3049	H(216)...H(227)	483.1(79)	44.1(fixed)	—	–21.9	44.1
*u*2621	Si(3)...H(41)	483.2(44)	26.7(fixed)	—	–4.8	26.7
*u*2625	H(155)...H(169)	483.4(32)	33.6(fixed)	—	2.6	33.6
*u*2398	H(14)...H(44)	483.5(69)	35.2(fixed)	—	14.4	35.2
*u*2563	Si(50)...C(64)	483.6(33)	12.7(tied to *u*2587)	—	–1.0	11.1
*u*2857	H(79)...H(93)	483.8(66)	63.8(fixed)	—	–12.1	63.8
*u*2495	H(255)...H(263)	484.0(76)	41.9(fixed)	—	9.3	41.9
*u*2601	Si(3)...C(17)	484.0(31)	12.5(tied to *u*2587)	—	–0.9	10.8
*u*2676	H(253)...H(257)	484.0(8)	16.2(fixed)	—	–7.8	16.2
*u*2624	Si(143)...H(184)	484.1(22)	22.1(fixed)	—	–3.3	22.1
*u*2707	Si(192)...H(209)	484.1(19)	22.5(fixed)	—	–4.0	22.5
*u*2751	H(77)...H(86)	484.3(47)	54.5(fixed)	—	–10.8	54.5
*u*2595	Si(97)...C(111)	484.4(31)	12.5(tied to *u*2587)	—	–0.8	10.9
*u*2541	H(109)...H(117)	484.5(83)	32.0(fixed)	—	1.8	32.0
*u*2958	H(207)...H(224)	484.5(42)	47.0(fixed)	—	–5.8	47.0
*u*2692	Si(239)...H(256)	484.6(20)	20.9(fixed)	—	–3.4	20.9
*u*2683	Si(51)...H(68)	484.8(23)	23.0(fixed)	—	–3.8	23.0
*u*2838	H(208)...H(226)	484.9(51)	45.5(fixed)	—	–5.5	45.5
*u*2725	C(104)...H(116)	484.9(42)	29.2(fixed)	—	2.3	29.2
*u*2656	H(23)...H(47)	485.2(8)	16.5(fixed)	—	–7.2	16.5
*u*2667	H(112)...H(116)	485.2(8)	16.1(fixed)	—	–6.8	16.1
*u*2553	H(15)...H(23)	485.3(83)	37.3(fixed)	—	3.9	37.3
*u*2941	H(166)...H(177)	485.5(50)	48.2(fixed)	—	–6.2	48.2
*u*2640	H(211)...H(235)	485.5(8)	16.3(fixed)	—	–6.7	16.3
*u*2643	H(70)...H(94)	485.5(8)	16.3(fixed)	—	–6.5	16.3
*u*2648	H(18)...H(22)	485.5(8)	16.2(fixed)	—	–6.8	16.2
*u*2575	Si(2)...H(25)	485.6(26)	23.0(fixed)	—	–3.8	23.0
*u*2586	C(63)...H(61)	485.8(35)	23.5(fixed)	—	–1.4	23.5

*u*2649	H(206)...H(210)	485.8(8)	15.9(fixed)	—	–6.3	15.9
*u*2651	H(117)...H(141)	485.9(8)	16.1(fixed)	—	–6.1	16.1
*u*2565	Si(52)...C(56)	485.9(29)	13.1(tied to *u*2587)	—	–0.9	11.4
*u*2654	H(258)...H(282)	485.9(8)	16.0(fixed)	—	–6.0	16.0
*u*2652	H(126)...H(129)	486.0(8)	16.0(fixed)	—	–6.0	16.0
*u*3086	H(126)...H(140)	486.0(72)	35.6(fixed)	—	–7.1	35.6
*u*2786	H(162)...H(169)	486.2(45)	52.7(fixed)	—	–9.5	52.7
*u*2638	H(65)...H(69)	486.2(8)	15.7(fixed)	—	–5.8	15.7
*u*2718	Si(143)...H(168)	486.3(17)	21.2(fixed)	—	–4.2	21.2
*u*2617	C(147)...H(156)	486.4(33)	22.8(fixed)	—	–1.3	22.8
*u*2474	Si(237)...H(260)	486.6(27)	23.6(fixed)	—	–3.6	23.6
*u*2610	Si(192)...H(226)	486.6(25)	22.2(fixed)	—	–3.6	22.2
*u*2895	H(28)...H(44)	487.1(82)	56.4(fixed)	—	–15.3	56.4
*u*2741	H(255)...H(276)	487.3(70)	54.5(fixed)	—	–7.9	54.5
*u*2482	H(26)...H(39)	487.4(111)	47.3(fixed)	—	5.3	47.3
*u*2538	H(114)...H(122)	487.7(83)	40.3(fixed)	—	7.4	40.3
*u*2897	H(73)...H(91)	487.8(103)	41.2(fixed)	—	–6.7	41.2
*u*2890	H(122)...H(137)	487.8(74)	56.6(fixed)	—	–13.3	56.6
*u*2705	H(40)...H(47)	488.1(102)	45.3(fixed)	—	6.1	45.3
*u*2564	C(102)...H(108)	488.1(38)	23.2(fixed)	—	–1.2	23.2
*u*2582	Si(145)...H(166)	488.4(22)	22.7(fixed)	—	–3.8	22.7
*u*2818	H(75)...H(83)	488.6(90)	64.1(fixed)	—	–17.1	64.1
*u*2704	H(133)...H(141)	488.6(58)	39.5(fixed)	—	4.6	39.5
*u*2555	C(16)...H(14)	489.0(57)	22.9(fixed)	—	–1.4	22.9
*u*2492	H(208)...H(214)	489.3(46)	45.1(fixed)	—	4.1	45.1
*u*2708	C(197)...H(223)	490.1(41)	30.3(fixed)	—	3.0	30.3
*u*2544	H(69)...H(78)	490.1(74)	41.2(fixed)	—	12.9	41.2
*u*2798	H(81)...H(94)	490.6(116)	46.1(fixed)	—	–5.8	46.1
*u*2518	H(36)...H(47)	490.9(119)	43.4(fixed)	—	3.4	43.4
*u*2605	Si(98)...H(132)	490.9(26)	22.3(fixed)	—	–3.7	22.3
*u*2529	H(15)...H(20)	491.1(62)	33.2(fixed)	—	1.9	33.2
*u*2877	H(31)...H(39)	491.2(97)	44.0(fixed)	—	–11.1	44.0
*u*2775	H(65)...H(78)	491.4(64)	58.5(fixed)	—	12.2	58.5
*u*2696	C(7)...H(31)	491.5(43)	30.2(fixed)	—	8.1	30.2
*u*2608	Si(5)...H(38)	492.0(39)	22.0(fixed)	—	–3.2	22.0
*u*2711	C(10)...H(22)	492.0(36)	30.0(fixed)	—	4.5	30.0
*u*2770	Si(99)...H(135)	492.3(16)	22.6(fixed)	—	–3.8	22.6
*u*2597	H(20)...H(28)	492.4(86)	39.2(fixed)	—	4.6	39.2
*u*2724	C(56)...H(82)	492.4(66)	31.0(fixed)	—	3.1	31.0
*u*3226	H(113)...H(132)	492.4(41)	41.7(fixed)	—	–9.2	41.7
*u*2728	C(242)...H(266)	492.6(54)	29.2(fixed)	—	2.1	29.2
*u*2800	C(111)...H(108)	492.6(37)	21.8(fixed)	—	–1.3	21.8
*u*3065	H(257)...H(260)	492.7(51)	45.3(fixed)	—	–5.7	45.3
*u*2904	H(254)...H(274)	492.8(74)	49.9(fixed)	—	–8.3	49.9
*u*2891	H(78)...H(86)	492.8(43)	54.1(fixed)	—	–13.1	54.1
*u*2659	Si(97)...H(113)	493.0(54)	22.2(fixed)	—	–5.0	22.2

*u*2488	H(83)...H(94)	493.6(92)	53.1(fixed)	—	14.5	53.1
*u*2579	C(149)...H(176)	493.6(47)	34.5(fixed)	—	3.0	34.5
*u*2727	Si(99)...H(121)	493.7(54)	22.6(fixed)	—	–4.7	22.6
*u*2748	C(58)...H(75)	494.0(86)	32.8(fixed)	—	5.4	32.8
*u*2983	H(256)...H(261)	494.1(57)	45.7(fixed)	—	–5.4	45.7
*u*2522	H(109)...H(114)	494.2(61)	34.4(fixed)	—	4.3	34.4
*u*2774	C(195)...H(219)	494.3(46)	30.1(fixed)	—	2.7	30.1
*u*2710	H(37)...H(44)	494.4(109)	62.3(fixed)	—	17.3	62.3
*u*3015	H(27)...H(43)	494.4(64)	57.0(fixed)	—	–17.2	57.0
*u*2731	C(13)...H(47)	494.5(68)	36.6(fixed)	—	2.5	36.6
*u*3090	H(132)...H(139)	494.7(88)	38.7(fixed)	—	–7.7	38.7
*u*2945	H(41)...H(42)	494.9(48)	68.5(fixed)	—	–16.0	68.5
*u*2833	H(122)...H(138)	494.9(82)	54.8(fixed)	—	–13.3	54.8
*u*2757	H(18)...H(31)	495.0(37)	51.0(fixed)	—	9.6	51.0
*u*2865	H(208)...H(224)	495.1(47)	40.1(fixed)	—	–6.4	40.1
*u*3111	H(74)...H(85)	495.3(71)	59.1(fixed)	—	–21.9	59.1
*u*2737	Si(5)...H(27)	495.4(54)	22.8(fixed)	—	–4.4	22.8
*u*2703	C(241)...H(263)	495.4(53)	31.6(fixed)	—	2.9	31.6
*u*2861	H(167)...H(177)	495.4(55)	44.6(fixed)	—	–6.6	44.6
*u*2896	H(163)...H(169)	495.5(36)	48.0(fixed)	—	–11.3	48.0
*u*3027	H(76)...H(90)	495.6(110)	48.8(fixed)	—	–10.3	48.8
*u*2787	C(107)...H(141)	495.7(46)	31.3(fixed)	—	2.6	31.3
*u*2789	C(60)...H(65)	495.7(28)	33.8(fixed)	—	1.7	33.8
*u*3143	H(74)...H(87)	496.0(72)	42.8(fixed)	—	–12.3	42.8
*u*2573	C(59)...H(94)	496.0(74)	35.0(fixed)	—	2.6	35.0
*u*2755	C(150)...H(180)	496.1(43)	32.9(fixed)	—	2.3	32.9
*u*2778	C(63)...H(62)	496.2(30)	18.3(fixed)	—	–1.5	18.3
*u*2420	H(134)...H(138)	496.4(40)	58.8(fixed)	—	18.1	58.8
*u*2679	Si(3)...H(19)	496.5(54)	21.4(fixed)	—	–3.3	21.4
*u*2783	C(13)...H(18)	496.5(21)	32.1(fixed)	—	1.5	32.1
*u*2606	C(12)...H(47)	496.7(78)	35.7(fixed)	—	1.6	35.7
*u*2368	C(243)...H(271)	496.8(81)	38.1(fixed)	—	2.4	38.1
*u*2832	H(112)...H(125)	496.9(37)	39.7(fixed)	—	6.2	39.7
*u*2885	H(175)...H(188)	497.1(92)	48.1(fixed)	—	–6.4	48.1
*u*2490	H(163)...H(172)	497.2(37)	41.1(fixed)	—	16.7	41.1
*u*2874	H(164)...H(175)	497.3(42)	59.1(fixed)	—	–12.0	59.1
*u*2949	H(82)...H(93)	497.6(111)	47.4(fixed)	—	–6.3	47.4
*u*3129	H(121)...H(127)	497.6(78)	39.1(fixed)	—	–9.5	39.1
*u*2840	Si(4)...H(37)	497.7(37)	23.2(fixed)	—	–0.9	23.2
*u*2871	Si(51)...H(65)	497.8(25)	21.9(fixed)	—	–0.4	21.9
*u*3083	H(117)...H(128)	497.9(41)	37.5(fixed)	—	–7.8	37.5
*u*3134	H(262)...H(268)	497.9(72)	37.5(fixed)	—	–8.3	37.5
*u*2615	Si(52)...H(72)	498.1(61)	22.4(fixed)	—	–3.6	22.4
*u*2549	Si(50)...H(66)	498.4(54)	23.3(fixed)	—	–3.2	23.3
*u*2726	C(57)...H(69)	498.5(60)	30.0(fixed)	—	2.7	30.0
*u*3048	H(121)...H(137)	498.6(64)	56.5(fixed)	—	–17.1	56.5

*u*3080	H(23)...H(34)	498.8(41)	44.5(fixed)	—	–10.3	44.5
*u*2629	C(152)...H(167)	499.0(57)	31.3(fixed)	—	2.7	31.3
*u*2637	C(244)...H(255)	499.1(64)	30.9(fixed)	—	6.6	30.9
*u*3115	H(213)...H(221)	499.3(71)	40.4(fixed)	—	–8.0	40.4
*u*3317	H(72)...H(90)	499.4(72)	41.3(fixed)	—	–8.5	41.3
*u*3009	H(77)...H(88)	499.4(35)	55.5(fixed)	—	–14.5	55.5
*u*2821	Si(4)...H(18)	499.6(15)	22.2(fixed)	—	–0.4	22.2
*u*2943	C(100)...H(125)	499.6(34)	30.4(fixed)	—	2.4	30.4
*u*2613	C(8)...H(39)	499.7(98)	38.7(fixed)	—	2.7	38.7
*u*2812	Si(97)...H(131)	499.7(20)	21.8(fixed)	—	–0.5	21.8
*u*2803	C(197)...H(211)	499.8(31)	35.9(fixed)	—	2.5	35.9
*u*2810	H(34)...H(47)	499.8(92)	45.5(fixed)	—	–5.6	45.5
*u*2796	C(100)...H(108)	499.8(24)	18.4(fixed)	—	–1.5	18.4
*u*2753	H(161)...H(165)	499.9(48)	40.8(fixed)	—	5.7	40.8
*u*3031	H(30)...H(41)	499.9(63)	51.1(fixed)	—	–11.3	51.1
*u*2719	Si(98)...H(134)	500.0(26)	23.2(fixed)	—	–0.1	23.2
*u*2713	C(199)...H(216)	500.1(40)	31.7(fixed)	—	9.6	31.7
*u*3131	H(27)...H(33)	500.2(66)	39.1(fixed)	—	–8.6	39.1
*u*2714	H(120)...H(131)	500.2(51)	42.8(fixed)	—	7.6	42.8
*u*2959	H(22)...H(25)	500.2(84)	51.0(fixed)	—	–7.1	51.0
*u*2687	H(87)...H(94)	500.3(49)	46.1(fixed)	—	7.1	46.1
*u*3138	H(77)...H(93)	500.3(59)	46.4(fixed)	—	–14.8	46.4
*u*2736	C(107)...H(126)	500.4(33)	31.2(fixed)	—	1.8	31.2
*u*3078	C(101)...H(131)	500.4(42)	33.7(fixed)	—	2.6	33.7
*u*2939	C(9)...H(37)	500.4(39)	37.8(fixed)	—	1.6	37.8
*u*2930	H(66)...H(84)	500.5(39)	67.1(fixed)	—	–16.9	67.1
*u*2559	C(196)...H(208)	500.6(43)	34.2(fixed)	—	2.4	34.2
*u*3007	H(256)...H(264)	500.7(58)	41.3(fixed)	—	–7.0	41.3
*u*2790	C(242)...H(250)	500.7(28)	18.6(fixed)	—	–1.6	18.6
*u*2905	H(21)...H(26)	500.7(78)	51.7(fixed)	—	–7.3	51.7
*u*2957	H(255)...H(274)	500.8(73)	42.3(fixed)	—	–9.8	42.3
*u*3108	H(211)...H(222)	500.9(50)	36.9(fixed)	—	–8.1	36.9
*u*2984	C(63)...H(92)	501.1(37)	31.4(fixed)	—	2.9	31.4
*u*2868	Si(5)...H(40)	501.1(42)	21.9(fixed)	—	0.2	21.9
*u*2771	Si(49)...H(70)	501.2(24)	23.7(fixed)	—	–0.4	23.7
*u*2892	Si(49)...H(71)	501.3(35)	20.7(fixed)	—	–0.5	20.7
*u*3077	H(258)...H(269)	501.3(55)	37.1(fixed)	—	–7.4	37.1
*u*2827	Si(145)...H(159)	501.5(15)	22.7(fixed)	—	–0.6	22.7
*u*2628	H(215)...H(229)	501.5(73)	62.7(fixed)	—	–16.7	62.7
*u*2799	C(150)...H(183)	501.6(24)	33.3(fixed)	—	1.8	33.3
*u*2830	Si(190)...H(212)	501.6(17)	21.6(fixed)	—	–0.6	21.6
*u*2856	Si(98)...H(112)	501.7(15)	21.9(fixed)	—	0.6	21.9
*u*2754	Si(97)...H(126)	501.8(20)	21.4(fixed)	—	–0.3	21.4
*u*2733	H(159)...H(172)	501.8(32)	56.5(fixed)	—	10.6	56.5
*u*3133	H(30)...H(46)	501.9(56)	40.6(fixed)	—	–11.6	40.6
*u*2723	H(207)...H(228)	501.9(45)	67.2(fixed)	—	–9.8	67.2

*u*2963	C(16)...H(45)	502.0(33)	30.4(fixed)	—	2.2	30.4
*u*2986	H(71)...H(86)	502.1(100)	47.4(fixed)	—	6.6	47.4
*u*2695	C(54)...H(78)	502.3(57)	32.2(fixed)	—	11.2	32.2
*u*2882	Si(145)...H(178)	502.3(15)	21.7(fixed)	—	–0.5	21.7
*u*2848	H(24)...H(35)	502.4(49)	42.7(fixed)	—	6.8	42.7
*u*3060	H(162)...H(168)	502.4(32)	50.0(fixed)	—	–12.3	50.0
*u*2864	C(6)...H(31)	502.5(32)	39.7(fixed)	—	8.1	39.7
*u*2745	C(194)...H(202)	502.6(27)	17.9(fixed)	—	–1.3	17.9
*u*2831	H(206)...H(219)	502.7(37)	42.2(fixed)	—	6.1	42.2
*u*2876	C(53)...H(78)	502.8(46)	46.9(fixed)	—	10.8	46.9
*u*2893	Si(192)...H(206)	503.0(16)	21.5(fixed)	—	–0.1	21.5
*u*2717	C(105)...H(108)	503.2(20)	21.1(fixed)	—	–0.9	21.1
*u*2732	C(102)...H(136)	503.2(33)	53.9(fixed)	—	12.5	53.9
*u*2772	C(56)...H(61)	503.5(46)	18.2(fixed)	—	–1.4	18.2
*u*2716	C(103)...H(134)	503.5(37)	31.0(fixed)	—	2.9	31.0
*u*2845	Si(52)...H(89)	503.5(18)	22.0(fixed)	—	0.2	22.0
*u*2816	Si(50)...H(79)	503.6(18)	23.2(fixed)	—	3.2	23.2
*u*2630	C(13)...H(26)	503.6(75)	35.1(fixed)	—	2.5	35.1
*u*2980	C(110)...H(139)	503.6(34)	31.5(fixed)	—	2.7	31.5
*u*2927	Si(4)...H(24)	503.6(17)	20.9(fixed)	—	–0.6	20.9
*u*2785	Si(2)...H(23)	503.6(15)	23.5(fixed)	—	0.4	23.5
*u*2761	Si(3)...H(32)	503.7(16)	22.8(fixed)	—	2.0	22.8
*u*2742	C(100)...H(122)	503.8(70)	31.4(fixed)	—	3.1	31.4
*u*2873	H(222)...H(235)	503.8(101)	46.3(fixed)	—	–6.1	46.3
*u*2824	C(7)...H(14)	503.9(32)	21.8(fixed)	—	–1.1	21.8
*u*2836	Si(96)...H(117)	504.0(15)	22.1(fixed)	—	–0.3	22.1
*u*2645	C(194)...H(214)	504.1(34)	33.7(fixed)	—	2.3	33.7
*u*2862	Si(143)...H(174)	504.4(21)	21.8(fixed)	—	0.1	21.8
*u*2712	C(60)...H(94)	504.4(50)	36.6(fixed)	—	3.8	36.6
*u*2829	Si(52)...H(87)	504.4(26)	21.5(fixed)	—	0.2	21.5
*u*2791	Si(190)...H(211)	504.5(16)	23.5(fixed)	—	–0.2	23.5
*u*2801	Si(49)...H(80)	504.5(23)	22.1(fixed)	—	0.0	22.1
*u*2841	Si(239)...H(253)	504.6(18)	22.2(fixed)	—	1.3	22.2
*u*2760	Si(237)...H(258)	504.8(17)	21.8(fixed)	—	–0.2	21.8
*u*2766	C(149)...H(164)	504.9(30)	40.2(fixed)	—	9.2	40.2
*u*2820	Si(190)...H(221)	504.9(22)	21.7(fixed)	—	–0.1	21.7
*u*2940	H(128)...H(141)	505.0(94)	45.3(fixed)	—	–6.1	45.3
*u*2886	C(199)...H(203)	505.1(26)	21.9(fixed)	—	–1.4	21.9
*u*2863	Si(237)...H(268)	505.1(22)	21.9(fixed)	—	–0.1	21.9
*u*2670	H(208)...H(217)	505.2(29)	50.3(fixed)	—	10.1	50.3
*u*2805	H(253)...H(266)	505.3(40)	42.1(fixed)	—	8.0	42.1
*u*2806	Si(96)...H(127)	505.5(23)	21.8(fixed)	—	–0.3	21.8
*u*2814	Si(2)...H(29)	505.6(29)	21.8(fixed)	—	0.2	21.8
*u*2819	Si(2)...H(33)	505.7(21)	22.0(fixed)	—	0.0	22.0
*u*2744	C(12)...H(32)	505.7(31)	40.0(fixed)	—	8.7	40.0
*u*2902	H(253)...H(260)	505.7(53)	53.0(fixed)	—	–8.9	53.0

*u*2631	C(148)...H(172)	505.9(30)	30.5(fixed)	—	8.9	30.5
*u*2709	C(103)...H(114)	506.0(77)	30.0(fixed)	—	4.3	30.0
*u*2851	C(149)...H(155)	506.0(31)	19.4(fixed)	—	–1.6	19.4
*u*2503	H(130)...H(138)	506.1(60)	49.3(fixed)	—	13.4	49.3
*u*2776	Si(143)...H(164)	506.1(14)	22.8(fixed)	—	2.2	22.8
*u*2511	H(67)...H(73)	506.3(108)	41.7(fixed)	—	4.0	41.7
*u*3095	H(72)...H(80)	506.3(74)	41.2(fixed)	—	–7.8	41.2
*u*3235	H(74)...H(90)	506.4(69)	43.6(fixed)	—	–12.1	43.6
*u*2911	H(22)...H(26)	506.4(62)	45.8(fixed)	—	–7.9	45.8
*u*2881	Si(51)...H(84)	506.5(15)	25.3(fixed)	—	3.2	25.3
*u*3032	C(101)...C(104)	506.5(38)	21.4(tied to *u*3057)	—	–0.9	19.1
*u*2793	C(54)...H(61)	506.5(22)	22.1(fixed)	—	–1.4	22.1
*u*3188	H(132)...H(140)	506.5(68)	38.5(fixed)	—	–8.4	38.5
*u*2879	H(269)...H(282)	506.6(106)	43.4(fixed)	—	–5.5	43.4
*u*3093	C(57)...H(71)	506.6(46)	31.0(fixed)	—	2.4	31.0
*u*2956	Si(239)...H(259)	506.7(17)	21.2(fixed)	—	–0.8	21.2
*u*2813	Si(237)...H(264)	506.7(26)	21.7(fixed)	—	–0.1	21.7
*u*2975	H(257)...H(261)	506.7(54)	38.9(fixed)	—	–6.0	38.9
*u*2788	C(199)...H(202)	506.7(19)	20.7(fixed)	—	–1.0	20.7
*u*2942	C(53)...H(80)	506.8(36)	32.8(fixed)	—	3.3	32.8
*u*2929	C(111)...H(133)	506.9(43)	32.5(fixed)	—	1.5	32.5
*u*2752	C(59)...H(79)	506.9(32)	43.4(fixed)	—	11.2	43.4
*u*2763	Si(96)...H(123)	506.9(27)	22.2(fixed)	—	0.3	22.2
*u*2765	H(69)...H(89)	507.1(47)	40.8(fixed)	—	7.0	40.8
*u*2910	H(35)...H(46)	507.1(98)	44.3(fixed)	—	–5.5	44.3
*u*3097	H(41)...H(43)	507.1(34)	54.7(fixed)	—	–17.0	54.7
*u*2878	Si(99)...H(136)	507.1(19)	27.2(fixed)	—	2.9	27.2
*u*3075	C(55)...H(86)	507.1(69)	39.0(fixed)	—	3.9	39.0
*u*2722	C(243)...H(277)	507.2(26)	38.4(fixed)	—	6.8	38.4
*u*2901	C(11)...H(40)	507.2(51)	30.7(fixed)	—	4.5	30.7
*u*3100	C(246)...H(272)	507.2(39)	33.3(fixed)	—	2.2	33.3
*u*3157	H(124)...H(140)	507.3(60)	34.9(fixed)	—	–7.1	34.9
*u*2734	C(8)...H(42)	507.3(32)	45.5(fixed)	—	15.4	45.5
*u*2937	C(8)...H(35)	507.4(31)	33.1(fixed)	—	4.0	33.1
*u*2934	Si(98)...H(118)	507.5(15)	21.2(fixed)	—	–0.4	21.2
*u*2872	H(82)...H(94)	507.5(115)	39.6(fixed)	—	–6.9	39.6
*u*2870	Si(50)...H(92)	507.6(41)	21.7(fixed)	—	–0.3	21.7
*u*2768	Si(192)...H(228)	507.8(23)	22.0(fixed)	—	2.8	22.0
*u*2834	Si(145)...H(170)	507.9(22)	21.9(fixed)	—	–0.3	21.9
*u*2758	C(6)...H(28)	508.0(73)	32.0(fixed)	—	2.5	32.0
*u*2966	C(6)...H(33)	508.1(35)	34.3(fixed)	—	3.3	34.3
*u*2682	C(197)...H(208)	508.2(30)	33.6(fixed)	—	3.5	33.6
*u*2954	C(147)...H(174)	508.3(34)	31.4(fixed)	—	3.2	31.4
*u*2781	C(106)...H(120)	508.4(41)	32.6(fixed)	—	4.5	32.6
*u*3001	H(75)...H(79)	508.4(61)	55.7(fixed)	—	13.3	55.7
*u*3016	C(100)...H(127)	508.4(38)	33.6(fixed)	—	3.1	33.6

*u*2888	C(149)...H(161)	508.5(45)	32.6(fixed)	—	2.5	32.6
*u*2950	H(259)...H(270)	508.5(52)	40.8(fixed)	—	5.7	40.8
*u*2951	C(194)...H(219)	508.6(21)	33.3(fixed)	—	3.3	33.3
*u*2938	H(66)...H(85)	508.6(25)	60.5(fixed)	—	–16.0	60.5
*u*2907	C(241)...H(266)	508.6(21)	31.5(fixed)	—	2.8	31.5
*u*2828	Si(5)...H(42)	508.9(16)	23.7(fixed)	—	4.5	23.7
*u*2889	C(58)...H(62)	508.9(44)	21.0(fixed)	—	–1.3	21.0
*u*2898	Si(3)...H(45)	509.0(35)	21.8(fixed)	—	–0.4	21.8
*u*2698	H(170)...H(176)	509.0(30)	49.9(fixed)	—	6.5	49.9
*u*2991	C(194)...H(221)	509.1(36)	33.3(fixed)	—	3.0	33.3
*u*2859	H(176)...H(188)	509.2(93)	38.6(fixed)	—	–7.4	38.6
*u*3063	C(57)...H(75)	509.2(59)	43.6(fixed)	—	5.4	43.6
*u*2973	C(241)...H(268)	509.2(37)	32.6(fixed)	—	2.6	32.6
*u*2743	C(106)...H(109)	509.3(24)	21.4(fixed)	—	–1.1	21.4
*u*2691	C(17)...H(36)	509.3(104)	32.7(fixed)	—	1.8	32.7
*u*2912	C(152)...H(181)	509.3(46)	31.8(fixed)	—	3.6	31.8
*u*2509	C(107)...H(138)	509.4(36)	45.9(fixed)	—	16.5	45.9
*u*3079	C(195)...H(225)	509.5(31)	32.7(fixed)	—	2.5	32.7
*u*3304	H(207)...H(226)	509.5(33)	40.5(fixed)	—	–7.9	40.5
*u*2837	C(241)...H(250)	509.5(37)	21.0(fixed)	—	–1.3	21.0
*u*3121	H(118)...H(135)	509.6(74)	34.2(fixed)	—	–7.7	34.2
*u*2970	C(7)...C(10)	509.6(32)	21.1(tied to *u*3057)	—	–1.0	18.9
*u*2968	C(243)...H(270)	509.7(34)	32.1(fixed)	—	3.2	32.1
*u*3099	H(70)...H(81)	509.8(71)	36.5(fixed)	—	–8.2	36.5
*u*2747	C(9)...H(20)	509.8(78)	30.9(fixed)	—	1.7	30.9
*u*2777	C(12)...H(44)	509.9(75)	49.6(fixed)	—	15.7	49.6
*u*2903	C(58)...H(87)	510.1(46)	31.3(fixed)	—	4.4	31.3
*u*2855	Si(97)...H(139)	510.1(35)	21.8(fixed)	—	0.0	21.8
*u*2825	C(59)...H(91)	510.2(47)	34.0(fixed)	—	3.9	34.0
*u*3221	H(81)...H(93)	510.2(88)	42.2(fixed)	—	–8.0	42.2
*u*2767	C(104)...H(109)	510.4(28)	22.6(fixed)	—	–0.8	22.6
*u*3123	H(108)...H(139)	510.5(44)	36.8(fixed)	—	–1.4	36.8
*u*2880	H(129)...H(140)	510.5(105)	47.5(fixed)	—	–5.9	47.5
*u*2916	C(110)...H(116)	510.5(30)	31.9(fixed)	—	2.7	31.9
*u*2721	C(150)...H(176)	510.6(22)	40.3(fixed)	—	3.9	40.3
*u*3072	H(115)...H(123)	510.6(89)	41.8(fixed)	—	–7.5	41.8
*u*2738	H(84)...H(91)	511.2(48)	47.8(fixed)	—	16.4	47.8
*u*2955	H(62)...H(91)	511.3(43)	37.9(fixed)	—	–1.1	37.9
*u*3436	H(166)...H(179)	511.3(42)	42.5(fixed)	—	–9.2	42.5
*u*2935	C(102)...H(129)	511.4(29)	32.1(fixed)	—	4.1	32.1
*u*3047	H(209)...H(212)	511.4(38)	37.5(fixed)	—	–7.7	37.5
*u*2792	H(29)...H(39)	511.5(84)	50.8(fixed)	—	6.7	50.8
*u*2854	C(8)...H(14)	511.6(57)	20.6(fixed)	—	–1.5	20.6
*u*2982	H(116)...H(119)	511.6(81)	44.8(fixed)	—	–6.3	44.8
*u*3449	H(256)...H(260)	511.6(40)	41.9(fixed)	—	–7.6	41.9
*u*2914	C(10)...H(29)	511.9(47)	30.6(fixed)	—	3.9	30.6

*u*3089	H(166)...H(181)	511.9(46)	44.1(fixed)	—	–8.0	44.1
*u*3064	H(254)...H(276)	512.0(52)	47.2(fixed)	—	–10.1	47.2
*u*2852	H(118)...H(129)	512.1(41)	40.8(fixed)	—	7.3	40.8
*u*2817	C(147)...H(172)	512.1(20)	44.8(fixed)	—	9.0	44.8
*u*2762	C(244)...H(249)	512.1(22)	21.4(fixed)	—	–1.3	21.4
*u*3107	H(88)...H(89)	512.1(52)	39.3(fixed)	—	–9.3	39.3
*u*2844	C(10)...H(15)	512.3(26)	22.9(fixed)	—	–0.8	22.9
*u*2756	H(109)...H(126)	512.4(40)	30.8(fixed)	—	1.2	30.8
*u*2809	C(148)...H(155)	512.4(21)	21.4(fixed)	—	–1.1	21.4
*u*2913	C(63)...H(69)	512.7(36)	32.5(fixed)	—	3.5	32.5
*u*2795	C(7)...H(15)	512.7(66)	18.9(fixed)	—	–1.5	18.9
*u*2931	H(202)...H(212)	512.8(21)	32.2(fixed)	—	1.2	32.2
*u*2693	C(110)...H(130)	512.9(45)	31.7(fixed)	—	2.0	31.7
*u*3213	H(74)...H(88)	513.0(74)	41.8(fixed)	—	–12.4	41.8
*u*2780	Si(52)...H(76)	513.1(38)	22.4(fixed)	—	1.6	22.4
*u*2779	C(101)...H(109)	513.1(66)	18.5(fixed)	—	–1.4	18.5
*u*3057	C(56)...C(58)	513.1(56)	23.0(7)	20.6(20)	–1.2	20.6
*u*2953	C(150)...H(155)	513.3(27)	21.6(fixed)	—	–1.4	21.6
*u*2928	C(55)...H(84)	513.3(25)	54.4(fixed)	—	13.3	54.4
*u*3084	H(21)...H(29)	513.4(93)	40.7(fixed)	—	–9.8	40.7
*u*3010	H(160)...H(178)	513.6(33)	36.5(fixed)	—	–6.8	36.5
*u*2900	C(16)...H(22)	513.9(24)	34.6(fixed)	—	5.4	34.6
*u*2835	C(9)...H(39)	513.9(76)	42.2(fixed)	—	3.7	42.2
*u*2884	C(104)...H(123)	513.9(45)	32.1(fixed)	—	4.4	32.1
*u*2619	C(64)...H(83)	514.0(68)	38.9(fixed)	—	14.9	38.9
*u*2995	C(197)...C(199)	514.3(28)	19.6(fixed)	—	–1.1	19.6
*u*3023	C(242)...C(245)	514.4(42)	21.5(tied to *u*3057)	—	–0.9	19.3
*u*3105	H(162)...H(175)	514.7(50)	45.3(fixed)	—	–13.4	45.3
*u*3082	C(195)...C(198)	515.0(36)	22.0(tied to *u*3057)	—	–1.0	19.7
*u*3140	H(159)...H(168)	515.2(41)	33.9(fixed)	—	–7.3	33.9
*u*2946	C(242)...H(275)	515.2(42)	30.4(fixed)	—	4.2	30.4
*u*2853	H(223)...H(235)	515.4(101)	41.6(fixed)	—	–6.8	41.6
*u*2899	C(196)...H(202)	515.4(18)	23.5(fixed)	—	–1.2	23.5
*u*2875	H(115)...H(120)	515.5(69)	46.9(fixed)	—	–5.4	46.9
*u*2826	H(116)...H(136)	515.6(50)	44.3(fixed)	—	13.3	44.3
*u*2531	C(106)...H(138)	515.6(52)	37.4(fixed)	—	14.0	37.4
*u*2962	C(241)...C(244)	515.7(42)	22.3(tied to *u*3057)	—	–1.1	19.9
*u*2979	C(54)...C(57)	515.7(44)	21.5(tied to *u*3057)	—	–1.0	19.3
*u*3241	H(175)...H(187)	515.8(80)	42.7(fixed)	—	–8.2	42.7
*u*3204	H(256)...H(262)	515.9(38)	37.4(fixed)	—	–8.1	37.4
*u*3139	H(21)...H(34)	516.1(47)	41.7(fixed)	—	–10.1	41.7
*u*2702	H(261)...H(275)	516.2(68)	41.5(fixed)	—	5.9	41.5
*u*2811	C(56)...H(70)	516.3(87)	36.2(fixed)	—	2.5	36.2
*u*2866	C(149)...C(152)	516.4(37)	24.9(tied to *u*3057)	—	–1.2	22.3
*u*3209	H(207)...H(229)	516.6(24)	38.7(fixed)	—	–14.9	38.7
*u*3220	H(34)...H(46)	516.6(78)	42.0(fixed)	—	–7.6	42.0

*u*2920	C(58)...H(61)	516.6(28)	23.1(fixed)	—	–1.1	23.1
*u*2948	C(152)...H(155)	516.7(25)	22.9(fixed)	—	–1.1	22.9
*u*3154	H(115)...H(128)	516.9(49)	36.1(fixed)	—	–8.0	36.1
*u*2846	H(35)...H(47)	517.1(96)	38.1(fixed)	—	–6.3	38.1
*u*2782	C(242)...H(249)	517.2(26)	23.2(fixed)	—	–0.8	23.2
*u*2607	C(243)...C(247)	517.7(63)	29.7(tied to *u*3057)	—	–1.3	26.5
*u*2797	H(22)...H(42)	517.7(38)	49.4(fixed)	—	16.5	49.4
*u*3187	H(213)...H(222)	517.8(43)	40.3(fixed)	—	–8.4	40.3
*u*2842	H(15)...H(32)	517.8(33)	31.6(fixed)	—	5.4	31.6
*u*3113	H(121)...H(128)	517.8(54)	39.4(fixed)	—	–8.7	39.4
*u*3124	H(27)...H(34)	517.9(49)	40.0(fixed)	—	–8.1	40.0
*u*2960	H(211)...H(227)	518.1(38)	57.0(fixed)	—	9.6	57.0
*u*3071	C(246)...H(274)	518.1(33)	35.6(fixed)	—	3.4	35.6
*u*3096	H(61)...H(75)	518.2(64)	48.1(fixed)	—	–2.4	48.1
*u*2839	C(59)...C(64)	518.2(52)	25.2(tied to *u*3057)	—	–1.2	22.6
*u*2869	H(270)...H(282)	518.2(106)	38.8(fixed)	—	–6.2	38.8
*u*3013	H(263)...H(280)	518.6(41)	44.3(fixed)	—	5.9	44.3
*u*2689	C(244)...H(271)	518.8(51)	31.4(fixed)	—	3.5	31.4
*u*3183	H(254)...H(260)	518.8(36)	38.7(fixed)	—	–10.9	38.7
*u*3085	C(150)...C(154)	518.8(32)	21.8(fixed)	—	–1.4	21.8
*u*2589	C(55)...H(67)	518.9(84)	32.9(fixed)	—	2.0	32.9
*u*2964	H(249)...H(266)	519.1(34)	35.5(fixed)	—	–1.4	35.5
*u*2867	C(6)...H(15)	519.1(48)	21.4(fixed)	—	–1.3	21.4
*u*3167	H(209)...H(222)	519.2(51)	38.8(fixed)	—	–8.4	38.8
*u*2919	C(148)...C(151)	519.3(25)	18.6(fixed)	—	–0.9	18.6
*u*2672	C(53)...H(73)	519.3(96)	32.4(fixed)	—	2.2	32.4
*u*2967	Si(96)...H(129)	519.5(10)	20.5(fixed)	—	–1.1	20.5
*u*3216	H(72)...H(81)	519.6(50)	37.6(fixed)	—	–8.4	37.6
*u*2972	Si(143)...H(176)	519.6(10)	23.3(fixed)	—	–1.4	23.3
*u*3005	Si(96)...H(116)	519.6(11)	21.0(fixed)	—	–1.1	21.0
*u*3256	H(128)...H(140)	519.7(81)	40.7(fixed)	—	–8.2	40.7
*u*2969	Si(190)...H(223)	519.8(10)	21.3(fixed)	—	–1.0	21.3
*u*2998	Si(2)...H(35)	519.8(10)	20.8(fixed)	—	–1.0	20.8
*u*2999	Si(97)...H(125)	519.8(11)	19.9(fixed)	—	–1.2	19.9
*u*2822	C(100)...H(109)	519.9(47)	20.2(fixed)	—	–1.2	20.2
*u*3003	Si(237)...H(270)	519.9(10)	21.0(fixed)	—	–0.9	21.0
*u*2690	C(196)...H(228)	519.9(34)	36.9(fixed)	—	13.7	36.9
*u*3234	H(222)...H(234)	519.9(85)	41.3(fixed)	—	–8.6	41.3
*u*3022	Si(3)...H(31)	519.9(11)	24.2(fixed)	—	–1.1	24.2
*u*3000	Si(49)...H(82)	519.9(10)	21.5(fixed)	—	–1.3	21.5
*u*3141	H(262)...H(269)	519.9(50)	38.1(fixed)	—	–8.0	38.1
*u*2808	C(103)...H(108)	520.0(39)	23.0(fixed)	—	–0.9	23.0
*u*2987	Si(2)...H(22)	520.0(11)	22.2(fixed)	—	–1.1	22.2
*u*3051	H(24)...H(38)	520.0(83)	35.9(fixed)	—	–6.4	35.9
*u*2769	H(249)...H(258)	520.0(34)	31.5(fixed)	—	1.5	31.5
*u*2750	H(164)...H(177)	520.1(36)	42.4(fixed)	—	11.3	42.4

*u*2749	H(23)...H(36)	520.2(48)	40.2(fixed)	—	7.7	40.2
*u*3042	Si(50)...H(78)	520.3(11)	28.2(fixed)	—	–0.6	28.2
*u*2993	Si(49)...H(69)	520.3(11)	20.9(fixed)	—	–1.2	20.9
*u*3098	Si(192)...H(227)	520.3(15)	25.0(fixed)	—	–2.5	25.0
*u*2894	H(116)...H(120)	520.3(55)	40.3(fixed)	—	–6.3	40.3
*u*3120	C(107)...C(111)	520.4(33)	23.6(tied to *u*3057)	—	–1.3	21.1
*u*3028	H(117)...H(133)	520.4(37)	43.7(fixed)	—	4.9	43.7
*u*2823	H(202)...H(208)	520.4(30)	36.3(fixed)	—	–0.9	36.3
*u*3055	Si(2)...H(28)	520.6(18)	21.7(fixed)	—	–1.7	21.7
*u*2802	C(148)...H(177)	520.6(37)	30.5(fixed)	—	4.1	30.5
*u*2858	C(194)...C(196)	520.6(26)	25.3(tied to *u*3057)	—	–1.2	22.7
*u*3044	Si(5)...H(44)	520.7(14)	28.9(fixed)	—	–0.5	28.9
*u*3144	H(256)...H(269)	520.7(51)	35.6(fixed)	—	–7.4	35.6
*u*2994	Si(143)...H(163)	520.8(12)	27.0(fixed)	—	–1.2	27.0
*u*2909	C(8)...C(13)	520.8(65)	28.1(tied to *u*3057)	—	–1.6	25.2
*u*3061	Si(98)...H(114)	520.9(13)	21.7(fixed)	—	–0.9	21.7
*u*2933	H(61)...H(80)	521.0(43)	31.5(fixed)	—	1.9	31.5
*u*2989	Si(237)...H(257)	521.0(12)	20.6(fixed)	—	–1.3	20.6
*u*2978	H(155)...H(174)	521.0(38)	31.8(fixed)	—	2.0	31.8
*u*3052	Si(4)...H(20)	521.0(13)	20.4(fixed)	—	–1.2	20.4
*u*3030	Si(190)...H(210)	521.1(12)	21.2(fixed)	—	–1.1	21.2
*u*2915	H(129)...H(141)	521.1(100)	40.3(fixed)	—	–6.7	40.3
*u*2906	C(12)...C(17)	521.1(66)	26.2(tied to *u*3057)	—	–1.4	23.5
*u*3040	Si(5)...H(39)	521.2(16)	22.6(fixed)	—	–1.9	22.6
*u*2700	H(70)...H(83)	521.2(65)	58.6(fixed)	—	20.4	58.6
*u*2784	C(64)...H(62)	521.2(58)	21.0(fixed)	—	–1.2	21.0
*u*3033	Si(52)...H(91)	521.2(13)	21.7(fixed)	—	–1.0	21.7
*u*3020	Si(51)...H(67)	521.2(13)	20.9(fixed)	—	–1.1	20.9
*u*3059	H(108)...H(114)	521.3(30)	40.3(fixed)	—	–1.5	40.3
*u*3039	Si(96)...H(122)	521.5(17)	21.4(fixed)	—	–1.7	21.4
*u*2815	H(214)...H(233)	521.5(36)	40.1(fixed)	—	6.8	40.1
*u*2926	C(11)...H(14)	521.8(39)	23.7(fixed)	—	–1.0	23.7
*u*3068	Si(52)...H(86)	521.9(15)	22.2(fixed)	—	–1.8	22.2
*u*3101	H(65)...H(88)	521.9(37)	40.0(fixed)	—	3.0	40.0
*u*2921	H(119)...H(135)	521.9(70)	41.4(fixed)	—	–5.9	41.4
*u*3132	H(68)...H(81)	522.1(57)	39.6(fixed)	—	–7.9	39.6
*u*3006	H(112)...H(119)	522.1(66)	47.3(fixed)	—	–9.1	47.3
*u*2976	Si(99)...H(138)	522.2(14)	25.9(fixed)	—	1.0	25.9
*u*2997	Si(192)...H(208)	522.2(15)	21.2(fixed)	—	–1.0	21.2
*u*3062	Si(98)...H(133)	522.3(16)	20.4(fixed)	—	–1.9	20.4
*u*3018	H(209)...H(213)	522.3(28)	37.9(fixed)	—	–6.9	37.9
*u*3043	Si(145)...H(161)	522.3(15)	20.7(fixed)	—	–1.2	20.7
*u*3054	Si(239)...H(255)	522.3(15)	22.6(fixed)	—	–0.8	22.6
*u*3224	H(269)...H(281)	522.4(89)	39.1(fixed)	—	–7.7	39.1
*u*3025	Si(49)...H(73)	522.6(18)	21.2(fixed)	—	–1.4	21.2
*u*3012	Si(237)...H(263)	522.6(18)	21.1(fixed)	—	–1.7	21.1

*u*3056	C(195)...H(227)	522.6(29)	45.5(fixed)	—	7.9	45.5
*u*2908	C(199)...H(224)	522.8(31)	30.7(fixed)	—	3.7	30.7
*u*3069	Si(145)...H(169)	522.9(15)	20.0(fixed)	—	–1.5	20.0
*u*3104	H(18)...H(41)	522.9(29)	38.0(fixed)	—	2.4	38.0
*u*2990	Si(97)...H(130)	523.0(18)	19.6(fixed)	—	–1.2	19.6
*u*2626	H(67)...H(76)	523.1(97)	43.3(fixed)	—	8.3	43.3
*u*3106	H(88)...H(90)	523.3(34)	39.7(fixed)	—	–8.7	39.7
*u*3014	Si(97)...H(141)	523.6(20)	22.1(fixed)	—	–1.1	22.1
*u*3008	Si(98)...H(120)	523.7(16)	20.9(fixed)	—	–0.8	20.9
*u*3037	Si(4)...H(26)	523.7(16)	21.1(fixed)	—	–1.2	21.1
*u*3198	H(202)...H(233)	523.7(29)	37.7(fixed)	—	–1.9	37.7
*u*3035	Si(145)...H(177)	523.8(16)	20.8(fixed)	—	–1.1	20.8
*u*3053	Si(4)...H(36)	523.8(15)	19.7(fixed)	—	–1.2	19.7
*u*3002	Si(190)...H(214)	523.8(18)	20.5(fixed)	—	–1.4	20.5
*u*2974	H(134)...H(136)	523.9(45)	75.8(fixed)	—	2.9	75.8
*u*3094	C(17)...H(24)	524.0(67)	33.0(fixed)	—	2.3	33.0
*u*2981	Si(3)...H(47)	524.0(21)	21.6(fixed)	—	–1.3	21.6
*u*3222	H(65)...H(79)	524.3(63)	63.8(fixed)	—	4.6	63.8
*u*2807	H(108)...H(123)	524.4(51)	31.4(fixed)	—	2.6	31.4
*u*2952	Si(50)...H(94)	524.5(21)	22.0(fixed)	—	–1.2	22.0
*u*3045	Si(51)...H(83)	524.6(16)	25.7(fixed)	—	0.2	25.7
*u*2971	Si(239)...H(261)	524.7(16)	20.5(fixed)	—	–1.0	20.5
*u*2985	H(155)...H(167)	524.8(32)	36.6(fixed)	—	–1.0	36.6
*u*3114	H(124)...H(131)	524.9(48)	36.3(fixed)	—	–7.4	36.3
*u*2860	H(73)...H(92)	524.9(91)	41.3(fixed)	—	6.1	41.3
*u*3026	C(100)...C(103)	525.1(62)	22.6(tied to *u*3057)	—	–1.1	20.2
*u*2961	H(160)...H(179)	525.5(25)	37.6(fixed)	—	–6.1	37.6
*u*2847	C(106)...C(110)	525.6(34)	23.3(tied to *u*3057)	—	–1.2	20.9
*u*3127	H(160)...H(168)	525.6(28)	38.2(fixed)	—	–6.8	38.2
*u*3058	H(68)...H(71)	525.7(124)	35.8(fixed)	—	–7.2	35.8
*u*2850	C(7)...H(36)	525.8(58)	29.6(fixed)	—	3.2	29.6
*u*3231	H(37)...H(42)	525.8(99)	73.4(fixed)	—	4.0	73.4
*u*3073	Si(52)...H(75)	525.9(22)	24.8(fixed)	—	–2.0	24.8
*u*3122	C(101)...H(133)	526.4(32)	35.9(fixed)	—	2.2	35.9
*u*2947	H(14)...H(33)	526.8(44)	31.6(fixed)	—	2.1	31.6
*u*3180	H(18)...H(32)	526.8(39)	59.3(fixed)	—	4.0	59.3
*u*3103	C(111)...H(118)	526.9(66)	33.8(fixed)	—	2.4	33.8
*u*3322	H(166)...H(182)	527.0(43)	37.6(fixed)	—	–9.0	37.6
*u*3074	H(25)...H(38)	527.1(66)	38.9(fixed)	—	–6.2	38.9
*u*3214	C(57)...H(65)	527.1(55)	30.2(fixed)	—	1.2	30.2
*u*3189	H(27)...H(37)	527.1(42)	43.5(fixed)	—	2.8	43.5
*u*2701	C(56)...H(67)	527.2(77)	33.8(fixed)	—	2.9	33.8
*u*3034	H(126)...H(135)	527.4(43)	36.9(fixed)	—	2.5	36.9
*u*3041	H(28)...H(45)	527.5(74)	45.9(fixed)	—	5.3	45.9
*u*3184	H(113)...H(134)	527.8(55)	38.0(fixed)	—	–9.2	38.0
*u*3165	C(16)...H(37)	527.8(88)	32.6(fixed)	—	0.9	32.6

*u*2804	H(127)...H(130)	527.9(45)	38.9(fixed)	—	7.3	38.9
*u*2988	H(15)...H(22)	528.3(67)	41.8(fixed)	—	–1.1	41.8
*u*3463	H(115)...H(131)	528.7(52)	38.9(fixed)	—	3.5	38.9
*u*3087	C(17)...H(28)	528.8(69)	36.9(fixed)	—	2.9	36.9
*u*2965	H(109)...H(116)	528.8(66)	35.1(fixed)	—	–1.3	35.1
*u*2883	C(110)...H(134)	529.1(35)	33.2(fixed)	—	1.7	33.2
*u*3340	H(21)...H(25)	529.1(104)	46.2(fixed)	—	–10.3	46.2
*u*3442	H(40)...H(45)	529.1(100)	41.1(fixed)	—	3.9	41.1
*u*3288	H(115)...H(125)	529.2(61)	36.6(fixed)	—	1.1	36.6
*u*3211	C(17)...H(40)	529.2(88)	31.1(fixed)	—	2.3	31.1
*u*3070	C(6)...C(9)	529.4(63)	23.5(tied to *u*3057)	—	–1.3	21.0
*u*3117	H(159)...H(182)	529.4(33)	38.5(fixed)	—	3.2	38.5
*u*3395	H(113)...H(135)	529.5(30)	41.2(fixed)	—	–9.6	41.2
*u*3319	H(90)...H(92)	529.9(38)	36.9(fixed)	—	3.9	36.9
*u*3125	H(211)...H(215)	529.9(40)	41.4(fixed)	—	6.5	41.4
*u*2764	C(54)...H(83)	530.0(49)	44.4(fixed)	—	18.1	44.4
*u*2925	C(64)...H(73)	530.0(82)	31.7(fixed)	—	3.2	31.7
*u*2977	H(121)...H(134)	530.2(32)	36.7(fixed)	—	4.4	36.7
*u*3175	C(10)...H(18)	530.2(32)	29.9(fixed)	—	1.1	29.9
*u*2924	C(105)...H(130)	530.5(36)	29.4(fixed)	—	3.9	29.4
*u*3081	C(111)...H(122)	530.9(69)	35.5(fixed)	—	3.5	35.5
*u*3102	H(18)...H(25)	530.9(66)	36.7(fixed)	—	–6.9	36.7
*u*3116	H(249)...H(277)	531.0(47)	46.9(fixed)	—	–1.3	46.9
*u*3036	H(19)...H(37)	531.0(111)	33.1(fixed)	—	–5.5	33.1
*u*3164	H(62)...H(80)	531.2(54)	37.6(fixed)	—	–1.6	37.6
*u*3017	H(119)...H(136)	531.6(43)	58.9(fixed)	—	15.8	58.9
*u*3004	H(124)...H(132)	531.7(34)	37.6(fixed)	—	–6.3	37.6
*u*3021	H(122)...H(139)	531.8(74)	44.4(fixed)	—	6.2	44.4
*u*3212	C(13)...C(17)	532.8(56)	23.9(tied to *u*3057)	—	–1.3	21.4
*u*3109	H(164)...H(166)	532.8(39)	45.5(fixed)	—	11.4	45.5
*u*2996	H(19)...H(38)	532.9(68)	35.7(fixed)	—	–4.8	35.7
*u*3147	C(8)...C(16)	533.5(24)	21.4(tied to *u*3057)	—	–1.2	19.1
*u*3066	H(32)...H(38)	533.6(41)	45.4(fixed)	—	10.6	45.4
*u*3153	C(53)...C(60)	533.7(21)	20.0(tied to *u*3057)	—	–1.4	17.9
*u*3402	H(112)...H(126)	533.8(41)	39.7(fixed)	—	4.8	39.7
*u*3268	C(53)...C(57)	533.8(38)	21.8(tied to *u*3057)	—	–1.0	19.5
*u*3118	C(102)...C(110)	534.1(26)	20.3(tied to *u*3057)	—	–0.9	18.2
*u*3293	H(43)...H(45)	534.1(32)	36.0(fixed)	—	5.8	36.0
*u*3382	H(215)...H(223)	534.5(45)	43.8(fixed)	—	0.0	43.8
*u*3246	C(6)...C(10)	534.6(26)	21.1(tied to *u*3057)	—	–0.9	18.9
*u*3326	C(101)...C(106)	534.8(32)	18.6(tied to *u*3057)	—	–0.9	16.6
*u*3284	C(104)...H(112)	534.9(33)	27.8(fixed)	—	3.0	27.8
*u*3166	C(6)...C(13)	535.1(13)	19.7(tied to *u*3057)	—	–1.5	17.6
*u*3238	H(14)...H(24)	535.3(70)	35.4(fixed)	—	–2.1	35.4
*u*3191	H(155)...H(170)	535.4(27)	38.4(fixed)	—	–1.5	38.4
*u*3352	H(137)...H(139)	535.5(32)	37.0(fixed)	—	5.5	37.0

*u*3050	H(25)...H(42)	535.6(41)	50.8(fixed)	—	18.7	50.8
*u*3252	H(116)...H(124)	535.7(40)	36.8(fixed)	—	1.8	36.8
*u*3011	C(107)...C(110)	535.8(27)	22.2(fixed)	—	–1.0	22.2
*u*3019	H(253)...H(273)	535.8(36)	43.4(fixed)	—	8.6	43.4
*u*3219	H(159)...H(173)	535.9(29)	59.0(fixed)	—	3.7	59.0
*u*2887	C(53)...C(55)	536.1(70)	24.7(tied to *u*3057)	—	–1.1	22.1
*u*3346	C(100)...C(104)	536.2(28)	19.9(tied to *u*3057)	—	–0.8	17.8
*u*3174	C(148)...C(149)	536.3(18)	21.3(tied to *u*3057)	—	–1.1	19.1
*u*3259	H(21)...H(27)	536.5(112)	40.3(fixed)	—	–10.7	40.3
*u*3169	C(57)...C(59)	536.6(20)	21.6(tied to *u*3057)	—	–1.3	19.3
*u*3176	H(34)...H(40)	536.6(63)	35.9(fixed)	—	5.9	35.9
*u*3247	C(63)...C(64)	536.8(35)	18.5(tied to *u*3057)	—	–0.8	16.6
*u*3232	H(66)...H(80)	536.8(35)	37.4(fixed)	—	4.0	37.4
*u*3218	C(12)...C(16)	536.9(57)	22.7(tied to *u*3057)	—	–1.2	20.4
*u*3498	H(259)...H(281)	536.9(47)	38.5(fixed)	—	3.0	38.5
*u*3177	C(148)...H(183)	536.9(26)	31.0(fixed)	—	1.1	31.0
*u*3223	H(115)...H(121)	537.0(111)	38.8(fixed)	—	–8.5	38.8
*u*3264	C(102)...H(131)	537.1(48)	29.1(fixed)	—	1.5	29.1
*u*3182	C(195)...C(197)	537.1(20)	21.0(tied to *u*3057)	—	–1.4	18.8
*u*3491	H(71)...H(77)	537.5(56)	36.6(fixed)	—	4.7	36.6
*u*3160	C(10)...C(12)	537.6(19)	21.4(tied to *u*3057)	—	–1.5	19.2
*u*3233	C(9)...C(12)	537.8(36)	23.0(tied to *u*3057)	—	–1.4	20.6
*u*3227	C(16)...C(17)	537.9(31)	18.2(tied to *u*3057)	—	–0.9	16.3
*u*3170	C(147)...C(154)	538.1(14)	20.1(tied to *u*3057)	—	–1.2	18.0
*u*3146	C(103)...C(107)	538.2(31)	19.3(tied to *u*3057)	—	–0.9	17.2
*u*3149	C(104)...C(107)	538.4(22)	20.2(tied to *u*3057)	—	–1.4	18.1
*u*3126	H(109)...H(112)	538.5(44)	40.6(fixed)	—	–1.3	40.6
*u*3365	H(115)...H(119)	538.7(101)	40.7(fixed)	—	–8.4	40.7
*u*3301	H(109)...H(127)	538.7(38)	28.3(fixed)	—	–4.3	28.3
*u*3161	H(15)...H(18)	538.8(46)	33.9(fixed)	—	–1.6	33.9
*u*3250	H(41)...H(47)	538.8(67)	45.6(fixed)	—	1.3	45.6
*u*3283	H(19)...H(33)	538.8(34)	39.0(fixed)	—	4.1	39.0
*u*3245	H(160)...H(174)	538.9(33)	36.5(fixed)	—	3.9	36.5
*u*3290	C(110)...C(111)	539.0(31)	18.5(tied to *u*3057)	—	–1.0	16.6
*u*3574	H(118)...H(131)	539.1(64)	43.4(fixed)	—	2.0	43.4
*u*3197	H(170)...H(187)	539.1(56)	37.1(fixed)	—	4.7	37.1
*u*3215	C(11)...C(13)	539.1(42)	17.9(tied to *u*3057)	—	–0.5	16.0
*u*3092	H(79)...H(85)	539.2(42)	49.0(fixed)	—	18.0	49.0
*u*3473	H(206)...H(220)	539.3(30)	42.3(fixed)	—	3.1	42.3
*u*3464	C(60)...H(71)	539.4(86)	30.7(fixed)	—	1.3	30.7
*u*3185	C(64)...H(87)	539.4(49)	30.3(fixed)	—	2.4	30.3
*u*3135	C(241)...C(247)	539.5(17)	20.7(tied to *u*3057)	—	–1.1	18.5
*u*3308	C(195)...H(230)	539.5(30)	28.2(fixed)	—	1.7	28.2
*u*3297	H(74)...H(82)	539.6(63)	41.0(fixed)	—	1.5	41.0
*u*3171	H(21)...H(31)	539.6(49)	41.2(fixed)	—	8.2	41.2
*u*3392	C(11)...H(24)	539.6(36)	29.8(fixed)	—	1.2	29.8

*u*3276	C(147)...H(165)	539.6(35)	29.4(fixed)	—	1.6	29.4
*u*3384	H(135)...H(141)	539.8(53)	38.8(fixed)	—	2.0	38.8
*u*3434	H(209)...H(225)	540.0(39)	38.1(fixed)	—	3.4	38.1
*u*3024	H(85)...H(94)	540.1(83)	54.7(fixed)	—	1.6	54.7
*u*3192	H(81)...H(87)	540.1(56)	36.5(fixed)	—	6.0	36.5
*u*3381	H(113)...H(127)	540.2(39)	38.2(fixed)	—	4.6	38.2
*u*3194	C(60)...C(64)	540.2(43)	23.0(tied to *u*3057)	—	–1.0	20.6
*u*3353	H(207)...H(221)	540.3(36)	37.9(fixed)	—	3.9	37.9
*u*3578	H(24)...H(33)	540.5(40)	47.1(fixed)	—	2.3	47.1
*u*3282	H(22)...H(30)	540.8(36)	43.4(fixed)	—	2.7	43.4
*u*3563	H(71)...H(87)	541.1(99)	46.3(fixed)	—	2.9	46.3
*u*3321	H(254)...H(268)	541.3(37)	37.4(fixed)	—	4.5	37.4
*u*3067	H(38)...H(47)	541.5(77)	45.4(fixed)	—	1.3	45.4
*u*3424	H(87)...H(92)	541.6(69)	41.4(fixed)	—	4.0	41.4
*u*3374	C(55)...C(57)	541.8(35)	19.4(tied to *u*3057)	—	–1.0	17.4
*u*3349	C(243)...C(252)	541.8(28)	19.2(tied to *u*3057)	—	–1.0	17.2
*u*3208	C(55)...C(59)	541.9(22)	22.7(tied to *u*3057)	—	–1.2	20.3
*u*3262	C(53)...C(58)	542.0(32)	19.2(tied to *u*3057)	—	–1.1	17.2
*u*3029	H(166)...H(176)	542.0(47)	43.9(fixed)	—	3.2	43.9
*u*3285	H(249)...H(280)	542.0(36)	28.0(fixed)	—	–4.0	28.0
*u*3388	C(8)...C(11)	542.0(22)	21.6(tied to *u*3057)	—	–1.2	19.3
*u*3286	C(102)...C(106)	542.0(37)	20.4(tied to *u*3057)	—	–1.0	18.3
*u*3261	C(150)...C(158)	542.1(33)	18.4(tied to *u*3057)	—	–0.8	16.4
*u*3314	C(8)...H(44)	542.2(35)	70.4(fixed)	—	–1.2	70.4
*u*3243	C(58)...C(60)	542.2(33)	18.1(tied to *u*3057)	—	–0.6	16.2
*u*3480	C(55)...C(60)	542.2(57)	23.8(tied to *u*3057)	—	–1.1	21.3
*u*3202	H(109)...H(128)	542.3(33)	30.8(fixed)	—	–3.6	30.8
*u*3236	C(147)...C(151)	542.3(17)	22.0(tied to *u*3057)	—	–0.9	19.7
*u*3225	C(147)...C(152)	542.5(31)	18.7(tied to *u*3057)	—	–1.0	16.8
*u*3278	C(242)...H(277)	542.7(31)	28.0(fixed)	—	4.4	28.0
*u*3650	H(259)...H(268)	542.7(43)	44.4(fixed)	—	1.8	44.4
*u*3359	H(15)...H(33)	542.9(33)	28.0(fixed)	—	–4.4	28.0
*u*3368	C(194)...C(198)	542.9(18)	20.2(tied to *u*3057)	—	–0.9	18.1
*u*3186	H(72)...H(84)	542.9(21)	60.0(fixed)	—	16.7	60.0
*u*3260	H(254)...H(263)	542.9(54)	44.2(fixed)	—	1.3	44.2
*u*3410	C(56)...C(57)	542.9(46)	21.4(tied to *u*3057)	—	–0.9	19.1
*u*3272	C(6)...C(11)	543.0(32)	18.9(tied to *u*3057)	—	–1.1	16.9
*u*3332	C(241)...C(245)	543.2(18)	19.8(tied to *u*3057)	—	–0.9	17.7
*u*3251	H(256)...H(266)	543.2(56)	36.3(fixed)	—	1.8	36.3
*u*3362	C(195)...C(200)	543.3(20)	19.9(tied to *u*3057)	—	–1.1	17.8
*u*3310	H(75)...H(81)	543.5(98)	41.8(fixed)	—	5.4	41.8
*u*3205	H(29)...H(30)	543.5(58)	35.6(fixed)	—	6.3	35.6
*u*3152	C(194)...C(197)	543.6(21)	21.6(tied to *u*3057)	—	–1.0	19.3
*u*3306	C(100)...C(105)	543.6(34)	18.6(tied to *u*3057)	—	–0.9	16.6
*u*3289	C(194)...C(199)	543.6(33)	18.4(tied to *u*3057)	—	–0.9	16.5
*u*3151	C(196)...C(201)	543.8(31)	20.7(tied to *u*3057)	—	–1.0	18.5

*u*3506	H(159)...H(165)	543.8(46)	42.1(fixed)	—	2.5	42.1
*u*3495	C(246)...H(259)	544.0(38)	28.7(fixed)	—	0.9	28.7
*u*3038	H(68)...H(72)	544.0(121)	38.3(fixed)	—	–6.8	38.3
*u*3279	C(241)...C(246)	544.0(33)	18.1(tied to *u*3057)	—	–0.9	16.2
*u*3407	H(253)...H(267)	544.1(31)	39.9(fixed)	—	6.9	39.9
*u*3432	C(243)...C(246)	544.1(24)	20.7(tied to *u*3057)	—	–1.2	18.5
*u*3356	H(209)...H(219)	544.2(47)	39.7(fixed)	—	1.9	39.7
*u*3329	C(147)...C(149)	544.2(31)	21.7(tied to *u*3057)	—	–1.1	19.4
*u*3269	C(9)...C(10)	544.3(32)	18.6(tied to *u*3057)	—	–0.7	16.7
*u*3397	Si(51)...H(85)	544.4(8)	17.4(fixed)	—	–7.5	17.4
*u*3265	C(54)...H(89)	544.6(42)	28.0(fixed)	—	2.4	28.0
*u*3448	Si(50)...H(77)	544.7(9)	17.1(fixed)	—	–6.5	17.1
*u*3292	C(59)...C(63)	544.7(33)	20.8(tied to *u*3057)	—	–1.2	18.6
*u*3420	H(70)...H(84)	544.8(66)	74.4(fixed)	—	2.4	74.4
*u*3549	H(113)...H(125)	544.9(43)	36.9(fixed)	—	1.2	36.9
*u*3172	H(123)...H(124)	544.9(56)	36.5(fixed)	—	5.5	36.5
*u*3203	C(150)...C(152)	544.9(19)	24.3(tied to *u*3057)	—	–1.1	21.8
*u*3193	H(113)...H(119)	545.0(89)	37.2(fixed)	—	–10.3	37.2
*u*3334	C(101)...C(110)	545.0(25)	20.1(tied to *u*3057)	—	–0.9	18.0
*u*3350	H(168)...H(180)	545.2(45)	41.0(fixed)	—	1.5	41.0
*u*3389	C(102)...C(105)	545.4(21)	20.8(tied to *u*3057)	—	–1.0	18.6
*u*3444	Si(5)...H(43)	545.5(11)	17.5(fixed)	—	–7.5	17.5
*u*3484	Si(99)...H(137)	545.7(12)	16.7(fixed)	—	–7.6	16.7
*u*3248	C(103)...C(104)	545.7(31)	18.7(tied to *u*3057)	—	–0.8	16.7
*u*3316	C(7)...C(16)	545.9(20)	19.9(tied to *u*3057)	—	–0.8	17.8
*u*3328	H(69)...H(77)	546.0(65)	46.1(fixed)	—	–0.2	46.1
*u*3190	C(152)...H(170)	546.0(29)	31.2(fixed)	—	1.6	31.2
*u*3360	C(56)...H(79)	546.2(50)	29.8(fixed)	—	7.7	29.8
*u*3300	C(242)...C(248)	546.2(30)	18.7(tied to *u*3057)	—	–0.7	16.8
*u*3179	C(59)...H(70)	546.3(53)	30.9(fixed)	—	1.6	30.9
*u*3254	H(256)...H(275)	546.4(53)	35.1(fixed)	—	5.3	35.1
*u*3162	C(102)...H(138)	546.4(38)	59.7(fixed)	—	1.6	59.7
*u*3335	C(54)...C(63)	546.4(30)	20.2(tied to *u*3057)	—	–0.8	18.1
*u*3357	Si(5)...H(41)	546.4(15)	17.1(fixed)	—	–4.3	17.1
*u*3148	C(194)...H(217)	546.4(24)	32.7(fixed)	—	6.5	32.7
*u*3258	H(14)...H(42)	546.5(51)	41.1(fixed)	—	–8.7	41.1
*u*3355	Si(3)...H(30)	546.6(9)	16.6(fixed)	—	–5.1	16.6
*u*2636	H(260)...H(271)	546.6(81)	46.5(fixed)	—	2.5	46.5
*u*3267	H(15)...H(34)	546.6(33)	32.4(fixed)	—	–4.0	32.4
*u*3405	H(62)...H(87)	546.9(47)	28.4(fixed)	—	–4.3	28.4
*u*3240	Si(98)...H(135)	547.0(9)	17.5(fixed)	—	–3.6	17.5
*u*3303	Si(192)...H(229)	547.0(8)	18.3(fixed)	—	–5.0	18.3
*u*3371	Si(4)...H(38)	547.0(13)	15.7(fixed)	—	–3.7	15.7
*u*3299	Si(97)...H(132)	547.2(12)	15.7(fixed)	—	–3.3	15.7
*u*3401	H(170)...H(174)	547.3(38)	41.4(fixed)	—	3.3	41.4
*u*3390	Si(49)...H(72)	547.5(16)	15.6(fixed)	—	–3.4	15.6

*u*3418	C(105)...H(118)	547.6(28)	28.4(fixed)	—	1.6	28.4
*u*3446	Si(51)...H(66)	547.6(14)	15.4(fixed)	—	–3.4	15.4
*u*3478	C(101)...H(130)	547.8(47)	33.2(fixed)	—	–0.1	33.2
*u*3287	C(107)...H(136)	547.8(39)	66.7(fixed)	—	–3.4	66.7
*u*3320	Si(52)...H(88)	547.8(11)	17.0(fixed)	—	–3.9	17.0
*u*3333	Si(49)...H(68)	547.8(7)	16.0(fixed)	—	–3.9	16.0
*u*3337	Si(2)...H(27)	547.8(15)	16.8(fixed)	—	–3.8	16.8
*u*3136	H(70)...H(74)	547.9(111)	41.9(fixed)	—	4.5	41.9
*u*3369	Si(2)...H(21)	547.9(5)	16.1(fixed)	—	–4.3	16.1
*u*3076	H(25)...H(39)	548.2(111)	48.3(fixed)	—	2.8	48.3
*u*3150	H(255)...H(262)	548.2(71)	39.2(fixed)	—	6.5	39.2
*u*3195	H(249)...H(281)	548.2(36)	31.9(fixed)	—	–3.7	31.9
*u*3199	H(108)...H(129)	548.3(26)	25.4(fixed)	—	–1.5	25.4
*u*3273	Si(96)...H(121)	548.3(14)	17.0(fixed)	—	–3.8	17.0
*u*3417	Si(145)...H(179)	548.3(8)	15.7(fixed)	—	–3.6	15.7
*u*3483	Si(98)...H(113)	548.4(12)	15.5(fixed)	—	–3.8	15.5
*u*3393	Si(143)...H(175)	548.4(7)	16.0(fixed)	—	–4.0	16.0
*u*3439	Si(4)...H(19)	548.5(12)	15.5(fixed)	—	–3.2	15.5
*u*3607	H(118)...H(127)	548.6(36)	45.5(fixed)	—	2.4	45.5
*u*3465	H(70)...H(89)	548.7(53)	42.5(fixed)	—	3.6	42.5
*u*3351	Si(143)...H(162)	548.7(8)	16.8(fixed)	—	–5.6	16.8
*u*3398	Si(4)...H(25)	548.8(8)	15.6(fixed)	—	–3.6	15.6
*u*3291	C(9)...C(13)	548.9(63)	24.8(tied to *u*3057)	—	–1.0	22.2
*u*3181	C(54)...C(56)	548.9(65)	21.0(tied to *u*3057)	—	–1.2	18.8
*u*3457	Si(52)...H(90)	548.9(11)	15.6(fixed)	—	–3.7	15.6
*u*3386	Si(49)...H(81)	548.9(7)	16.0(fixed)	—	–3.5	16.0
*u*3325	Si(97)...H(124)	549.1(9)	15.7(fixed)	—	–3.0	15.7
*u*3206	H(19)...H(25)	549.2(89)	37.1(fixed)	—	–7.2	37.1
*u*3228	C(54)...C(59)	549.2(36)	20.8(tied to *u*3057)	—	–0.9	18.7
*u*3367	Si(2)...H(34)	549.2(7)	15.9(fixed)	—	–3.6	15.9
*u*3376	Si(190)...H(222)	549.3(7)	15.7(fixed)	—	–3.6	15.7
*u*2992	H(208)...H(213)	549.3(52)	42.0(fixed)	—	2.6	42.0
*u*3532	C(53)...H(79)	549.4(47)	54.8(fixed)	—	–0.5	54.8
*u*3469	Si(96)...H(115)	549.4(5)	15.3(fixed)	—	–3.3	15.3
*u*3453	Si(237)...H(269)	549.4(7)	15.3(fixed)	—	–3.4	15.3
*u*3242	C(63)...H(84)	549.6(36)	31.4(fixed)	—	10.2	31.4
*u*3377	Si(98)...H(119)	549.6(7)	15.7(fixed)	—	–3.6	15.7
*u*3311	Si(96)...H(128)	549.7(7)	15.7(fixed)	—	–3.4	15.7
*u*2936	H(213)...H(228)	549.8(31)	42.2(fixed)	—	16.4	42.2
*u*3399	H(62)...H(88)	549.8(59)	32.2(fixed)	—	–4.7	32.2
*u*3178	H(88)...H(94)	549.8(63)	44.4(fixed)	—	3.1	44.4
*u*3441	C(59)...H(78)	550.0(26)	60.3(fixed)	—	–1.6	60.3
*u*3526	C(6)...H(32)	550.0(33)	50.4(fixed)	—	–0.7	50.4
*u*3277	C(13)...H(29)	550.1(76)	30.9(fixed)	—	2.2	30.9
*u*3312	Si(190)...H(213)	550.1(12)	16.0(fixed)	—	–3.4	16.0
*u*3505	H(18)...H(40)	550.1(42)	36.4(fixed)	—	0.5	36.4

*u*3416	C(149)...H(163)	550.2(21)	57.1(fixed)	—	–1.6	57.1
*u*3496	H(19)...H(31)	550.3(38)	42.3(fixed)	—	8.6	42.3
*u*3471	Si(239)...H(254)	550.4(13)	15.7(fixed)	—	–4.5	15.7
*u*3110	H(167)...H(175)	550.5(62)	40.7(fixed)	—	2.3	40.7
*u*3512	H(65)...H(87)	550.6(36)	38.1(fixed)	—	0.3	38.1
*u*3257	Si(237)...H(262)	550.6(13)	16.5(fixed)	—	–3.6	16.5
*u*3163	C(243)...C(248)	550.7(44)	20.4(tied to *u*3057)	—	–1.1	18.3
*u*3364	H(61)...H(89)	550.7(38)	29.1(fixed)	—	–4.3	29.1
*u*3445	C(244)...C(252)	550.8(25)	20.8(tied to *u*3057)	—	–0.7	18.6
*u*3302	C(60)...H(67)	550.8(36)	31.9(fixed)	—	–1.1	31.9
*u*3281	C(148)...C(153)	550.9(25)	19.4(tied to *u*3057)	—	–0.8	17.4
*u*3404	Si(190)...H(209)	551.0(9)	15.7(fixed)	—	–3.9	15.7
*u*3411	Si(145)...H(160)	551.0(12)	15.4(fixed)	—	–3.3	15.4
*u*3270	H(202)...H(223)	551.1(25)	25.2(fixed)	—	–1.4	25.2
*u*3155	H(68)...H(78)	551.1(60)	42.3(fixed)	—	12.1	42.3
*u*3379	H(76)...H(79)	551.1(68)	47.4(fixed)	—	12.8	47.4
*u*3217	C(243)...H(275)	551.2(61)	28.6(fixed)	—	1.6	28.6
*u*3629	C(13)...H(45)	551.2(69)	32.5(fixed)	—	–1.6	32.5
*u*3488	Si(192)...H(207)	551.5(13)	15.1(fixed)	—	–3.4	15.1
*u*3394	Si(239)...H(260)	551.6(9)	15.5(fixed)	—	–3.5	15.5
*u*3345	Si(145)...H(168)	551.7(9)	16.3(fixed)	—	–3.3	16.3
*u*3363	Si(237)...H(256)	551.7(9)	15.7(fixed)	—	–3.1	15.7
*u*3207	C(197)...H(220)	551.7(27)	31.4(fixed)	—	2.0	31.4
*u*3324	H(14)...H(43)	551.9(62)	43.0(fixed)	—	–9.4	43.0
*u*3296	C(195)...C(201)	551.9(20)	22.5(tied to *u*3057)	—	–0.9	20.2
*u*3342	H(14)...H(22)	552.0(25)	26.0(fixed)	—	–1.5	26.0
*u*3415	H(108)...H(118)	552.1(38)	27.3(fixed)	—	–4.5	27.3
*u*3409	H(155)...H(183)	552.1(35)	25.9(fixed)	—	–3.7	25.9
*u*3670	H(72)...H(86)	552.2(68)	42.7(fixed)	—	3.3	42.7
*u*3130	H(26)...H(41)	552.2(70)	43.1(fixed)	—	1.7	43.1
*u*3298	C(101)...H(136)	552.3(43)	30.9(fixed)	—	9.1	30.9
*u*3544	H(25)...H(35)	552.3(32)	38.5(fixed)	—	3.0	38.5
*u*3517	H(66)...H(78)	552.5(50)	48.2(fixed)	—	11.6	48.2
*u*3542	C(12)...H(42)	552.7(69)	61.8(fixed)	—	–1.5	61.8
*u*3275	H(206)...H(217)	552.8(32)	43.0(fixed)	—	10.5	43.0
*u*3430	H(14)...H(23)	552.8(37)	26.9(fixed)	—	–2.3	26.9
*u*3481	C(11)...H(39)	552.9(66)	39.1(fixed)	—	–0.7	39.1
*u*3229	H(108)...H(128)	553.0(23)	26.6(fixed)	—	–1.6	26.6
*u*3479	H(14)...H(21)	553.0(39)	27.5(fixed)	—	–2.4	27.5
*u*3421	C(244)...H(280)	553.3(36)	28.1(fixed)	—	1.8	28.1
*u*3459	C(103)...H(133)	553.3(41)	33.4(fixed)	—	–1.4	33.4
*u*3201	H(216)...H(222)	553.4(41)	41.2(fixed)	—	10.6	41.2
*u*3347	C(196)...C(205)	553.5(21)	19.4(tied to *u*3057)	—	–0.8	17.4
*u*3358	C(150)...H(185)	553.6(20)	32.3(fixed)	—	–1.0	32.3
*u*3378	C(63)...H(94)	553.6(58)	36.8(fixed)	—	–0.4	36.8
*u*3244	C(243)...H(279)	553.7(26)	48.1(fixed)	—	–0.8	48.1

*u*3253	C(149)...H(173)	553.7(25)	28.5(fixed)	—	6.1	28.5
*u*3656	C(100)...H(126)	553.8(37)	31.2(fixed)	—	–1.1	31.2
*u*3271	C(7)...H(42)	553.9(34)	30.7(fixed)	—	10.4	30.7
*u*3327	H(61)...H(90)	553.9(29)	32.3(fixed)	—	–4.2	32.3
*u*3274	H(155)...H(156)	553.9(41)	17.5(fixed)	—	–2.3	17.5
*u*3280	H(108)...H(127)	554.0(23)	25.9(fixed)	—	–2.3	25.9
*u*3590	H(260)...H(270)	554.1(36)	36.9(fixed)	—	2.2	36.9
*u*3354	C(8)...C(17)	554.2(48)	19.9(tied to *u*3057)	—	–1.2	17.8
*u*3501	H(259)...H(275)	554.3(75)	41.7(fixed)	—	2.9	41.7
*u*3648	H(117)...H(131)	554.4(37)	34.9(fixed)	—	1.6	34.9
*u*3492	H(85)...H(91)	554.4(57)	46.7(fixed)	—	0.9	46.7
*u*3561	H(116)...H(137)	554.4(28)	43.5(fixed)	—	–0.4	43.5
*u*3338	H(61)...H(69)	554.5(28)	25.9(fixed)	—	–1.8	25.9
*u*3385	H(61)...H(70)	554.8(23)	27.6(fixed)	—	–2.6	27.6
*u*3313	H(126)...H(134)	554.8(32)	35.3(fixed)	—	0.8	35.3
*u*3550	H(119)...H(129)	554.8(35)	37.8(fixed)	—	2.8	37.8
*u*3158	H(162)...H(172)	554.8(31)	45.1(fixed)	—	7.8	45.1
*u*3427	H(120)...H(132)	554.9(41)	36.8(fixed)	—	3.8	36.8
*u*3366	C(13)...H(20)	555.0(27)	32.1(fixed)	—	–1.4	32.1
*u*3361	C(16)...H(47)	555.1(50)	33.7(fixed)	—	–0.6	33.7
*u*3128	H(207)...H(214)	555.1(40)	40.9(fixed)	—	2.2	40.9
*u*3621	H(75)...H(77)	555.1(73)	52.2(fixed)	—	4.2	52.2
*u*3507	H(211)...H(216)	555.1(32)	38.2(fixed)	—	–1.0	38.2
*u*3343	C(196)...H(233)	555.2(29)	27.5(fixed)	—	2.0	27.5
*u*3570	C(196)...H(227)	555.2(43)	58.7(fixed)	—	–4.3	58.7
*u*3344	H(155)...H(184)	555.2(27)	31.1(fixed)	—	–3.6	31.1
*u*3119	H(211)...H(228)	555.4(31)	64.8(fixed)	—	8.1	64.8
*u*3454	C(9)...H(36)	555.4(57)	32.9(fixed)	—	–1.0	32.9
*u*3456	C(12)...H(31)	555.4(29)	52.5(fixed)	—	–2.0	52.5
*u*3422	C(197)...H(210)	555.5(30)	35.1(fixed)	—	–1.2	35.1
*u*3396	C(55)...H(92)	555.6(73)	28.6(fixed)	—	1.5	28.6
*u*3323	H(109)...H(131)	555.6(23)	25.8(fixed)	—	–2.4	25.8
*u*3601	H(44)...H(45)	555.7(38)	35.4(fixed)	—	–1.7	35.4
*u*3239	C(12)...H(23)	555.7(42)	29.6(fixed)	—	3.3	29.6
*u*3330	H(113)...H(122)	555.7(84)	40.9(fixed)	—	2.2	40.9
*u*3597	H(71)...H(92)	555.7(79)	41.6(fixed)	—	2.6	41.6
*u*3534	H(161)...H(166)	555.8(55)	37.8(fixed)	—	1.2	37.8
*u*3528	H(211)...H(217)	555.9(25)	40.8(fixed)	—	–0.4	40.8
*u*3486	C(110)...H(141)	556.1(51)	36.8(fixed)	—	–0.9	36.8
*u*3294	C(7)...C(12)	556.1(44)	19.8(tied to *u*3057)	—	–0.8	17.7
*u*3091	H(208)...H(215)	556.1(42)	45.3(fixed)	—	4.5	45.3
*u*3519	H(65)...H(86)	556.1(27)	34.6(fixed)	—	–1.0	34.6
*u*3413	H(61)...H(68)	556.2(26)	27.6(fixed)	—	–2.8	27.6
*u*3584	H(29)...H(37)	556.2(57)	41.1(fixed)	—	0.4	41.1
*u*3461	H(84)...H(89)	556.2(48)	46.9(fixed)	—	14.2	46.9
*u*3518	H(254)...H(266)	556.3(20)	39.2(fixed)	—	1.7	39.2

*u*3348	C(102)...C(111)	556.4(46)	19.1(tied to *u*3057)	—	–1.1	17.1
*u*3435	H(29)...H(40)	556.5(99)	40.8(fixed)	—	4.5	40.8
*u*3595	H(138)...H(139)	556.6(41)	36.4(fixed)	—	–0.2	36.4
*u*3429	H(120)...H(136)	556.7(24)	60.3(fixed)	—	6.8	60.3
*u*3336	Si(52)...H(74)	556.7(37)	17.8(fixed)	—	–4.8	17.8
*u*3426	H(117)...H(136)	556.8(50)	44.6(fixed)	—	13.1	44.6
*u*3200	H(168)...H(176)	556.8(26)	45.2(fixed)	—	3.9	45.2
*u*3613	H(207)...H(219)	557.0(20)	38.1(fixed)	—	2.2	38.1
*u*3230	H(249)...H(263)	557.1(21)	25.9(fixed)	—	–1.8	25.9
*u*3428	C(107)...H(117)	557.1(31)	29.8(fixed)	—	1.4	29.8
*u*3196	H(108)...H(119)	557.2(37)	33.3(fixed)	—	–3.6	33.3
*u*3425	H(202)...H(222)	557.2(21)	26.1(fixed)	—	–2.1	26.1
*u*3372	Si(50)...H(93)	557.2(39)	15.7(fixed)	—	–3.9	15.7
*u*3508	H(18)...H(39)	557.5(31)	33.7(fixed)	—	–1.4	33.7
*u*3509	H(164)...H(178)	557.5(33)	44.5(fixed)	—	8.5	44.5
*u*3497	H(264)...H(280)	557.6(46)	42.4(fixed)	—	4.0	42.4
*u*3482	H(24)...H(46)	557.6(85)	38.7(fixed)	—	2.9	38.7
*u*3423	H(202)...H(221)	557.9(21)	25.5(fixed)	—	–2.3	25.5
*u*3520	H(29)...H(45)	558.0(53)	42.7(fixed)	—	3.2	42.7
*u*3460	Si(3)...H(46)	558.1(38)	15.3(fixed)	—	–3.5	15.3
*u*3159	C(53)...C(56)	558.1(56)	21.7(tied to *u*3057)	—	–0.9	19.4
*u*3447	Si(97)...H(140)	558.1(38)	15.4(fixed)	—	–3.6	15.4
*u*3375	C(55)...C(64)	558.1(63)	19.9(tied to *u*3057)	—	–1.1	17.8
*u*3598	H(89)...H(92)	558.2(41)	33.7(fixed)	—	1.7	33.7
*u*3502	C(101)...C(107)	558.2(23)	22.2(tied to *u*3057)	—	–1.0	19.9
*u*3266	H(109)...H(132)	558.2(28)	26.8(fixed)	—	–1.8	26.8
*u*3305	H(155)...H(163)	558.2(22)	26.2(fixed)	—	–1.3	26.2
*u*3466	C(9)...H(45)	558.3(56)	29.8(fixed)	—	1.3	29.8
*u*3210	H(114)...H(121)	558.3(91)	39.1(fixed)	—	3.6	39.1
*u*3142	C(53)...H(76)	558.5(75)	29.6(fixed)	—	4.6	29.6
*u*3523	H(159)...H(180)	558.5(30)	35.2(fixed)	—	–0.6	35.2
*u*3516	H(159)...H(181)	558.5(24)	37.1(fixed)	—	0.2	37.1
*u*3475	C(9)...C(17)	558.5(52)	21.8(tied to *u*3057)	—	–1.0	19.5
*u*3414	H(23)...H(42)	558.7(40)	49.6(fixed)	—	14.7	49.6
*u*3255	H(109)...H(130)	558.7(30)	25.9(fixed)	—	–1.7	25.9
*u*3383	H(32)...H(37)	558.8(47)	38.1(fixed)	—	7.4	38.1
*u*3527	C(58)...H(86)	559.0(49)	38.4(fixed)	—	–0.9	38.4
*u*3649	H(91)...H(92)	559.0(38)	34.8(fixed)	—	0.4	34.8
*u*3380	C(105)...C(106)	559.2(26)	19.9(tied to *u*3057)	—	–0.9	17.8
*u*3467	C(103)...C(111)	559.2(51)	20.8(tied to *u*3057)	—	–0.9	18.6
*u*3541	C(147)...H(173)	559.3(22)	49.8(fixed)	—	–0.9	49.8
*u*3511	H(22)...H(43)	559.3(23)	47.4(fixed)	—	3.3	47.4
*u*3533	C(195)...H(224)	559.4(27)	36.2(fixed)	—	–0.9	36.2
*u*3600	H(28)...H(37)	559.4(32)	38.4(fixed)	—	–0.9	38.4
*u*2932	H(135)...H(138)	559.4(47)	50.1(fixed)	—	18.0	50.1
*u*3476	C(246)...H(271)	559.5(40)	33.9(fixed)	—	–0.4	33.9

*u*3339	C(55)...H(83)	559.6(36)	66.4(fixed)	—	1.4	66.4
*u*3535	C(152)...H(180)	559.7(48)	34.3(fixed)	—	–0.9	34.3
*u*3309	H(123)...H(134)	560.0(48)	35.2(fixed)	—	1.7	35.2
*u*3451	C(107)...H(125)	560.1(34)	31.9(fixed)	—	–1.7	31.9
*u*3504	H(123)...H(139)	560.1(52)	44.3(fixed)	—	3.9	44.3
*u*3373	H(27)...H(39)	560.2(87)	49.0(fixed)	—	3.3	49.0
*u*3604	H(42)...H(45)	560.2(29)	34.8(fixed)	—	0.1	34.8
*u*3558	H(212)...H(233)	560.4(34)	42.1(fixed)	—	3.1	42.1
*u*3531	H(133)...H(140)	560.4(47)	41.8(fixed)	—	0.4	41.8
*u*3633	C(60)...H(92)	560.5(59)	33.2(fixed)	—	–1.5	33.2
*u*3370	C(106)...H(127)	560.6(36)	28.3(fixed)	—	1.9	28.3
*u*3331	H(19)...H(28)	560.6(86)	40.9(fixed)	—	2.1	40.9
*u*3713	H(71)...H(79)	560.7(57)	34.1(fixed)	—	0.7	34.1
*u*3450	H(164)...H(165)	560.8(31)	38.5(fixed)	—	8.1	38.5
*u*3403	H(38)...H(44)	561.0(75)	49.9(fixed)	—	17.3	49.9
*u*3431	C(103)...H(139)	561.0(56)	28.4(fixed)	—	1.8	28.4
*u*3515	H(126)...H(133)	561.0(32)	33.1(fixed)	—	–0.7	33.1
*u*3391	C(147)...H(176)	561.1(50)	39.5(fixed)	—	–0.9	39.5
*u*3490	H(79)...H(83)	561.1(24)	52.1(fixed)	—	4.7	52.1
*u*3680	C(194)...H(220)	561.3(22)	33.8(fixed)	—	–1.2	33.8
*u*3543	H(69)...H(90)	561.3(43)	39.1(fixed)	—	2.3	39.1
*u*3500	H(118)...H(140)	561.4(83)	38.9(fixed)	—	3.2	38.9
*u*3173	H(130)...H(137)	561.5(51)	50.9(fixed)	—	–0.6	50.9
*u*3263	H(65)...H(76)	561.6(81)	40.1(fixed)	—	6.8	40.1
*u*3738	H(116)...H(131)	561.6(43)	37.5(fixed)	—	–0.1	37.5
*u*3767	C(8)...H(33)	561.6(29)	37.4(fixed)	—	–2.0	37.4
*u*3437	H(155)...H(164)	561.7(23)	25.8(fixed)	—	–1.8	25.8
*u*3318	H(249)...H(262)	561.7(27)	27.0(fixed)	—	–2.2	27.0
*u*3521	C(57)...H(73)	561.7(52)	36.2(fixed)	—	–0.6	36.2
*u*3721	H(259)...H(282)	561.7(49)	36.4(fixed)	—	0.0	36.4
*u*3477	H(122)...H(134)	561.9(32)	33.4(fixed)	—	–0.1	33.4
*u*3827	C(243)...H(268)	562.0(31)	35.1(fixed)	—	–1.9	35.1
*u*3654	C(241)...H(267)	562.0(22)	31.4(fixed)	—	–1.1	31.4
*u*3307	H(20)...H(27)	562.0(91)	39.2(fixed)	—	0.6	39.2
*u*3452	H(249)...H(264)	562.1(32)	26.1(fixed)	—	–2.5	26.1
*u*3438	H(79)...H(84)	562.1(34)	42.0(fixed)	—	8.6	42.0
*u*3784	C(106)...H(118)	562.2(51)	33.8(fixed)	—	–2.2	33.8
*u*3669	H(114)...H(127)	562.2(39)	37.5(fixed)	—	0.4	37.5
*u*3631	H(136)...H(139)	562.3(31)	35.0(fixed)	—	0.3	35.0
*u*3568	H(65)...H(80)	562.3(40)	34.6(fixed)	—	2.3	34.6
*u*3773	C(55)...H(87)	562.7(70)	37.2(fixed)	—	–1.4	37.2
*u*3514	H(164)...H(167)	562.7(23)	45.5(fixed)	—	5.2	45.5
*u*3605	C(242)...H(274)	562.8(42)	38.1(fixed)	—	–1.4	38.1
*u*3468	C(194)...H(223)	562.9(51)	36.0(fixed)	—	–0.4	36.0
*u*3145	H(36)...H(46)	562.9(118)	40.6(fixed)	—	1.3	40.6
*u*3341	H(253)...H(271)	563.4(24)	43.7(fixed)	—	3.5	43.7

*u*3472	H(155)...H(162)	563.5(23)	27.2(fixed)	—	–2.6	27.2
*u*3462	C(241)...H(270)	563.5(51)	34.1(fixed)	—	–0.5	34.1
*u*3408	C(56)...H(69)	563.5(73)	34.3(fixed)	—	–1.0	34.3
*u*3470	H(160)...H(172)	563.6(20)	45.9(fixed)	—	9.6	45.9
*u*3419	H(24)...H(42)	563.6(39)	42.4(fixed)	—	14.6	42.4
*u*3562	C(10)...H(28)	563.6(42)	37.5(fixed)	—	–1.2	37.5
*u*3639	C(57)...H(76)	563.7(62)	39.2(fixed)	—	–0.3	39.2
*u*3583	H(35)...H(40)	563.7(49)	34.4(fixed)	—	1.8	34.4
*u*3569	H(159)...H(174)	563.8(31)	34.2(fixed)	—	2.0	34.2
*u*3647	H(20)...H(33)	564.0(38)	37.7(fixed)	—	0.8	37.7
*u*3433	H(26)...H(42)	564.1(25)	51.6(fixed)	—	9.9	51.6
*u*3732	H(117)...H(125)	564.3(47)	30.4(fixed)	—	–2.0	30.4
*u*3412	H(118)...H(136)	564.3(40)	49.0(fixed)	—	12.0	49.0
*u*3487	C(53)...H(82)	564.3(54)	37.8(fixed)	—	–0.9	37.8
*u*3611	H(255)...H(268)	564.4(40)	37.3(fixed)	—	–0.2	37.3
*u*3573	H(170)...H(188)	564.4(50)	36.0(fixed)	—	0.7	36.0
*u*2922	H(132)...H(138)	564.4(61)	46.9(fixed)	—	16.2	46.9
*u*3624	C(150)...H(174)	564.5(27)	33.2(fixed)	—	–1.5	33.2
*u*3503	H(23)...H(37)	564.6(67)	43.3(fixed)	—	4.8	43.3
*u*3661	H(263)...H(281)	564.7(38)	40.2(fixed)	—	2.8	40.2
*u*3659	C(54)...H(84)	564.7(48)	64.0(fixed)	—	–3.8	64.0
*u*3576	H(82)...H(87)	564.9(51)	36.1(fixed)	—	1.4	36.1
*u*3443	H(253)...H(272)	564.9(31)	36.9(fixed)	—	5.4	36.9
*u*3636	H(208)...H(221)	564.9(39)	37.3(fixed)	—	0.3	37.3
*u*3553	C(197)...H(206)	565.1(30)	33.3(fixed)	—	–1.4	33.3
*u*3651	H(211)...H(225)	565.1(29)	34.8(fixed)	—	1.3	34.8
*u*3249	H(62)...H(94)	565.2(48)	26.0(fixed)	—	–1.7	26.0
*u*3792	C(102)...H(127)	565.3(30)	36.6(fixed)	—	–2.0	36.6
*u*3539	H(33)...H(40)	565.3(56)	33.2(fixed)	—	3.1	33.2
*u*3567	C(104)...H(122)	565.3(40)	37.9(fixed)	—	–1.4	37.9
*u*3485	C(6)...H(35)	565.5(53)	35.9(fixed)	—	–0.6	35.9
*u*3714	H(71)...H(78)	565.5(36)	35.2(fixed)	—	–0.7	35.2
*u*3112	H(261)...H(276)	565.6(48)	39.0(fixed)	—	3.3	39.0
*u*3592	H(67)...H(80)	565.6(39)	36.3(fixed)	—	1.0	36.3
*u*3493	C(100)...H(129)	565.6(56)	35.7(fixed)	—	–0.3	35.7
*u*3618	H(253)...H(268)	565.8(40)	34.5(fixed)	—	0.9	34.5
*u*3644	C(110)...H(117)	565.8(33)	32.8(fixed)	—	–1.1	32.8
*u*3489	H(32)...H(36)	565.9(32)	45.4(fixed)	—	5.3	45.4
*u*3655	C(16)...H(23)	566.0(28)	39.8(fixed)	—	–1.5	39.8
*u*3575	H(18)...H(33)	566.1(33)	35.7(fixed)	—	2.3	35.7
*u*3698	C(149)...H(159)	566.3(41)	32.7(fixed)	—	–1.7	32.7
*u*3603	H(206)...H(221)	566.4(37)	34.5(fixed)	—	2.1	34.5
*u*3671	C(59)...H(89)	566.5(43)	35.6(fixed)	—	–1.7	35.6
*u*3640	H(161)...H(174)	566.6(39)	34.4(fixed)	—	0.9	34.4
*u*3745	H(259)...H(280)	566.7(32)	35.0(fixed)	—	0.8	35.0
*u*3638	H(112)...H(127)	567.0(39)	35.3(fixed)	—	1.7	35.3

*u*3513	H(117)...H(134)	567.0(43)	40.7(fixed)	—	3.0	40.7
*u*3697	H(116)...H(126)	567.1(40)	30.4(fixed)	—	–1.2	30.4
*u*3088	H(83)...H(93)	567.4(70)	49.1(fixed)	—	16.9	49.1
*u*3746	H(210)...H(225)	567.5(33)	35.8(fixed)	—	0.2	35.8
*u*3585	H(217)...H(223)	567.5(36)	40.4(fixed)	—	–5.1	40.4
*u*3566	H(84)...H(94)	567.6(64)	43.4(fixed)	—	–10.7	43.4
*u*3571	H(29)...H(31)	567.7(38)	35.3(fixed)	—	0.8	35.3
*u*3406	H(162)...H(177)	568.0(46)	41.3(fixed)	—	2.5	41.3
*u*3627	H(127)...H(131)	568.1(43)	44.6(fixed)	—	2.5	44.6
*u*3687	C(63)...H(70)	568.2(42)	33.8(fixed)	—	–1.4	33.8
*u*3556	H(170)...H(186)	568.4(36)	33.4(fixed)	—	2.6	33.4
*u*3560	H(29)...H(32)	568.5(49)	33.4(fixed)	—	2.0	33.4
*u*3455	H(62)...H(92)	568.5(60)	25.6(fixed)	—	–2.3	25.6
*u*3652	H(22)...H(32)	568.7(33)	37.4(fixed)	—	–3.3	37.4
*u*3538	H(80)...H(87)	568.7(36)	32.7(fixed)	—	3.0	32.7
*u*3582	H(123)...H(125)	568.8(39)	35.8(fixed)	—	2.0	35.8
*u*3615	H(73)...H(84)	568.9(44)	60.7(fixed)	—	7.2	60.7
*u*3494	C(17)...H(26)	569.7(44)	36.7(fixed)	—	–0.6	36.7
*u*3612	H(257)...H(275)	570.1(37)	34.3(fixed)	—	1.7	34.3
*u*3548	H(71)...H(84)	570.7(39)	49.0(fixed)	—	13.2	49.0
*u*3524	H(214)...H(234)	571.0(39)	36.5(fixed)	—	2.8	36.5
*u*3672	H(23)...H(31)	571.2(38)	33.6(fixed)	—	1.3	33.6
*u*3699	C(148)...H(178)	571.2(32)	34.9(fixed)	—	–1.8	34.9
*u*3805	C(104)...H(115)	571.3(43)	27.7(fixed)	—	–3.2	27.7
*u*3510	H(70)...H(76)	571.3(84)	39.1(fixed)	—	1.3	39.1
*u*3635	C(244)...H(272)	571.4(58)	33.3(fixed)	—	–2.0	33.3
*u*3295	H(212)...H(228)	571.7(39)	36.0(fixed)	—	11.9	36.0
*u*3537	H(70)...H(75)	571.8(80)	38.5(fixed)	—	–1.0	38.5
*u*3137	H(66)...H(73)	572.0(113)	41.1(fixed)	—	1.8	41.1
*u*3522	H(123)...H(126)	572.1(47)	33.8(fixed)	—	3.2	33.8
*u*3046	H(67)...H(72)	572.2(94)	40.9(fixed)	—	1.9	40.9
*u*3685	H(76)...H(82)	572.4(61)	35.7(fixed)	—	–2.8	35.7
*u*3440	C(195)...H(228)	572.5(25)	55.3(fixed)	—	1.3	55.3
*u*3565	H(258)...H(275)	572.7(44)	32.6(fixed)	—	2.9	32.6
*u*3645	C(9)...H(40)	572.8(84)	33.4(fixed)	—	–0.9	33.4
*u*3715	C(10)...H(21)	572.9(36)	30.6(fixed)	—	–4.2	30.6
*u*3474	C(111)...H(120)	573.1(41)	36.7(fixed)	—	–0.1	36.7
*u*3692	C(246)...H(275)	573.3(34)	34.4(fixed)	—	–0.6	34.4
*u*3795	C(7)...H(30)	573.4(30)	33.4(fixed)	—	–6.1	33.4
*u*3682	H(69)...H(79)	573.5(52)	39.0(fixed)	—	–5.8	39.0
*u*3620	H(209)...H(227)	573.5(32)	47.8(fixed)	—	9.0	47.8
*u*3653	H(253)...H(263)	573.5(47)	37.2(fixed)	—	–4.1	37.2
*u*3797	C(101)...H(124)	573.8(35)	27.4(fixed)	—	–3.0	27.4
*u*3912	C(199)...H(215)	573.8(30)	32.8(fixed)	—	–7.6	32.8
*u*3711	H(257)...H(267)	573.9(49)	30.9(fixed)	—	–1.7	30.9
*u*3577	H(109)...H(124)	574.0(27)	28.0(fixed)	—	–2.9	28.0

*u*3777	C(7)...H(32)	574.0(32)	35.4(fixed)	—	–6.1	35.4
*u*3610	H(15)...H(31)	574.2(23)	32.3(fixed)	—	–4.7	32.3
*u*3753	H(75)...H(80)	574.4(75)	35.1(fixed)	—	–0.1	35.1
*u*3580	H(165)...H(176)	574.4(42)	35.3(fixed)	—	–1.9	35.3
*u*3622	H(15)...H(30)	574.6(27)	30.7(fixed)	—	–4.7	30.7
*u*3400	H(62)...H(93)	574.7(71)	26.3(fixed)	—	–2.5	26.3
*u*3798	H(210)...H(220)	575.0(42)	31.5(fixed)	—	–1.4	31.5
*u*3547	H(109)...H(125)	575.1(25)	26.2(fixed)	—	–2.6	26.2
*u*3902	C(101)...H(126)	575.3(38)	23.9(fixed)	—	–3.2	23.9
*u*3551	C(64)...H(85)	575.4(58)	45.9(fixed)	—	–7.7	45.9
*u*3678	H(39)...H(47)	575.5(59)	37.0(fixed)	—	–2.5	37.0
*u*3877	C(58)...H(74)	575.9(49)	31.8(fixed)	—	–5.5	31.8
*u*3788	C(64)...H(71)	576.2(67)	32.3(fixed)	—	–1.7	32.3
*u*3761	C(199)...H(225)	576.3(27)	33.6(fixed)	—	–1.7	33.6
*u*3664	C(16)...H(25)	576.4(32)	25.8(fixed)	—	–1.9	25.8
*u*3679	C(53)...H(88)	576.4(30)	25.2(fixed)	—	–2.2	25.2
*u*3499	H(21)...H(36)	576.4(78)	37.5(fixed)	—	1.7	37.5
*u*3904	C(104)...H(117)	576.5(32)	25.1(fixed)	—	–3.5	25.1
*u*3703	C(17)...H(29)	576.8(46)	33.8(fixed)	—	–0.8	33.8
*u*3705	C(111)...H(123)	576.8(45)	36.0(fixed)	—	–0.9	36.0
*u*3751	H(169)...H(181)	577.1(38)	35.0(fixed)	—	–2.3	35.0
*u*3594	C(110)...H(119)	577.2(34)	25.0(fixed)	—	–1.5	25.0
*u*3156	H(67)...H(74)	577.5(90)	45.3(fixed)	—	1.6	45.3
*u*3564	C(56)...H(65)	577.7(60)	30.8(fixed)	—	–1.3	30.8
*u*3237	H(259)...H(271)	577.7(75)	38.2(fixed)	—	–2.3	38.2
*u*3854	C(10)...H(23)	577.8(28)	28.7(fixed)	—	–5.0	28.7
*u*3806	H(115)...H(133)	577.8(37)	41.1(fixed)	—	1.1	41.1
*u*3822	C(54)...H(77)	577.9(47)	37.0(fixed)	—	–7.4	37.0
*u*3696	C(6)...H(41)	577.9(20)	24.7(fixed)	—	–2.7	24.7
*u*3762	C(64)...H(84)	578.0(45)	42.9(fixed)	—	–11.9	42.9
*u*3710	H(216)...H(221)	578.2(37)	34.1(fixed)	—	3.2	34.1
*u*3844	C(56)...H(81)	578.2(63)	30.1(fixed)	—	–3.9	30.1
*u*3589	H(37)...H(47)	578.4(67)	34.9(fixed)	—	–2.5	34.9
*u*3785	C(54)...H(79)	578.4(40)	38.3(fixed)	—	–6.9	38.3
*u*3752	H(118)...H(141)	578.4(64)	37.3(fixed)	—	–0.2	37.3
*u*3704	H(28)...H(46)	578.6(85)	41.7(fixed)	—	2.1	41.7
*u*3778	H(134)...H(141)	578.8(40)	32.0(fixed)	—	–1.0	32.0
*u*3315	H(214)...H(228)	578.9(39)	43.0(fixed)	—	9.6	43.0
*u*3949	C(106)...H(115)	578.9(41)	23.0(fixed)	—	–1.9	23.0
*u*3779	C(244)...H(254)	578.9(41)	33.0(fixed)	—	–5.4	33.0
*u*3641	H(167)...H(174)	579.1(51)	32.0(fixed)	—	–1.7	32.0
*u*3718	H(24)...H(47)	579.2(64)	36.1(fixed)	—	–0.2	36.1
*u*3716	H(24)...H(45)	579.3(62)	35.1(fixed)	—	1.3	35.1
*u*3609	H(202)...H(214)	579.4(20)	27.7(fixed)	—	–3.3	27.7
*u*3619	H(155)...H(176)	579.4(25)	28.4(fixed)	—	–3.5	28.4
*u*3626	H(61)...H(82)	579.4(27)	27.9(fixed)	—	–3.5	27.9

*u*3700	C(57)...H(68)	579.5(45)	30.1(fixed)	—	–3.6	30.1
*u*3602	H(255)...H(264)	579.5(55)	33.1(fixed)	—	1.4	33.1
*u*3756	H(155)...H(175)	579.8(21)	29.9(fixed)	—	–4.2	29.9
*u*3675	H(122)...H(140)	579.8(84)	40.8(fixed)	—	2.8	40.8
*u*3614	H(24)...H(39)	579.8(85)	38.5(fixed)	—	–2.4	38.5
*u*3730	C(148)...H(166)	579.9(27)	26.1(fixed)	—	–1.9	26.1
*u*3695	C(199)...H(217)	580.0(26)	39.7(fixed)	—	–6.2	39.7
*u*3903	H(114)...H(125)	580.0(30)	34.1(fixed)	—	–2.2	34.1
*u*3545	H(249)...H(257)	580.1(25)	27.2(fixed)	—	–2.9	27.2
*u*3674	H(202)...H(213)	580.1(19)	28.8(fixed)	—	–3.6	28.8
*u*3706	H(61)...H(81)	580.1(23)	29.5(fixed)	—	–3.7	29.5
*u*3724	C(241)...H(262)	580.3(46)	28.7(fixed)	—	–3.9	28.7
*u*3665	H(26)...H(44)	580.4(32)	72.2(fixed)	—	3.9	72.2
*u*3893	C(197)...H(221)	580.6(28)	26.8(fixed)	—	–4.3	26.8
*u*3591	H(163)...H(173)	580.6(28)	38.3(fixed)	—	–0.1	38.3
*u*3634	C(110)...H(120)	580.6(18)	24.0(fixed)	—	–1.3	24.0
*u*3809	C(12)...H(27)	580.6(42)	27.5(fixed)	—	–2.4	27.5
*u*3554	H(208)...H(212)	580.7(35)	34.6(fixed)	—	–2.3	34.6
*u*3540	H(128)...H(130)	580.7(44)	35.5(fixed)	—	2.9	35.5
*u*3559	C(152)...H(166)	580.7(35)	32.9(fixed)	—	–3.4	32.9
*u*3546	H(73)...H(93)	580.9(101)	37.6(fixed)	—	2.0	37.6
*u*3529	H(120)...H(138)	581.0(30)	60.0(fixed)	—	6.4	60.0
*u*3709	C(57)...H(85)	581.1(30)	26.7(fixed)	—	–1.0	26.7
*u*3863	C(195)...H(218)	581.1(36)	30.0(fixed)	—	–3.7	30.0
*u*3881	C(58)...H(76)	581.1(56)	31.0(fixed)	—	–4.8	31.0
*u*3691	C(10)...H(38)	581.2(28)	26.7(fixed)	—	–2.6	26.7
*u*3642	C(107)...H(121)	581.2(28)	24.3(fixed)	—	–1.6	24.3
*u*3701	C(7)...H(37)	581.2(62)	32.8(fixed)	—	–1.5	32.8
*u*3934	C(111)...H(135)	581.2(37)	29.1(fixed)	—	–3.8	29.1
*u*3782	C(242)...H(265)	581.2(42)	27.1(fixed)	—	–3.1	27.1
*u*3830	H(25)...H(44)	581.4(45)	78.8(fixed)	—	–2.9	78.8
*u*3726	H(112)...H(122)	581.5(59)	35.5(fixed)	—	–2.5	35.5
*u*3914	C(56)...H(80)	581.7(47)	27.6(fixed)	—	–4.2	27.6
*u*3596	H(249)...H(256)	581.8(27)	28.8(fixed)	—	–3.0	28.8
*u*3771	C(244)...H(253)	581.8(40)	33.4(fixed)	—	–5.7	33.4
*u*3662	H(208)...H(216)	581.8(25)	37.6(fixed)	—	–6.5	37.6
*u*3734	C(197)...H(222)	581.8(28)	29.6(fixed)	—	–3.8	29.6
*u*3387	H(68)...H(83)	581.9(54)	46.3(fixed)	—	19.2	46.3
*u*3747	C(195)...H(215)	582.0(29)	26.0(fixed)	—	–1.2	26.0
*u*3894	C(64)...H(90)	582.0(37)	23.2(fixed)	—	–1.9	23.2
*u*3599	H(108)...H(122)	582.0(35)	27.7(fixed)	—	–3.7	27.7
*u*3666	C(104)...H(135)	582.1(32)	25.0(fixed)	—	–2.5	25.0
*u*3694	C(148)...H(171)	582.1(25)	34.7(fixed)	—	–6.1	34.7
*u*3702	C(147)...H(182)	582.3(23)	24.6(fixed)	—	–1.8	24.6
*u*3676	H(70)...H(78)	582.3(50)	33.1(fixed)	—	5.3	33.1
*u*3906	C(242)...H(267)	582.6(39)	24.9(fixed)	—	–3.4	24.9

*u*3787	H(116)...H(130)	582.7(47)	36.4(fixed)	—	1.4	36.4
*u*3586	C(17)...H(38)	582.7(61)	33.9(fixed)	—	–3.5	33.9
*u*3937	C(195)...H(220)	582.8(34)	25.2(fixed)	—	–3.7	25.2
*u*3668	H(130)...H(136)	582.8(39)	42.6(fixed)	—	–9.5	42.6
*u*3688	C(16)...H(26)	582.8(20)	25.5(fixed)	—	–1.6	25.5
*u*3737	C(148)...H(173)	582.9(25)	34.6(fixed)	—	–6.4	34.6
*u*3717	C(53)...H(86)	582.9(19)	22.2(fixed)	—	–2.2	22.2
*u*3725	C(106)...H(136)	582.9(33)	44.7(fixed)	—	–10.4	44.7
*u*3810	H(35)...H(39)	583.0(62)	44.6(fixed)	—	1.1	44.6
*u*3579	H(108)...H(121)	583.0(39)	30.9(fixed)	—	–3.6	30.9
*u*3758	C(195)...H(216)	583.1(22)	23.2(fixed)	—	–2.1	23.2
*u*3763	H(83)...H(91)	583.3(39)	44.4(fixed)	—	–6.3	44.4
*u*3786	C(149)...H(174)	583.3(34)	26.5(fixed)	—	–4.3	26.5
*u*3630	H(14)...H(35)	583.4(33)	27.7(fixed)	—	–3.2	27.7
*u*3689	H(161)...H(180)	583.4(26)	37.8(fixed)	—	0.2	37.8
*u*3768	C(17)...H(44)	583.5(39)	23.0(fixed)	—	–0.9	23.0
*u*3808	H(67)...H(78)	583.6(41)	47.8(fixed)	—	5.7	47.8
*u*3581	C(149)...H(175)	583.6(40)	32.8(fixed)	—	–3.9	32.8
*u*3834	H(20)...H(31)	583.6(28)	41.0(fixed)	—	3.6	41.0
*u*3168	C(243)...H(273)	583.6(61)	35.8(fixed)	—	–3.3	35.8
*u*3739	C(147)...H(180)	583.7(18)	22.7(fixed)	—	–1.9	22.7
*u*3858	C(105)...H(131)	583.8(33)	35.2(fixed)	—	–2.1	35.2
*u*3901	C(106)...H(116)	583.8(33)	22.4(fixed)	—	–1.5	22.4
*u*3632	C(241)...H(273)	583.9(26)	25.5(fixed)	—	–1.9	25.5
*u*3907	C(150)...H(182)	584.0(32)	29.9(fixed)	—	–4.1	29.9
*u*3646	H(206)...H(214)	584.0(30)	34.8(fixed)	—	–2.1	34.8
*u*3882	C(17)...H(43)	584.1(29)	23.0(fixed)	—	–1.7	23.0
*u*3818	C(64)...H(91)	584.2(40)	22.6(fixed)	—	–1.3	22.6
*u*3783	C(111)...H(138)	584.2(41)	23.6(fixed)	—	0.1	23.6
*u*3673	H(86)...H(94)	584.2(42)	37.8(fixed)	—	–1.5	37.8
*u*3677	H(114)...H(123)	584.3(65)	32.5(fixed)	—	–0.6	32.5
*u*3978	H(75)...H(78)	584.4(50)	48.9(fixed)	—	–3.5	48.9
*u*3625	H(26)...H(40)	584.5(70)	35.9(fixed)	—	–2.0	35.9
*u*3815	C(241)...H(264)	584.5(37)	26.9(fixed)	—	–3.9	26.9
*u*3855	C(16)...H(24)	584.5(28)	22.0(fixed)	—	–2.6	22.0
*u*3729	H(118)...H(139)	584.7(58)	35.3(fixed)	—	1.3	35.3
*u*3804	C(152)...H(165)	584.7(36)	26.9(fixed)	—	–4.7	26.9
*u*3819	C(13)...H(35)	584.7(40)	22.3(fixed)	—	–1.1	22.3
*u*3802	C(13)...H(34)	584.8(54)	22.3(fixed)	—	–1.2	22.3
*u*3820	H(116)...H(138)	584.8(28)	40.3(fixed)	—	–5.5	40.3
*u*3898	C(6)...H(40)	584.8(33)	23.8(fixed)	—	–2.3	23.8
*u*3660	H(67)...H(86)	584.9(35)	37.9(fixed)	—	0.3	37.9
*u*3887	C(57)...H(70)	585.0(40)	24.4(fixed)	—	–3.9	24.4
*u*3744	C(101)...H(134)	585.0(33)	31.4(fixed)	—	–1.0	31.4
*u*3936	C(111)...H(137)	585.0(30)	23.9(fixed)	—	–2.5	23.9
*u*3923	H(133)...H(139)	585.1(39)	34.0(fixed)	—	–2.7	34.0

*u*3593	C(13)...H(25)	585.2(74)	35.6(fixed)	—	–3.9	35.6
*u*3837	C(10)...H(37)	585.2(33)	22.5(fixed)	—	–2.9	22.5
*u*3880	H(122)...H(133)	585.2(40)	38.5(fixed)	—	–0.5	38.5
*u*3555	C(59)...H(93)	585.2(50)	32.5(fixed)	—	–3.7	32.5
*u*3719	C(6)...H(39)	585.2(29)	22.5(fixed)	—	–2.5	22.5
*u*3770	C(59)...H(92)	585.3(51)	26.6(fixed)	—	–4.3	26.6
*u*3860	H(22)...H(44)	585.3(23)	43.9(fixed)	—	–5.5	43.9
*u*3832	C(12)...H(28)	585.3(31)	23.4(fixed)	—	–2.1	23.4
*u*3862	C(53)...H(87)	585.3(27)	24.0(fixed)	—	–2.6	24.0
*u*3637	C(8)...H(41)	585.3(57)	34.1(fixed)	—	–4.6	34.1
*u*3552	C(194)...H(213)	585.3(31)	31.5(fixed)	—	–3.2	31.5
*u*3764	C(107)...H(122)	585.4(30)	21.9(fixed)	—	–2.1	21.9
*u*3962	C(107)...H(139)	585.4(32)	27.1(fixed)	—	–4.0	27.1
*u*3536	C(243)...H(272)	585.5(60)	30.3(fixed)	—	–4.8	30.3
*u*3754	C(148)...H(167)	585.7(13)	24.4(fixed)	—	–1.6	24.4
*u*3749	C(57)...H(83)	585.7(14)	26.2(fixed)	—	–1.4	26.2
*u*3865	C(243)...H(282)	585.8(37)	22.8(fixed)	—	–1.2	22.8
*u*3690	H(91)...H(94)	585.9(62)	41.2(fixed)	—	1.4	41.2
*u*3760	C(59)...H(72)	586.1(18)	27.2(fixed)	—	–1.9	27.2
*u*3867	H(255)...H(266)	586.1(22)	35.7(fixed)	—	–3.2	35.7
*u*3557	H(255)...H(271)	586.3(30)	51.5(fixed)	—	2.1	51.5
*u*3755	H(163)...H(167)	586.3(18)	59.0(fixed)	—	1.7	59.0
*u*3608	C(241)...H(271)	586.3(18)	25.2(fixed)	—	–1.4	25.2
*u*3708	H(14)...H(34)	586.3(46)	30.5(fixed)	—	–3.8	30.5
*u*3961	C(106)...H(117)	586.4(24)	22.1(fixed)	—	–2.0	22.1
*u*3643	H(119)...H(138)	586.5(50)	68.1(fixed)	—	0.0	68.1
*u*3876	C(148)...H(165)	586.8(18)	22.5(fixed)	—	–2.5	22.5
*u*3920	C(150)...H(181)	586.9(29)	28.8(fixed)	—	–4.4	28.8
*u*3816	C(12)...H(45)	586.9(55)	26.9(fixed)	—	–4.1	26.9
*u*3658	H(44)...H(47)	587.0(59)	40.6(fixed)	—	4.0	40.6
*u*3841	C(60)...H(82)	587.0(40)	22.6(fixed)	—	–1.5	22.6
*u*3835	C(150)...H(188)	587.0(38)	23.1(fixed)	—	–1.7	23.1
*u*3712	H(138)...H(141)	587.0(63)	43.4(fixed)	—	4.5	43.4
*u*3975	C(55)...H(77)	587.1(46)	24.1(fixed)	—	–2.4	24.1
*u*3875	C(57)...H(84)	587.1(21)	22.6(fixed)	—	–3.4	22.6
*u*3775	H(18)...H(28)	587.3(60)	32.2(fixed)	—	–1.4	32.2
*u*3722	H(210)...H(216)	587.3(33)	41.1(fixed)	—	1.9	41.1
*u*3588	C(196)...H(207)	587.5(26)	30.7(fixed)	—	–3.3	30.7
*u*3617	C(106)...H(137)	587.5(34)	42.2(fixed)	—	–8.3	42.2
*u*3707	H(261)...H(282)	587.7(53)	38.1(fixed)	—	1.4	38.1
*u*3757	H(28)...H(36)	587.7(47)	36.4(fixed)	—	0.4	36.4
*u*3965	C(243)...H(281)	587.9(35)	23.8(fixed)	—	–2.1	23.8
*u*3765	C(196)...H(206)	588.0(26)	28.2(fixed)	—	–4.2	28.2
*u*3733	C(104)...H(134)	588.0(21)	24.7(fixed)	—	–2.1	24.7
*u*3866	C(150)...H(187)	588.1(43)	22.9(fixed)	—	–2.0	22.9
*u*3681	H(36)...H(45)	588.3(89)	32.9(fixed)	—	–2.0	32.9

*u*3859	H(208)...H(219)	588.3(21)	35.8(fixed)	—	–0.6	35.8
*u*3807	C(110)...H(118)	588.4(29)	21.9(fixed)	—	–2.4	21.9
*u*3861	C(60)...H(81)	588.4(43)	22.5(fixed)	—	–1.4	22.5
*u*3874	H(26)...H(35)	588.4(27)	35.3(fixed)	—	–0.1	35.3
*u*3899	H(82)...H(86)	588.4(60)	43.1(fixed)	—	0.9	43.1
*u*3884	C(58)...H(66)	588.5(32)	23.3(fixed)	—	–2.3	23.3
*u*3990	H(115)...H(130)	588.5(57)	39.6(fixed)	—	–1.1	39.6
*u*3791	C(194)...H(212)	588.5(22)	27.3(fixed)	—	–4.5	27.3
*u*3803	C(104)...H(133)	588.6(22)	21.8(fixed)	—	–2.5	21.8
*u*3972	H(73)...H(86)	588.6(62)	40.9(fixed)	—	–0.3	40.9
*u*3667	C(197)...H(226)	588.6(28)	25.5(fixed)	—	–1.5	25.5
*u*3727	H(20)...H(29)	588.6(65)	32.6(fixed)	—	–2.2	32.6
*u*3525	C(110)...H(132)	588.7(38)	30.6(fixed)	—	–3.2	30.6
*u*3766	H(78)...H(83)	588.7(21)	64.2(fixed)	—	5.3	64.2
*u*3873	C(105)...H(114)	588.7(39)	22.2(fixed)	—	–1.3	22.2
*u*3845	C(13)...H(24)	588.9(56)	28.3(fixed)	—	–5.0	28.3
*u*3458	H(133)...H(138)	589.1(30)	46.1(fixed)	—	10.2	46.1
*u*3813	H(161)...H(167)	589.1(38)	35.6(fixed)	—	–1.1	35.6
*u*3892	H(169)...H(188)	589.1(56)	39.3(fixed)	—	0.6	39.3
*u*3929	C(64)...H(89)	589.1(33)	21.8(fixed)	—	–2.0	21.8
*u*3759	C(10)...H(36)	589.4(29)	24.7(fixed)	—	–1.8	24.7
*u*3789	C(8)...H(40)	589.5(66)	29.4(fixed)	—	–4.5	29.4
*u*3839	C(152)...H(160)	589.5(30)	23.1(fixed)	—	–2.1	23.1
*u*3958	C(196)...H(218)	589.5(27)	24.8(fixed)	—	–2.5	24.8
*u*3895	C(195)...H(217)	589.6(15)	24.1(fixed)	—	–3.1	24.1
*u*3952	C(107)...H(140)	589.6(33)	30.7(fixed)	—	–4.2	30.7
*u*3826	C(199)...H(208)	589.6(39)	22.7(fixed)	—	–1.5	22.7
*u*3735	H(120)...H(130)	589.7(41)	35.2(fixed)	—	0.4	35.2
*u*3868	C(11)...H(20)	589.7(38)	22.5(fixed)	—	–1.6	22.5
*u*3878	C(103)...H(112)	589.8(51)	30.4(fixed)	—	–4.7	30.4
*u*3684	H(169)...H(176)	589.8(19)	40.7(fixed)	—	–0.8	40.7
*u*3742	H(36)...H(44)	589.9(66)	50.8(fixed)	—	9.7	50.8
*u*3824	C(246)...H(255)	589.9(40)	22.7(fixed)	—	–1.1	22.7
*u*3935	C(196)...H(219)	590.0(22)	23.0(fixed)	—	–1.5	23.0
*u*3989	H(108)...H(140)	590.1(35)	25.0(fixed)	—	–6.3	25.0
*u*3829	C(152)...H(161)	590.2(39)	22.9(fixed)	—	–1.6	22.9
*u*3686	H(20)...H(39)	590.3(55)	37.6(fixed)	—	–0.2	37.6
*u*3900	C(11)...H(19)	590.3(30)	23.0(fixed)	—	–2.2	23.0
*u*3793	C(101)...H(108)	590.5(21)	15.7(fixed)	—	–1.9	15.7
*u*3886	C(100)...H(123)	590.5(49)	27.5(fixed)	—	–4.1	27.5
*u*3940	C(12)...H(29)	590.5(44)	26.0(fixed)	—	–2.4	26.0
*u*3616	C(12)...H(46)	590.6(75)	31.8(fixed)	—	–3.5	31.8
*u*3910	C(244)...H(266)	590.7(27)	22.5(fixed)	—	–1.5	22.5
*u*3883	H(261)...H(270)	590.7(28)	33.9(fixed)	—	–0.4	33.9
*u*3889	C(103)...H(125)	590.8(28)	22.1(fixed)	—	–1.5	22.1
*u*3869	C(9)...H(31)	590.9(26)	22.5(fixed)	—	–1.2	22.5

*u*3833	C(17)...H(37)	591.0(61)	25.8(fixed)	—	–4.3	25.8
*u*3890	C(147)...H(181)	591.1(17)	23.7(fixed)	—	–2.6	23.7
*u*3828	C(58)...H(67)	591.1(39)	23.0(fixed)	—	–1.4	23.0
*u*3897	C(9)...H(30)	591.1(43)	23.2(fixed)	—	–1.6	23.2
*u*3927	C(199)...H(207)	591.2(32)	22.4(fixed)	—	–2.0	22.4
*u*3776	H(161)...H(172)	591.2(21)	46.2(fixed)	—	4.2	46.2
*u*3796	C(59)...H(73)	591.2(44)	25.6(fixed)	—	–1.9	25.6
*u*3944	C(58)...H(65)	591.3(31)	22.3(fixed)	—	–2.1	22.3
*u*3943	C(105)...H(113)	591.3(35)	22.8(fixed)	—	–1.8	22.8
*u*3911	H(210)...H(224)	591.4(30)	39.6(fixed)	—	0.9	39.6
*u*3848	H(67)...H(88)	591.4(49)	36.8(fixed)	—	–2.2	36.8
*u*3908	C(55)...H(78)	591.5(26)	23.4(fixed)	—	–0.7	23.4
*u*3769	C(107)...H(123)	591.5(40)	23.4(fixed)	—	–1.9	23.4
*u*3849	H(69)...H(91)	591.5(32)	35.3(fixed)	—	–0.7	35.3
*u*3856	H(120)...H(129)	591.6(25)	34.9(fixed)	—	0.0	34.9
*u*3921	C(246)...H(254)	591.6(33)	22.7(fixed)	—	–1.9	22.7
*u*3986	C(17)...H(41)	591.6(54)	31.7(fixed)	—	–4.1	31.7
*u*3971	H(257)...H(274)	591.6(40)	42.4(fixed)	—	–0.1	42.4
*u*3928	H(163)...H(166)	591.7(29)	64.2(fixed)	—	–2.8	64.2
*u*3926	C(17)...H(42)	591.7(25)	21.7(fixed)	—	–2.1	21.7
*u*3836	C(197)...H(225)	591.7(32)	21.9(fixed)	—	–2.3	21.9
*u*3814	C(195)...H(202)	591.9(23)	15.8(fixed)	—	–2.1	15.8
*u*3871	C(241)...H(272)	591.9(20)	21.6(fixed)	—	–2.7	21.6
*u*3939	H(78)...H(85)	592.0(36)	68.1(fixed)	—	–2.2	68.1
*u*3960	C(111)...H(134)	592.0(28)	24.4(fixed)	—	–3.4	24.4
*u*3918	C(59)...H(71)	592.0(32)	23.2(fixed)	—	–2.5	23.2
*u*3987	C(55)...H(79)	592.1(39)	22.3(fixed)	—	–1.9	22.3
*u*3811	C(57)...H(62)	592.1(22)	15.7(fixed)	—	–1.8	15.7
*u*3964	H(214)...H(227)	592.1(52)	62.8(fixed)	—	–1.4	62.8
*u*3840	C(103)...H(113)	592.2(72)	30.3(fixed)	—	–4.4	30.3
*u*3967	C(111)...H(136)	592.2(26)	22.5(fixed)	—	–3.0	22.5
*u*3825	C(246)...H(249)	592.2(22)	15.7(fixed)	—	–1.9	15.7
*u*3623	H(83)...H(92)	592.3(62)	36.9(fixed)	—	8.4	36.9
*u*3916	C(152)...H(159)	592.5(25)	22.4(fixed)	—	–2.3	22.4
*u*3794	C(100)...H(121)	592.6(73)	29.6(fixed)	—	–4.2	29.6
*u*3846	H(28)...H(39)	592.7(67)	42.2(fixed)	—	–1.2	42.2
*u*3917	C(13)...H(33)	593.0(39)	21.5(fixed)	—	–1.8	21.5
*u*3857	C(103)...H(124)	593.1(41)	22.9(fixed)	—	–1.7	22.9
*u*3800	C(111)...H(109)	593.2(24)	15.7(fixed)	—	–1.7	15.7
*u*3817	C(17)...H(15)	593.6(24)	15.8(fixed)	—	–2.0	15.8
*u*3731	H(208)...H(223)	593.6(59)	40.0(fixed)	—	1.3	40.0
*u*3723	H(161)...H(176)	593.6(58)	44.3(fixed)	—	0.7	44.3
*u*3922	C(244)...H(265)	593.7(40)	23.0(fixed)	—	–1.6	23.0
*u*3780	C(54)...H(75)	593.7(61)	23.3(fixed)	—	–2.3	23.3
*u*3852	C(55)...H(61)	593.7(25)	15.6(fixed)	—	–2.4	15.6
*u*3743	C(197)...H(224)	593.8(38)	24.7(fixed)	—	–1.8	24.7

*u*3831	H(31)...H(36)	593.9(54)	55.1(fixed)	—	1.0	55.1
*u*3799	C(110)...H(131)	593.9(29)	25.7(fixed)	—	–4.7	25.7
*u*3931	C(11)...H(18)	594.1(26)	22.4(fixed)	—	–2.1	22.4
*u*4003	H(62)...H(90)	594.1(28)	20.9(fixed)	—	–7.0	20.9
*u*3853	C(9)...H(14)	594.1(26)	15.4(fixed)	—	–2.2	15.4
*u*3748	H(69)...H(75)	594.2(78)	39.1(fixed)	—	0.9	39.1
*u*3932	H(121)...H(133)	594.4(42)	38.8(fixed)	—	–2.2	38.8
*u*3530	H(131)...H(138)	594.5(43)	36.2(fixed)	—	7.8	36.2
*u*3959	H(122)...H(125)	594.6(42)	42.1(fixed)	—	0.0	42.1
*u*4000	H(108)...H(113)	594.6(24)	21.8(fixed)	—	–7.7	21.8
*u*3720	H(255)...H(270)	594.6(59)	39.3(fixed)	—	2.2	39.3
*u*3956	C(199)...H(206)	594.9(30)	21.8(fixed)	—	–2.0	21.8
*u*3891	H(125)...H(133)	594.9(36)	36.3(fixed)	—	–1.0	36.3
*u*3968	C(196)...H(220)	594.9(18)	23.0(fixed)	—	–2.3	23.0
*u*3915	C(6)...H(29)	594.9(50)	26.5(fixed)	—	–3.8	26.5
*u*3781	H(163)...H(177)	595.0(33)	37.9(fixed)	—	–3.6	37.9
*u*3950	C(246)...H(253)	595.1(32)	21.3(fixed)	—	–2.2	21.3
*u*3963	C(105)...H(112)	595.2(30)	21.9(fixed)	—	–2.1	21.9
*u*3772	H(114)...H(129)	595.3(61)	39.6(fixed)	—	1.9	39.6
*u*4051	C(57)...H(66)	595.3(40)	25.9(fixed)	—	–3.5	25.9
*u*4036	C(10)...H(19)	595.5(31)	25.2(fixed)	—	–3.2	25.2
*u*3741	C(54)...H(74)	595.5(87)	25.8(fixed)	—	–2.2	25.8
*u*3925	C(9)...H(18)	595.5(50)	24.4(fixed)	—	–3.6	24.4
*u*3919	C(60)...H(80)	595.6(22)	21.5(fixed)	—	–1.8	21.5
*u*3924	H(28)...H(31)	595.8(37)	42.6(fixed)	—	1.7	42.6
*u*3948	C(150)...H(186)	595.8(22)	21.6(fixed)	—	–1.7	21.6
*u*3993	C(243)...H(280)	595.9(21)	22.4(fixed)	—	–2.3	22.4
*u*3953	H(27)...H(36)	595.9(74)	39.3(fixed)	—	–2.3	39.3
*u*3905	H(161)...H(182)	596.0(27)	37.9(fixed)	—	–1.9	37.9
*u*3933	C(9)...H(32)	596.0(32)	21.9(fixed)	—	–1.8	21.9
*u*3896	H(20)...H(41)	596.0(32)	37.7(fixed)	—	–2.7	37.7
*u*4083	C(104)...H(113)	596.1(34)	25.3(fixed)	—	–3.6	25.3
*u*3587	H(67)...H(71)	596.2(71)	33.6(fixed)	—	–2.2	33.6
*u*3740	H(255)...H(273)	596.2(34)	55.4(fixed)	—	–2.0	55.4
*u*3821	H(20)...H(35)	596.5(59)	40.0(fixed)	—	1.0	40.0
*u*3683	C(110)...H(135)	596.6(34)	31.0(fixed)	—	–3.3	31.0
*u*3941	H(31)...H(38)	596.7(35)	60.8(fixed)	—	–3.8	60.8
*u*3970	H(263)...H(282)	597.0(28)	37.3(fixed)	—	–0.6	37.3
*u*3864	C(6)...H(27)	597.2(73)	29.9(fixed)	—	–4.1	29.9
*u*3973	H(34)...H(39)	597.2(84)	43.6(fixed)	—	–1.6	43.6
*u*3976	H(61)...H(74)	597.4(40)	23.6(fixed)	—	–9.7	23.6
*u*3628	H(261)...H(274)	597.4(50)	32.7(fixed)	—	–1.4	32.7
*u*4024	H(213)...H(227)	597.4(40)	65.8(fixed)	—	–5.7	65.8
*u*3945	H(90)...H(94)	597.5(64)	42.3(fixed)	—	–1.6	42.3
*u*3888	C(102)...H(141)	597.5(43)	23.3(fixed)	—	–1.5	23.3
*u*3657	H(65)...H(73)	597.6(79)	32.2(fixed)	—	–1.5	32.2

*u*3851	C(9)...H(19)	597.6(72)	30.2(fixed)	—	–3.5	30.2
*u*3909	C(103)...H(126)	597.9(30)	21.8(fixed)	—	–1.8	21.8
*u*3870	C(8)...H(47)	597.9(43)	23.7(fixed)	—	–1.8	23.7
*u*4008	C(16)...H(38)	598.1(56)	25.9(fixed)	—	–3.8	25.9
*u*3693	H(73)...H(83)	598.3(68)	65.5(fixed)	—	6.2	65.5
*u*3774	H(67)...H(82)	598.4(64)	41.6(fixed)	—	0.9	41.6
*u*3801	H(73)...H(78)	598.5(41)	40.7(fixed)	—	3.6	40.7
*u*3974	H(210)...H(215)	598.5(39)	41.1(fixed)	—	–2.1	41.1
*u*3942	C(244)...H(267)	598.7(28)	22.0(fixed)	—	–1.7	22.0
*u*3750	H(26)...H(47)	598.7(48)	40.7(fixed)	—	0.9	40.7
*u*4005	H(249)...H(265)	598.8(27)	20.4(fixed)	—	–6.0	20.4
*u*3736	H(120)...H(141)	598.9(47)	40.7(fixed)	—	1.8	40.7
*u*3954	C(64)...H(88)	599.4(51)	30.3(fixed)	—	–3.6	30.3
*u*3977	H(210)...H(227)	599.7(26)	46.8(fixed)	—	2.4	46.8
*u*3823	C(53)...H(71)	600.2(61)	26.2(fixed)	—	–4.2	26.2
*u*3951	H(43)...H(47)	600.3(50)	39.7(fixed)	—	–1.8	39.7
*u*3879	C(54)...H(76)	600.4(58)	24.3(fixed)	—	–1.9	24.3
*u*3980	H(202)...H(207)	600.5(27)	19.9(fixed)	—	–6.2	19.9
*u*3850	H(214)...H(235)	600.6(27)	33.6(fixed)	—	–0.7	33.6
*u*4104	C(56)...H(77)	600.7(56)	32.1(fixed)	—	–6.1	32.1
*u*3847	H(72)...H(83)	600.8(31)	75.9(fixed)	—	–0.2	75.9
*u*3663	H(67)...H(75)	600.9(64)	37.0(fixed)	—	–3.8	37.0
*u*4091	C(11)...H(25)	601.0(24)	25.8(fixed)	—	–3.8	25.8
*u*4055	C(63)...H(85)	601.0(41)	32.3(fixed)	—	–7.4	32.3
*u*4026	C(17)...H(39)	601.2(47)	25.5(fixed)	—	–4.4	25.5
*u*3790	C(55)...H(65)	601.4(55)	25.1(fixed)	—	–3.6	25.1
*u*4127	C(60)...H(72)	601.4(54)	26.7(fixed)	—	–3.5	26.7
*u*4006	H(137)...H(141)	601.4(51)	44.6(fixed)	—	–2.6	44.6
*u*4098	C(101)...H(137)	601.8(23)	30.5(fixed)	—	–7.2	30.5
*u*3812	H(22)...H(36)	602.0(47)	33.7(fixed)	—	–1.7	33.7
*u*4012	H(202)...H(234)	602.0(26)	25.4(fixed)	—	–6.5	25.4
*u*4014	H(249)...H(278)	602.3(33)	24.9(fixed)	—	–9.1	24.9
*u*4041	C(102)...H(132)	602.4(34)	24.3(fixed)	—	–3.2	24.3
*u*3947	H(125)...H(135)	602.7(45)	37.5(fixed)	—	–3.1	37.5
*u*4112	C(246)...H(260)	603.1(27)	24.5(fixed)	—	–3.6	24.5
*u*4021	C(57)...H(67)	603.1(33)	23.9(fixed)	—	–2.8	23.9
*u*4044	H(155)...H(166)	603.2(30)	21.2(fixed)	—	–6.9	21.2
*u*4094	C(105)...H(119)	603.2(26)	25.4(fixed)	—	–3.8	25.4
*u*4063	C(7)...H(43)	603.3(19)	32.6(fixed)	—	–6.7	32.6
*u*3838	C(194)...H(215)	603.3(29)	33.7(fixed)	—	–3.5	33.7
*u*3955	C(8)...H(46)	603.6(63)	24.3(fixed)	—	–2.5	24.3
*u*4039	H(209)...H(224)	603.6(32)	43.7(fixed)	—	–2.5	43.7
*u*4002	H(116)...H(133)	603.7(28)	37.4(fixed)	—	–1.4	37.4
*u*4033	C(10)...H(20)	603.9(22)	23.5(fixed)	—	–2.8	23.5
*u*4071	C(104)...H(114)	604.0(24)	26.0(fixed)	—	–3.5	26.0
*u*3913	C(110)...H(133)	604.1(21)	24.7(fixed)	—	–3.7	24.7

*u*4070	C(242)...H(278)	604.3(17)	27.1(fixed)	—	–4.1	27.1
*u*3606	C(55)...H(66)	604.3(83)	31.5(fixed)	—	–3.3	31.5
*u*4027	H(81)...H(86)	604.4(59)	43.6(fixed)	—	–1.8	43.6
*u*4020	H(62)...H(81)	604.5(41)	24.2(fixed)	—	–6.3	24.2
*u*3572	C(53)...H(72)	604.6(75)	31.3(fixed)	—	–3.2	31.3
*u*3996	H(261)...H(281)	604.6(47)	40.1(fixed)	—	–1.8	40.1
*u*3966	C(152)...H(168)	604.9(21)	29.3(fixed)	—	–3.1	29.3
*u*4018	H(169)...H(187)	605.1(58)	40.5(fixed)	—	–2.2	40.5
*u*3994	C(8)...H(45)	605.1(44)	23.0(fixed)	—	–2.3	23.0
*u*4081	C(147)...H(166)	605.2(38)	25.3(fixed)	—	–3.7	25.3
*u*4113	C(195)...H(231)	605.2(17)	24.4(fixed)	—	–3.4	24.4
*u*4046	H(73)...H(77)	605.3(69)	43.1(fixed)	—	–2.4	43.1
*u*4043	C(194)...H(216)	605.5(15)	29.1(fixed)	—	–7.9	29.1
*u*4030	C(148)...H(184)	605.5(17)	25.6(fixed)	—	–3.2	25.6
*u*3969	H(28)...H(47)	605.8(57)	37.9(fixed)	—	–0.9	37.9
*u*4017	C(16)...H(36)	606.5(48)	24.1(fixed)	—	–2.9	24.1
*u*3981	H(14)...H(25)	606.6(51)	24.9(fixed)	—	–6.4	24.9
*u*3842	H(73)...H(94)	606.6(67)	34.1(fixed)	—	–0.9	34.1
*u*4066	C(7)...H(44)	606.6(21)	36.1(fixed)	—	–7.5	36.1
*u*4101	H(24)...H(44)	606.6(32)	65.5(fixed)	—	–5.9	65.5
*u*3957	C(102)...H(140)	606.7(61)	23.3(fixed)	—	–2.3	23.3
*u*3728	H(69)...H(83)	606.7(43)	45.8(fixed)	—	11.5	45.8
*u*4105	C(56)...H(78)	606.9(35)	34.2(fixed)	—	–6.0	34.2
*u*3872	H(129)...H(130)	607.0(31)	32.4(fixed)	—	–0.3	32.4
*u*3938	H(160)...H(176)	607.0(50)	44.7(fixed)	—	–2.2	44.7
*u*3979	H(122)...H(141)	607.1(57)	37.5(fixed)	—	–0.7	37.5
*u*4035	C(64)...H(86)	607.5(33)	25.7(fixed)	—	–4.3	25.7
*u*4045	C(63)...H(83)	607.7(23)	35.9(fixed)	—	–7.0	35.9
*u*3946	H(69)...H(74)	607.9(94)	40.0(fixed)	—	–2.3	40.0
*u*4068	C(242)...H(279)	608.4(19)	26.9(fixed)	—	–4.3	26.9
*u*4085	C(54)...H(90)	608.4(33)	25.9(fixed)	—	–3.6	25.9
*u*4009	C(13)...H(27)	608.4(69)	31.4(fixed)	—	–3.6	31.4
*u*4037	C(101)...H(138)	608.5(24)	33.1(fixed)	—	–5.3	33.1
*u*3984	C(102)...H(139)	608.5(41)	22.2(fixed)	—	–2.1	22.2
*u*4011	H(15)...H(21)	608.7(65)	22.2(fixed)	—	–8.5	22.2
*u*4065	H(155)...H(168)	609.3(27)	23.4(fixed)	—	–6.2	23.4
*u*4100	H(256)...H(274)	609.3(54)	43.7(fixed)	—	–2.6	43.7
*u*4025	C(148)...H(185)	609.5(19)	24.2(fixed)	—	–2.8	24.2
*u*4072	H(28)...H(30)	609.7(54)	43.2(fixed)	—	–2.6	43.2
*u*4048	C(195)...H(232)	609.7(19)	24.6(fixed)	—	–2.9	24.6
*u*3983	H(207)...H(223)	609.8(52)	41.6(fixed)	—	–1.5	41.6
*u*3997	H(254)...H(270)	610.2(53)	40.2(fixed)	—	–1.8	40.2
*u*3985	H(66)...H(82)	610.2(58)	44.0(fixed)	—	–2.3	44.0
*u*4120	H(78)...H(84)	610.3(23)	57.9(fixed)	—	–9.1	57.9
*u*4078	C(11)...H(26)	610.7(18)	24.8(fixed)	—	–3.4	24.8
*u*4117	C(244)...H(281)	611.1(28)	25.3(fixed)	—	–3.2	25.3

*u*4049	C(102)...H(130)	611.1(36)	23.5(fixed)	—	–3.2	23.5
*u*3885	C(243)...H(276)	611.2(39)	27.5(fixed)	—	–3.1	27.5
*u*4029	C(149)...H(171)	611.3(32)	29.2(fixed)	—	–5.0	29.2
*u*4109	C(60)...H(73)	611.4(50)	26.8(fixed)	—	–3.3	26.8
*u*4015	C(59)...H(68)	611.6(39)	25.4(fixed)	—	–3.6	25.4
*u*4038	C(152)...H(169)	611.6(16)	24.7(fixed)	—	–3.8	24.7
*u*4001	H(109)...H(115)	611.8(65)	20.4(fixed)	—	–5.8	20.4
*u*4050	C(147)...H(167)	612.1(23)	25.7(fixed)	—	–3.1	25.7
*u*4060	H(122)...H(124)	612.2(51)	43.7(fixed)	—	–2.6	43.7
*u*4059	C(54)...H(91)	612.3(26)	25.1(fixed)	—	–3.1	25.1
*u*4028	H(118)...H(138)	612.5(35)	57.2(fixed)	—	–3.2	57.2
*u*4074	C(246)...H(261)	612.7(19)	23.3(fixed)	—	–3.0	23.3
*u*3992	H(19)...H(35)	612.7(55)	41.8(fixed)	—	–2.0	41.8
*u*3991	H(108)...H(116)	612.8(24)	26.9(fixed)	—	–1.0	26.9
*u*4040	H(109)...H(139)	612.9(28)	26.8(fixed)	—	–1.0	26.8
*u*4093	H(61)...H(71)	613.3(32)	25.4(fixed)	—	–2.1	25.4
*u*4058	C(149)...H(172)	613.3(19)	31.4(fixed)	—	–5.7	31.4
*u*4123	H(117)...H(130)	613.3(37)	33.9(fixed)	—	–2.8	33.9
*u*4023	H(202)...H(211)	613.4(26)	28.9(fixed)	—	–1.5	28.9
*u*4007	H(113)...H(129)	613.5(61)	41.7(fixed)	—	–1.5	41.7
*u*4073	C(105)...H(120)	613.5(16)	24.8(fixed)	—	–3.0	24.8
*u*3998	H(109)...H(141)	613.6(23)	28.4(fixed)	—	–0.8	28.4
*u*4064	H(15)...H(45)	613.6(29)	26.1(fixed)	—	–1.6	26.1
*u*4114	H(163)...H(165)	613.7(17)	54.1(fixed)	—	–5.4	54.1
*u*4062	C(197)...H(218)	613.8(22)	27.5(fixed)	—	–3.8	27.5
*u*3982	H(15)...H(47)	614.2(23)	28.2(fixed)	—	–1.3	28.2
*u*4080	H(133)...H(136)	614.2(32)	65.0(fixed)	—	–4.0	65.0
*u*4047	H(249)...H(268)	614.3(29)	27.3(fixed)	—	–1.3	27.3
*u*4013	H(62)...H(79)	614.7(29)	32.1(fixed)	—	2.0	32.1
*u*4075	C(13)...H(28)	615.0(54)	26.0(fixed)	—	–3.9	26.0
*u*4077	C(196)...H(234)	615.1(27)	24.7(fixed)	—	–3.3	24.7
*u*4234	H(37)...H(43)	615.3(88)	40.3(fixed)	—	–17.1	40.3
*u*4032	H(202)...H(210)	615.3(25)	27.4(fixed)	—	–1.1	27.4
*u*4069	H(135)...H(136)	615.4(47)	71.9(fixed)	—	–9.1	71.9
*u*4031	C(59)...H(69)	615.4(29)	23.9(fixed)	—	–3.1	23.9
*u*3999	H(109)...H(113)	615.4(49)	23.8(fixed)	—	–7.3	23.8
*u*4042	H(108)...H(117)	615.7(28)	26.7(fixed)	—	–1.5	26.7
*u*4082	H(67)...H(87)	615.8(33)	32.9(fixed)	—	–3.8	32.9
*u*4200	H(39)...H(45)	615.8(66)	37.3(fixed)	—	–4.3	37.3
*u*4004	H(249)...H(270)	616.0(24)	27.2(fixed)	—	–0.8	27.2
*u*4119	H(31)...H(37)	616.4(20)	48.8(fixed)	—	–5.7	48.8
*u*4019	C(243)...H(274)	616.6(44)	22.9(fixed)	—	–4.2	22.9
*u*4121	H(67)...H(79)	616.7(44)	53.2(fixed)	—	–0.5	53.2
*u*4185	H(212)...H(227)	616.8(41)	53.8(fixed)	—	–8.0	53.8
*u*4010	H(15)...H(19)	616.9(50)	23.7(fixed)	—	–5.2	23.7
*u*4097	C(244)...H(282)	617.0(19)	24.4(fixed)	—	–2.8	24.4

*u*4227	H(66)...H(79)	617.2(49)	59.6(fixed)	—	–5.7	59.6
*u*4210	H(19)...H(32)	617.2(37)	55.1(fixed)	—	–5.3	55.1
*u*3995	H(26)...H(46)	617.3(56)	42.9(fixed)	—	–1.9	42.9
*u*4057	C(197)...H(219)	617.5(16)	24.9(fixed)	—	–3.1	24.9
*u*4129	H(20)...H(32)	617.5(29)	49.7(fixed)	—	–1.3	49.7
*u*4264	H(41)...H(45)	617.8(67)	40.3(fixed)	—	–6.0	40.3
*u*4052	H(134)...H(137)	617.9(34)	41.6(fixed)	—	–15.0	41.6
*u*4111	H(20)...H(40)	618.2(20)	32.9(fixed)	—	–3.8	32.9
*u*4076	H(14)...H(28)	618.3(31)	28.4(fixed)	—	–1.7	28.4
*u*4056	H(14)...H(29)	618.4(36)	25.8(fixed)	—	–1.1	25.8
*u*4192	H(114)...H(126)	618.4(31)	39.1(fixed)	—	–3.5	39.1
*u*4089	H(42)...H(47)	618.5(41)	35.4(fixed)	—	–5.7	35.4
*u*4096	H(89)...H(94)	618.5(50)	36.8(fixed)	—	–3.4	36.8
*u*4067	C(196)...H(235)	618.5(17)	24.1(fixed)	—	–3.2	24.1
*u*4140	H(136)...H(141)	618.5(42)	38.3(fixed)	—	–6.8	38.3
*u*4084	H(255)...H(272)	618.8(23)	45.7(fixed)	—	–4.4	45.7
*u*4016	C(53)...H(75)	618.8(42)	27.8(fixed)	—	–5.4	27.8
*u*4131	H(33)...H(39)	619.0(56)	38.5(fixed)	—	–3.9	38.5
*u*4054	C(12)...H(21)	619.2(57)	26.1(fixed)	—	–4.0	26.1
*u*4106	H(210)...H(217)	619.4(21)	35.5(fixed)	—	–5.5	35.5
*u*4022	H(62)...H(78)	619.5(27)	36.4(fixed)	—	1.1	36.4
*u*4053	C(12)...H(22)	619.5(31)	25.9(fixed)	—	–3.7	25.9
*u*4102	H(161)...H(181)	619.5(18)	33.2(fixed)	—	–3.9	33.2
*u*4115	H(123)...H(133)	619.6(43)	33.9(fixed)	—	–4.0	33.9
*u*4292	H(65)...H(77)	619.7(55)	35.8(fixed)	—	–12.8	35.8
*u*4199	C(8)...H(43)	619.8(22)	27.6(fixed)	—	–17.6	27.6
*u*4225	H(38)...H(42)	619.9(67)	66.1(fixed)	—	–7.8	66.1
*u*4139	H(36)...H(42)	620.6(67)	59.1(fixed)	—	–0.7	59.1
*u*4361	H(113)...H(126)	620.7(44)	36.5(fixed)	—	–5.4	36.5
*u*3930	C(53)...H(74)	621.0(66)	32.4(fixed)	—	–4.3	32.4
*u*4126	H(29)...H(36)	621.2(56)	33.8(fixed)	—	–3.4	33.8
*u*4034	H(61)...H(73)	621.5(34)	27.0(fixed)	—	–1.6	27.0
*u*4099	H(71)...H(83)	621.6(27)	62.8(fixed)	—	–3.4	62.8
*u*4180	C(102)...H(137)	621.6(23)	28.4(fixed)	—	–16.4	28.4
*u*4087	C(107)...H(137)	621.6(24)	34.8(fixed)	—	–15.8	34.8
*u*4061	C(55)...H(94)	621.6(45)	24.0(fixed)	—	–3.3	24.0
*u*4237	C(12)...H(43)	621.9(53)	32.7(fixed)	—	–16.9	32.7
*u*4124	C(103)...H(140)	622.0(64)	26.0(fixed)	—	–3.6	26.0
*u*4110	C(107)...H(116)	622.1(18)	25.3(fixed)	—	–3.0	25.3
*u*4226	H(206)...H(216)	622.2(23)	43.0(fixed)	—	–8.6	43.0
*u*4154	C(107)...H(115)	622.2(26)	26.1(fixed)	—	–3.5	26.1
*u*4141	C(9)...H(46)	622.2(64)	26.1(fixed)	—	–3.5	26.1
*u*4086	C(106)...H(128)	622.3(31)	24.6(fixed)	—	–3.3	24.6
*u*3988	H(120)...H(140)	622.3(51)	42.6(fixed)	—	–1.5	42.6
*u*4203	H(23)...H(44)	622.5(31)	56.6(fixed)	—	–7.6	56.6
*u*4088	C(9)...H(47)	622.5(37)	24.5(fixed)	—	–3.0	24.5

*u*4092	C(55)...H(93)	622.6(77)	25.2(fixed)	—	–3.8	25.2
*u*4079	C(106)...H(129)	622.7(19)	23.9(fixed)	—	–3.2	23.9
*u*4107	C(103)...H(141)	622.7(37)	25.1(fixed)	—	–3.2	25.1
*u*4095	H(125)...H(134)	622.9(26)	32.7(fixed)	—	–3.7	32.7
*u*4202	H(255)...H(267)	623.2(26)	40.2(fixed)	—	–4.2	40.2
*u*4142	H(73)...H(79)	623.3(49)	37.0(fixed)	—	–4.7	37.0
*u*4279	C(53)...H(77)	623.3(35)	28.2(fixed)	—	–13.4	28.2
*u*4198	H(76)...H(78)	623.8(48)	52.1(fixed)	—	–4.9	52.1
*u*4147	H(211)...H(224)	623.8(22)	35.7(fixed)	—	–3.9	35.7
*u*4138	H(161)...H(173)	623.9(25)	49.5(fixed)	—	–1.3	49.5
*u*4103	H(159)...H(176)	623.9(41)	38.8(fixed)	—	–3.7	38.8
*u*4220	H(86)...H(92)	624.2(45)	38.7(fixed)	—	–4.3	38.7
*u*4151	H(80)...H(86)	624.3(36)	37.9(fixed)	—	–3.9	37.9
*u*4183	H(83)...H(89)	624.3(34)	54.3(fixed)	—	–6.8	54.3
*u*4165	H(208)...H(220)	624.5(25)	39.2(fixed)	—	–2.6	39.2
*u*4166	H(169)...H(186)	625.1(35)	33.9(fixed)	—	–3.5	33.9
*u*4158	H(117)...H(138)	625.4(36)	49.0(fixed)	—	–5.2	49.0
*u*4135	H(261)...H(280)	625.4(29)	34.4(fixed)	—	–3.2	34.4
*u*4267	C(55)...H(85)	625.6(22)	28.4(fixed)	—	–18.7	28.4
*u*4118	H(253)...H(270)	625.8(44)	34.7(fixed)	—	–4.1	34.7
*u*4213	C(59)...H(77)	625.8(19)	27.6(fixed)	—	–14.0	27.6
*u*4137	H(65)...H(82)	626.1(45)	37.1(fixed)	—	–3.5	37.1
*u*4255	H(18)...H(30)	626.1(32)	33.9(fixed)	—	–10.0	33.9
*u*4128	H(206)...H(223)	626.1(43)	36.1(fixed)	—	–3.1	36.1
*u*4160	H(28)...H(32)	626.2(36)	37.4(fixed)	—	–4.8	37.4
*u*4301	H(76)...H(77)	626.6(75)	50.0(fixed)	—	–8.7	50.0
*u*4268	C(6)...H(30)	627.1(24)	25.4(fixed)	—	–10.7	25.4
*u*4242	H(88)...H(92)	627.2(69)	40.1(fixed)	—	–5.8	40.1
*u*4265	H(118)...H(130)	627.2(50)	38.4(fixed)	—	–3.6	38.4
*u*4245	H(26)...H(33)	627.4(27)	41.4(fixed)	—	–3.5	41.4
*u*4108	H(69)...H(76)	627.5(57)	35.0(fixed)	—	–3.8	35.0
*u*4187	H(258)...H(274)	627.5(35)	37.1(fixed)	—	–3.9	37.1
*u*4219	C(149)...H(162)	627.6(18)	25.1(fixed)	—	–12.1	25.1
*u*4384	H(117)...H(137)	627.9(29)	43.5(fixed)	—	–10.6	43.5
*u*4132	H(112)...H(129)	628.1(47)	35.9(fixed)	—	–3.5	35.9
*u*4478	H(25)...H(33)	628.2(32)	41.0(fixed)	—	–6.2	41.0
*u*4125	H(18)...H(35)	628.3(43)	35.5(fixed)	—	–3.2	35.5
*u*4520	H(260)...H(268)	628.4(35)	38.4(fixed)	—	–5.8	38.4
*u*4335	H(23)...H(43)	628.4(25)	50.5(fixed)	—	–11.2	50.5
*u*4376	H(85)...H(89)	628.4(51)	45.9(fixed)	—	–11.9	45.9
*u*4240	H(261)...H(268)	628.5(29)	38.4(fixed)	—	–3.1	38.4
*u*4205	C(12)...H(30)	628.8(20)	25.7(fixed)	—	–11.4	25.7
*u*4215	H(169)...H(174)	628.8(25)	36.4(fixed)	—	–3.6	36.4
*u*4249	H(163)...H(178)	629.0(27)	47.9(fixed)	—	–6.3	47.9
*u*4247	H(73)...H(87)	629.0(68)	41.2(fixed)	—	–2.8	41.2
*u*4228	H(160)...H(173)	629.1(21)	54.2(fixed)	—	–5.7	54.2

*u*4484	H(72)...H(87)	629.2(66)	40.8(fixed)	—	–5.4	40.8
*u*4161	H(122)...H(126)	629.3(33)	36.8(fixed)	—	–3.8	36.8
*u*4197	H(159)...H(167)	629.5(33)	38.9(fixed)	—	–3.2	38.9
*u*4201	H(69)...H(84)	629.6(43)	62.7(fixed)	—	–3.3	62.7
*u*4195	H(70)...H(91)	629.8(38)	40.0(fixed)	—	–3.1	40.0
*u*4338	H(254)...H(267)	629.9(21)	39.1(fixed)	—	–6.2	39.1
*u*4504	H(119)...H(127)	630.5(37)	40.4(fixed)	—	–6.5	40.4
*u*4475	H(118)...H(132)	630.5(51)	37.0(fixed)	—	–6.1	37.0
*u*4152	C(6)...C(16)	630.6(20)	14.8(tied to *u*4168)	—	–1.5	13.3
*u*4144	H(206)...H(215)	630.7(39)	47.9(fixed)	—	–7.0	47.9
*u*4146	C(100)...C(110)	630.7(20)	15.1(tied to *u*4168)	—	–1.5	13.5
*u*4207	C(13)...H(46)	630.7(52)	26.5(fixed)	—	–5.5	26.5
*u*4252	H(40)...H(46)	630.8(87)	34.7(fixed)	—	–2.8	34.7
*u*4155	C(53)...C(63)	630.8(20)	14.8(tied to *u*4168)	—	–1.6	13.3
*u*4163	C(147)...C(157)	631.1(21)	14.9(tied to *u*4168)	—	–1.7	13.3
*u*4448	H(207)...H(220)	631.1(21)	37.5(fixed)	—	–5.1	37.5
*u*4148	C(194)...C(204)	631.3(21)	14.7(tied to *u*4168)	—	–1.5	13.1
*u*4248	H(159)...H(171)	631.3(27)	36.2(fixed)	—	–10.9	36.2
*u*4244	H(120)...H(127)	631.4(25)	41.2(fixed)	—	–3.2	41.2
*u*4238	H(168)...H(174)	631.5(30)	39.2(fixed)	—	–5.1	39.2
*u*4149	C(241)...C(251)	631.6(21)	14.6(tied to *u*4168)	—	–1.4	13.1
*u*4212	C(54)...H(85)	632.2(31)	35.6(fixed)	—	–17.1	35.6
*u*4211	C(60)...H(66)	632.2(18)	21.2(fixed)	—	–5.7	21.2
*u*4177	C(11)...C(12)	632.3(8)	14.8(tied to *u*4168)	—	–2.0	13.2
*u*4162	C(105)...C(107)	632.5(8)	14.5(tied to *u*4168)	—	–1.8	12.9
*u*4173	C(7)...C(13)	632.5(8)	14.7(tied to *u*4168)	—	–1.9	13.2
*u*4224	H(70)...H(85)	632.5(51)	42.0(fixed)	—	–17.1	42.0
*u*4218	C(13)...H(19)	632.7(14)	20.7(fixed)	—	–5.7	20.7
*u*4174	C(149)...C(158)	632.9(5)	14.9(tied to *u*4168)	—	–1.9	13.3
*u*4176	C(54)...C(60)	633.0(6)	14.7(tied to *u*4168)	—	–1.9	13.1
*u*4171	C(8)...C(10)	633.0(6)	14.8(tied to *u*4168)	—	–1.8	13.2
*u*4340	H(68)...H(84)	633.2(50)	67.8(fixed)	—	–10.1	67.8
*u*4143	H(26)...H(45)	633.2(36)	36.5(fixed)	—	–3.3	36.5
*u*4175	C(58)...C(59)	633.2(5)	14.7(tied to *u*4168)	—	–1.8	13.1
*u*4164	C(197)...C(205)	633.3(6)	14.4(tied to *u*4168)	—	–1.6	12.9
*u*4254	C(147)...H(171)	633.4(17)	27.9(fixed)	—	–11.5	27.9
*u*4172	C(102)...C(104)	633.5(6)	14.4(tied to *u*4168)	—	–1.7	12.9
*u*4186	H(65)...H(75)	633.6(52)	39.8(fixed)	—	–5.5	39.8
*u*4170	C(148)...C(154)	633.7(6)	14.6(tied to *u*4168)	—	–1.7	13.1
*u*4159	C(242)...C(247)	633.7(6)	14.8(tied to *u*4168)	—	–1.8	13.2
*u*4157	C(196)...H(229)	633.7(27)	29.7(fixed)	—	–12.5	29.7
*u*4251	H(259)...H(274)	634.0(59)	37.0(fixed)	—	–4.9	37.0
*u*4375	C(101)...H(132)	634.0(28)	19.1(fixed)	—	–5.9	19.1
*u*4184	C(243)...H(278)	634.2(16)	23.0(fixed)	—	–9.4	23.0
*u*4231	C(197)...H(209)	634.2(18)	22.5(fixed)	—	–6.5	22.5
*u*4307	C(63)...H(93)	634.5(28)	18.8(fixed)	—	–6.0	18.8

*u*4341	H(21)...H(30)	634.6(35)	45.4(fixed)	—	–10.2	45.4
*u*4168	C(56)...C(64)	634.7(7)	14.9(0.9627)	—	–1.8	13.3
*u*4325	C(100)...H(124)	634.9(26)	21.1(fixed)	—	–4.7	21.1
*u*4190	C(196)...C(200)	635.4(28)	14.2(tied to *u*4168)	—	–2.1	12.7
*u*4182	C(107)...H(124)	635.5(19)	21.5(fixed)	—	–5.4	21.5
*u*4449	H(159)...H(166)	635.5(48)	36.1(fixed)	—	–5.8	36.1
*u*4181	C(103)...C(106)	635.6(28)	14.3(tied to *u*4168)	—	–1.8	12.8
*u*4230	H(28)...H(40)	635.7(72)	37.5(fixed)	—	–3.2	37.5
*u*4246	H(71)...H(94)	636.0(50)	37.2(fixed)	—	–3.3	37.2
*u*4189	C(244)...C(248)	636.0(30)	14.4(tied to *u*4168)	—	–1.8	12.9
*u*4409	C(57)...H(74)	636.1(40)	25.5(fixed)	—	–9.0	25.5
*u*4277	C(9)...H(38)	636.1(31)	23.2(fixed)	—	–6.0	23.2
*u*4287	C(16)...H(46)	636.4(25)	18.4(fixed)	—	–5.2	18.4
*u*4334	C(110)...H(140)	636.4(25)	19.2(fixed)	—	–6.2	19.2
*u*4188	C(60)...H(93)	636.6(38)	27.2(fixed)	—	–6.0	27.2
*u*4130	H(120)...H(139)	636.7(32)	36.6(fixed)	—	–2.9	36.6
*u*4364	H(21)...H(32)	636.8(36)	44.9(fixed)	—	–10.3	44.9
*u*4253	C(11)...H(41)	636.8(35)	19.6(fixed)	—	–6.2	19.6
*u*4179	C(103)...H(135)	636.9(30)	21.3(fixed)	—	–5.4	21.3
*u*4090	H(210)...H(228)	637.0(24)	52.1(fixed)	—	0.4	52.1
*u*4258	H(119)...H(131)	637.0(46)	33.9(fixed)	—	–4.6	33.9
*u*4223	C(150)...H(184)	637.1(14)	21.0(fixed)	—	–5.5	21.0
*u*4362	H(115)...H(124)	637.3(40)	36.7(fixed)	—	–5.6	36.7
*u*4295	C(53)...H(81)	637.3(25)	20.1(fixed)	—	–6.4	20.1
*u*4209	H(264)...H(282)	637.4(29)	38.3(fixed)	—	–2.1	38.3
*u*4348	H(112)...H(124)	637.4(32)	29.7(fixed)	—	–1.7	29.7
*u*4257	H(212)...H(235)	637.8(24)	38.8(fixed)	—	–3.4	38.8
*u*4420	C(55)...H(88)	637.9(52)	25.2(fixed)	—	–6.8	25.2
*u*4214	C(106)...H(119)	638.0(32)	25.6(fixed)	—	–6.1	25.6
*u*4318	C(8)...H(34)	638.1(20)	24.0(fixed)	—	–6.6	24.0
*u*4424	H(70)...H(90)	638.1(46)	38.3(fixed)	—	–5.7	38.3
*u*4377	H(162)...H(178)	638.1(38)	43.3(fixed)	—	–8.4	43.3
*u*4367	H(23)...H(32)	638.2(27)	38.8(fixed)	—	–8.1	38.8
*u*4312	C(6)...H(34)	638.2(24)	20.5(fixed)	—	–6.7	20.5
*u*4194	H(29)...H(47)	638.5(34)	37.5(fixed)	—	–2.2	37.5
*u*4263	C(58)...H(88)	638.7(28)	20.6(fixed)	—	–6.5	20.6
*u*4405	C(57)...H(72)	638.8(30)	19.0(fixed)	—	–5.8	19.0
*u*4216	H(123)...H(141)	638.8(33)	40.1(fixed)	—	–2.6	40.1
*u*4222	H(22)...H(37)	638.9(43)	40.5(fixed)	—	–3.9	40.5
*u*4281	C(147)...H(175)	638.9(26)	19.2(fixed)	—	–6.6	19.2
*u*4477	H(71)...H(88)	639.3(84)	33.2(fixed)	—	–5.4	33.2
*u*4447	H(74)...H(81)	639.3(55)	42.6(fixed)	—	–9.0	42.6
*u*4359	C(100)...H(128)	639.3(27)	19.5(fixed)	—	–6.2	19.5
*u*4206	H(259)...H(276)	639.3(55)	40.0(fixed)	—	–5.6	40.0
*u*4271	C(152)...H(182)	639.4(28)	20.3(fixed)	—	–5.9	20.3
*u*4463	H(215)...H(222)	639.4(28)	43.5(fixed)	—	–11.6	43.5

*u*4332	H(68)...H(77)	639.4(47)	48.6(fixed)	—	–10.9	48.6
*u*4153	H(209)...H(228)	639.6(27)	63.1(fixed)	—	–4.5	63.1
*u*4400	C(246)...H(273)	639.7(24)	19.2(fixed)	—	–5.8	19.2
*u*4413	H(24)...H(34)	639.7(36)	32.5(fixed)	—	–5.1	32.5
*u*4221	H(87)...H(93)	639.8(46)	34.8(fixed)	—	–3.5	34.8
*u*4122	H(85)...H(93)	639.8(54)	58.6(fixed)	—	–11.2	58.6
*u*4259	H(27)...H(40)	639.8(94)	40.8(fixed)	—	–5.2	40.8
*u*4169	C(197)...H(207)	639.9(18)	25.1(fixed)	—	–5.5	25.1
*u*4441	H(117)...H(126)	639.9(31)	28.8(fixed)	—	–4.9	28.8
*u*4260	C(59)...H(90)	640.0(29)	24.0(fixed)	—	–6.5	24.0
*u*4339	C(194)...H(218)	640.1(17)	22.7(fixed)	—	–5.7	22.7
*u*4489	H(115)...H(126)	640.2(45)	30.7(fixed)	—	–5.9	30.7
*u*4336	C(194)...H(222)	640.2(27)	19.6(fixed)	—	–6.3	19.6
*u*4290	C(16)...H(21)	640.2(18)	24.0(fixed)	—	–7.4	24.0
*u*4532	H(215)...H(221)	640.5(33)	36.5(fixed)	—	–10.6	36.5
*u*4266	C(10)...H(27)	640.6(30)	20.3(fixed)	—	–6.0	20.3
*u*4411	H(264)...H(281)	640.6(37)	39.4(fixed)	—	–4.6	39.4
*u*4373	H(206)...H(218)	640.8(30)	31.0(fixed)	—	–3.9	31.0
*u*4422	H(84)...H(92)	640.8(38)	42.8(fixed)	—	–12.2	42.8
*u*4304	H(160)...H(165)	640.9(34)	31.5(fixed)	—	–3.1	31.5
*u*4354	C(195)...H(229)	641.0(18)	24.5(fixed)	—	–12.9	24.5
*u*4324	C(241)...H(269)	641.0(28)	19.2(fixed)	—	–5.9	19.2
*u*4275	C(149)...H(160)	641.1(28)	23.0(fixed)	—	–5.1	23.0
*u*4305	C(241)...H(265)	641.1(17)	21.7(fixed)	—	–5.0	21.7
*u*4196	C(150)...H(175)	641.2(17)	29.0(fixed)	—	–6.5	29.0
*u*4386	C(195)...H(226)	641.3(19)	19.9(fixed)	—	–6.1	19.9
*u*4250	C(104)...H(121)	641.3(28)	21.3(fixed)	—	–6.6	21.3
*u*4355	C(243)...H(269)	641.4(22)	22.9(fixed)	—	–5.9	22.9
*u*4346	H(68)...H(79)	641.6(44)	48.0(fixed)	—	–10.9	48.0
*u*4315	C(102)...H(128)	641.6(19)	23.4(fixed)	—	–6.0	23.4
*u*4365	H(254)...H(262)	641.7(42)	42.5(fixed)	—	–9.1	42.5
*u*4317	C(110)...H(115)	642.1(23)	21.7(fixed)	—	–5.2	21.7
*u*4291	C(63)...H(68)	642.4(26)	23.0(fixed)	—	–5.5	23.0
*u*4494	H(23)...H(30)	642.4(27)	39.4(fixed)	—	–10.6	39.4
*u*4435	H(74)...H(79)	642.7(48)	33.9(fixed)	—	–2.3	33.9
*u*4286	H(164)...H(173)	642.8(26)	40.1(fixed)	—	–9.5	40.1
*u*4303	H(217)...H(221)	642.8(23)	39.8(fixed)	—	–7.4	39.8
*u*4381	H(70)...H(79)	643.0(33)	38.8(fixed)	—	–7.7	38.8
*u*4283	H(162)...H(171)	643.1(26)	48.8(fixed)	—	–12.3	48.8
*u*4284	C(242)...H(276)	643.2(26)	20.2(fixed)	—	–6.1	20.2
*u*4314	H(129)...H(131)	643.4(28)	39.7(fixed)	—	–3.6	39.7
*u*4261	C(9)...H(41)	643.4(55)	28.5(fixed)	—	–6.7	28.5
*u*4296	H(85)...H(92)	643.6(61)	44.2(fixed)	—	–11.1	44.2
*u*4208	H(116)...H(134)	644.0(29)	36.6(fixed)	—	–2.4	36.6
*u*4306	H(84)...H(93)	644.1(47)	52.7(fixed)	—	–16.7	52.7
*u*4337	H(253)...H(265)	644.2(32)	30.4(fixed)	—	–1.1	30.4

*u*4481	H(117)...H(124)	644.2(30)	31.8(fixed)	—	–6.0	31.8
*u*4316	H(211)...H(229)	644.4(26)	34.8(fixed)	—	–11.8	34.8
*u*4480	H(211)...H(220)	644.9(31)	29.9(fixed)	—	–5.4	29.9
*u*4432	H(76)...H(80)	645.0(41)	34.1(fixed)	—	–6.3	34.1
*u*4511	H(74)...H(80)	645.0(45)	36.1(fixed)	—	–8.8	36.1
*u*4217	H(132)...H(136)	645.0(44)	53.6(fixed)	—	–14.2	53.6
*u*4454	H(258)...H(267)	645.1(35)	29.1(fixed)	—	–4.9	29.1
*u*4308	H(68)...H(89)	645.1(40)	30.7(fixed)	—	–3.1	30.7
*u*4486	H(259)...H(269)	645.4(38)	31.2(fixed)	—	–4.7	31.2
*u*4352	H(253)...H(264)	645.5(29)	35.5(fixed)	—	–7.0	35.5
*u*4469	H(212)...H(234)	645.5(32)	38.3(fixed)	—	–5.7	38.3
*u*4428	H(123)...H(140)	645.7(55)	41.3(fixed)	—	–5.1	41.3
*u*4388	H(131)...H(136)	645.8(23)	46.0(fixed)	—	–11.3	46.0
*u*4204	H(207)...H(217)	645.9(24)	36.7(fixed)	—	0.0	36.7
*u*4440	H(165)...H(174)	645.9(28)	30.3(fixed)	—	–6.5	30.3
*u*4408	H(209)...H(218)	645.9(37)	41.1(fixed)	—	–6.8	41.1
*u*4416	C(246)...H(276)	646.1(22)	22.6(fixed)	—	–6.1	22.6
*u*4371	H(162)...H(173)	646.1(24)	47.6(fixed)	—	–12.3	47.6
*u*4236	H(170)...H(175)	646.3(27)	36.3(fixed)	—	–4.8	36.3
*u*4467	H(76)...H(81)	646.3(70)	39.1(fixed)	—	–8.3	39.1
*u*4529	H(135)...H(139)	646.3(40)	33.6(fixed)	—	–6.9	33.6
*u*4353	H(253)...H(262)	646.6(49)	41.5(fixed)	—	–9.1	41.5
*u*4134	H(166)...H(175)	646.8(37)	45.2(fixed)	—	–6.4	45.2
*u*4233	C(148)...H(179)	646.9(22)	23.0(fixed)	—	–5.7	23.0
*u*4330	H(256)...H(265)	647.0(42)	36.1(fixed)	—	–5.5	36.1
*u*4156	C(244)...H(273)	647.0(39)	24.7(fixed)	—	–5.6	24.7
*u*4262	H(217)...H(222)	647.1(28)	49.6(fixed)	—	–9.8	49.6
*u*4461	H(29)...H(46)	647.2(56)	38.3(fixed)	—	–4.6	38.3
*u*4298	H(166)...H(174)	647.3(34)	35.4(fixed)	—	–7.1	35.4
*u*4232	C(56)...H(68)	647.3(64)	22.3(fixed)	—	–6.2	22.3
*u*4239	H(259)...H(272)	647.5(54)	32.8(fixed)	—	–7.5	32.8
*u*4193	H(65)...H(74)	647.6(66)	41.6(fixed)	—	–6.8	41.6
*u*4456	C(11)...H(37)	647.9(27)	26.9(fixed)	—	–1.9	26.9
*u*4503	H(71)...H(93)	647.9(83)	37.0(fixed)	—	–5.8	37.0
*u*4280	H(84)...H(90)	648.0(35)	34.7(fixed)	—	2.8	34.7
*u*4133	H(132)...H(137)	648.0(34)	54.4(fixed)	—	–11.2	54.4
*u*4419	H(118)...H(128)	648.1(28)	31.4(fixed)	—	–4.4	31.4
*u*4167	H(25)...H(41)	648.2(64)	46.6(fixed)	—	–7.4	46.6
*u*4492	H(168)...H(182)	648.4(33)	38.3(fixed)	—	–7.5	38.3
*u*4321	H(38)...H(45)	648.5(55)	35.9(fixed)	—	–6.8	35.9
*u*4349	C(16)...H(18)	648.7(25)	24.9(fixed)	—	–1.2	24.9
*u*4453	H(254)...H(264)	648.7(39)	37.0(fixed)	—	–8.4	37.0
*u*3843	H(260)...H(273)	648.7(60)	46.9(fixed)	—	–5.6	46.9
*u*4407	C(63)...H(65)	648.7(28)	24.8(fixed)	—	–1.3	24.8
*u*4518	H(70)...H(77)	648.8(46)	37.2(fixed)	—	–10.6	37.2
*u*4272	C(199)...H(226)	648.8(19)	22.6(fixed)	—	–5.5	22.6

*u*4522	H(135)...H(140)	648.8(36)	40.0(fixed)	—	–7.2	40.0
*u*4425	H(206)...H(212)	649.1(19)	31.5(fixed)	—	–6.4	31.5
*u*4524	H(209)...H(220)	649.2(35)	33.2(fixed)	—	–7.0	33.2
*u*4328	H(29)...H(41)	649.3(72)	35.2(fixed)	—	–4.3	35.2
*u*4444	H(37)...H(45)	649.5(42)	29.3(fixed)	—	–6.2	29.3
*u*4311	C(110)...H(112)	649.7(26)	27.1(fixed)	—	–0.2	27.1
*u*4482	H(256)...H(267)	649.7(41)	31.2(fixed)	—	–6.0	31.2
*u*4465	H(170)...H(181)	649.9(28)	32.7(fixed)	—	–6.3	32.7
*u*4293	C(105)...H(134)	650.2(26)	24.9(fixed)	—	–0.9	24.9
*u*4485	H(134)...H(139)	650.5(25)	29.7(fixed)	—	–5.0	29.7
*u*4421	H(112)...H(123)	650.6(36)	33.8(fixed)	—	–6.3	33.8
*u*4136	H(207)...H(213)	650.7(27)	41.4(fixed)	—	–5.6	41.4
*u*4150	H(38)...H(46)	650.8(68)	43.6(fixed)	—	–5.9	43.6
*u*4403	C(147)...H(183)	650.9(25)	25.5(fixed)	—	–1.5	25.5
*u*4241	C(7)...H(38)	651.0(35)	22.1(fixed)	—	–5.0	22.1
*u*4450	H(24)...H(40)	651.3(52)	31.3(fixed)	—	–6.7	31.3
*u*4379	C(194)...H(230)	651.3(26)	24.9(fixed)	—	–1.0	24.9
*u*4116	H(259)...H(273)	651.3(61)	38.8(fixed)	—	–7.4	38.8
*u*4326	H(21)...H(42)	651.3(33)	34.2(fixed)	—	1.6	34.2
*u*4458	C(152)...H(178)	651.7(15)	26.0(fixed)	—	–1.6	26.0
*u*4243	H(260)...H(275)	651.9(59)	32.5(fixed)	—	–4.0	32.5
*u*4396	C(17)...H(25)	652.1(50)	19.7(fixed)	—	–6.5	19.7
*u*4512	H(168)...H(181)	652.3(32)	36.3(fixed)	—	–7.3	36.3
*u*4351	C(102)...H(126)	652.4(12)	24.3(fixed)	—	–1.1	24.3
*u*4418	H(21)...H(37)	652.4(77)	38.1(fixed)	—	–6.4	38.1
*u*4357	H(165)...H(175)	652.5(42)	35.3(fixed)	—	–8.1	35.3
*u*4446	C(7)...H(40)	652.6(28)	24.1(fixed)	—	–0.5	24.1
*u*4313	C(241)...H(277)	652.7(26)	28.4(fixed)	—	0.6	28.4
*u*4368	H(115)...H(136)	652.8(42)	32.5(fixed)	—	2.9	32.5
*u*4466	C(101)...H(135)	652.9(18)	22.9(fixed)	—	–5.4	22.9
*u*4274	H(206)...H(213)	653.2(36)	35.7(fixed)	—	–6.8	35.7
*u*4468	H(262)...H(280)	653.4(34)	30.5(fixed)	—	–4.4	30.5
*u*4490	C(56)...H(92)	653.5(21)	24.4(fixed)	—	–1.3	24.4
*u*4270	C(105)...H(132)	653.5(22)	22.9(fixed)	—	–5.5	22.9
*u*4278	H(164)...H(179)	653.6(24)	31.8(fixed)	—	–0.4	31.8
*u*4398	C(111)...H(119)	653.7(49)	19.4(fixed)	—	–6.6	19.4
*u*4310	C(53)...H(91)	653.7(31)	26.8(fixed)	—	–0.5	26.8
*u*4487	C(10)...H(24)	653.8(13)	24.2(fixed)	—	–1.5	24.2
*u*4509	C(103)...H(131)	653.8(32)	24.7(fixed)	—	–1.6	24.7
*u*4517	C(242)...H(272)	653.9(13)	24.7(fixed)	—	–1.8	24.7
*u*4343	C(107)...H(129)	653.9(17)	24.6(fixed)	—	–0.6	24.6
*u*4438	C(60)...H(70)	653.9(17)	26.6(fixed)	—	–1.5	26.6
*u*4358	C(100)...H(136)	654.0(28)	38.1(fixed)	—	1.5	38.1
*u*4319	C(243)...H(267)	654.1(11)	25.0(fixed)	—	–1.1	25.0
*u*4382	C(53)...H(89)	654.2(27)	26.1(fixed)	—	–0.8	26.1
*u*4390	C(12)...H(35)	654.2(16)	25.8(fixed)	—	–0.9	25.8

*u*4299	H(25)...H(40)	654.2(81)	38.5(fixed)	—	–7.4	38.5
*u*4235	C(194)...H(232)	654.2(30)	26.0(fixed)	—	–0.5	26.0
*u*4397	H(24)...H(41)	654.3(52)	36.0(fixed)	—	–8.6	36.0
*u*4356	C(147)...H(185)	654.3(30)	25.3(fixed)	—	–1.0	25.3
*u*4459	C(64)...H(75)	654.3(19)	31.7(fixed)	—	–1.2	31.7
*u*4460	C(58)...H(84)	654.7(16)	35.3(fixed)	—	1.6	35.3
*u*4320	C(6)...H(44)	654.8(30)	36.8(fixed)	—	2.4	36.8
*u*4527	H(128)...H(131)	654.8(38)	39.1(fixed)	—	–6.1	39.1
*u*4294	C(241)...H(279)	655.2(30)	28.5(fixed)	—	0.5	28.5
*u*4498	C(196)...H(225)	655.3(35)	24.7(fixed)	—	–1.8	24.7
*u*4363	H(213)...H(233)	655.3(28)	30.6(fixed)	—	–3.7	30.6
*u*4285	C(64)...H(72)	655.4(61)	23.1(fixed)	—	–5.6	23.1
*u*4333	C(8)...H(32)	655.4(10)	29.0(fixed)	—	1.2	29.0
*u*4464	H(18)...H(29)	655.4(35)	29.0(fixed)	—	–5.2	29.0
*u*4439	C(17)...H(27)	655.4(53)	23.3(fixed)	—	–6.2	23.3
*u*4297	C(56)...H(94)	655.4(21)	27.2(fixed)	—	–0.8	27.2
*u*4434	C(54)...H(87)	655.5(21)	24.1(fixed)	—	–0.7	24.1
*u*4394	C(150)...H(173)	655.5(8)	28.7(fixed)	—	1.2	28.7
*u*4276	C(110)...H(114)	655.6(31)	27.1(fixed)	—	–0.1	27.1
*u*4525	H(35)...H(37)	655.6(35)	37.2(fixed)	—	0.9	37.2
*u*4178	C(56)...H(66)	655.6(56)	24.6(fixed)	—	–4.9	24.6
*u*4323	C(16)...H(20)	655.7(31)	25.3(fixed)	—	–0.9	25.3
*u*4457	C(149)...H(186)	655.7(9)	24.7(fixed)	—	–0.9	24.7
*u*4269	H(23)...H(38)	655.7(37)	31.7(fixed)	—	–1.9	31.7
*u*4429	C(111)...H(121)	655.7(53)	22.7(fixed)	—	–6.5	22.7
*u*4406	C(59)...H(80)	655.7(10)	25.5(fixed)	—	–1.0	25.5
*u*4327	C(149)...H(188)	655.8(10)	29.4(fixed)	—	–1.1	29.4
*u*4445	C(197)...H(233)	655.8(12)	25.2(fixed)	—	–1.1	25.2
*u*4380	C(13)...H(22)	655.9(14)	27.0(fixed)	—	–0.5	27.0
*u*4427	C(148)...H(180)	655.9(10)	24.7(fixed)	—	–1.1	24.7
*u*4395	C(148)...H(181)	655.9(15)	25.1(fixed)	—	–1.0	25.1
*u*4519	C(104)...H(118)	656.0(13)	24.4(fixed)	—	–1.5	24.4
*u*4385	C(243)...H(266)	656.0(9)	25.1(fixed)	—	–1.5	25.1
*u*4329	C(197)...H(235)	656.2(13)	25.9(fixed)	—	–0.4	25.9
*u*4378	C(59)...H(82)	656.3(11)	26.6(fixed)	—	–1.0	26.6
*u*4417	C(13)...H(23)	656.5(16)	27.9(fixed)	—	–0.8	27.9
*u*4374	H(207)...H(212)	656.6(27)	34.2(fixed)	—	–7.3	34.2
*u*4229	C(100)...H(138)	656.7(30)	33.0(fixed)	—	4.1	33.0
*u*4289	C(63)...H(67)	656.7(30)	25.9(fixed)	—	–0.7	25.9
*u*4443	H(112)...H(121)	656.7(62)	38.4(fixed)	—	–8.2	38.4
*u*4282	C(199)...H(228)	657.0(22)	27.6(fixed)	—	2.7	27.6
*u*4402	H(72)...H(92)	657.1(73)	31.7(fixed)	—	–3.9	31.7
*u*4342	C(64)...H(76)	657.2(27)	26.5(fixed)	—	0.9	26.5
*u*4508	C(199)...H(227)	657.2(9)	32.2(fixed)	—	–1.0	32.2
*u*4345	C(6)...H(42)	657.2(27)	32.3(fixed)	—	3.4	32.3
*u*4471	H(117)...H(135)	657.2(28)	31.6(fixed)	—	–3.6	31.6

*u*4497	H(113)...H(123)	657.3(58)	35.7(fixed)	—	–7.8	35.7
*u*4488	C(107)...H(127)	657.3(11)	24.8(fixed)	—	–1.7	24.8
*u*4505	H(115)...H(134)	657.3(37)	35.6(fixed)	—	–4.8	35.6
*u*4370	H(129)...H(134)	657.3(38)	34.0(fixed)	—	2.1	34.0
*u*4452	C(12)...H(33)	657.3(13)	25.7(fixed)	—	–1.3	25.7
*u*4451	C(54)...H(86)	657.4(13)	28.0(fixed)	—	–1.2	28.0
*u*4322	C(104)...H(120)	657.7(14)	25.4(fixed)	—	–0.3	25.4
*u*4387	C(150)...H(172)	657.7(8)	33.2(fixed)	—	0.3	33.2
*u*4414	C(60)...H(69)	657.7(13)	25.3(fixed)	—	–0.8	25.3
*u*4455	H(65)...H(91)	657.7(42)	35.7(fixed)	—	1.5	35.7
*u*4433	C(102)...H(125)	657.9(10)	23.9(fixed)	—	–1.3	23.9
*u*4256	C(242)...H(271)	657.9(14)	25.3(fixed)	—	–0.7	25.3
*u*4426	H(131)...H(137)	658.0(34)	41.5(fixed)	—	–12.6	41.5
*u*4389	C(7)...H(39)	658.0(14)	29.3(fixed)	—	–1.3	29.3
*u*4436	C(8)...H(31)	658.1(10)	30.2(fixed)	—	–0.2	30.2
*u*4470	C(244)...H(275)	658.2(37)	24.2(fixed)	—	–0.7	24.2
*u*4331	C(10)...H(26)	658.3(14)	26.1(fixed)	—	–0.7	26.1
*u*4437	H(65)...H(71)	658.7(41)	28.7(fixed)	—	–5.7	28.7
*u*4499	C(106)...H(122)	658.7(35)	26.1(fixed)	—	–1.4	26.1
*u*4410	H(113)...H(121)	659.0(85)	40.4(fixed)	—	–8.1	40.4
*u*4566	H(25)...H(43)	659.2(31)	35.4(fixed)	—	–19.6	35.4
*u*4502	C(105)...H(133)	659.3(10)	25.4(fixed)	—	–1.8	25.4
*u*4347	C(152)...H(177)	659.4(11)	25.2(fixed)	—	–0.8	25.2
*u*4555	H(75)...H(92)	659.4(40)	38.9(fixed)	—	1.7	38.9
*u*4491	C(244)...H(274)	659.6(39)	26.1(fixed)	—	–1.4	26.1
*u*4500	H(27)...H(45)	659.6(57)	32.1(fixed)	—	–4.7	32.1
*u*4191	H(66)...H(76)	660.0(76)	32.6(fixed)	—	–0.5	32.6
*u*4360	H(127)...H(132)	660.0(35)	31.1(fixed)	—	–3.8	31.1
*u*4366	H(206)...H(232)	660.1(39)	35.2(fixed)	—	1.6	35.2
*u*4476	H(159)...H(185)	660.1(39)	35.6(fixed)	—	0.6	35.6
*u*4495	H(165)...H(188)	660.3(23)	39.1(fixed)	—	1.0	39.1
*u*4401	C(11)...H(36)	660.6(13)	23.9(fixed)	—	–1.1	23.9
*u*4442	C(196)...H(224)	660.8(40)	24.6(fixed)	—	–1.6	24.6
*u*4556	H(119)...H(137)	661.1(33)	36.3(fixed)	—	–18.3	36.3
*u*4430	C(106)...H(123)	661.2(42)	25.2(fixed)	—	–0.6	25.2
*u*4548	H(257)...H(272)	661.4(19)	34.7(fixed)	—	0.0	34.7
*u*4412	H(18)...H(44)	661.5(39)	40.8(fixed)	—	7.1	40.8
*u*4474	H(121)...H(139)	661.7(57)	30.8(fixed)	—	–4.8	30.8
*u*4392	H(120)...H(126)	661.9(20)	34.1(fixed)	—	1.9	34.1
*u*4391	H(37)...H(46)	662.3(76)	32.9(fixed)	—	–7.1	32.9
*u*4510	H(22)...H(40)	662.7(32)	34.9(fixed)	—	3.1	34.9
*u*4496	H(19)...H(29)	662.9(59)	34.1(fixed)	—	–6.6	34.1
*u*4372	C(58)...H(83)	663.0(11)	32.5(fixed)	—	3.3	32.5
*u*4541	H(134)...H(140)	663.0(31)	31.8(fixed)	—	–6.8	31.8
*u*4565	H(122)...H(131)	663.1(43)	35.7(fixed)	—	0.6	35.7
*u*4514	H(18)...H(27)	663.3(61)	31.5(fixed)	—	–6.8	31.5

*u*4288	H(258)...H(271)	663.6(21)	34.7(fixed)	—	1.6	34.7
*u*4273	H(112)...H(138)	663.8(40)	41.2(fixed)	—	9.6	41.2
*u*4423	C(103)...H(130)	663.9(42)	23.3(fixed)	—	–0.9	23.3
*u*4350	H(253)...H(279)	664.0(39)	39.7(fixed)	—	5.9	39.7
*u*4501	H(164)...H(180)	664.1(14)	38.8(fixed)	—	4.7	38.8
*u*4344	H(76)...H(94)	664.2(48)	37.9(fixed)	—	4.3	37.9
*u*4530	H(70)...H(86)	664.4(27)	38.5(fixed)	—	1.2	38.5
*u*4431	H(19)...H(27)	665.0(85)	40.1(fixed)	—	–6.8	40.1
*u*4521	H(82)...H(84)	665.0(26)	47.3(fixed)	—	6.1	47.3
*u*4558	H(118)...H(125)	665.6(23)	33.9(fixed)	—	0.3	33.9
*u*4596	H(24)...H(43)	666.1(27)	32.9(fixed)	—	–17.3	32.9
*u*4543	H(24)...H(31)	666.1(21)	36.7(fixed)	—	2.9	36.7
*u*4393	H(114)...H(136)	666.3(43)	49.5(fixed)	—	6.7	49.5
*u*4415	H(67)...H(89)	666.4(44)	36.8(fixed)	—	1.7	36.8
*u*4603	H(72)...H(85)	666.4(18)	36.4(fixed)	—	–20.9	36.4
*u*4515	H(69)...H(87)	666.4(31)	34.5(fixed)	—	2.2	34.5
*u*4302	H(217)...H(235)	667.0(32)	38.6(fixed)	—	7.4	38.6
*u*4552	H(216)...H(233)	667.1(18)	39.3(fixed)	—	3.3	39.3
*u*4540	H(212)...H(224)	667.3(50)	34.4(fixed)	—	0.3	34.4
*u*4369	H(26)...H(32)	667.3(20)	39.7(fixed)	—	5.0	39.7
*u*4578	H(77)...H(85)	667.3(31)	35.8(fixed)	—	–14.5	35.8
*u*4473	H(163)...H(181)	667.4(18)	39.8(fixed)	—	4.2	39.8
*u*4539	H(263)...H(275)	667.8(47)	34.9(fixed)	—	1.7	34.9
*u*4507	H(167)...H(186)	667.9(15)	34.1(fixed)	—	1.9	34.1
*u*4583	H(162)...H(166)	668.2(29)	32.9(fixed)	—	–13.6	32.9
*u*4493	H(23)...H(39)	668.6(36)	41.0(fixed)	—	2.1	41.0
*u*4551	H(62)...H(77)	668.8(21)	19.3(fixed)	—	–10.1	19.3
*u*4383	H(66)...H(71)	668.9(78)	34.1(fixed)	—	–7.0	34.1
*u*4571	H(30)...H(38)	669.4(30)	33.8(fixed)	—	–13.3	33.8
*u*4404	H(20)...H(42)	669.7(42)	42.9(fixed)	—	7.6	42.9
*u*4572	H(127)...H(133)	670.0(19)	35.8(fixed)	—	0.0	35.8
*u*4300	H(65)...H(72)	670.2(63)	32.7(fixed)	—	–6.1	32.7
*u*4538	H(75)...H(94)	670.3(29)	44.9(fixed)	—	–0.1	44.9
*u*4581	H(30)...H(37)	670.4(43)	30.9(fixed)	—	–11.6	30.9
*u*4650	H(71)...H(85)	670.4(40)	32.6(fixed)	—	–18.1	32.6
*u*4545	H(108)...H(115)	671.2(21)	17.7(fixed)	—	–5.3	17.7
*u*4577	H(120)...H(137)	671.3(16)	30.0(fixed)	—	–17.5	30.0
*u*4594	H(118)...H(137)	671.5(27)	32.9(fixed)	—	–16.5	32.9
*u*4526	H(33)...H(36)	671.6(32)	35.1(fixed)	—	1.3	35.1
*u*4309	H(208)...H(232)	672.0(36)	37.8(fixed)	—	0.8	37.8
*u*4588	H(26)...H(43)	672.1(17)	30.3(fixed)	—	–19.2	30.3
*u*4523	H(161)...H(185)	672.1(36)	35.4(fixed)	—	0.1	35.4
*u*4591	H(77)...H(84)	672.1(21)	32.7(fixed)	—	–13.8	32.7
*u*4145	H(66)...H(72)	672.4(88)	42.1(fixed)	—	–5.6	42.1
*u*4595	H(162)...H(165)	672.7(19)	30.3(fixed)	—	–12.2	30.3
*u*4576	H(66)...H(88)	672.7(28)	29.7(fixed)	—	–6.6	29.7

*u*4506	H(255)...H(279)	672.9(36)	44.6(fixed)	—	2.2	44.6
*u*4544	H(14)...H(27)	673.1(25)	18.0(fixed)	—	–6.2	18.0
*u*4579	H(19)...H(41)	673.3(22)	28.8(fixed)	—	–7.1	28.8
*u*4547	H(202)...H(209)	673.6(23)	17.8(fixed)	—	–6.1	17.8
*u*4553	H(249)...H(269)	673.6(21)	17.8(fixed)	—	–5.6	17.8
*u*4542	H(61)...H(72)	673.9(24)	18.2(fixed)	—	–5.7	18.2
*u*4516	H(20)...H(44)	673.9(37)	51.5(fixed)	—	3.1	51.5
*u*4462	H(67)...H(91)	674.1(37)	38.1(fixed)	—	0.7	38.1
*u*4472	H(80)...H(83)	674.1(16)	38.6(fixed)	—	8.6	38.6
*u*4557	H(163)...H(180)	675.1(13)	45.6(fixed)	—	0.7	45.6
*u*4574	H(216)...H(235)	675.3(14)	45.8(fixed)	—	–0.3	45.8
*u*4513	H(123)...H(130)	676.0(59)	34.0(fixed)	—	2.2	34.0
*u*4619	H(19)...H(40)	676.0(44)	27.8(fixed)	—	–6.0	27.8
*u*4564	H(212)...H(229)	676.1(29)	35.7(fixed)	—	–12.2	35.7
*u*4561	H(254)...H(273)	676.1(27)	30.5(fixed)	—	–10.8	30.5
*u*4535	H(22)...H(39)	676.1(14)	42.5(fixed)	—	0.3	42.5
*u*4563	H(129)...H(133)	676.2(16)	36.2(fixed)	—	–0.3	36.2
*u*4537	H(213)...H(229)	676.4(25)	37.5(fixed)	—	–13.7	37.5
*u*4399	H(114)...H(138)	676.4(37)	48.0(fixed)	—	5.5	48.0
*u*4479	H(257)...H(271)	676.5(13)	36.2(fixed)	—	–0.1	36.2
*u*4703	H(115)...H(132)	676.6(40)	26.0(fixed)	—	–7.3	26.0
*u*4559	H(124)...H(135)	676.8(31)	29.5(fixed)	—	–6.7	29.5
*u*4618	H(27)...H(38)	676.9(34)	31.4(fixed)	—	–7.3	31.4
*u*4584	H(209)...H(215)	677.0(29)	30.8(fixed)	—	–6.2	30.8
*u*4534	H(135)...H(137)	677.0(31)	46.1(fixed)	—	–17.6	46.1
*u*4546	H(109)...H(140)	677.3(29)	17.8(fixed)	—	–5.6	17.8
*u*4560	H(69)...H(86)	677.3(14)	39.1(fixed)	—	0.0	39.1
*u*4695	H(38)...H(43)	677.4(54)	41.6(fixed)	—	–19.1	41.6
*u*4606	H(77)...H(83)	677.5(13)	29.9(fixed)	—	–16.0	29.9
*u*4673	H(90)...H(93)	677.5(30)	26.0(fixed)	—	–7.3	26.0
*u*4602	H(66)...H(87)	677.6(27)	28.3(fixed)	—	–6.6	28.3
*u*4549	H(15)...H(46)	677.7(29)	17.9(fixed)	—	–5.5	17.9
*u*4533	H(35)...H(36)	677.9(15)	35.5(fixed)	—	0.4	35.5
*u*4483	H(167)...H(188)	678.0(14)	40.4(fixed)	—	0.4	40.4
*u*4550	H(121)...H(135)	678.2(27)	29.3(fixed)	—	–6.1	29.3
*u*4536	H(26)...H(31)	678.3(13)	43.6(fixed)	—	1.0	43.6
*u*4637	H(73)...H(85)	678.5(39)	30.9(fixed)	—	–20.1	30.9
*u*4531	H(120)...H(125)	678.6(13)	35.8(fixed)	—	0.4	35.8
*u*4562	H(124)...H(134)	678.6(22)	29.2(fixed)	—	–5.6	29.2
*u*4592	H(263)...H(274)	678.8(51)	38.6(fixed)	—	–1.3	38.6
*u*4580	H(160)...H(182)	679.3(24)	28.5(fixed)	—	–6.2	28.5
*u*4730	H(66)...H(77)	679.6(38)	37.0(fixed)	—	–15.7	37.0
*u*4585	H(112)...H(136)	680.1(34)	48.3(fixed)	—	–1.7	48.3
*u*4682	H(117)...H(132)	680.1(19)	25.2(fixed)	—	–6.4	25.2
*u*4658	H(65)...H(81)	680.1(29)	26.3(fixed)	—	–6.8	26.3
*u*4692	H(137)...H(140)	680.1(25)	26.5(fixed)	—	–8.0	26.5

*u*4617	H(162)...H(167)	680.4(12)	27.4(fixed)	—	–13.3	27.4
*u*4664	H(43)...H(46)	680.4(24)	25.7(fixed)	—	–6.2	25.7
*u*4610	H(209)...H(217)	680.8(16)	29.0(fixed)	—	–7.7	29.0
*u*4604	H(34)...H(41)	680.8(48)	26.7(fixed)	—	–7.1	26.7
*u*4554	H(214)...H(224)	680.8(51)	35.7(fixed)	—	–0.6	35.7
*u*4659	H(89)...H(93)	681.0(27)	24.9(fixed)	—	–6.6	24.9
*u*4607	H(254)...H(272)	681.3(22)	27.2(fixed)	—	–10.1	27.2
*u*4654	H(66)...H(81)	681.4(25)	26.8(fixed)	—	–8.1	26.8
*u*4528	H(82)...H(83)	681.4(14)	48.7(fixed)	—	4.6	48.7
*u*4624	H(206)...H(230)	682.1(34)	32.2(fixed)	—	–2.1	32.2
*u*4633	H(159)...H(183)	682.1(33)	31.7(fixed)	—	–2.9	31.7
*u*4712	H(72)...H(77)	682.2(42)	26.3(fixed)	—	–7.7	26.3
*u*4567	H(122)...H(130)	682.4(48)	36.2(fixed)	—	–0.1	36.2
*u*4575	H(253)...H(277)	682.7(34)	41.2(fixed)	—	–0.7	41.2
*u*4635	H(159)...H(175)	682.7(20)	26.2(fixed)	—	–7.4	26.2
*u*4656	H(29)...H(38)	682.7(41)	29.3(fixed)	—	–6.5	29.3
*u*4622	H(81)...H(88)	682.9(41)	27.8(fixed)	—	–7.6	27.8
*u*4720	H(19)...H(30)	683.0(29)	33.3(fixed)	—	–12.9	33.3
*u*4665	H(19)...H(34)	683.0(23)	27.3(fixed)	—	–8.2	27.3
*u*4587	H(18)...H(42)	683.0(33)	41.7(fixed)	—	–0.3	41.7
*u*4640	H(18)...H(34)	683.0(19)	27.1(fixed)	—	–7.1	27.1
*u*4625	H(65)...H(89)	683.2(32)	32.5(fixed)	—	–2.2	32.5
*u*4694	H(72)...H(79)	683.2(36)	24.7(fixed)	—	–5.7	24.7
*u*4626	H(168)...H(187)	683.4(41)	27.6(fixed)	—	–7.5	27.6
*u*4621	H(209)...H(216)	683.4(19)	24.7(fixed)	—	–8.4	24.7
*u*4675	H(33)...H(37)	683.5(13)	33.5(fixed)	—	–3.1	33.5
*u*4709	H(260)...H(281)	683.8(34)	26.3(fixed)	—	–7.3	26.3
*u*4638	H(160)...H(175)	684.0(26)	26.1(fixed)	—	–7.9	26.1
*u*4655	H(80)...H(84)	684.1(13)	44.5(fixed)	—	–2.3	44.5
*u*4616	H(30)...H(36)	684.2(23)	27.7(fixed)	—	–12.5	27.7
*u*4570	H(254)...H(271)	684.3(16)	26.8(fixed)	—	–10.4	26.8
*u*4611	H(160)...H(181)	684.4(20)	27.6(fixed)	—	–6.5	27.6
*u*4641	H(41)...H(46)	684.4(51)	37.8(fixed)	—	–8.1	37.8
*u*4568	H(123)...H(135)	684.4(40)	28.6(fixed)	—	–5.7	28.6
*u*4661	H(258)...H(272)	684.4(12)	31.7(fixed)	—	–2.7	31.7
*u*4693	H(113)...H(128)	684.6(27)	26.3(fixed)	—	–7.5	26.3
*u*4685	H(165)...H(186)	684.6(13)	32.3(fixed)	—	–2.6	32.3
*u*4683	H(136)...H(140)	684.7(22)	25.9(fixed)	—	–7.1	25.9
*u*4600	H(66)...H(86)	684.7(17)	23.4(fixed)	—	–7.2	23.4
*u*4672	H(118)...H(126)	684.8(12)	31.1(fixed)	—	–2.7	31.1
*u*4627	H(44)...H(46)	684.9(35)	23.9(fixed)	—	–6.3	23.9
*u*4628	H(138)...H(140)	684.9(37)	24.4(fixed)	—	–6.0	24.4
*u*4620	H(33)...H(41)	685.0(31)	26.5(fixed)	—	–7.0	26.5
*u*4660	H(42)...H(46)	685.0(20)	24.7(fixed)	—	–5.5	24.7
*u*4681	H(112)...H(128)	685.1(23)	25.5(fixed)	—	–6.7	25.5
*u*4639	H(35)...H(41)	685.3(35)	23.5(fixed)	—	–7.5	23.5

*u*4644	H(91)...H(93)	685.3(35)	23.8(fixed)	—	–6.9	23.8
*u*4629	H(24)...H(32)	685.3(12)	37.0(fixed)	—	–1.5	37.0
*u*4623	H(127)...H(134)	685.3(15)	31.9(fixed)	—	–2.6	31.9
*u*4678	H(206)...H(222)	685.5(25)	25.6(fixed)	—	–6.7	25.6
*u*4636	H(76)...H(92)	685.6(19)	33.6(fixed)	—	–1.0	33.6
*u*4691	H(207)...H(222)	685.6(28)	26.0(fixed)	—	–7.8	26.0
*u*4630	H(27)...H(30)	685.6(42)	27.5(fixed)	—	–7.0	27.5
*u*4684	H(116)...H(132)	685.7(29)	23.5(fixed)	—	–6.8	23.5
*u*4699	H(209)...H(226)	685.9(28)	27.2(fixed)	—	–8.0	27.2
*u*4608	H(160)...H(180)	686.0(17)	23.8(fixed)	—	–6.7	23.8
*u*4671	H(253)...H(269)	686.3(28)	24.9(fixed)	—	–6.4	24.9
*u*4601	H(164)...H(181)	686.3(11)	38.1(fixed)	—	–1.1	38.1
*u*4614	H(27)...H(32)	686.4(29)	26.6(fixed)	—	–6.0	26.6
*u*4613	H(80)...H(88)	686.5(18)	26.9(fixed)	—	–6.9	26.9
*u*4589	H(214)...H(229)	686.5(35)	29.6(fixed)	—	–14.7	29.6
*u*4687	H(254)...H(269)	686.6(29)	26.2(fixed)	—	–7.1	26.2
*u*4598	H(19)...H(39)	686.6(23)	23.6(fixed)	—	–7.2	23.6
*u*4605	H(121)...H(124)	686.6(40)	28.1(fixed)	—	–7.8	28.1
*u*4698	H(212)...H(225)	686.7(42)	31.6(fixed)	—	–3.3	31.6
*u*4643	H(70)...H(87)	686.8(11)	32.8(fixed)	—	–2.3	32.8
*u*4646	H(23)...H(40)	686.8(11)	34.3(fixed)	—	–1.8	34.3
*u*4653	H(28)...H(38)	686.8(29)	24.5(fixed)	—	–7.2	24.5
*u*4648	H(82)...H(88)	686.9(35)	24.2(fixed)	—	–8.0	24.2
*u*4612	H(122)...H(135)	687.1(29)	23.4(fixed)	—	–7.2	23.4
*u*4676	H(211)...H(226)	687.1(18)	26.2(fixed)	—	–6.6	26.2
*u*4669	H(260)...H(282)	687.3(33)	23.9(fixed)	—	–6.4	23.9
*u*4590	H(121)...H(126)	687.3(29)	27.7(fixed)	—	–6.8	27.7
*u*4634	H(168)...H(186)	687.5(16)	26.6(fixed)	—	–5.9	26.6
*u*4582	H(217)...H(233)	687.5(13)	38.1(fixed)	—	0.1	38.1
*u*4642	H(168)...H(188)	687.8(34)	24.5(fixed)	—	–7.3	24.5
*u*4704	H(260)...H(280)	688.0(20)	25.0(fixed)	—	–6.6	25.0
*u*4674	H(114)...H(128)	688.7(34)	23.5(fixed)	—	–7.1	23.5
*u*4657	H(256)...H(276)	689.0(38)	27.1(fixed)	—	–7.2	27.1
*u*4670	H(20)...H(34)	689.2(33)	24.0(fixed)	—	–7.6	24.0
*u*4788	H(74)...H(77)	689.5(50)	38.1(fixed)	—	–13.6	38.1
*u*4679	H(68)...H(85)	689.5(35)	45.6(fixed)	—	–19.2	45.6
*u*4632	H(124)...H(133)	689.6(19)	23.2(fixed)	—	–7.0	23.2
*u*4686	H(123)...H(131)	689.8(41)	32.6(fixed)	—	–2.5	32.6
*u*4609	H(258)...H(276)	689.8(25)	26.9(fixed)	—	–6.3	26.9
*u*4647	H(208)...H(222)	690.0(35)	24.0(fixed)	—	–7.3	24.0
*u*4666	H(121)...H(125)	690.2(24)	23.8(fixed)	—	–7.8	23.8
*u*4744	H(113)...H(124)	690.3(32)	29.4(fixed)	—	–7.0	29.4
*u*4662	H(264)...H(275)	690.3(42)	32.1(fixed)	—	–1.4	32.1
*u*4652	H(161)...H(175)	690.3(34)	24.1(fixed)	—	–7.5	24.1
*u*4663	H(27)...H(31)	690.4(22)	23.8(fixed)	—	–7.5	23.8
*u*4651	H(255)...H(269)	690.5(35)	23.9(fixed)	—	–6.7	23.9

*u*4645	H(67)...H(81)	690.6(33)	24.1(fixed)	—	–7.2	24.1
*u*4597	H(88)...H(93)	690.8(45)	38.0(fixed)	—	–8.0	38.0
*u*4677	H(257)...H(276)	691.0(23)	23.6(fixed)	—	–7.4	23.6
*u*4696	H(210)...H(226)	691.1(20)	24.0(fixed)	—	–6.9	24.0
*u*4649	H(133)...H(137)	691.2(18)	33.3(fixed)	—	–18.4	33.3
*u*4689	H(72)...H(78)	691.6(22)	24.4(fixed)	—	–6.4	24.4
*u*4710	H(160)...H(171)	691.6(17)	36.2(fixed)	—	–13.5	36.2
*u*4725	H(25)...H(34)	692.1(23)	32.2(fixed)	—	–8.7	32.2
*u*4793	H(72)...H(88)	692.2(50)	32.5(fixed)	—	–8.9	32.5
*u*4707	H(85)...H(90)	692.5(38)	37.3(fixed)	—	–11.1	37.3
*u*4586	H(68)...H(74)	692.5(89)	30.7(fixed)	—	–7.4	30.7
*u*4726	H(36)...H(43)	693.0(40)	31.6(fixed)	—	–18.2	31.6
*u*4599	H(68)...H(76)	693.3(60)	28.6(fixed)	—	–6.2	28.6
*u*4667	H(119)...H(132)	693.5(28)	33.4(fixed)	—	–7.6	33.4
*u*4735	H(67)...H(77)	693.6(29)	28.6(fixed)	—	–14.8	28.6
*u*4722	H(21)...H(43)	693.9(18)	38.0(fixed)	—	–12.1	38.0
*u*4631	H(68)...H(75)	694.6(57)	24.7(fixed)	—	–8.1	24.7
*u*4723	H(119)...H(128)	694.8(24)	31.6(fixed)	—	–8.3	31.6
*u*4753	H(115)...H(137)	695.0(21)	33.5(fixed)	—	–10.4	33.5
*u*4573	H(207)...H(215)	695.5(27)	37.8(fixed)	—	–6.9	37.8
*u*4743	H(260)...H(269)	695.9(26)	30.4(fixed)	—	–7.9	30.4
*u*4615	H(168)...H(175)	696.4(19)	38.0(fixed)	—	–8.0	38.0
*u*4721	H(160)...H(166)	696.8(37)	30.4(fixed)	—	–7.3	30.4
*u*4741	H(20)...H(30)	696.9(20)	27.0(fixed)	—	–12.2	27.0
*u*4702	H(25)...H(45)	697.0(48)	25.8(fixed)	—	–7.0	25.8
*u*4777	H(207)...H(218)	697.8(17)	30.3(fixed)	—	–8.0	30.3
*u*4690	H(27)...H(41)	697.8(60)	39.1(fixed)	—	–9.0	39.1
*u*4680	H(119)...H(141)	697.9(41)	24.6(fixed)	—	–7.4	24.6
*u*4769	H(209)...H(229)	698.0(22)	32.4(fixed)	—	–15.9	32.4
*u*4729	H(254)...H(265)	698.1(17)	31.1(fixed)	—	–7.7	31.1
*u*4668	H(25)...H(47)	698.6(41)	24.7(fixed)	—	–7.3	24.7
*u*4717	H(69)...H(85)	699.2(23)	33.9(fixed)	—	–18.8	33.9
*u*4714	H(39)...H(46)	699.4(40)	27.5(fixed)	—	–8.8	27.5
*u*4734	H(68)...H(90)	699.5(29)	31.9(fixed)	—	–8.0	31.9
*u*4697	H(119)...H(139)	699.9(46)	25.3(fixed)	—	–7.1	25.3
*u*4705	H(25)...H(46)	700.4(68)	26.8(fixed)	—	–8.2	26.8
*u*4800	H(74)...H(78)	700.7(29)	34.8(fixed)	—	–13.6	34.8
*u*4732	H(161)...H(171)	701.1(18)	28.4(fixed)	—	–13.1	28.4
*u*4752	H(21)...H(44)	701.4(18)	35.7(fixed)	—	–13.9	35.7
*u*4797	H(262)...H(281)	701.9(26)	30.4(fixed)	—	–8.3	30.4
*u*4724	H(207)...H(216)	702.4(12)	30.4(fixed)	—	–12.2	30.4
*u*4757	H(114)...H(124)	702.7(21)	26.4(fixed)	—	–7.4	26.4
*u*4706	H(119)...H(140)	702.7(67)	26.2(fixed)	—	–8.3	26.2
*u*4569	H(260)...H(276)	703.0(34)	34.6(fixed)	—	–7.1	34.6
*u*4736	H(83)...H(90)	703.6(18)	34.6(fixed)	—	–12.5	34.6
*u*4688	H(162)...H(179)	703.7(30)	34.7(fixed)	—	–8.9	34.7

*u*4715	H(86)...H(93)	703.9(29)	28.4(fixed)	—	–9.3	28.4
*u*4733	H(115)...H(138)	705.5(21)	32.0(fixed)	—	–9.5	32.0
*u*4780	C(6)...H(43)	705.7(14)	16.9(tied to *u*4766)	—	–11.4	18.2
*u*4711	H(213)...H(234)	706.0(26)	30.9(fixed)	—	–7.5	30.9
*u*4776	C(100)...H(137)	706.1(14)	17.3(tied to *u*4766)	—	–11.4	18.7
*u*4755	H(255)...H(265)	706.4(18)	27.4(fixed)	—	–8.4	27.4
*u*4751	H(26)...H(34)	706.7(15)	26.4(fixed)	—	–8.7	26.4
*u*4767	H(210)...H(229)	706.7(13)	27.6(fixed)	—	–14.1	27.6
*u*4739	H(208)...H(218)	706.9(18)	26.1(fixed)	—	–7.8	26.1
*u*4798	H(73)...H(88)	707.0(42)	27.8(fixed)	—	–9.0	27.8
*u*4716	H(119)...H(130)	707.2(31)	26.7(fixed)	—	–8.4	26.7
*u*4770	C(58)...H(85)	707.3(5)	17.4(tied to *u*4766)	—	–11.6	18.7
*u*4718	H(169)...H(175)	707.4(15)	28.5(fixed)	—	–9.2	28.5
*u*4742	H(68)...H(91)	708.4(22)	26.6(fixed)	—	–7.9	26.6
*u*4754	H(28)...H(41)	709.1(45)	28.9(fixed)	—	–9.6	28.9
*u*4728	H(163)...H(179)	709.2(16)	31.5(fixed)	—	–10.6	31.5
*u*4738	H(160)...H(167)	709.2(18)	26.5(fixed)	—	–7.2	26.5
*u*4746	H(120)...H(128)	709.2(14)	26.3(fixed)	—	–8.1	26.3
*u*4700	H(21)...H(38)	709.5(48)	31.3(fixed)	—	–7.6	31.3
*u*4745	H(261)...H(269)	709.5(16)	25.1(fixed)	—	–7.7	25.1
*u*4756	C(199)...H(229)	710.7(5)	16.6(tied to *u*4766)	—	–8.4	17.8
*u*4785	C(53)...H(90)	711.2(15)	14.9(tied to *u*4766)	—	–5.7	16.0
*u*4795	H(262)...H(282)	711.6(15)	25.8(fixed)	—	–7.9	25.8
*u*4804	H(115)...H(135)	711.8(23)	30.4(fixed)	—	–7.7	30.4
*u*4794	C(8)...H(30)	711.8(8)	15.6(tied to *u*4766)	—	–8.1	16.8
*u*4790	C(13)...H(21)	712.0(15)	15.1(tied to *u*4766)	—	–6.7	16.3
*u*4762	C(7)...H(41)	712.1(6)	15.2(tied to *u*4766)	—	–6.3	16.3
*u*4708	H(128)...H(132)	712.1(28)	30.8(fixed)	—	–7.4	30.8
*u*4778	C(241)...H(278)	712.1(16)	15.0(tied to *u*4766)	—	–6.9	16.1
*u*4771	C(110)...H(113)	712.2(14)	14.7(tied to *u*4766)	—	–6.0	15.9
*u*4701	H(260)...H(274)	712.4(37)	26.3(fixed)	—	–8.7	26.3
*u*4760	C(54)...H(88)	712.4(5)	15.3(tied to *u*4766)	—	–6.0	16.4
*u*4789	C(12)...H(34)	712.6(13)	15.1(tied to *u*4766)	—	–6.0	16.2
*u*4784	C(150)...H(171)	712.6(9)	15.4(tied to *u*4766)	—	–8.6	16.6
*u*4775	C(63)...H(66)	712.8(14)	14.8(tied to *u*4766)	—	–5.0	15.9
*u*4758	C(10)...H(25)	713.1(6)	15.3(tied to *u*4766)	—	–5.4	16.4
*u*4772	C(16)...H(19)	713.1(14)	15.7(fixed)	—	–4.8	15.7
*u*4768	C(11)...H(38)	713.1(7)	15.0(tied to *u*4766)	—	–5.5	16.1
*u*4747	C(107)...H(128)	713.2(12)	15.4(tied to *u*4766)	—	–5.3	16.6
*u*4782	C(152)...H(179)	713.3(5)	15.0(tied to *u*4766)	—	–5.6	16.2
*u*4750	C(104)...H(119)	713.3(7)	15.4(tied to *u*4766)	—	–5.4	16.6
*u*4737	H(213)...H(235)	713.3(13)	25.9(fixed)	—	–7.8	25.9
*u*4748	C(105)...H(135)	713.4(5)	15.2(tied to *u*4766)	—	–5.3	16.4
*u*4791	C(149)...H(187)	713.5(8)	15.1(tied to *u*4766)	—	–6.1	16.2
*u*4781	C(147)...H(184)	713.5(15)	16.0(fixed)	—	–5.0	16.0
*u*4779	C(60)...H(68)	713.8(10)	14.9(tied to *u*4766)	—	–5.7	16.1

*u*4774	C(194)...H(231)	713.9(15)	15.7(fixed)	—	–5.0	15.7
*u*4765	C(106)...H(121)	714.0(19)	15.2(tied to *u*4766)	—	–5.8	16.3
*u*4796	C(59)...H(81)	714.1(8)	14.7(tied to *u*4766)	—	–5.6	15.8
*u*4727	H(22)...H(38)	714.4(25)	26.8(fixed)	—	–8.0	26.8
*u*4773	C(197)...H(234)	714.4(10)	14.9(tied to *u*4766)	—	–5.4	16.0
*u*4593	H(66)...H(74)	714.6(71)	37.7(fixed)	—	–7.7	37.7
*u*4761	C(148)...H(182)	714.7(6)	14.8(tied to *u*4766)	—	–5.2	15.9
*u*4749	C(242)...H(273)	714.9(6)	15.7(tied to *u*4766)	—	–5.2	16.9
*u*4801	H(121)...H(140)	715.0(69)	31.1(fixed)	—	–9.0	31.1
*u*4803	H(27)...H(46)	715.4(69)	31.3(fixed)	—	–8.6	31.3
*u*4766	C(64)...H(74)	715.5(18)	15.6(14)	16.8(17)	–7.5	16.8
*u*4759	C(103)...H(132)	715.7(21)	15.1(tied to *u*4766)	—	–5.1	16.3
*u*4783	C(196)...H(226)	715.8(20)	14.9(tied to *u*4766)	—	–5.4	16.1
*u*4786	C(102)...H(124)	715.9(8)	14.5(tied to *u*4766)	—	–4.7	15.6
*u*4713	H(66)...H(75)	716.1(38)	29.1(fixed)	—	–9.5	29.1
*u*4719	H(72)...H(93)	716.2(78)	31.5(fixed)	—	–7.9	31.5
*u*4764	C(244)...H(276)	716.3(22)	15.1(tied to *u*4766)	—	–5.5	16.2
*u*4792	C(243)...H(265)	716.3(8)	14.5(tied to *u*4766)	—	–5.1	15.6
*u*4740	H(129)...H(132)	716.5(15)	25.6(fixed)	—	–7.8	25.6
*u*4802	H(116)...H(135)	716.5(14)	26.1(fixed)	—	–7.3	26.1
*u*4799	H(121)...H(141)	717.9(37)	26.6(fixed)	—	–8.6	26.6
*u*4731	H(72)...H(94)	718.1(42)	26.0(fixed)	—	–7.8	26.0
*u*4787	H(27)...H(47)	718.2(37)	25.9(fixed)	—	–8.1	25.9
*u*4763	C(56)...H(93)	718.5(17)	15.3(tied to *u*4766)	—	–5.6	16.4
*u*4817	H(18)...H(43)	723.7(18)	29.1(fixed)	—	–11.0	29.1
*u*4811	H(112)...H(137)	725.3(19)	31.0(fixed)	—	–10.1	31.0
*u*4834	H(34)...H(37)	727.9(38)	28.8(fixed)	—	–5.7	28.8
*u*4830	H(65)...H(90)	728.8(26)	27.1(fixed)	—	–5.2	27.1
*u*4805	H(128)...H(134)	730.6(31)	28.1(fixed)	—	–4.2	28.1
*u*4815	H(80)...H(85)	730.7(17)	30.6(fixed)	—	–10.6	30.6
*u*4839	H(21)...H(40)	731.8(41)	26.6(fixed)	—	–5.2	26.6
*u*4849	H(121)...H(131)	732.1(27)	26.1(fixed)	—	–5.6	26.1
*u*4835	H(165)...H(187)	732.7(18)	27.8(fixed)	—	–5.6	27.8
*u*4864	H(24)...H(30)	732.7(16)	26.2(fixed)	—	–7.9	26.2
*u*4821	H(159)...H(184)	733.2(18)	27.6(fixed)	—	–4.7	27.6
*u*4807	H(119)...H(126)	733.2(17)	27.6(fixed)	—	–4.6	27.6
*u*4814	H(253)...H(278)	733.3(19)	28.9(fixed)	—	–5.0	28.9
*u*4823	H(70)...H(88)	733.6(24)	28.1(fixed)	—	–5.6	28.1
*u*4843	H(215)...H(233)	733.7(19)	26.2(fixed)	—	–8.5	26.2
*u*4824	H(206)...H(231)	734.1(19)	26.8(fixed)	—	–4.3	26.8
*u*4858	H(74)...H(92)	734.5(32)	26.1(fixed)	—	–7.0	26.1
*u*4829	H(162)...H(181)	735.2(21)	27.6(fixed)	—	–8.1	27.6
*u*4836	H(212)...H(226)	735.5(25)	26.8(fixed)	—	–4.9	26.8
*u*4859	H(82)...H(85)	735.5(10)	29.1(fixed)	—	–14.2	29.1
*u*4808	H(25)...H(32)	736.2(14)	29.3(fixed)	—	–2.2	29.3
*u*4806	H(258)...H(273)	736.3(14)	28.3(fixed)	—	–4.3	28.3

*u*4816	H(66)...H(89)	736.5(22)	27.7(fixed)	—	–4.0	27.7
*u*4828	H(68)...H(87)	736.5(27)	26.1(fixed)	—	–4.4	26.1
*u*4852	H(20)...H(43)	736.6(24)	27.9(fixed)	—	–13.6	27.9
*u*4819	H(23)...H(41)	736.6(18)	28.8(fixed)	—	–5.0	28.8
*u*4841	H(114)...H(137)	736.6(25)	29.7(fixed)	—	–12.8	29.7
*u*4842	H(81)...H(84)	737.0(18)	32.6(fixed)	—	–1.7	32.6
*u*4827	H(113)...H(136)	737.1(23)	35.5(fixed)	—	–2.6	35.5
*u*4833	H(166)...H(186)	737.1(15)	27.2(fixed)	—	–4.3	27.2
*u*4820	H(164)...H(182)	737.2(12)	28.0(fixed)	—	–2.3	28.0
*u*4872	H(256)...H(272)	737.3(17)	25.7(fixed)	—	–5.0	25.7
*u*4809	H(217)...H(234)	738.6(26)	27.4(fixed)	—	–1.4	27.4
*u*4837	H(262)...H(275)	738.9(31)	25.8(fixed)	—	–4.7	25.8
*u*4848	H(127)...H(135)	739.1(19)	25.7(fixed)	—	–5.2	25.7
*u*4825	H(33)...H(38)	739.2(17)	27.5(fixed)	—	–4.5	27.5
*u*4867	H(118)...H(124)	739.6(15)	25.6(fixed)	—	–4.4	25.6
*u*4832	H(215)...H(235)	739.8(11)	28.3(fixed)	—	–9.4	28.3
*u*4813	H(19)...H(42)	740.9(21)	30.2(fixed)	—	0.4	30.2
*u*4871	H(162)...H(180)	741.0(11)	26.1(fixed)	—	–10.0	26.1
*u*4810	H(76)...H(93)	741.5(34)	28.2(fixed)	—	–2.7	28.2
*u*4812	H(123)...H(132)	742.0(37)	27.3(fixed)	—	–3.6	27.3
*u*4838	H(129)...H(135)	742.1(15)	25.3(fixed)	—	–5.3	25.3
*u*4847	H(254)...H(279)	742.3(25)	28.6(fixed)	—	–6.9	28.6
*u*4860	H(35)...H(38)	742.4(14)	25.7(fixed)	—	–5.6	25.7
*u*4854	H(22)...H(41)	742.8(12)	27.1(fixed)	—	–6.3	27.1
*u*4831	H(74)...H(94)	743.0(13)	27.8(fixed)	—	–8.1	27.8
*u*4844	H(66)...H(91)	743.3(25)	26.8(fixed)	—	–5.0	26.8
*u*4845	H(166)...H(188)	743.4(9)	28.9(fixed)	—	–6.2	28.9
*u*4851	H(19)...H(44)	743.6(24)	35.1(fixed)	—	–3.3	35.1
*u*4850	H(26)...H(30)	743.6(15)	27.2(fixed)	—	–8.9	27.2
*u*4818	H(113)...H(138)	744.2(25)	32.1(fixed)	—	–2.9	32.1
*u*4822	H(207)...H(232)	744.3(25)	26.3(fixed)	—	–5.2	26.3
*u*4857	H(257)...H(273)	744.6(9)	25.6(fixed)	—	–6.1	25.6
*u*4856	H(160)...H(185)	744.6(25)	25.4(fixed)	—	–5.2	25.4
*u*4861	H(69)...H(88)	744.7(11)	25.7(fixed)	—	–6.3	25.7
*u*4875	H(75)...H(93)	744.8(16)	30.9(fixed)	—	–6.6	30.9
*u*4865	H(21)...H(39)	744.8(14)	28.8(fixed)	—	–7.7	28.8
*u*4878	H(216)...H(234)	745.0(10)	31.1(fixed)	—	–6.7	31.1
*u*4840	H(67)...H(90)	745.0(24)	26.1(fixed)	—	–6.0	26.1
*u*4870	H(25)...H(31)	745.1(9)	29.7(fixed)	—	–5.7	29.7
*u*4866	H(119)...H(125)	745.1(10)	24.6(fixed)	—	–6.3	24.6
*u*4873	H(68)...H(86)	745.6(13)	27.6(fixed)	—	–6.3	27.6
*u*4855	H(163)...H(182)	745.7(7)	32.0(fixed)	—	–5.0	32.0
*u*4876	H(122)...H(132)	746.2(28)	26.1(fixed)	—	–6.0	26.1
*u*4846	H(120)...H(124)	747.1(16)	25.6(fixed)	—	–4.4	25.6
*u*4853	H(167)...H(187)	747.2(12)	25.7(fixed)	—	–6.3	25.7
*u*4874	H(262)...H(274)	747.2(31)	26.1(fixed)	—	–6.4	26.1

*u*4877	H(128)...H(133)	747.6(11)	25.4(fixed)	—	–6.6	25.4
*u*4826	H(256)...H(271)	747.7(15)	25.5(fixed)	—	–5.0	25.5
*u*4868	H(34)...H(36)	748.5(14)	24.5(fixed)	—	–6.3	24.5
*u*4869	H(213)...H(224)	748.9(32)	25.0(fixed)	—	–6.1	25.0
*u*4862	H(81)...H(83)	749.7(13)	31.4(fixed)	—	–3.4	31.4
*u*4863	H(121)...H(130)	750.0(33)	24.3(fixed)	—	–6.2	24.3
*u*4898	H(113)...H(137)	782.3(13)	20.8(fixed)	—	–14.4	20.8
*u*4892	H(81)...H(85)	782.8(8)	21.3(fixed)	—	–13.7	21.3
*u*4895	H(19)...H(43)	783.0(13)	20.8(fixed)	—	–13.2	20.8
*u*4888	H(21)...H(41)	785.3(13)	20.5(fixed)	—	–10.3	20.5
*u*4890	H(25)...H(30)	785.9(10)	20.6(fixed)	—	–10.5	20.6
*u*4882	H(215)...H(234)	786.3(8)	21.6(fixed)	—	–10.7	21.6
*u*4883	H(68)...H(88)	786.8(9)	20.6(fixed)	—	–9.2	20.6
*u*4896	H(66)...H(90)	786.9(14)	19.2(fixed)	—	–8.7	19.2
*u*4891	H(34)...H(38)	786.9(12)	19.9(fixed)	—	–8.9	19.9
*u*4894	H(166)...H(187)	787.3(8)	19.7(fixed)	—	–9.3	19.7
*u*4897	H(254)...H(278)	787.4(14)	19.2(fixed)	—	–11.1	19.2
*u*4881	H(121)...H(132)	787.5(14)	20.8(fixed)	—	–8.3	20.8
*u*4879	H(128)...H(135)	787.7(9)	21.2(fixed)	—	–8.2	21.2
*u*4887	H(162)...H(182)	788.0(10)	20.6(fixed)	—	–10.7	20.6
*u*4885	H(119)...H(124)	789.2(10)	19.9(fixed)	—	–7.9	19.9
*u*4884	H(213)...H(226)	789.9(14)	20.1(fixed)	—	–8.1	20.1
*u*4893	H(160)...H(184)	789.9(14)	19.2(fixed)	—	–8.0	19.2
*u*4880	H(262)...H(276)	790.4(16)	20.9(fixed)	—	–8.3	20.9
*u*4899	H(207)...H(231)	790.4(14)	18.6(fixed)	—	–8.2	18.6
*u*4889	H(256)...H(273)	791.1(10)	19.9(fixed)	—	–8.0	19.9
*u*4886	H(74)...H(93)	793.8(31)	21.2(fixed)	—	–10.5	21.2

Table S12. Interatomic distances (r_a / pm), refined and calculated amplitudes of vibration (u_{h1} / pm) and perpendicular corrections (k_{h1} / pm) for the SARACEN-restrained GED structure of **2**

	Atom Pair	r_a	u_{hl} (GED)	Restraint	k_{hl}	u_{hl} (Calc.)
*u*37	C(16)–H(42)	109.6(3)	7.8(tied to *u*47)	—	0.4	7.9
*u*18	C(16)–H(44)	109.6(3)	7.8(tied to *u*47)	—	0.4	7.8
*u*85	C(16)–H(43)	109.6(3)	7.8(tied to *u*47)	—	0.4	7.8
*u*38	C(147)–H(161)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*40	C(17)–H(45)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*22	C(10)–H(32)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*25	C(148)–H(164)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*21	C(148)–H(163)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*17	C(10)–H(31)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*13	C(152)–H(176)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*16	C(60)–H(87)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*20	C(56)–H(76)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*19	C(53)–H(67)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*11	C(9)–H(29)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*8	C(103)–H(123)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*9	C(13)–H(40)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*83	C(53)–H(66)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*1	C(59)–H(83)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*12	C(57)–H(78)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*6	C(12)–H(36)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*5	C(8)–H(26)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*4	C(149)–H(167)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*10	C(150)–H(170)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*76	C(101)–H(115)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*3	C(102)–H(120)	109.6(3)	7.5(tied to *u*47)	—	0.4	7.6
*u*2	C(55)–H(73)	109.6(3)	7.5(tied to *u*47)	—	0.4	7.6
*u*72	C(103)–H(121)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*70	C(59)–H(85)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*71	C(13)–H(41)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*69	C(60)–H(88)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*65	C(102)–H(119)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*62	C(55)–H(72)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*64	C(8)–H(25)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*63	C(149)–H(166)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*66	C(150)–H(168)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*61	C(12)–H(38)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*68	C(56)–H(74)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*67	C(9)–H(27)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*58	C(55)–H(71)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*54	C(59)–H(84)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*56	C(63)–H(89)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*52	C(8)–H(24)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7

*u*59	C(12)–H(37)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*57	C(102)–H(118)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*47	C(7)–H(23)	109.6(3)	7.6(4)	—	0.4	7.7
*u*50	C(100)–H(112)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*60	C(149)–H(165)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*51	C(147)–H(159)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*55	C(150)–H(169)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*48	C(103)–H(122)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*43	C(9)–H(28)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*46	C(101)–H(117)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*41	C(53)–H(65)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*53	C(56)–H(75)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*49	C(60)–H(86)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*45	C(54)–H(70)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*35	C(7)–H(22)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*34	C(6)–H(18)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*44	C(54)–H(69)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*36	C(11)–H(33)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*33	C(64)–H(92)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*39	C(6)–H(20)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*24	C(58)–H(82)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*27	C(63)–H(91)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*32	C(13)–H(39)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*42	C(105)–H(129)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*26	C(58)–H(80)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*30	C(57)–H(79)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*23	C(11)–H(35)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*31	C(152)–H(174)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*29	C(105)–H(127)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*28	C(101)–H(116)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*90	C(148)–H(162)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*88	C(10)–H(30)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*89	C(57)–H(77)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*15	C(64)–H(94)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*82	C(17)–H(46)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*78	C(6)–H(19)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*87	C(152)–H(175)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*81	C(105)–H(128)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*74	C(7)–H(21)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*84	C(100)–H(113)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*75	C(11)–H(34)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*86	C(64)–H(93)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*79	C(54)–H(68)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*80	C(58)–H(81)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*7	C(17)–H(47)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6
*u*14	C(100)–H(114)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.6

*u*77	C(147)–H(160)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*73	C(63)–H(90)	109.6(3)	7.6(tied to *u*47)	—	0.4	7.7
*u*94	H(42)...H(44)	173.9(16)	12.6(fixed)	—	–0.4	12.6
*u*96	H(31)...H(32)	174.0(16)	12.6(fixed)	—	–0.3	12.6
*u*156	H(22)...H(23)	174.1(16)	12.6(fixed)	—	–0.3	12.6
*u*151	H(33)...H(35)	174.1(16)	12.6(fixed)	—	–0.3	12.6
*u*99	H(163)...H(164)	174.1(16)	12.7(fixed)	—	–0.3	12.7
*u*173	H(45)...H(47)	174.1(16)	12.6(fixed)	—	–0.2	12.6
*u*175	H(18)...H(20)	174.1(16)	12.6(fixed)	—	–0.2	12.6
*u*174	H(159)...H(161)	174.2(16)	12.6(fixed)	—	–0.2	12.6
*u*163	H(174)...H(176)	174.2(16)	12.6(fixed)	—	–0.2	12.6
*u*171	H(92)...H(94)	174.2(16)	12.6(fixed)	—	–0.2	12.6
*u*177	H(69)...H(70)	174.2(16)	12.6(fixed)	—	–0.2	12.6
*u*180	H(65)...H(67)	174.2(16)	12.6(fixed)	—	–0.2	12.6
*u*167	H(112)...H(114)	174.3(16)	12.6(fixed)	—	–0.2	12.6
*u*148	H(127)...H(129)	174.3(16)	12.6(fixed)	—	–0.2	12.6
*u*176	H(116)...H(117)	174.3(16)	12.6(fixed)	—	–0.2	12.6
*u*102	H(78)...H(79)	174.3(16)	12.7(fixed)	—	–0.2	12.7
*u*147	H(80)...H(82)	174.3(16)	12.6(fixed)	—	–0.2	12.6
*u*153	H(89)...H(91)	174.4(16)	12.6(fixed)	—	–0.2	12.6
*u*123	H(83)...H(84)	175.4(16)	12.7(fixed)	—	–0.3	12.7
*u*121	H(122)...H(123)	175.4(16)	12.7(fixed)	—	–0.3	12.7
*u*162	H(86)...H(87)	175.5(16)	12.6(fixed)	—	–0.2	12.6
*u*170	H(71)...H(73)	175.5(16)	12.6(fixed)	—	–0.2	12.6
*u*172	H(75)...H(76)	175.5(16)	12.6(fixed)	—	–0.2	12.6
*u*165	H(118)...H(120)	175.5(16)	12.6(fixed)	—	–0.2	12.6
*u*160	H(169)...H(170)	175.7(16)	12.6(fixed)	—	–0.2	12.6
*u*166	H(165)...H(167)	175.7(16)	12.6(fixed)	—	–0.2	12.6
*u*161	H(24)...H(26)	175.8(16)	12.6(fixed)	—	–0.2	12.6
*u*169	H(28)...H(29)	175.8(16)	12.6(fixed)	—	–0.2	12.6
*u*178	H(39)...H(40)	175.8(16)	12.6(fixed)	—	–0.2	12.6
*u*179	H(36)...H(37)	175.8(16)	12.6(fixed)	—	–0.2	12.6
*u*127	H(42)...H(43)	176.4(7)	12.7(fixed)	—	–0.5	12.7
*u*132	H(43)...H(44)	176.4(7)	12.6(fixed)	—	–0.4	12.6
*u*126	H(30)...H(32)	176.5(7)	12.7(fixed)	—	–0.3	12.7
*u*134	H(30)...H(31)	176.5(7)	12.6(fixed)	—	–0.3	12.6
*u*149	H(121)...H(123)	176.5(7)	12.7(fixed)	—	–0.3	12.7
*u*159	H(84)...H(85)	176.5(7)	12.7(fixed)	—	–0.3	12.7
*u*168	H(133)...H(135)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*122	H(162)...H(164)	176.6(7)	12.7(fixed)	—	–0.3	12.7
*u*158	H(83)...H(85)	176.6(7)	12.7(fixed)	—	–0.3	12.7
*u*95	H(33)...H(34)	176.6(7)	12.7(fixed)	—	–0.3	12.7
*u*93	H(112)...H(113)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*136	H(162)...H(163)	176.6(7)	12.7(fixed)	—	–0.3	12.7
*u*91	H(21)...H(23)	176.6(7)	12.7(fixed)	—	–0.3	12.7
*u*105	H(34)...H(35)	176.6(7)	12.6(fixed)	—	–0.3	12.6

*u*101	H(127)...H(128)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*100	H(80)...H(81)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*117	H(81)...H(82)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*109	H(21)...H(22)	176.6(7)	12.6(fixed)	—	–0.3	12.6
*u*139	H(118)...H(119)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*137	H(113)...H(114)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*111	H(128)...H(129)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*116	H(115)...H(117)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*124	H(115)...H(116)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*128	H(77)...H(79)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*140	H(130)...H(132)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*103	H(45)...H(46)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*146	H(24)...H(25)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*129	H(165)...H(166)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*110	H(68)...H(69)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*92	H(89)...H(90)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*130	H(25)...H(26)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*112	H(160)...H(161)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*98	H(174)...H(175)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*145	H(77)...H(78)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*97	H(92)...H(93)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*104	H(74)...H(76)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*107	H(159)...H(160)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*113	H(65)...H(66)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*120	H(27)...H(29)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*131	H(93)...H(94)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*106	H(68)...H(70)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*141	H(175)...H(176)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*144	H(71)...H(72)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*135	H(66)...H(67)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*152	H(86)...H(88)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*108	H(90)...H(91)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*118	H(87)...H(88)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*138	H(166)...H(167)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*125	H(168)...H(170)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*142	H(72)...H(73)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*157	H(27)...H(28)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*115	H(19)...H(20)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*119	H(40)...H(41)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*155	H(74)...H(75)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*154	H(168)...H(169)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*114	H(18)...H(19)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*143	H(46)...H(47)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*133	H(36)...H(38)	176.6(7)	12.6(fixed)	—	–0.2	12.6
*u*150	H(37)...H(38)	176.6(7)	12.7(fixed)	—	–0.2	12.7
*u*164	H(39)...H(41)	176.6(7)	12.6(fixed)	—	–0.2	12.6

*u*191	Si(144)–C(149)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.9
*u*186	Si(50)–C(55)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*188	Si(97)–C(102)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*187	Si(144)–C(150)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*189	Si(3)–C(8)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*185	Si(3)–C(9)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*183	Si(2)–C(13)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*182	Si(97)–C(103)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*184	Si(2)–C(12)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*181	Si(49)–C(59)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.8
*u*192	Si(50)–C(56)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.9
*u*190	Si(49)–C(60)	187.7(7)	5.8(tied to *u*195)	—	0.2	5.9
*u*208	Si(98)–C(105)	188.7(5)	5.9(tied to *u*195)	—	0.2	6.0
*u*207	Si(4)–C(11)	188.7(5)	5.9(tied to *u*195)	—	0.2	6.0
*u*202	Si(52)–C(54)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*206	Si(51)–C(58)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*201	Si(4)–C(16)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*205	Si(146)–C(147)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*200	Si(146)–C(148)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*197	Si(99)–C(101)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*199	Si(5)–C(6)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*198	Si(4)–C(10)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*195	Si(5)–C(17)	188.7(5)	5.9(1)	—	0.2	5.9
*u*193	Si(52)–C(53)	188.7(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*196	Si(145)–C(152)	188.7(5)	5.8(tied to *u*195)	—	0.2	5.9
*u*194	Si(51)–C(57)	188.8(5)	5.8(tied to *u*195)	—	0.2	5.9
*u*209	Si(5)–C(7)	188.8(5)	5.9(tied to *u*195)	—	0.2	6.0
*u*210	Si(51)–C(63)	188.8(5)	5.9(tied to *u*195)	—	0.2	6.0
*u*203	Si(52)–C(64)	188.8(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*204	Si(99)–C(100)	188.8(5)	5.9(tied to *u*195)	—	0.2	5.9
*u*213	C(48)–Si(50)	190.1(3)	6.3(tied to *u*195)	—	0.2	6.4
*u*215	C(142)–Si(143)	190.1(3)	6.3(tied to *u*195)	—	0.3	6.4
*u*216	C(1)–Si(2)	190.1(3)	6.3(tied to *u*195)	—	0.3	6.4
*u*214	C(48)–Si(49)	190.1(3)	6.3(tied to *u*195)	—	0.3	6.4
*u*211	C(1)–Si(3)	190.1(3)	6.3(tied to *u*195)	—	0.3	6.4
*u*212	C(95)–Si(96)	190.1(3)	6.3(tied to *u*195)	—	0.3	6.3
*u*2902	H(170)...H(181)	192.7(77)	29.4(fixed)	—	–5.1	29.4
*u*231	H(174)...H(186)	193.0(106)	37.3(fixed)	—	22.1	37.3
*u*218	C(1)–Si(4)	193.8(3)	6.6(tied to *u*195)	—	0.3	6.7
*u*220	C(1)–Si(5)	193.8(3)	6.7(tied to *u*195)	—	0.3	6.8
*u*221	C(142)–Si(145)	193.8(3)	6.7(tied to *u*195)	—	0.3	6.7
*u*219	C(95)–Si(98)	193.8(3)	6.6(tied to *u*195)	—	0.3	6.7
*u*222	C(48)–Si(52)	193.8(3)	6.8(tied to *u*195)	—	0.3	6.8
*u*217	C(48)–Si(51)	193.8(3)	6.6(tied to *u*195)	—	0.3	6.6
*u*258	H(70)...H(73)	196.9(65)	41.3(fixed)	—	10.5	41.3
*u*226	Si(96)–Cl(108)	207.5(2)	5.7(tied to *u*227)	—	0.3	6.3

*u*225	Si(50)–Cl(62)	207.5(2)	5.7(tied to *u*227)	—	0.3	6.3
*u*224	Si(49)–Cl(61)	208.4(2)	5.6(tied to *u*227)	—	0.3	6.2
*u*223	Si(143)–Cl(155)	208.5(2)	5.6(tied to *u*227)	—	0.3	6.2
*u*227	Si(2)–Cl(14)	208.5(2)	5.7(2)	—	0.3	6.3
*u*228	Si(3)–Cl(15)	208.5(2)	5.7(tied to *u*227)	—	0.3	6.3
*u*1123	H(112)...H(130)	208.7(45)	37.8(fixed)	—	3.0	37.8
*u*2317	H(117)...H(123)	208.9(56)	34.2(fixed)	—	0.6	34.2
*u*229	H(80)...H(92)	209.6(100)	35.5(fixed)	—	20.6	35.5
*u*243	H(69)...H(73)	210.9(66)	43.1(fixed)	—	12.3	43.1
*u*1247	H(159)...H(178)	212.4(62)	42.6(fixed)	—	–2.4	42.6
*u*304	H(116)...H(127)	213.9(64)	42.2(fixed)	—	9.0	42.2
*u*2297	H(164)...H(167)	215.7(39)	40.1(fixed)	—	3.2	40.1
*u*253	H(65)...H(83)	218.2(45)	44.1(fixed)	—	14.8	44.1
*u*270	H(20)...H(24)	219.7(58)	46.0(fixed)	—	11.9	46.0
*u*299	H(18)...H(36)	222.9(49)	45.6(fixed)	—	9.6	45.6
*u*248	H(71)...H(82)	223.2(54)	42.2(fixed)	—	13.9	42.2
*u*233	H(23)...H(24)	225.6(56)	33.7(fixed)	—	22.5	33.7
*u*234	H(33)...H(45)	227.2(95)	34.2(fixed)	—	23.4	34.2
*u*2397	H(163)...H(167)	228.2(30)	49.6(fixed)	—	1.8	49.6
*u*230	H(127)...H(139)	228.5(120)	34.6(fixed)	—	16.8	34.6
*u*249	H(87)...H(91)	228.8(62)	41.0(fixed)	—	10.5	41.0
*u*3120	H(118)...H(131)	229.9(88)	32.5(fixed)	—	–2.2	32.5
*u*2587	H(114)...H(122)	231.3(40)	36.1(fixed)	—	–2.6	36.1
*u*296	H(23)...H(28)	231.4(68)	46.5(fixed)	—	13.1	46.5
*u*2731	H(122)...H(131)	231.7(42)	41.8(fixed)	—	–4.2	41.8
*u*267	H(75)...H(89)	231.8(55)	41.1(fixed)	—	10.3	41.1
*u*261	H(26)...H(37)	232.1(56)	41.4(fixed)	—	12.7	41.4
*u*1847	H(114)...H(123)	232.7(71)	42.8(fixed)	—	8.0	42.8
*u*2356	H(169)...H(183)	233.5(60)	36.0(fixed)	—	–0.1	36.0
*u*254	H(31)...H(45)	234.8(48)	42.1(fixed)	—	19.2	42.1
*u*247	H(78)...H(94)	235.1(55)	46.3(fixed)	—	13.7	46.3
*u*268	H(22)...H(28)	235.4(63)	48.5(fixed)	—	14.4	48.5
*u*245	H(29)...H(35)	235.8(60)	44.7(fixed)	—	16.3	44.7
*u*238	H(79)...H(87)	235.9(46)	36.8(fixed)	—	18.5	36.8
*u*306	H(116)...H(129)	236.4(48)	45.6(fixed)	—	10.3	45.6
*u*235	H(32)...H(40)	236.8(52)	33.8(fixed)	—	27.2	33.8
*u*255	H(22)...H(33)	237.2(35)	47.8(fixed)	—	15.1	47.8
*u*244	H(67)...H(83)	239.1(47)	44.4(fixed)	—	16.4	44.4
*u*310	H(28)...H(35)	239.3(38)	50.2(fixed)	—	15.8	50.2
*u*1825	H(114)...H(130)	239.8(48)	36.6(fixed)	—	–6.0	36.6
*u*269	H(78)...H(92)	240.0(49)	42.3(fixed)	—	12.0	42.3
*u*2405	H(178)...H(188)	240.6(54)	32.2(fixed)	—	–1.4	32.2
*u*2447	H(161)...H(180)	240.7(40)	40.2(fixed)	—	0.7	40.2
*u*265	H(31)...H(47)	240.9(55)	43.7(fixed)	—	19.1	43.7
*u*287	H(163)...H(176)	241.5(42)	51.6(fixed)	—	18.3	51.6
*u*313	H(86)...H(91)	242.7(36)	46.1(fixed)	—	10.5	46.1

*u*273	Si(50)...H(72)	243.1(8)	14.1(tied to *u*278)	—	–0.4	13.2
*u*290	Si(144)...H(166)	243.1(8)	14.2(tied to *u*278)	—	–0.4	13.3
*u*284	Si(49)...H(88)	243.1(8)	14.1(tied to *u*278)	—	–0.4	13.2
*u*285	Si(50)...H(74)	243.1(8)	14.1(tied to *u*278)	—	–0.4	13.2
*u*289	Si(144)...H(168)	243.1(8)	14.1(tied to *u*278)	—	–0.4	13.1
*u*272	Si(2)...H(41)	243.2(8)	14.2(tied to *u*278)	—	–0.4	13.2
*u*274	Si(97)...H(119)	243.2(8)	14.1(tied to *u*278)	—	–0.4	13.1
*u*275	Si(3)...H(27)	243.2(8)	14.2(tied to *u*278)	—	–0.4	13.2
*u*283	Si(49)...H(85)	243.2(8)	14.1(tied to *u*278)	—	–0.4	13.2
*u*276	Si(2)...H(38)	243.2(8)	14.1(tied to *u*278)	—	–0.4	13.1
*u*280	Si(97)...H(121)	243.2(8)	14.1(tied to *u*278)	—	–0.4	13.2
*u*281	Si(3)...H(25)	243.2(8)	14.2(tied to *u*278)	—	–0.4	13.2
*u*279	Si(52)...H(66)	244.0(6)	14.3(tied to *u*278)	—	–0.4	13.3
*u*291	Si(52)...H(68)	244.0(6)	14.4(tied to *u*278)	—	–0.4	13.4
*u*277	Si(52)...H(93)	244.0(6)	14.3(tied to *u*278)	—	–0.4	13.4
*u*308	Si(51)...H(90)	244.0(6)	14.3(tied to *u*278)	—	–0.4	13.4
*u*282	Si(145)...H(175)	244.0(6)	14.4(tied to *u*278)	—	–0.4	13.4
*u*302	Si(146)...H(160)	244.0(6)	14.4(tied to *u*278)	—	–0.4	13.4
*u*301	Si(51)...H(81)	244.0(6)	14.4(tied to *u*278)	—	–0.4	13.4
*u*297	Si(51)...H(77)	244.1(6)	14.2(tied to *u*278)	—	–0.4	13.3
*u*294	Si(146)...H(162)	244.1(6)	14.4(tied to *u*278)	—	–0.4	13.5
*u*288	Si(99)...H(113)	244.1(6)	14.3(tied to *u*278)	—	–0.4	13.4
*u*293	Si(98)...H(128)	244.1(6)	14.4(tied to *u*278)	—	–0.4	13.4
*u*298	Si(4)...H(34)	244.1(6)	14.5(tied to *u*278)	—	–0.4	13.5
*u*278	Si(5)...H(46)	244.1(6)	14.3(6)	—	–0.4	13.4
*u*300	Si(5)...H(19)	244.1(6)	14.3(tied to *u*278)	—	–0.4	13.3
*u*292	Si(99)...H(115)	244.1(6)	14.3(tied to *u*278)	—	–0.4	13.3
*u*303	Si(5)...H(21)	244.1(6)	14.5(tied to *u*278)	—	–0.4	13.6
*u*305	Si(4)...H(43)	244.1(6)	14.6(tied to *u*278)	—	–0.3	13.7
*u*295	Si(4)...H(30)	244.2(6)	14.4(tied to *u*278)	—	–0.3	13.4
*u*312	H(69)...H(80)	244.4(50)	46.7(fixed)	—	10.2	46.7
*u*264	H(20)...H(36)	246.1(42)	42.5(fixed)	—	11.4	42.5
*u*383	C(54)...H(73)	246.2(58)	31.0(tied to *u*278)	—	9.0	28.9
*u*240	H(76)...H(84)	246.3(29)	38.0(fixed)	—	20.1	38.0
*u*331	H(20)...H(26)	247.8(57)	49.7(fixed)	—	11.7	49.7
*u*328	H(69)...H(82)	248.3(51)	51.8(fixed)	—	10.8	51.8
*u*318	Si(3)...H(28)	249.3(8)	14.3(tied to *u*278)	—	–0.4	13.3
*u*315	Si(2)...H(37)	249.3(8)	14.2(tied to *u*278)	—	–0.4	13.2
*u*314	Si(2)...H(39)	249.3(8)	14.1(tied to *u*278)	—	–0.4	13.2
*u*322	Si(3)...H(24)	249.3(8)	14.3(tied to *u*278)	—	–0.3	13.3
*u*330	Si(144)...H(165)	249.3(8)	14.5(tied to *u*278)	—	–0.4	13.6
*u*319	Si(144)...H(169)	249.4(8)	14.2(tied to *u*278)	—	–0.4	13.3
*u*307	H(39)...H(44)	249.5(43)	45.1(fixed)	—	29.8	45.1
*u*353	H(22)...H(35)	249.6(52)	56.2(fixed)	—	13.8	56.2
*u*316	Si(97)...H(122)	249.8(8)	14.2(tied to *u*278)	—	–0.4	13.3
*u*324	Si(97)...H(118)	249.8(8)	14.1(tied to *u*278)	—	–0.4	13.2

*u*320	Si(50)...H(71)	249.8(8)	14.2(tied to *u*278)	—	–0.4	13.2
*u*323	Si(49)...H(86)	249.9(8)	14.1(tied to *u*278)	—	–0.3	13.2
*u*325	Si(50)...H(75)	249.9(8)	14.0(tied to *u*278)	—	–0.4	13.0
*u*321	Si(49)...H(84)	249.9(8)	14.1(tied to *u*278)	—	–0.3	13.1
*u*252	H(40)...H(44)	250.6(69)	41.4(fixed)	—	27.9	41.4
*u*334	Si(50)...H(73)	251.1(8)	14.0(tied to *u*278)	—	–0.4	13.0
*u*354	Si(50)...H(76)	251.1(8)	13.9(tied to *u*278)	—	–0.4	13.0
*u*347	Si(49)...H(87)	251.1(8)	13.9(tied to *u*278)	—	–0.4	12.9
*u*332	Si(49)...H(83)	251.2(8)	14.0(tied to *u*278)	—	–0.3	13.1
*u*337	Si(144)...H(167)	251.2(8)	14.0(tied to *u*278)	—	–0.4	13.1
*u*335	Si(3)...H(29)	251.2(8)	14.1(tied to *u*278)	—	–0.4	13.1
*u*340	Si(144)...H(170)	251.2(8)	14.0(tied to *u*278)	—	–0.4	13.0
*u*338	Si(97)...H(120)	251.2(8)	13.9(tied to *u*278)	—	–0.4	12.9
*u*336	Si(2)...H(36)	251.2(8)	13.9(tied to *u*278)	—	–0.4	12.9
*u*346	Si(2)...H(40)	251.2(8)	13.9(tied to *u*278)	—	–0.4	12.9
*u*352	Si(97)...H(123)	251.2(8)	13.9(tied to *u*278)	—	–0.3	13.0
*u*341	Si(3)...H(26)	251.3(8)	13.8(tied to *u*278)	—	–0.3	12.9
*u*368	Si(51)...H(82)	252.0(6)	14.1(tied to *u*278)	—	–0.4	13.2
*u*355	Si(51)...H(78)	252.0(6)	14.0(tied to *u*278)	—	–0.4	13.1
*u*376	Si(51)...H(89)	252.0(6)	14.0(tied to *u*278)	—	–0.4	13.1
*u*371	Si(51)...H(91)	252.0(6)	14.1(tied to *u*278)	—	–0.3	13.2
*u*365	Si(51)...H(80)	252.0(6)	14.0(tied to *u*278)	—	–0.3	13.1
*u*364	Si(51)...H(79)	252.1(6)	14.0(tied to *u*278)	—	–0.3	13.0
*u*333	Si(99)...H(117)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*349	Si(99)...H(114)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.2
*u*357	Si(52)...H(70)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*350	Si(146)...H(163)	252.1(6)	14.3(tied to *u*278)	—	–0.4	13.3
*u*351	Si(52)...H(65)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*339	Si(52)...H(94)	252.1(6)	14.2(tied to *u*278)	—	–0.4	13.2
*u*375	Si(99)...H(112)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.2
*u*345	Si(146)...H(159)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*361	Si(98)...H(129)	252.1(6)	14.0(tied to *u*278)	—	–0.4	13.1
*u*360	Si(52)...H(69)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*359	Si(5)...H(45)	252.1(6)	14.2(tied to *u*278)	—	–0.4	13.3
*u*362	Si(145)...H(174)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.2
*u*343	Si(52)...H(67)	252.1(6)	14.0(tied to *u*278)	—	–0.4	13.0
*u*377	Si(52)...H(92)	252.1(6)	14.0(tied to *u*278)	—	–0.4	13.1
*u*348	Si(145)...H(176)	252.1(6)	14.0(tied to *u*278)	—	–0.4	13.1
*u*380	Si(5)...H(23)	252.1(6)	14.3(tied to *u*278)	—	–0.4	13.4
*u*379	Si(146)...H(164)	252.1(6)	14.3(tied to *u*278)	—	–0.3	13.3
*u*374	Si(146)...H(161)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*378	Si(98)...H(127)	252.1(6)	14.1(tied to *u*278)	—	–0.3	13.2
*u*342	Si(5)...H(18)	252.1(6)	14.1(tied to *u*278)	—	–0.4	13.1
*u*369	Si(4)...H(33)	252.1(6)	14.4(tied to *u*278)	—	–0.3	13.4
*u*366	Si(99)...H(116)	252.1(6)	13.9(tied to *u*278)	—	–0.3	12.9
*u*367	Si(5)...H(22)	252.1(6)	14.2(tied to *u*278)	—	–0.3	13.3

*u*344	Si(5)...H(47)	252.1(6)	14.0(tied to *u*278)	—	–0.4	13.0
*u*372	Si(4)...H(35)	252.2(6)	14.1(tied to *u*278)	—	–0.3	13.2
*u*363	Si(5)...H(20)	252.2(6)	13.9(tied to *u*278)	—	–0.4	13.0
*u*356	Si(4)...H(31)	252.2(6)	14.2(tied to *u*278)	—	–0.3	13.2
*u*373	Si(4)...H(32)	252.2(6)	14.1(tied to *u*278)	—	–0.3	13.2
*u*358	Si(4)...H(44)	252.3(6)	14.9(tied to *u*278)	—	–0.1	13.9
*u*370	Si(4)...H(42)	252.3(6)	14.9(tied to *u*278)	—	–0.1	13.9
*u*266	H(163)...H(174)	253.1(53)	47.0(fixed)	—	17.3	47.0
*u*431	Cl(62)...H(67)	256.1(53)	30.4(fixed)	—	8.8	30.4
*u*1984	Cl(109)...H(129)	258.6(50)	32.1(fixed)	—	2.9	32.1
*u*2483	H(122)...H(130)	261.4(49)	46.7(fixed)	—	1.2	46.7
*u*259	H(26)...H(36)	262.5(37)	41.0(fixed)	—	13.6	41.0
*u*257	H(76)...H(86)	262.6(60)	41.0(fixed)	—	11.3	41.0
*u*309	H(73)...H(82)	264.7(44)	47.0(fixed)	—	13.4	47.0
*u*2415	C(148)...H(167)	265.4(26)	23.3(fixed)	—	–1.5	23.3
*u*1507	C(110)...H(120)	265.5(29)	32.8(fixed)	—	–2.4	32.8
*u*415	C(105)...H(116)	267.6(35)	30.0(fixed)	—	7.1	30.0
*u*1882	Cl(156)...H(161)	268.4(40)	30.1(fixed)	—	2.7	30.1
*u*1654	H(177)...H(188)	268.8(41)	39.2(fixed)	—	6.2	39.2
*u*237	H(29)...H(42)	269.0(72)	38.1(fixed)	—	38.4	38.1
*u*562	C(55)...H(70)	270.5(56)	35.9(fixed)	—	3.3	35.9
*u*381	C(53)...H(83)	272.1(24)	30.4(fixed)	—	13.2	30.4
*u*459	C(158)...H(174)	272.5(80)	30.6(fixed)	—	9.5	30.6
*u*1922	C(103)...H(114)	273.3(49)	32.2(fixed)	—	3.2	32.2
*u*436	Cl(62)...H(70)	273.5(51)	34.7(fixed)	—	6.6	34.7
*u*241	H(71)...H(89)	273.5(64)	36.6(fixed)	—	15.6	36.6
*u*329	H(75)...H(86)	274.2(35)	47.7(fixed)	—	10.8	47.7
*u*425	C(8)...H(20)	274.6(49)	30.5(fixed)	—	8.9	30.5
*u*396	C(60)...H(91)	276.2(43)	28.6(fixed)	—	7.9	28.6
*u*410	C(7)...H(28)	277.4(62)	31.8(fixed)	—	10.8	31.8
*u*311	H(75)...H(91)	277.6(44)	44.5(fixed)	—	10.7	44.5
*u*405	H(38)...H(41)	277.9(30)	33.7(fixed)	—	7.7	33.7
*u*402	H(72)...H(74)	278.0(31)	35.0(fixed)	—	6.5	35.0
*u*399	C(6)...H(36)	278.1(32)	29.6(fixed)	—	7.9	29.6
*u*391	C(9)...H(35)	278.2(40)	31.3(fixed)	—	13.1	31.3
*u*394	H(25)...H(27)	279.1(30)	34.5(fixed)	—	9.0	34.5
*u*428	H(119)...H(121)	279.1(31)	37.2(fixed)	—	8.6	37.2
*u*408	H(85)...H(88)	279.4(31)	37.2(fixed)	—	8.5	37.2
*u*413	H(166)...H(168)	279.6(31)	35.8(fixed)	—	7.2	35.8
*u*2510	C(157)...H(169)	279.8(38)	22.7(fixed)	—	–1.8	22.7
*u*387	C(64)...H(78)	280.4(37)	29.2(fixed)	—	10.4	29.2
*u*386	C(17)...H(31)	280.6(41)	27.9(fixed)	—	16.5	27.9
*u*2538	C(154)...H(170)	281.6(57)	25.2(fixed)	—	–3.5	25.2
*u*393	Cl(14)...H(47)	283.7(44)	29.7(fixed)	—	10.2	29.7
*u*388	C(55)...H(82)	283.8(34)	30.1(fixed)	—	11.1	30.1
*u*448	C(58)...H(92)	285.1(76)	29.3(fixed)	—	8.0	29.3

*u*2300	C(106)...H(122)	286.6(39)	43.2(fixed)	—	–1.1	43.2
*u*389	C(13)...H(44)	287.2(48)	40.0(fixed)	—	26.3	40.0
*u*385	C(12)...H(26)	287.3(29)	28.7(fixed)	—	10.8	28.7
*u*447	C(64)...H(80)	287.6(77)	29.7(fixed)	—	9.2	29.7
*u*414	C(11)...H(22)	287.8(29)	32.3(fixed)	—	11.1	32.3
*u*427	H(66)...H(68)	287.8(23)	36.9(fixed)	—	6.0	36.9
*u*424	H(68)...H(93)	287.9(23)	37.2(fixed)	—	6.2	37.2
*u*421	H(124)...H(128)	288.4(23)	35.3(fixed)	—	5.6	35.3
*u*404	H(77)...H(90)	288.7(23)	36.2(fixed)	—	6.7	36.2
*u*401	H(124)...H(137)	288.8(23)	34.9(fixed)	—	5.9	34.9
*u*432	H(77)...H(81)	289.4(23)	38.0(fixed)	—	7.9	38.0
*u*518	Cl(156)...H(164)	289.6(28)	46.5(fixed)	—	6.4	46.5
*u*426	H(160)...H(162)	289.6(23)	40.2(fixed)	—	9.1	40.2
*u*433	H(19)...H(21)	289.7(23)	38.3(fixed)	—	7.7	38.3
*u*463	C(8)...H(23)	289.8(49)	31.7(fixed)	—	9.8	31.7
*u*434	C(58)...H(69)	289.9(38)	31.6(fixed)	—	7.6	31.6
*u*435	Cl(14)...H(18)	290.5(45)	34.9(fixed)	—	7.9	34.9
*u*423	H(171)...H(175)	290.6(23)	40.4(fixed)	—	10.2	40.4
*u*398	H(21)...H(46)	290.7(23)	37.2(fixed)	—	8.4	37.2
*u*397	C(152)...H(163)	290.8(32)	33.3(fixed)	—	14.9	33.3
*u*574	C(59)...H(65)	291.6(30)	37.7(fixed)	—	3.6	37.7
*u*608	C(101)...H(127)	291.6(42)	37.1(fixed)	—	3.6	37.1
*u*403	Cl(61)...H(94)	292.7(52)	30.0(fixed)	—	9.7	30.0
*u*2562	C(101)...H(123)	293.4(41)	22.4(fixed)	—	–1.9	22.4
*u*430	H(30)...H(34)	293.7(23)	40.1(fixed)	—	12.2	40.1
*u*683	C(55)...H(69)	293.7(56)	37.9(fixed)	—	3.0	37.9
*u*627	C(6)...H(24)	294.1(48)	41.6(fixed)	—	4.6	41.6
*u*1894	C(103)...H(117)	294.5(41)	30.1(fixed)	—	2.0	30.1
*u*475	C(7)...H(24)	294.6(50)	31.1(fixed)	—	8.9	31.1
*u*400	H(128)...H(137)	294.9(43)	36.4(fixed)	—	6.1	36.4
*u*480	C(11)...H(45)	295.2(72)	31.7(fixed)	—	8.2	31.7
*u*419	H(81)...H(90)	295.3(43)	36.7(fixed)	—	7.1	36.7
*u*411	H(175)...H(184)	295.3(43)	38.3(fixed)	—	7.9	38.3
*u*600	C(9)...H(23)	295.3(60)	42.3(fixed)	—	4.5	42.3
*u*390	H(66)...H(93)	295.6(43)	35.7(fixed)	—	7.2	35.7
*u*1764	C(149)...H(176)	295.7(37)	29.6(fixed)	—	3.5	29.6
*u*412	C(63)...H(75)	296.2(37)	29.4(fixed)	—	8.1	29.4
*u*406	H(19)...H(46)	296.8(43)	35.3(fixed)	—	7.6	35.3
*u*1396	C(147)...H(178)	297.5(46)	35.2(fixed)	—	–2.7	35.2
*u*483	C(106)...H(112)	297.5(30)	30.6(fixed)	—	7.4	30.6
*u*701	Si(50)...H(70)	297.6(34)	31.0(fixed)	—	3.1	31.0
*u*439	Cl(61)...H(65)	298.3(47)	34.7(fixed)	—	7.4	34.7
*u*622	C(12)...H(18)	298.5(34)	40.6(fixed)	—	3.7	40.6
*u*524	Cl(61)...H(79)	298.7(17)	41.8(fixed)	—	4.7	41.8
*u*533	Cl(15)...H(42)	299.0(25)	61.3(fixed)	—	11.4	61.3
*u*594	C(153)...H(159)	299.4(46)	38.0(fixed)	—	3.7	38.0

*u*601	C(10)...H(45)	299.6(37)	38.4(fixed)	—	4.0	38.4
*u*444	C(111)...H(127)	299.6(91)	29.4(fixed)	—	7.1	29.4
*u*420	H(30)...H(43)	299.7(23)	41.7(fixed)	—	18.7	41.7
*u*445	C(151)...C(152)	300.1(16)	12.6(tied to *u*519)	—	–0.2	11.7
*u*468	C(147)...C(148)	300.1(16)	12.8(tied to *u*519)	—	–0.1	11.9
*u*606	Si(3)...H(23)	300.1(33)	33.5(fixed)	—	5.1	33.5
*u*454	C(53)...C(54)	300.2(16)	12.8(tied to *u*519)	—	–0.2	11.9
*u*450	C(54)...C(64)	300.3(16)	12.7(tied to *u*519)	—	–0.1	11.8
*u*456	C(57)...C(58)	300.3(16)	12.5(tied to *u*519)	—	–0.1	11.7
*u*451	C(57)...C(63)	300.3(16)	12.5(tied to *u*519)	—	–0.1	11.6
*u*461	C(10)...C(16)	300.5(16)	12.8(tied to *u*519)	—	–0.1	11.9
*u*438	C(7)...C(17)	300.5(16)	12.7(tied to *u*519)	—	–0.2	11.8
*u*452	C(6)...C(7)	300.5(16)	12.8(tied to *u*519)	—	–0.1	11.9
*u*446	C(10)...C(11)	300.5(16)	12.5(tied to *u*519)	—	–0.1	11.6
*u*443	C(100)...C(101)	300.5(16)	12.6(tied to *u*519)	—	–0.1	11.7
*u*464	C(104)...C(105)	300.5(16)	12.6(tied to *u*519)	—	–0.1	11.8
*u*474	C(17)...H(33)	300.6(73)	30.1(fixed)	—	11.6	30.1
*u*1842	C(149)...H(164)	300.9(28)	34.5(fixed)	—	6.6	34.5
*u*2029	Cl(108)...H(112)	301.1(55)	30.5(fixed)	—	2.9	30.5
*u*462	C(102)...C(103)	301.5(28)	12.3(tied to *u*519)	—	–0.1	11.4
*u*593	C(58)...H(71)	301.9(37)	37.0(fixed)	—	3.9	37.0
*u*457	C(55)...C(56)	302.6(28)	12.3(tied to *u*519)	—	–0.1	11.4
*u*466	C(59)...C(60)	302.7(28)	12.2(tied to *u*519)	—	–0.1	11.4
*u*460	C(12)...C(13)	302.9(27)	12.5(tied to *u*519)	—	–0.1	11.7
*u*465	C(8)...C(9)	302.9(27)	12.4(tied to *u*519)	—	–0.1	11.5
*u*458	C(149)...C(150)	303.3(28)	12.5(tied to *u*519)	—	–0.1	11.7
*u*417	H(34)...H(43)	303.3(43)	43.2(fixed)	—	16.3	43.2
*u*429	Cl(15)...H(39)	303.4(39)	28.4(fixed)	—	11.3	28.4
*u*470	C(10)...H(40)	303.6(38)	32.2(fixed)	—	9.3	32.2
*u*531	Cl(62)...H(84)	303.7(27)	44.1(fixed)	—	5.4	44.1
*u*522	Si(3)...Si(5)	304.0(20)	10.8(tied to *u*519)	—	0.0	10.0
*u*613	Si(50)...Si(52)	304.1(20)	10.3(tied to *u*519)	—	0.1	9.6
*u*469	Cl(15)...H(37)	305.3(37)	35.7(fixed)	—	6.4	35.7
*u*2449	Cl(155)...H(170)	305.6(25)	34.9(fixed)	—	–0.9	34.9
*u*553	C(63)...H(87)	306.1(44)	35.6(fixed)	—	4.0	35.6
*u*442	C(152)...C(157)	306.6(36)	12.7(tied to *u*519)	—	–0.2	11.8
*u*440	C(53)...C(64)	306.8(36)	12.6(tied to *u*519)	—	–0.2	11.7
*u*441	C(58)...C(63)	306.9(36)	12.5(tied to *u*519)	—	–0.1	11.6
*u*603	C(8)...H(37)	306.9(37)	36.8(fixed)	—	3.5	36.8
*u*449	C(11)...C(16)	307.0(36)	13.0(tied to *u*519)	—	–0.2	12.1
*u*453	C(6)...C(17)	307.0(36)	12.7(tied to *u*519)	—	–0.2	11.8
*u*437	C(105)...C(110)	307.1(36)	12.5(tied to *u*519)	—	–0.1	11.6
*u*557	C(103)...H(119)	307.4(27)	24.7(fixed)	—	0.7	24.7
*u*545	C(13)...H(38)	307.4(26)	24.2(fixed)	—	0.6	24.2
*u*542	C(11)...H(29)	307.5(42)	40.2(fixed)	—	5.0	40.2
*u*588	C(7)...H(33)	307.6(27)	44.1(fixed)	—	5.9	44.1

*u*610	C(57)...H(92)	307.7(36)	37.3(fixed)	—	3.7	37.3
*u*537	C(9)...H(25)	307.9(26)	25.4(fixed)	—	1.3	25.4
*u*543	C(56)...H(72)	308.1(27)	25.1(fixed)	—	0.7	25.1
*u*517	C(102)...H(121)	308.2(27)	27.6(fixed)	—	1.9	27.6
*u*497	C(12)...H(41)	308.3(26)	25.6(fixed)	—	1.7	25.6
*u*544	C(60)...H(85)	308.4(27)	27.7(fixed)	—	1.5	27.7
*u*491	C(8)...H(27)	308.5(26)	25.4(fixed)	—	1.8	25.4
*u*471	Cl(109)...H(117)	308.5(26)	35.7(fixed)	—	5.9	35.7
*u*487	C(57)...H(87)	308.5(33)	30.1(fixed)	—	7.0	30.1
*u*416	C(56)...H(86)	308.6(37)	30.2(fixed)	—	8.4	30.2
*u*505	C(59)...H(88)	308.6(27)	24.1(fixed)	—	1.1	24.1
*u*473	C(13)...H(32)	308.7(38)	33.9(fixed)	—	14.8	33.9
*u*490	C(55)...H(74)	308.7(27)	23.9(fixed)	—	1.1	23.9
*u*565	C(55)...Cl(62)	308.8(12)	12.9(tied to *u*519)	—	–0.2	12.0
*u*548	C(56)...Cl(62)	308.8(12)	12.8(tied to *u*519)	—	–0.2	11.9
*u*567	C(16)...H(40)	308.8(48)	37.2(fixed)	—	4.8	37.2
*u*573	C(12)...Cl(14)	308.9(12)	13.0(tied to *u*519)	—	–0.2	12.1
*u*549	C(8)...Cl(15)	308.9(12)	12.9(tied to *u*519)	—	–0.2	12.0
*u*564	C(9)...Cl(15)	308.9(12)	12.9(tied to *u*519)	—	–0.2	12.0
*u*552	C(13)...Cl(14)	308.9(12)	12.8(tied to *u*519)	—	–0.2	11.9
*u*550	C(150)...H(166)	308.9(26)	25.8(fixed)	—	0.8	25.8
*u*498	C(60)...H(79)	309.0(32)	30.4(fixed)	—	8.9	30.4
*u*556	C(106)...Cl(108)	309.1(12)	12.7(tied to *u*519)	—	–0.1	11.8
*u*586	C(107)...Cl(108)	309.1(12)	12.8(tied to *u*519)	—	–0.1	11.9
*u*602	C(56)...H(89)	309.1(41)	35.2(fixed)	—	3.5	35.2
*u*476	Si(143)...Si(144)	309.2(6)	10.4(tied to *u*519)	—	0.0	9.7
*u*539	Si(96)...Si(97)	309.2(6)	10.1(tied to *u*519)	—	0.0	9.4
*u*523	Cl(14)...H(32)	309.2(29)	48.0(fixed)	—	7.8	48.0
*u*504	C(149)...H(168)	309.5(26)	24.4(fixed)	—	1.2	24.4
*u*555	C(153)...Cl(155)	309.6(12)	12.9(tied to *u*519)	—	–0.2	12.0
*u*566	C(154)...Cl(155)	309.6(12)	12.9(tied to *u*519)	—	–0.2	12.0
*u*577	C(59)...Cl(61)	309.6(12)	12.7(tied to *u*519)	—	–0.1	11.9
*u*551	C(60)...Cl(61)	309.6(12)	12.7(tied to *u*519)	—	–0.1	11.8
*u*1893	C(154)...H(159)	310.9(42)	32.5(fixed)	—	2.7	32.5
*u*554	C(151)...H(175)	311.4(17)	28.6(fixed)	—	0.8	28.6
*u*2169	C(100)...H(123)	311.6(49)	28.5(fixed)	—	3.9	28.5
*u*2959	C(106)...H(118)	311.7(66)	24.8(fixed)	—	–1.0	24.8
*u*502	Si(49)...Si(50)	311.7(6)	10.3(tied to *u*519)	—	0.0	9.6
*u*568	C(53)...H(68)	311.7(17)	25.8(fixed)	—	0.4	25.8
*u*519	Si(2)...Si(3)	311.8(6)	10.1(2)	—	0.0	9.4
*u*576	C(54)...H(93)	311.8(17)	26.8(fixed)	—	0.6	26.8
*u*605	H(79)...H(91)	311.8(42)	41.5(fixed)	—	4.7	41.5
*u*575	C(147)...H(162)	312.0(17)	29.6(fixed)	—	1.6	29.6
*u*583	C(57)...H(81)	312.0(17)	27.5(fixed)	—	0.9	27.5
*u*511	H(114)...H(117)	312.1(42)	38.6(fixed)	—	3.9	38.6
*u*541	C(7)...H(46)	312.1(17)	27.3(fixed)	—	0.6	27.3

*u*589	C(6)...H(21)	312.2(17)	28.4(fixed)	—	0.9	28.4
*u*520	Si(97)...Si(98)	312.2(4)	10.7(tied to *u*519)	—	0.0	10.0
*u*547	C(63)...H(77)	312.2(17)	26.3(fixed)	—	0.9	26.3
*u*546	C(100)...H(115)	312.2(17)	24.8(fixed)	—	0.3	24.8
*u*621	Si(144)...Si(145)	312.3(4)	10.2(tied to *u*519)	—	0.1	9.5
*u*506	C(54)...H(66)	312.3(17)	25.8(fixed)	—	0.9	25.8
*u*512	C(148)...H(160)	312.3(17)	25.4(fixed)	—	1.2	25.4
*u*496	C(64)...H(68)	312.4(17)	25.0(fixed)	—	0.8	25.0
*u*578	C(104)...H(128)	312.4(17)	25.3(fixed)	—	0.6	25.3
*u*630	H(125)...H(127)	312.5(42)	37.0(fixed)	—	4.0	37.0
*u*535	H(67)...H(70)	312.6(42)	37.9(fixed)	—	4.3	37.9
*u*489	C(57)...H(90)	312.6(17)	24.1(fixed)	—	1.0	24.1
*u*615	C(148)...H(174)	312.6(36)	39.5(fixed)	—	4.6	39.5
*u*509	C(58)...H(77)	312.6(17)	25.8(fixed)	—	1.3	25.8
*u*536	C(10)...H(34)	312.7(17)	28.9(fixed)	—	1.5	28.9
*u*507	C(7)...H(19)	312.7(17)	26.2(fixed)	—	1.1	26.2
*u*561	H(69)...H(92)	312.8(42)	39.0(fixed)	—	4.8	39.0
*u*501	C(111)...H(115)	312.8(17)	24.2(fixed)	—	0.8	24.2
*u*500	C(152)...H(171)	312.8(17)	28.0(fixed)	—	2.1	28.0
*u*525	C(11)...H(30)	312.9(17)	30.9(fixed)	—	2.1	30.9
*u*560	H(78)...H(80)	312.9(42)	42.1(fixed)	—	6.0	42.1
*u*481	C(101)...H(113)	313.1(17)	24.7(fixed)	—	1.1	24.7
*u*671	H(173)...H(185)	313.2(42)	44.7(fixed)	—	6.8	44.7
*u*534	C(16)...H(30)	313.3(17)	29.8(fixed)	—	2.3	29.8
*u*478	C(17)...H(21)	313.4(17)	26.5(fixed)	—	1.7	26.5
*u*743	Si(143)...H(159)	313.6(15)	31.5(fixed)	—	3.6	31.5
*u*689	C(59)...H(67)	313.8(37)	38.9(fixed)	—	2.9	38.9
*u*770	C(16)...H(39)	313.8(39)	47.4(fixed)	—	2.9	47.4
*u*515	H(22)...H(45)	313.8(42)	41.3(fixed)	—	6.2	41.3
*u*730	Si(146)...H(174)	313.9(19)	31.6(fixed)	—	5.3	31.6
*u*569	H(20)...H(23)	314.0(42)	40.2(fixed)	—	6.1	40.2
*u*510	H(172)...H(174)	314.1(42)	45.0(fixed)	—	7.8	45.0
*u*668	C(54)...H(80)	314.1(36)	41.5(fixed)	—	4.3	41.5
*u*2231	C(149)...H(163)	314.2(25)	46.4(fixed)	—	–0.7	46.4
*u*530	C(10)...H(43)	314.3(17)	34.0(fixed)	—	4.1	34.0
*u*2578	C(152)...H(165)	314.3(37)	26.4(fixed)	—	–4.2	26.4
*u*528	Si(50)...Si(51)	314.8(4)	10.7(tied to *u*519)	—	0.0	9.9
*u*596	Si(49)...Si(51)	314.8(4)	10.5(tied to *u*519)	—	0.0	9.8
*u*590	Si(2)...Si(4)	314.8(4)	10.6(tied to *u*519)	—	0.0	9.8
*u*595	Si(3)...Si(4)	314.8(4)	10.4(tied to *u*519)	—	0.0	9.7
*u*612	Si(2)...Si(5)	314.8(4)	10.4(tied to *u*519)	—	0.0	9.7
*u*591	Si(143)...Si(145)	314.8(4)	10.5(tied to *u*519)	—	0.0	9.8
*u*617	Si(96)...Si(98)	314.9(4)	10.3(tied to *u*519)	—	0.1	9.5
*u*607	Si(49)...Si(52)	314.9(4)	10.3(tied to *u*519)	—	0.1	9.6
*u*609	Si(98)...Si(99)	315.3(5)	10.9(tied to *u*519)	—	0.1	10.2
*u*619	Si(145)...Si(146)	315.3(5)	10.7(tied to *u*519)	—	0.1	10.0

*u*2612	C(107)...H(118)	315.5(32)	21.5(fixed)	—	–2.2	21.5
*u*704	C(10)...H(47)	315.8(47)	42.7(fixed)	—	3.0	42.7
*u*720	Si(49)...H(65)	315.8(15)	31.9(fixed)	—	3.6	31.9
*u*705	Si(99)...H(127)	316.1(22)	30.9(fixed)	—	3.7	30.9
*u*618	C(1)...C(7)	316.3(8)	11.9(tied to *u*519)	—	–0.1	11.0
*u*636	C(95)...C(105)	316.3(8)	11.8(tied to *u*519)	—	–0.1	10.9
*u*631	C(1)...C(16)	316.3(8)	12.0(tied to *u*519)	—	–0.1	11.2
*u*670	C(1)...C(17)	316.3(8)	12.1(tied to *u*519)	—	–0.1	11.2
*u*639	C(1)...C(11)	316.3(8)	12.0(tied to *u*519)	—	–0.1	11.2
*u*663	C(95)...C(100)	316.3(8)	11.8(tied to *u*519)	—	0.0	11.0
*u*646	C(1)...C(6)	316.3(8)	11.8(tied to *u*519)	—	–0.1	11.0
*u*628	C(1)...C(10)	316.3(8)	11.8(tied to *u*519)	—	–0.1	11.0
*u*642	C(95)...C(101)	316.3(8)	11.6(tied to *u*519)	—	0.0	10.8
*u*719	C(9)...H(22)	316.4(56)	45.4(fixed)	—	3.2	45.4
*u*624	C(48)...C(54)	316.5(8)	12.0(tied to *u*519)	—	–0.1	11.2
*u*667	C(48)...C(53)	316.5(8)	12.0(tied to *u*519)	—	–0.1	11.1
*u*638	C(48)...C(58)	316.5(8)	11.7(tied to *u*519)	—	–0.1	10.9
*u*654	C(48)...C(64)	316.5(8)	11.8(tied to *u*519)	—	–0.1	11.0
*u*634	C(48)...C(57)	316.5(8)	11.8(tied to *u*519)	—	0.0	11.0
*u*632	C(48)...C(63)	316.5(8)	11.5(tied to *u*519)	—	0.0	10.7
*u*657	C(142)...C(152)	316.6(8)	12.2(tied to *u*519)	—	–0.1	11.3
*u*620	C(142)...C(148)	316.6(8)	11.9(tied to *u*519)	—	–0.1	11.0
*u*640	C(142)...C(147)	316.7(8)	11.7(tied to *u*519)	—	0.0	10.9
*u*712	Si(51)...H(92)	316.7(21)	30.9(fixed)	—	4.2	30.9
*u*495	C(59)...H(76)	316.8(22)	30.6(fixed)	—	7.0	30.6
*u*739	Si(2)...H(18)	316.9(14)	32.6(fixed)	—	3.9	32.6
*u*503	H(31)...H(33)	316.9(42)	44.3(fixed)	—	10.1	44.3
*u*633	H(32)...H(44)	316.9(42)	54.2(fixed)	—	13.3	54.2
*u*1539	Si(143)...H(170)	317.0(13)	27.7(fixed)	—	–1.6	27.7
*u*759	Si(5)...H(24)	317.1(32)	32.9(fixed)	—	4.8	32.9
*u*666	Cl(62)...H(74)	317.4(12)	26.7(fixed)	—	0.6	26.7
*u*558	C(158)...H(160)	317.4(37)	27.0(fixed)	—	0.5	27.0
*u*655	Cl(109)...H(121)	317.5(12)	30.4(fixed)	—	1.8	30.4
*u*687	C(57)...H(94)	317.5(47)	41.5(fixed)	—	3.1	41.5
*u*571	Cl(109)...H(119)	317.6(12)	26.1(fixed)	—	1.1	26.1
*u*749	Si(4)...H(45)	317.8(21)	31.6(fixed)	—	4.4	31.6
*u*665	Cl(61)...H(88)	317.9(12)	27.6(fixed)	—	0.6	27.6
*u*623	Si(4)...Si(5)	317.9(6)	10.9(tied to *u*519)	—	0.1	10.1
*u*614	Si(51)...Si(52)	317.9(6)	10.9(tied to *u*519)	—	0.1	10.1
*u*570	C(58)...H(90)	317.9(36)	25.1(fixed)	—	0.4	25.1
*u*581	Cl(62)...H(72)	318.0(12)	26.6(fixed)	—	1.2	26.6
*u*529	C(64)...H(66)	318.0(36)	25.7(fixed)	—	0.6	25.7
*u*674	Cl(15)...H(27)	318.1(12)	29.9(fixed)	—	0.9	29.9
*u*641	Cl(14)...H(41)	318.2(12)	30.3(fixed)	—	1.1	30.3
*u*672	Si(96)...H(112)	318.2(18)	29.8(fixed)	—	4.0	29.8
*u*540	C(111)...H(113)	318.3(36)	26.0(fixed)	—	0.5	26.0

*u*664	Cl(156)...H(168)	318.3(12)	27.5(fixed)	—	0.8	27.5
*u*559	C(17)...H(19)	318.5(36)	25.9(fixed)	—	0.7	25.9
*u*484	C(157)...H(175)	318.6(37)	26.4(fixed)	—	1.6	26.4
*u*598	Cl(14)...H(38)	318.8(12)	26.1(fixed)	—	0.9	26.1
*u*479	C(110)...H(128)	318.8(36)	25.1(fixed)	—	0.9	25.1
*u*486	C(63)...H(81)	318.8(36)	26.5(fixed)	—	1.5	26.5
*u*477	C(53)...H(93)	318.8(36)	25.0(fixed)	—	1.3	25.0
*u*592	Cl(15)...H(25)	318.9(12)	28.4(fixed)	—	1.4	28.4
*u*648	C(95)...C(103)	318.9(7)	11.5(tied to *u*519)	—	0.0	10.7
*u*644	C(95)...C(102)	318.9(7)	11.4(tied to *u*519)	—	0.0	10.6
*u*645	C(142)...C(149)	318.9(7)	11.7(tied to *u*519)	—	0.0	10.8
*u*661	C(142)...C(150)	318.9(7)	11.6(tied to *u*519)	—	0.0	10.8
*u*611	Cl(61)...H(85)	318.9(12)	29.1(fixed)	—	1.9	29.1
*u*584	Cl(156)...H(166)	319.0(12)	27.2(fixed)	—	1.4	27.2
*u*508	C(16)...H(34)	319.0(36)	28.6(fixed)	—	1.7	28.6
*u*653	C(48)...C(60)	319.1(7)	11.6(tied to *u*519)	—	0.0	10.8
*u*659	C(48)...C(55)	319.1(7)	11.6(tied to *u*519)	—	0.0	10.8
*u*643	C(48)...C(59)	319.1(7)	11.5(tied to *u*519)	—	0.0	10.7
*u*650	C(48)...C(56)	319.1(7)	11.4(tied to *u*519)	—	0.0	10.6
*u*877	C(54)...C(55)	319.1(50)	22.0(tied to *u*519)	—	0.9	20.5
*u*762	C(11)...H(28)	319.2(35)	46.2(fixed)	—	3.0	46.2
*u*488	C(6)...H(46)	319.2(36)	25.6(fixed)	—	1.4	25.6
*u*521	C(56)...H(84)	319.6(21)	31.5(fixed)	—	10.4	31.5
*u*758	C(148)...H(176)	319.7(35)	47.6(fixed)	—	2.9	47.6
*u*538	C(11)...H(43)	319.7(37)	35.0(fixed)	—	3.6	35.0
*u*775	C(101)...H(129)	319.8(39)	40.3(fixed)	—	2.6	40.3
*u*673	C(1)...C(13)	320.0(7)	11.8(tied to *u*519)	—	0.0	11.0
*u*482	C(16)...H(29)	320.0(51)	30.7(fixed)	—	9.4	30.7
*u*656	C(1)...C(9)	320.1(7)	11.6(tied to *u*519)	—	0.0	10.8
*u*662	C(1)...C(8)	320.1(7)	11.4(tied to *u*519)	—	0.0	10.6
*u*647	C(1)...C(12)	320.1(7)	11.4(tied to *u*519)	—	0.0	10.6
*u*736	Si(52)...H(80)	320.4(21)	32.7(fixed)	—	5.0	32.7
*u*748	Si(97)...H(117)	320.5(18)	29.0(fixed)	—	3.0	29.0
*u*691	Si(144)...H(164)	320.7(16)	33.3(fixed)	—	7.8	33.3
*u*2703	C(100)...H(122)	321.1(37)	26.4(fixed)	—	–4.3	26.4
*u*1579	Si(145)...H(165)	321.8(16)	29.3(fixed)	—	–2.0	29.3
*u*724	C(10)...H(44)	322.1(26)	41.9(fixed)	—	1.4	41.9
*u*2008	Cl(155)...H(169)	322.3(33)	34.0(fixed)	—	3.3	34.0
*u*1912	Si(96)...H(118)	322.5(16)	21.1(fixed)	—	–0.4	21.1
*u*721	Si(5)...H(33)	322.8(22)	35.7(fixed)	—	6.6	35.7
*u*694	C(158)...H(163)	323.0(26)	32.7(fixed)	—	0.5	32.7
*u*725	C(58)...H(78)	323.4(26)	28.5(fixed)	—	0.1	28.5
*u*972	H(70)...H(72)	323.4(60)	46.3(fixed)	—	2.3	46.3
*u*726	C(147)...H(164)	323.5(26)	32.3(fixed)	—	1.0	32.3
*u*742	C(57)...H(91)	323.5(26)	26.2(fixed)	—	–0.1	26.2
*u*688	C(63)...H(79)	323.6(26)	29.1(fixed)	—	0.5	29.1

*u*709	C(17)...H(22)	323.7(26)	29.2(fixed)	—	0.2	29.2
*u*713	C(101)...H(114)	323.7(26)	27.1(fixed)	—	–0.1	27.1
*u*773	C(148)...H(161)	323.7(26)	26.6(fixed)	—	0.1	26.6
*u*738	Si(49)...H(79)	323.7(17)	30.8(fixed)	—	5.1	30.8
*u*717	C(54)...H(67)	323.8(26)	26.3(fixed)	—	0.0	26.3
*u*727	C(64)...H(69)	323.9(26)	25.7(fixed)	—	0.0	25.7
*u*680	C(11)...H(31)	323.9(26)	33.2(fixed)	—	1.2	33.2
*u*732	C(16)...H(32)	323.9(26)	32.7(fixed)	—	1.1	32.7
*u*682	C(57)...H(80)	324.0(26)	28.4(fixed)	—	0.7	28.4
*u*740	Cl(61)...H(78)	324.0(22)	46.0(fixed)	—	2.9	46.0
*u*729	C(7)...H(20)	324.0(26)	26.7(fixed)	—	0.1	26.7
*u*761	C(111)...H(116)	324.1(26)	24.8(fixed)	—	–0.1	24.8
*u*1003	H(69)...H(71)	324.1(61)	48.8(fixed)	—	2.1	48.8
*u*669	C(151)...H(174)	324.1(26)	28.1(fixed)	—	0.8	28.1
*u*676	C(53)...H(70)	324.2(26)	25.6(fixed)	—	0.3	25.6
*u*679	C(54)...H(92)	324.2(26)	27.4(fixed)	—	0.6	27.4
*u*747	C(12)...H(20)	324.2(36)	40.0(fixed)	—	3.0	40.0
*u*1518	Cl(109)...H(116)	324.3(28)	35.2(fixed)	—	–2.3	35.2
*u*635	C(100)...H(117)	324.3(26)	25.3(fixed)	—	0.2	25.3
*u*681	C(6)...H(23)	324.3(26)	29.2(fixed)	—	0.8	29.2
*u*698	C(104)...H(127)	324.4(26)	25.9(fixed)	—	0.4	25.9
*u*677	C(10)...H(33)	324.4(26)	29.8(fixed)	—	1.0	29.8
*u*637	C(7)...H(45)	324.4(26)	27.6(fixed)	—	0.7	27.6
*u*1869	Si(99)...H(123)	324.7(13)	22.0(fixed)	—	1.2	22.0
*u*782	Cl(15)...H(26)	324.9(23)	30.8(fixed)	—	0.2	30.8
*u*801	Cl(14)...H(36)	325.2(23)	27.7(fixed)	—	–0.1	27.7
*u*745	C(1)...Cl(14)	325.2(12)	12.3(tied to *u*519)	—	–0.2	11.5
*u*750	C(1)...Cl(15)	325.2(12)	12.3(tied to *u*519)	—	–0.1	11.4
*u*787	C(63)...H(86)	325.4(32)	41.5(fixed)	—	2.3	41.5
*u*751	Cl(14)...H(40)	325.7(23)	30.0(fixed)	—	0.8	30.0
*u*746	Cl(15)...H(29)	325.7(23)	30.2(fixed)	—	0.9	30.2
*u*804	Cl(62)...H(73)	326.1(23)	28.2(fixed)	—	0.0	28.2
*u*767	C(48)...Cl(62)	326.2(12)	12.2(tied to *u*519)	—	–0.1	11.3
*u*675	Si(50)...H(89)	326.2(18)	28.7(fixed)	—	3.3	28.7
*u*1020	H(39)...H(42)	326.3(60)	88.7(fixed)	—	–1.7	88.7
*u*737	Cl(62)...H(76)	326.5(23)	28.2(fixed)	—	0.4	28.2
*u*792	Cl(156)...H(167)	326.5(23)	29.8(fixed)	—	0.0	29.8
*u*794	Cl(61)...H(83)	326.5(23)	32.3(fixed)	—	0.5	32.3
*u*585	H(118)...H(122)	326.7(66)	41.6(fixed)	—	5.9	41.6
*u*771	C(142)...Cl(155)	326.8(12)	12.2(tied to *u*519)	—	–0.1	11.3
*u*752	Cl(62)...H(83)	326.9(28)	52.9(fixed)	—	3.1	52.9
*u*777	Cl(156)...H(170)	326.9(23)	29.1(fixed)	—	0.4	29.1
*u*756	C(48)...Cl(61)	327.0(12)	12.1(tied to *u*519)	—	–0.1	11.3
*u*527	H(82)...H(89)	327.2(74)	40.4(fixed)	—	5.1	40.4
*u*516	H(65)...H(94)	327.3(74)	39.9(fixed)	—	4.8	39.9
*u*741	Cl(61)...H(87)	327.3(23)	27.6(fixed)	—	0.5	27.6

*u*791	Cl(109)...H(120)	327.3(23)	28.1(fixed)	—	0.0	28.1
*u*703	Si(4)...H(40)	327.4(12)	32.1(fixed)	—	5.4	32.1
*u*789	Cl(109)...H(123)	327.4(23)	32.9(fixed)	—	1.0	32.9
*u*513	H(129)...H(136)	327.5(74)	38.5(fixed)	—	4.6	38.5
*u*760	C(95)...Cl(108)	327.5(12)	12.2(tied to *u*519)	—	–0.1	11.3
*u*776	Si(3)...H(37)	327.6(14)	31.2(fixed)	—	3.1	31.2
*u*711	Si(51)...H(87)	327.6(12)	29.5(fixed)	—	4.0	29.5
*u*572	H(18)...H(47)	327.8(74)	39.6(fixed)	—	4.9	39.6
*u*499	H(176)...H(183)	327.9(74)	40.6(fixed)	—	5.7	40.6
*u*1489	C(106)...H(114)	328.0(39)	33.5(fixed)	—	–2.4	33.5
*u*707	Si(2)...H(32)	328.5(17)	35.2(fixed)	—	9.1	35.2
*u*714	Si(4)...H(29)	328.5(12)	32.6(fixed)	—	5.4	32.6
*u*629	Si(49)...H(76)	328.8(15)	29.2(fixed)	—	3.9	29.2
*u*2220	C(154)...H(161)	329.0(35)	35.7(fixed)	—	–0.6	35.7
*u*810	Cl(14)...H(31)	329.0(33)	61.4(fixed)	—	2.8	61.4
*u*597	H(165)...H(169)	329.0(65)	41.3(fixed)	—	4.8	41.3
*u*604	H(71)...H(75)	329.3(65)	38.6(fixed)	—	4.2	38.6
*u*723	C(102)...H(122)	330.0(43)	30.7(fixed)	—	0.3	30.7
*u*807	C(7)...H(35)	330.2(43)	51.1(fixed)	—	2.7	51.1
*u*1004	H(175)...H(186)	330.3(70)	41.9(fixed)	—	6.1	41.9
*u*652	H(84)...H(86)	330.4(65)	40.2(fixed)	—	5.7	40.2
*u*781	Cl(15)...H(44)	330.6(41)	73.1(fixed)	—	5.0	73.1
*u*967	C(53)...Cl(62)	330.7(44)	21.1(tied to *u*897)	—	0.9	21.8
*u*693	C(103)...H(118)	330.8(43)	25.8(fixed)	—	0.3	25.8
*u*563	C(60)...H(76)	330.9(41)	35.4(fixed)	—	4.1	35.4
*u*658	H(24)...H(28)	331.1(64)	42.4(fixed)	—	5.4	42.4
*u*580	H(37)...H(39)	331.1(64)	39.7(fixed)	—	4.8	39.7
*u*763	Si(50)...H(84)	331.5(14)	32.6(fixed)	—	5.9	32.6
*u*796	C(6)...H(26)	331.6(48)	44.7(fixed)	—	2.9	44.7
*u*587	H(35)...H(42)	331.8(75)	52.9(fixed)	—	12.6	52.9
*u*798	C(54)...H(82)	332.2(44)	46.3(fixed)	—	2.8	46.3
*u*778	Si(51)...H(71)	332.3(16)	32.0(fixed)	—	3.6	32.0
*u*753	C(55)...H(75)	332.5(42)	26.3(fixed)	—	–0.2	26.3
*u*733	C(149)...H(169)	332.5(42)	27.6(fixed)	—	–0.1	27.6
*u*853	H(30)...H(44)	332.5(26)	66.0(fixed)	—	–3.5	66.0
*u*757	C(59)...H(86)	332.6(42)	25.7(fixed)	—	–0.1	25.7
*u*718	C(60)...H(84)	332.7(42)	29.6(fixed)	—	0.6	29.6
*u*690	C(150)...H(165)	332.9(42)	28.0(fixed)	—	0.3	28.0
*u*692	C(11)...H(42)	332.9(51)	41.9(fixed)	—	2.1	41.9
*u*766	C(8)...H(28)	332.9(41)	28.9(fixed)	—	–0.1	28.9
*u*686	C(56)...H(71)	332.9(42)	26.2(fixed)	—	0.3	26.2
*u*908	Si(50)...C(54)	333.0(31)	15.6(tied to *u*897)	—	0.2	16.2
*u*731	C(12)...H(39)	333.1(41)	28.5(fixed)	—	0.0	28.5
*u*710	C(9)...H(24)	333.4(41)	28.8(fixed)	—	0.3	28.8
*u*702	C(53)...H(94)	333.4(51)	27.8(fixed)	—	0.0	27.8
*u*715	C(63)...H(82)	333.4(51)	28.5(fixed)	—	0.2	28.5

*u*700	C(157)...H(176)	333.4(51)	28.7(fixed)	—	0.2	28.7
*u*492	C(9)...H(42)	333.5(55)	40.5(fixed)	—	23.7	40.5
*u*685	C(13)...H(37)	333.5(41)	26.2(fixed)	—	0.1	26.2
*u*735	C(6)...H(47)	333.6(51)	27.6(fixed)	—	–0.1	27.6
*u*716	C(16)...H(35)	333.7(51)	30.4(fixed)	—	0.5	30.4
*u*699	C(110)...H(129)	333.8(50)	26.0(fixed)	—	0.0	26.0
*u*651	C(58)...H(89)	334.0(51)	25.9(fixed)	—	0.4	25.9
*u*626	C(158)...H(159)	334.0(51)	26.5(fixed)	—	0.5	26.5
*u*660	C(64)...H(65)	334.0(51)	26.6(fixed)	—	0.4	26.6
*u*649	C(111)...H(112)	334.2(51)	26.8(fixed)	—	0.5	26.8
*u*678	C(17)...H(18)	334.2(50)	26.9(fixed)	—	0.4	26.9
*u*838	Si(3)...C(7)	334.5(30)	15.5(tied to *u*897)	—	0.1	16.1
*u*982	H(67)...H(84)	335.5(41)	58.0(fixed)	—	1.2	58.0
*u*849	H(32)...H(43)	336.0(26)	61.8(fixed)	—	–1.6	61.8
*u*728	Si(3)...H(42)	336.1(20)	43.0(fixed)	—	14.3	43.0
*u*1042	H(68)...H(73)	337.1(61)	31.2(fixed)	—	5.3	31.2
*u*514	C(55)...H(89)	337.2(49)	30.3(fixed)	—	6.3	30.3
*u*873	H(172)...H(175)	337.3(25)	51.7(fixed)	—	–2.9	51.7
*u*708	C(8)...H(36)	337.5(29)	37.0(fixed)	—	3.0	37.0
*u*839	H(31)...H(34)	337.6(25)	54.8(fixed)	—	–2.3	54.8
*u*2298	C(105)...Cl(109)	338.4(42)	18.4(tied to *u*897)	—	–0.9	19.0
*u*532	C(63)...H(71)	338.5(48)	32.0(fixed)	—	6.8	32.0
*u*817	H(30)...H(33)	338.6(25)	53.9(fixed)	—	–1.6	53.9
*u*954	H(32)...H(47)	339.1(53)	69.6(fixed)	—	1.1	69.6
*u*878	C(53)...C(59)	339.3(19)	19.9(tied to *u*897)	—	0.9	20.6
*u*1072	H(176)...H(186)	339.4(97)	40.7(fixed)	—	3.8	40.7
*u*999	H(23)...H(25)	339.6(54)	40.5(fixed)	—	6.7	40.5
*u*880	H(119)...H(122)	340.1(40)	45.7(fixed)	—	–2.4	45.7
*u*903	H(78)...H(81)	340.1(25)	45.0(fixed)	—	–2.2	45.0
*u*899	H(22)...H(46)	340.1(25)	45.2(fixed)	—	–2.5	45.2
*u*820	H(160)...H(164)	340.2(25)	48.3(fixed)	—	–1.1	48.3
*u*922	H(161)...H(162)	340.4(25)	45.2(fixed)	—	–1.7	45.2
*u*790	H(171)...H(174)	340.6(25)	48.6(fixed)	—	–0.6	48.6
*u*918	H(20)...H(21)	341.0(25)	43.5(fixed)	—	–2.1	43.5
*u*868	C(95)...H(127)	341.4(10)	23.3(fixed)	—	0.4	23.3
*u*861	C(1)...H(18)	341.4(10)	23.8(fixed)	—	0.5	23.8
*u*858	C(95)...H(117)	341.4(10)	21.9(fixed)	—	0.3	21.9
*u*764	C(58)...H(73)	341.5(36)	40.7(fixed)	—	2.6	40.7
*u*933	C(101)...C(105)	341.5(28)	21.2(tied to *u*897)	—	0.8	21.9
*u*852	C(48)...H(70)	341.5(10)	23.1(fixed)	—	0.3	23.1
*u*803	H(77)...H(80)	341.5(25)	45.1(fixed)	—	–0.7	45.1
*u*835	C(1)...H(47)	341.6(10)	24.9(fixed)	—	0.8	24.9
*u*891	C(95)...H(112)	341.6(10)	22.5(fixed)	—	0.5	22.5
*u*916	H(69)...H(93)	341.6(25)	40.4(fixed)	—	–1.9	40.4
*u*867	C(48)...H(65)	341.6(10)	23.5(fixed)	—	0.5	23.5
*u*828	C(95)...H(114)	341.6(10)	23.7(fixed)	—	0.7	23.7

*u*825	C(95)...H(116)	341.6(10)	22.4(fixed)	—	0.5	22.4
*u*856	C(1)...H(33)	341.6(10)	26.9(fixed)	—	1.2	26.9
*u*864	C(1)...H(23)	341.6(10)	24.6(fixed)	—	0.9	24.6
*u*885	C(1)...H(45)	341.7(10)	23.4(fixed)	—	0.7	23.4
*u*874	C(48)...H(89)	341.7(10)	21.7(fixed)	—	0.4	21.7
*u*826	C(95)...H(129)	341.7(10)	22.8(fixed)	—	0.7	22.8
*u*907	H(77)...H(91)	341.7(25)	40.4(fixed)	—	–1.7	40.4
*u*2934	H(168)...H(181)	341.7(48)	32.4(fixed)	—	–6.5	32.4
*u*886	H(67)...H(68)	341.7(25)	40.2(fixed)	—	–1.8	40.2
*u*819	C(48)...H(69)	341.7(10)	23.8(fixed)	—	0.6	23.8
*u*989	H(81)...H(92)	341.8(69)	42.0(fixed)	—	4.6	42.0
*u*866	C(48)...H(80)	341.8(10)	24.1(fixed)	—	0.8	24.1
*u*832	C(142)...H(176)	341.8(10)	26.6(fixed)	—	0.9	26.6
*u*793	H(19)...H(23)	341.8(25)	45.9(fixed)	—	–0.7	45.9
*u*834	C(48)...H(67)	341.8(10)	23.7(fixed)	—	0.7	23.7
*u*808	C(1)...H(22)	341.8(10)	25.7(fixed)	—	1.2	25.7
*u*859	C(142)...H(183)	341.8(10)	23.1(fixed)	—	0.4	23.1
*u*879	C(48)...H(92)	341.9(10)	22.9(fixed)	—	0.6	22.9
*u*822	C(48)...H(94)	341.9(10)	24.3(fixed)	—	0.9	24.3
*u*830	C(1)...H(20)	341.9(10)	23.6(fixed)	—	1.0	23.6
*u*809	H(118)...H(121)	341.9(40)	45.3(fixed)	—	–0.7	45.3
*u*821	C(48)...H(91)	341.9(10)	22.7(fixed)	—	0.7	22.7
*u*895	H(114)...H(115)	342.0(25)	39.7(fixed)	—	–2.0	39.7
*u*795	H(79)...H(90)	342.0(25)	42.7(fixed)	—	–0.8	42.7
*u*829	C(48)...H(78)	342.1(10)	24.3(fixed)	—	1.1	24.3
*u*824	C(48)...H(82)	342.1(10)	25.1(fixed)	—	1.2	25.1
*u*836	C(1)...H(31)	342.1(10)	28.3(fixed)	—	1.9	28.3
*u*827	C(142)...H(161)	342.1(10)	24.4(fixed)	—	0.9	24.4
*u*837	C(1)...H(35)	342.1(10)	25.7(fixed)	—	1.5	25.7
*u*854	C(48)...H(79)	342.1(10)	23.2(fixed)	—	1.0	23.2
*u*1032	C(152)...C(158)	342.2(64)	20.3(tied to *u*897)	—	0.5	21.0
*u*744	H(21)...H(45)	342.3(25)	45.7(fixed)	—	–0.3	45.7
*u*875	C(142)...H(174)	342.3(10)	23.5(fixed)	—	1.0	23.5
*u*818	C(142)...H(163)	342.4(10)	28.0(fixed)	—	1.7	28.0
*u*840	C(1)...H(32)	342.5(10)	27.6(fixed)	—	2.1	27.6
*u*906	H(25)...H(28)	342.5(39)	43.5(fixed)	—	–2.0	43.5
*u*786	H(68)...H(92)	342.5(25)	42.0(fixed)	—	–0.6	42.0
*u*797	H(66)...H(70)	342.7(25)	40.7(fixed)	—	–0.7	40.7
*u*930	H(125)...H(128)	342.7(25)	38.0(fixed)	—	–1.6	38.0
*u*887	H(38)...H(39)	342.8(39)	42.0(fixed)	—	–2.1	42.0
*u*846	C(142)...H(164)	342.8(10)	25.5(fixed)	—	1.8	25.5
*u*900	H(85)...H(86)	342.9(39)	44.0(fixed)	—	–1.7	44.0
*u*1038	H(23)...H(27)	343.0(63)	53.7(fixed)	—	3.4	53.7
*u*814	H(84)...H(88)	343.1(39)	45.4(fixed)	—	–1.2	45.4
*u*844	C(1)...H(42)	343.1(10)	32.3(fixed)	—	3.6	32.3
*u*2712	H(172)...H(178)	343.1(37)	45.0(fixed)	—	–4.3	45.0

*u*815	H(34)...H(42)	343.1(50)	64.3(fixed)	—	–2.7	64.3
*u*909	C(7)...C(9)	343.3(53)	20.8(tied to *u*897)	—	0.9	21.5
*u*977	Si(52)...Cl(62)	343.3(31)	17.0(tied to *u*897)	—	0.1	17.6
*u*2081	C(148)...C(149)	343.3(20)	16.3(tied to *u*897)	—	–0.9	16.8
*u*800	H(124)...H(127)	343.5(25)	39.5(fixed)	—	–0.5	39.5
*u*833	C(1)...H(44)	343.5(10)	31.9(fixed)	—	3.9	31.9
*u*805	H(24)...H(27)	343.5(39)	44.9(fixed)	—	–0.6	44.9
*u*892	H(166)...H(169)	343.5(39)	42.0(fixed)	—	–1.9	42.0
*u*755	H(126)...H(137)	343.6(25)	39.6(fixed)	—	–0.4	39.6
*u*915	H(72)...H(75)	343.6(39)	40.0(fixed)	—	–1.9	40.0
*u*894	C(10)...C(17)	344.1(34)	20.5(tied to *u*897)	—	0.9	21.3
*u*799	H(37)...H(41)	344.3(39)	42.3(fixed)	—	–0.5	42.3
*u*881	C(142)...H(165)	344.4(9)	24.0(fixed)	—	0.4	24.0
*u*806	H(165)...H(168)	344.6(39)	42.3(fixed)	—	–0.8	42.3
*u*848	C(142)...H(169)	344.6(9)	24.0(fixed)	—	0.6	24.0
*u*889	C(95)...H(118)	344.7(9)	22.8(fixed)	—	0.3	22.8
*u*1049	C(54)...Cl(62)	344.8(43)	24.5(tied to *u*897)	—	0.3	25.3
*u*1016	H(28)...H(33)	344.9(57)	62.6(fixed)	—	2.0	62.6
*u*788	H(71)...H(74)	344.9(39)	40.3(fixed)	—	–0.6	40.3
*u*896	C(48)...H(71)	345.0(9)	23.2(fixed)	—	0.3	23.2
*u*847	C(95)...H(122)	345.2(9)	26.0(fixed)	—	1.2	26.0
*u*845	C(48)...H(86)	345.2(9)	24.0(fixed)	—	0.5	24.0
*u*905	C(13)...C(16)	345.3(37)	21.5(tied to *u*897)	—	1.0	22.2
*u*842	C(48)...H(75)	345.4(9)	22.5(fixed)	—	0.6	22.5
*u*870	C(48)...H(84)	345.5(9)	24.8(fixed)	—	1.0	24.8
*u*882	C(1)...H(37)	345.7(9)	22.6(fixed)	—	0.1	22.6
*u*862	C(1)...H(39)	345.7(9)	25.9(fixed)	—	0.7	25.9
*u*890	C(1)...H(24)	345.8(9)	24.4(fixed)	—	0.5	24.4
*u*948	C(6)...C(8)	346.0(42)	21.1(tied to *u*897)	—	0.8	21.8
*u*863	H(35)...H(43)	346.0(50)	58.0(fixed)	—	–2.0	58.0
*u*843	C(1)...H(28)	346.0(9)	25.3(fixed)	—	0.9	25.3
*u*2036	C(147)...Cl(156)	346.3(32)	19.7(tied to *u*897)	—	–1.1	20.4
*u*850	C(142)...H(170)	346.5(9)	22.2(fixed)	—	0.8	22.2
*u*813	C(142)...H(167)	346.6(9)	23.6(fixed)	—	1.0	23.6
*u*855	C(48)...H(76)	346.6(9)	21.8(fixed)	—	0.6	21.8
*u*812	C(95)...H(120)	346.6(9)	22.2(fixed)	—	0.9	22.2
*u*851	C(48)...H(87)	346.6(9)	22.0(fixed)	—	0.7	22.0
*u*823	C(48)...H(73)	346.7(9)	23.1(fixed)	—	0.9	23.1
*u*1066	C(100)...C(106)	346.8(23)	21.1(tied to *u*897)	—	0.4	21.8
*u*944	Si(146)...C(152)	346.8(18)	16.1(tied to *u*897)	—	0.2	16.7
*u*1008	H(80)...H(93)	346.9(69)	40.2(fixed)	—	6.3	40.2
*u*841	C(95)...H(123)	347.1(9)	25.0(fixed)	—	1.8	25.0
*u*816	C(48)...H(83)	347.1(9)	25.6(fixed)	—	1.7	25.6
*u*901	C(9)...C(11)	347.2(31)	20.4(tied to *u*897)	—	1.0	21.1
*u*1036	H(21)...H(24)	347.3(55)	41.6(fixed)	—	5.5	41.6
*u*939	Si(143)...C(147)	347.5(14)	15.7(tied to *u*897)	—	0.2	16.2

*u*932	C(6)...C(12)	347.9(25)	21.0(tied to *u*897)	—	0.8	21.8
*u*857	C(1)...H(29)	348.0(9)	23.8(fixed)	—	1.1	23.8
*u*991	H(65)...H(85)	348.1(21)	53.0(fixed)	—	1.5	53.0
*u*811	C(1)...H(36)	348.1(9)	21.7(fixed)	—	0.9	21.7
*u*865	C(1)...H(40)	348.3(9)	22.9(fixed)	—	1.2	22.9
*u*831	C(1)...H(26)	348.4(9)	22.7(fixed)	—	1.3	22.7
*u*1116	H(117)...H(129)	348.6(43)	48.0(fixed)	—	2.2	48.0
*u*1051	H(19)...H(24)	348.7(51)	49.8(fixed)	—	3.9	49.8
*u*893	C(57)...C(64)	348.8(31)	19.6(tied to *u*897)	—	0.9	20.3
*u*888	H(176)...H(184)	348.9(49)	44.7(fixed)	—	–2.3	44.7
*u*2305	C(150)...Cl(155)	348.9(18)	18.5(tied to *u*897)	—	–0.9	19.2
*u*928	Si(49)...C(53)	349.0(14)	15.7(tied to *u*897)	—	0.2	16.3
*u*914	C(57)...Cl(61)	349.0(11)	22.6(tied to *u*897)	—	0.7	23.4
*u*923	C(60)...C(63)	349.1(33)	20.1(tied to *u*897)	—	0.8	20.8
*u*1014	H(115)...H(127)	349.5(33)	44.7(fixed)	—	3.1	44.7
*u*2197	C(100)...C(103)	349.7(38)	17.2(tied to *u*897)	—	–0.8	17.8
*u*911	H(82)...H(90)	349.7(49)	42.0(fixed)	—	–2.2	42.0
*u*1012	H(34)...H(45)	349.7(65)	43.5(fixed)	—	4.2	43.5
*u*871	H(66)...H(94)	349.9(49)	42.3(fixed)	—	–2.0	42.3
*u*912	Si(51)...C(64)	350.1(21)	15.3(tied to *u*897)	—	0.3	15.8
*u*1248	H(70)...H(71)	350.1(58)	39.9(fixed)	—	–2.0	39.9
*u*927	Si(144)...C(148)	350.1(13)	15.5(tied to *u*897)	—	0.2	16.1
*u*904	H(19)...H(47)	350.2(49)	42.5(fixed)	—	–2.1	42.5
*u*2438	C(107)...H(120)	350.3(43)	23.0(fixed)	—	–1.3	23.0
*u*940	Si(2)...C(6)	350.4(12)	15.9(tied to *u*897)	—	0.2	16.4
*u*1088	H(30)...H(45)	350.5(35)	55.8(fixed)	—	0.3	55.8
*u*883	H(129)...H(137)	350.8(49)	40.2(fixed)	—	–1.9	40.2
*u*769	H(175)...H(183)	351.0(49)	43.7(fixed)	—	–0.4	43.7
*u*3076	H(115)...H(123)	351.1(36)	25.5(fixed)	—	–5.4	25.5
*u*920	C(59)...Cl(62)	351.3(21)	23.7(tied to *u*897)	—	0.8	24.6
*u*958	Si(5)...C(8)	351.4(28)	15.8(tied to *u*897)	—	0.2	16.3
*u*774	H(81)...H(89)	351.4(49)	42.9(fixed)	—	–0.3	42.9
*u*947	Si(4)...C(17)	351.4(19)	15.9(tied to *u*897)	—	0.2	16.5
*u*772	H(65)...H(93)	351.4(49)	42.3(fixed)	—	–0.5	42.3
*u*925	Si(99)...C(105)	351.4(20)	15.6(tied to *u*897)	—	0.2	16.1
*u*783	H(18)...H(46)	351.6(49)	43.1(fixed)	—	–0.5	43.1
*u*765	H(128)...H(136)	351.7(49)	41.9(fixed)	—	–0.6	41.9
*u*979	H(79)...H(94)	352.1(47)	56.1(fixed)	—	2.4	56.1
*u*1184	Si(143)...C(150)	352.2(11)	15.1(tied to *u*897)	—	–0.1	15.6
*u*860	Si(96)...C(100)	352.3(16)	15.6(tied to *u*897)	—	0.2	16.1
*u*2834	H(112)...H(122)	352.4(58)	40.1(fixed)	—	–4.2	40.1
*u*1778	Si(99)...Cl(108)	352.6(20)	11.2(tied to *u*897)	—	–0.8	11.6
*u*926	C(148)...C(152)	352.6(25)	21.3(tied to *u*897)	—	0.8	22.1
*u*929	Cl(14)...C(17)	353.0(37)	20.2(tied to *u*897)	—	1.0	20.9
*u*1089	C(104)...Cl(108)	353.0(18)	25.7(tied to *u*897)	—	0.2	26.6
*u*3051	H(162)...H(167)	353.0(28)	25.3(fixed)	—	–10.0	25.3

*u*946	Si(5)...Cl(14)	353.1(21)	17.0(tied to *u*897)	—	0.1	17.6
*u*1948	H(160)...H(178)	353.4(41)	39.1(fixed)	—	–8.4	39.1
*u*1118	H(86)...H(89)	353.4(52)	50.3(fixed)	—	2.0	50.3
*u*754	C(56)...H(91)	353.6(38)	39.2(fixed)	—	2.5	39.2
*u*897	Si(2)...Cl(15)	353.7(21)	17.6(4)	—	0.0	18.2
*u*785	C(60)...H(75)	353.9(30)	41.3(fixed)	—	2.4	41.3
*u*1025	H(40)...H(43)	354.0(41)	65.4(fixed)	—	–1.2	65.4
*u*952	Si(52)...C(58)	354.0(19)	15.8(tied to *u*897)	—	0.2	16.3
*u*910	C(55)...C(58)	354.1(28)	20.1(tied to *u*897)	—	0.9	20.8
*u*998	H(159)...H(179)	354.3(41)	49.6(fixed)	—	2.5	49.6
*u*1067	H(82)...H(92)	354.3(90)	38.9(fixed)	—	2.4	38.9
*u*1103	H(20)...H(37)	354.4(48)	48.5(fixed)	—	2.5	48.5
*u*1052	Si(50)...H(69)	354.6(35)	32.0(fixed)	—	0.2	32.0
*u*1015	C(58)...C(64)	354.6(62)	19.6(tied to *u*897)	—	0.4	20.3
*u*941	Si(97)...C(101)	354.7(15)	15.4(tied to *u*897)	—	0.2	15.9
*u*983	H(128)...H(139)	354.8(82)	38.7(fixed)	—	4.7	38.7
*u*936	Cl(15)...C(16)	354.8(20)	24.5(tied to *u*897)	—	0.9	25.3
*u*1749	C(152)...H(167)	355.0(35)	29.6(fixed)	—	3.2	29.6
*u*902	C(8)...C(12)	355.1(23)	19.7(tied to *u*897)	—	1.0	20.3
*u*943	C(7)...C(11)	355.2(25)	21.8(tied to *u*897)	—	0.7	22.5
*u*2103	C(147)...C(154)	355.4(30)	16.4(tied to *u*897)	—	–0.9	16.9
*u*942	Si(4)...C(13)	355.5(12)	16.2(tied to *u*897)	—	0.2	16.7
*u*1046	H(80)...H(94)	355.5(91)	37.6(fixed)	—	4.2	37.6
*u*1023	Si(52)...H(73)	355.7(36)	27.3(fixed)	—	4.1	27.3
*u*960	Si(5)...C(11)	355.8(20)	16.4(tied to *u*897)	—	0.2	17.0
*u*962	Si(49)...C(57)	356.2(13)	15.6(tied to *u*897)	—	0.1	16.2
*u*1696	Si(99)...C(103)	356.2(11)	10.9(tied to *u*897)	—	–0.7	11.3
*u*1024	H(164)...H(176)	356.2(38)	70.2(fixed)	—	1.4	70.2
*u*985	Si(3)...H(22)	356.2(30)	37.5(fixed)	—	–0.1	37.5
*u*968	H(30)...H(40)	356.3(33)	48.8(fixed)	—	4.7	48.8
*u*1028	C(7)...C(8)	356.5(43)	20.9(tied to *u*897)	—	0.3	21.6
*u*1058	H(112)...H(132)	356.6(23)	39.3(fixed)	—	5.0	39.3
*u*1822	H(113)...H(130)	356.7(31)	42.9(fixed)	—	–5.4	42.9
*u*1336	Si(145)...Cl(155)	357.0(19)	16.7(tied to *u*897)	—	–0.2	17.3
*u*1670	Si(96)...C(102)	357.0(15)	10.6(tied to *u*897)	—	–0.7	11.0
*u*950	Si(4)...C(9)	357.3(11)	15.8(tied to *u*897)	—	0.3	16.3
*u*959	C(10)...Cl(14)	357.6(24)	24.6(tied to *u*897)	—	0.7	25.5
*u*963	Si(2)...C(10)	358.1(14)	15.9(tied to *u*897)	—	0.2	16.5
*u*2398	H(170)...H(180)	358.2(72)	31.4(fixed)	—	–1.5	31.4
*u*956	Si(51)...C(60)	358.2(10)	15.9(tied to *u*897)	—	0.2	16.5
*u*1000	H(18)...H(38)	358.3(25)	48.4(fixed)	—	3.3	48.4
*u*1952	C(150)...C(154)	358.4(45)	18.6(tied to *u*897)	—	–0.9	19.2
*u*1040	H(22)...H(29)	358.6(65)	58.2(fixed)	—	2.7	58.2
*u*872	Si(49)...C(56)	358.7(14)	15.6(tied to *u*897)	—	0.1	16.2
*u*1054	H(33)...H(46)	358.8(68)	39.7(fixed)	—	8.9	39.7
*u*965	C(54)...C(58)	358.9(31)	22.0(tied to *u*897)	—	0.7	22.8

*u*1007	C(6)...Cl(14)	359.2(36)	24.6(tied to *u*897)	—	0.3	25.5
*u*938	Si(3)...C(12)	359.4(14)	15.6(tied to *u*897)	—	0.2	16.1
*u*2060	H(117)...H(121)	359.6(36)	35.3(fixed)	—	3.6	35.3
*u*1062	H(171)...H(186)	359.8(29)	56.2(fixed)	—	2.1	56.2
*u*1126	H(116)...H(128)	360.1(38)	32.5(fixed)	—	3.0	32.5
*u*869	Si(50)...C(63)	360.3(16)	15.3(tied to *u*897)	—	0.1	15.9
*u*1047	H(77)...H(92)	360.4(32)	49.6(fixed)	—	2.4	49.6
*u*969	Si(52)...Cl(61)	360.5(19)	17.1(tied to *u*897)	—	0.1	17.7
*u*1033	H(73)...H(80)	360.7(51)	54.9(fixed)	—	1.7	54.9
*u*1251	Si(145)...C(149)	360.9(14)	14.8(tied to *u*897)	—	–0.1	15.4
*u*1122	H(114)...H(131)	361.1(44)	38.1(fixed)	—	2.4	38.1
*u*997	H(24)...H(36)	361.3(42)	51.7(fixed)	—	1.7	51.7
*u*966	Si(50)...C(59)	361.3(13)	15.7(tied to *u*897)	—	0.2	16.3
*u*1001	Si(3)...H(20)	361.3(31)	27.6(fixed)	—	4.1	27.6
*u*955	Cl(61)...C(64)	362.1(43)	20.4(tied to *u*897)	—	0.9	21.2
*u*1018	H(29)...H(34)	362.2(32)	51.5(fixed)	—	2.5	51.5
*u*964	Si(3)...C(16)	362.2(17)	16.3(tied to *u*897)	—	0.2	16.9
*u*1021	H(71)...H(81)	362.5(28)	49.5(fixed)	—	2.1	49.5
*u*1142	H(23)...H(35)	362.6(40)	61.0(fixed)	—	2.4	61.0
*u*1069	C(11)...C(17)	362.6(58)	21.4(tied to *u*897)	—	0.4	22.1
*u*1232	H(65)...H(84)	362.7(45)	43.7(fixed)	—	–3.6	43.7
*u*2040	H(164)...H(166)	363.1(22)	39.3(fixed)	—	8.4	39.3
*u*1039	H(66)...H(83)	363.9(26)	32.6(fixed)	—	9.2	32.6
*u*990	Si(49)...H(91)	363.9(29)	26.7(fixed)	—	3.5	26.7
*u*1002	H(21)...H(33)	363.9(26)	54.2(fixed)	—	4.9	54.2
*u*987	Si(3)...H(35)	364.0(24)	29.1(fixed)	—	6.4	29.1
*u*913	C(151)...Cl(155)	364.0(22)	23.6(tied to *u*897)	—	0.8	24.4
*u*986	H(87)...H(90)	364.1(36)	44.6(fixed)	—	3.2	44.6
*u*1151	Si(50)...H(67)	364.3(35)	27.8(fixed)	—	3.5	27.8
*u*2870	H(113)...H(123)	364.3(40)	31.5(fixed)	—	–1.9	31.5
*u*1030	H(77)...H(87)	364.4(30)	41.4(fixed)	—	4.1	41.4
*u*1128	Si(146)...H(176)	364.5(30)	39.4(fixed)	—	–0.3	39.4
*u*921	C(56)...C(63)	365.0(31)	20.4(tied to *u*897)	—	0.8	21.1
*u*1124	H(18)...H(26)	365.2(55)	52.8(fixed)	—	2.7	52.8
*u*1010	H(29)...H(43)	365.3(44)	52.9(fixed)	—	1.2	52.9
*u*1005	C(105)...C(111)	365.4(72)	19.8(tied to *u*897)	—	0.4	20.5
*u*961	Si(51)...C(55)	365.4(15)	16.3(tied to *u*897)	—	0.2	16.9
*u*1071	Si(98)...H(116)	365.4(22)	27.2(fixed)	—	3.1	27.2
*u*1129	Si(97)...H(114)	365.8(32)	27.6(fixed)	—	3.7	27.6
*u*2107	C(103)...C(106)	366.0(32)	16.2(tied to *u*897)	—	–0.8	16.7
*u*1133	H(35)...H(45)	366.1(84)	41.5(fixed)	—	1.9	41.5
*u*2101	C(101)...C(103)	366.2(32)	16.1(tied to *u*897)	—	–0.9	16.6
*u*971	Si(50)...H(82)	366.6(22)	28.3(fixed)	—	5.3	28.3
*u*1946	C(149)...C(152)	366.7(29)	18.3(tied to *u*897)	—	–0.9	19.0
*u*1019	H(25)...H(37)	366.8(26)	48.4(fixed)	—	1.8	48.4
*u*2698	H(116)...H(123)	366.9(51)	33.1(fixed)	—	–3.8	33.1

*u*1266	H(117)...H(127)	367.1(60)	40.7(fixed)	—	–1.1	40.7
*u*1138	Si(144)...H(163)	367.1(19)	44.2(fixed)	—	–0.6	44.2
*u*2062	H(159)...H(182)	367.2(33)	37.5(fixed)	—	3.7	37.5
*u*3087	H(121)...H(131)	367.6(29)	27.7(fixed)	—	–8.5	27.7
*u*1976	Si(146)...H(167)	367.6(18)	21.1(fixed)	—	–1.0	21.1
*u*1055	C(53)...Cl(61)	367.6(36)	24.5(tied to *u*897)	—	0.3	25.3
*u*2352	H(117)...H(122)	367.7(51)	33.5(fixed)	—	–1.1	33.5
*u*1137	Si(98)...H(120)	367.8(20)	32.7(fixed)	—	0.1	32.7
*u*951	C(13)...Cl(15)	368.0(31)	20.5(tied to *u*897)	—	1.0	21.2
*u*1065	C(10)...C(13)	368.1(30)	21.5(tied to *u*897)	—	0.3	22.3
*u*2700	H(161)...H(181)	368.1(47)	35.9(fixed)	—	–3.2	35.9
*u*994	Si(97)...H(129)	368.1(25)	27.0(fixed)	—	3.5	27.0
*u*2952	H(165)...H(175)	368.2(29)	34.6(fixed)	—	–7.7	34.6
*u*1027	H(79)...H(88)	368.2(28)	40.7(fixed)	—	6.6	40.7
*u*1107	H(22)...H(24)	368.2(47)	39.3(fixed)	—	2.8	39.3
*u*1082	Si(49)...H(67)	368.2(27)	32.8(fixed)	—	0.2	32.8
*u*1215	H(71)...H(80)	368.3(57)	42.8(fixed)	—	–2.4	42.8
*u*1064	Si(51)...H(94)	368.3(33)	34.3(fixed)	—	0.1	34.3
*u*1145	H(20)...H(25)	368.4(52)	30.5(fixed)	—	3.4	30.5
*u*3221	H(119)...H(131)	368.5(58)	26.4(fixed)	—	–4.2	26.4
*u*1097	Si(143)...H(161)	368.8(24)	34.5(fixed)	—	0.1	34.5
*u*1070	H(68)...H(80)	369.2(32)	49.9(fixed)	—	4.0	49.9
*u*1113	H(21)...H(28)	369.4(66)	31.1(fixed)	—	5.7	31.1
*u*2263	C(100)...Cl(108)	369.5(42)	16.0(tied to *u*897)	—	–0.9	16.5
*u*1099	H(23)...H(26)	369.6(48)	38.8(fixed)	—	4.1	38.8
*u*973	Si(2)...H(44)	369.9(31)	34.9(fixed)	—	14.4	34.9
*u*1109	H(19)...H(36)	370.0(35)	30.3(fixed)	—	3.3	30.3
*u*988	Si(52)...H(83)	370.5(17)	28.9(fixed)	—	6.7	28.9
*u*993	H(32)...H(41)	370.6(32)	43.7(fixed)	—	12.0	43.7
*u*1060	H(74)...H(89)	370.6(33)	44.2(fixed)	—	2.4	44.2
*u*1092	H(33)...H(47)	370.7(84)	38.1(fixed)	—	6.3	38.1
*u*1119	Si(4)...H(47)	370.8(29)	35.7(fixed)	—	0.1	35.7
*u*1263	H(18)...H(24)	370.8(51)	45.8(fixed)	—	–1.3	45.8
*u*2281	H(114)...H(121)	370.8(52)	40.1(fixed)	—	2.2	40.1
*u*1105	Si(2)...H(20)	370.9(22)	33.7(fixed)	—	0.2	33.7
*u*1146	H(70)...H(82)	371.0(48)	52.8(fixed)	—	3.0	52.8
*u*1112	H(88)...H(91)	371.1(45)	31.0(fixed)	—	3.7	31.0
*u*1176	H(32)...H(45)	371.3(45)	46.0(fixed)	—	–4.9	46.0
*u*1141	H(31)...H(40)	371.7(47)	41.4(fixed)	—	1.2	41.4
*u*3113	H(160)...H(180)	371.9(42)	24.0(fixed)	—	–7.5	24.0
*u*1169	Si(96)...H(122)	372.0(23)	40.9(fixed)	—	–0.9	40.9
*u*978	Si(2)...H(26)	372.1(19)	26.2(fixed)	—	5.1	26.2
*u*898	C(147)...C(153)	372.4(36)	20.2(tied to *u*897)	—	0.9	20.9
*u*1013	Si(5)...H(31)	372.4(24)	31.5(fixed)	—	8.5	31.5
*u*1056	H(76)...H(85)	372.7(23)	43.7(fixed)	—	3.3	43.7
*u*1152	Si(4)...H(39)	372.7(23)	37.6(fixed)	—	–0.4	37.6

*u*1061	C(12)...Cl(15)	372.7(26)	25.5(tied to *u*897)	—	0.2	26.4
*u*1094	C(57)...C(60)	373.0(25)	21.0(tied to *u*897)	—	0.3	21.7
*u*1085	H(27)...H(35)	373.1(42)	29.3(fixed)	—	7.6	29.3
*u*1026	Si(52)...H(78)	373.2(22)	27.9(fixed)	—	5.0	27.9
*u*1074	H(78)...H(93)	373.8(40)	31.7(fixed)	—	6.1	31.7
*u*1076	H(31)...H(46)	373.8(44)	29.4(fixed)	—	12.6	29.4
*u*1104	Si(5)...H(28)	373.9(36)	29.4(fixed)	—	5.1	29.4
*u*1269	H(18)...H(37)	374.0(47)	43.4(fixed)	—	–1.5	43.4
*u*924	C(56)...C(60)	374.5(28)	20.4(tied to *u*897)	—	0.9	21.2
*u*1178	H(40)...H(42)	374.9(63)	47.3(fixed)	—	–8.4	47.3
*u*1144	Si(52)...H(82)	375.1(30)	37.0(fixed)	—	–0.1	37.0
*u*1031	Si(5)...H(36)	375.2(22)	26.6(fixed)	—	3.6	26.6
*u*1114	Si(99)...H(129)	375.2(32)	32.0(fixed)	—	0.0	32.0
*u*2018	Si(145)...H(169)	375.3(22)	21.4(fixed)	—	–1.3	21.4
*u*1395	C(54)...H(71)	375.4(52)	32.3(fixed)	—	–2.2	32.3
*u*1073	H(129)...H(139)	375.5(104)	36.1(fixed)	—	2.8	36.1
*u*1006	Si(144)...H(161)	375.7(30)	28.8(fixed)	—	4.2	28.8
*u*1009	H(161)...H(178)	375.8(55)	54.3(fixed)	—	2.3	54.3
*u*1153	Si(4)...H(28)	376.3(21)	37.5(fixed)	—	–0.3	37.5
*u*1135	H(32)...H(39)	376.6(49)	35.7(fixed)	—	8.2	35.7
*u*1268	H(69)...H(72)	376.7(61)	42.9(fixed)	—	–1.8	42.9
*u*1252	H(24)...H(37)	377.1(56)	42.0(fixed)	—	–2.9	42.0
*u*1050	Si(4)...H(22)	377.4(16)	29.9(fixed)	—	5.4	29.9
*u*1165	Si(5)...H(35)	377.5(31)	40.2(fixed)	—	–0.4	40.2
*u*1017	Si(96)...H(114)	377.7(28)	33.7(fixed)	—	0.0	33.7
*u*1093	H(72)...H(82)	378.1(37)	32.2(fixed)	—	6.9	32.2
*u*2014	Si(99)...H(122)	378.2(21)	22.3(fixed)	—	–1.3	22.3
*u*1256	H(23)...H(29)	378.3(60)	45.4(fixed)	—	–2.4	45.4
*u*1173	H(29)...H(33)	378.4(57)	47.7(fixed)	—	–2.9	47.7
*u*1117	Si(144)...H(176)	378.9(23)	29.4(fixed)	—	4.9	29.4
*u*1079	Si(51)...H(69)	378.9(22)	28.8(fixed)	—	3.4	28.8
*u*1091	Si(97)...H(116)	379.1(22)	31.1(fixed)	—	0.2	31.1
*u*1022	Si(145)...H(163)	379.2(18)	30.8(fixed)	—	7.6	30.8
*u*1063	H(74)...H(84)	379.4(20)	41.1(fixed)	—	8.4	41.1
*u*1127	H(22)...H(34)	379.5(30)	31.2(fixed)	—	4.1	31.2
*u*1202	H(87)...H(89)	379.7(57)	39.9(fixed)	—	–0.9	39.9
*u*1029	Si(143)...H(169)	380.0(20)	28.3(fixed)	—	4.0	28.3
*u*1162	Si(51)...H(86)	380.1(19)	34.1(fixed)	—	–0.3	34.1
*u*2309	H(164)...H(165)	380.2(39)	35.1(fixed)	—	5.1	35.1
*u*1243	H(76)...H(89)	380.2(55)	40.2(fixed)	—	–1.5	40.2
*u*1139	H(78)...H(87)	380.2(40)	39.2(fixed)	—	1.7	39.2
*u*1163	Si(49)...H(78)	380.4(19)	35.8(fixed)	—	–0.2	35.8
*u*1100	C(56)...C(59)	380.7(17)	21.4(tied to *u*897)	—	0.2	22.2
*u*1170	Si(2)...H(31)	380.8(21)	45.4(fixed)	—	–1.1	45.4
*u*1157	H(79)...H(86)	381.1(40)	37.1(fixed)	—	4.0	37.1
*u*1086	C(9)...C(16)	381.2(41)	22.2(tied to *u*897)	—	0.3	23.0

*u*1044	H(76)...H(91)	381.2(49)	50.0(fixed)	—	2.1	50.0
*u*2739	C(102)...C(106)	381.3(52)	12.7(tied to *u*897)	—	–1.3	13.2
*u*1240	H(23)...H(33)	381.4(35)	48.6(fixed)	—	–1.6	48.6
*u*1150	Si(2)...H(47)	381.6(22)	28.2(fixed)	—	4.1	28.2
*u*1148	Si(5)...H(26)	381.6(30)	35.1(fixed)	—	0.1	35.1
*u*1084	Si(51)...H(75)	382.4(23)	26.6(fixed)	—	3.6	26.6
*u*1078	H(26)...H(38)	382.5(32)	28.3(fixed)	—	7.1	28.3
*u*1087	Si(49)...H(75)	382.8(24)	32.7(fixed)	—	–0.3	32.7
*u*1156	H(69)...H(81)	383.0(41)	34.2(fixed)	—	2.1	34.2
*u*1255	Si(52)...C(55)	383.2(30)	14.9(tied to *u*897)	—	–0.1	15.4
*u*1080	Si(3)...H(36)	384.0(24)	30.4(fixed)	—	0.4	30.4
*u*1110	H(163)...H(175)	384.0(34)	36.0(fixed)	—	9.9	36.0
*u*236	H(112)...H(131)	384.3(46)	36.4(fixed)	—	16.9	36.4
*u*1143	H(29)...H(44)	384.4(63)	54.0(fixed)	—	–3.0	54.0
*u*1035	Si(50)...H(86)	384.6(23)	28.3(fixed)	—	3.6	28.3
*u*2628	H(122)...H(132)	384.8(41)	49.8(fixed)	—	–2.4	49.8
*u*1134	Si(49)...H(94)	384.9(27)	28.0(fixed)	—	4.0	28.0
*u*1381	C(13)...H(42)	385.1(53)	60.5(fixed)	—	–8.1	60.5
*u*1168	Si(3)...H(44)	385.4(27)	55.9(fixed)	—	–0.8	55.9
*u*1937	Si(96)...H(120)	385.4(24)	20.2(fixed)	—	–0.8	20.2
*u*1254	H(79)...H(92)	385.6(45)	41.8(fixed)	—	–2.4	41.8
*u*1096	H(41)...H(44)	385.8(50)	30.0(fixed)	—	22.5	30.0
*u*1037	H(76)...H(88)	385.9(32)	44.9(fixed)	—	3.0	44.9
*u*1161	Si(50)...H(83)	386.1(22)	39.8(fixed)	—	–0.2	39.8
*u*1382	C(53)...H(84)	386.8(30)	39.6(fixed)	—	–3.6	39.6
*u*1149	H(76)...H(83)	387.1(24)	41.9(fixed)	—	0.7	41.9
*u*1179	Si(3)...C(6)	387.2(25)	15.7(tied to *u*1322)	—	–0.2	15.7
*u*2382	H(177)...H(186)	388.1(47)	32.1(fixed)	—	–1.6	32.1
*u*1048	Si(50)...H(91)	388.2(25)	31.7(fixed)	—	–0.1	31.7
*u*1172	Si(2)...C(16)	389.0(24)	16.0(tied to *u*1322)	—	–0.2	16.0
*u*1392	H(39)...H(43)	389.0(38)	45.2(fixed)	—	–10.5	45.2
*u*1121	H(75)...H(90)	389.4(42)	31.8(fixed)	—	4.4	31.8
*u*256	H(159)...H(177)	389.5(53)	44.0(fixed)	—	12.0	44.0
*u*2288	H(123)...H(130)	389.8(52)	39.5(fixed)	—	3.3	39.5
*u*1174	Si(3)...C(11)	389.9(18)	15.7(tied to *u*1322)	—	–0.2	15.6
*u*1314	Si(50)...C(53)	390.0(27)	15.1(tied to *u*1322)	—	–0.2	15.1
*u*1438	Cl(62)...H(65)	390.1(51)	33.3(fixed)	—	–2.3	33.3
*u*1238	C(10)...H(42)	390.5(14)	15.9(fixed)	—	–9.2	15.9
*u*1245	H(164)...H(174)	390.8(46)	46.5(fixed)	—	–3.8	46.5
*u*1166	H(75)...H(84)	391.2(24)	37.9(fixed)	—	5.4	37.9
*u*1108	H(72)...H(89)	391.3(45)	40.4(fixed)	—	3.7	40.4
*u*1183	Si(49)...C(63)	391.9(22)	15.1(tied to *u*1322)	—	–0.2	15.1
*u*1302	C(17)...H(32)	392.2(40)	47.4(fixed)	—	–4.5	47.4
*u*1171	Si(50)...C(58)	392.7(16)	15.2(tied to *u*1322)	—	–0.2	15.2
*u*2292	H(112)...H(123)	392.7(64)	41.0(fixed)	—	6.1	41.0
*u*1077	H(75)...H(87)	392.9(42)	50.8(fixed)	—	2.1	50.8

*u*1273	H(70)...H(80)	393.0(46)	44.8(fixed)	—	–0.9	44.8
*u*1283	Si(97)...C(100)	393.3(24)	15.0(tied to *u*1322)	—	–0.1	15.0
*u*2995	H(118)...H(130)	393.3(78)	33.8(fixed)	—	1.5	33.8
*u*1120	H(71)...H(90)	393.4(44)	40.5(fixed)	—	4.8	40.5
*u*1140	Si(51)...H(73)	393.6(24)	33.0(fixed)	—	0.1	33.0
*u*1221	C(11)...H(32)	393.6(14)	14.5(fixed)	—	–6.2	14.5
*u*1228	C(16)...H(31)	393.7(14)	13.2(fixed)	—	–6.1	13.2
*u*1236	C(147)...H(163)	393.8(14)	14.2(fixed)	—	–5.6	14.2
*u*2973	H(165)...H(174)	393.9(50)	31.4(fixed)	—	–6.0	31.4
*u*1219	C(158)...H(164)	393.9(14)	14.3(fixed)	—	–5.6	14.3
*u*1421	C(54)...H(72)	394.0(53)	31.9(fixed)	—	–2.5	31.9
*u*1261	Si(98)...C(101)	394.1(16)	15.8(tied to *u*1322)	—	–0.1	15.8
*u*1373	H(22)...H(27)	394.2(56)	48.5(fixed)	—	–3.0	48.5
*u*1177	Si(97)...C(105)	394.5(19)	15.6(tied to *u*1322)	—	–0.2	15.6
*u*1167	Si(3)...H(39)	394.5(27)	29.2(fixed)	—	4.5	29.2
*u*2082	H(166)...H(176)	394.6(40)	38.8(fixed)	—	3.2	38.8
*u*1230	C(102)...H(123)	394.6(23)	14.0(fixed)	—	–5.0	14.0
*u*1234	Si(52)...C(59)	394.6(13)	15.4(tied to *u*1322)	—	–0.1	15.4
*u*1415	C(105)...H(117)	394.7(41)	30.9(fixed)	—	–1.8	30.9
*u*1011	Si(145)...H(167)	394.9(23)	27.6(fixed)	—	4.7	27.6
*u*1208	C(10)...H(35)	395.0(14)	13.9(fixed)	—	–4.9	13.9
*u*1378	H(30)...H(47)	395.2(51)	43.0(fixed)	—	–5.8	43.0
*u*2306	H(159)...H(181)	395.2(55)	35.0(fixed)	—	1.6	35.0
*u*1191	C(151)...H(176)	395.2(14)	13.6(fixed)	—	–4.3	13.6
*u*1175	Si(2)...C(8)	395.3(14)	15.1(tied to *u*1322)	—	–0.2	15.0
*u*1187	C(17)...H(23)	395.4(14)	13.2(fixed)	—	–4.5	13.2
*u*1235	C(57)...H(82)	395.4(14)	13.5(fixed)	—	–4.3	13.5
*u*1226	C(6)...H(22)	395.4(14)	13.6(fixed)	—	–4.4	13.6
*u*1379	C(9)...H(33)	395.5(48)	41.8(fixed)	—	–3.6	41.8
*u*1229	C(58)...H(79)	395.6(14)	13.7(fixed)	—	–4.1	13.7
*u*1217	C(63)...H(78)	395.6(14)	13.4(fixed)	—	–4.1	13.4
*u*1386	H(162)...H(176)	395.6(42)	49.2(fixed)	—	–5.1	49.2
*u*1224	C(60)...H(83)	395.6(22)	13.5(fixed)	—	–4.7	13.5
*u*1041	H(27)...H(42)	395.6(49)	42.1(fixed)	—	21.1	42.1
*u*1214	C(11)...H(44)	395.7(28)	15.7(fixed)	—	–9.1	15.7
*u*1199	C(54)...H(94)	395.9(14)	13.4(fixed)	—	–3.8	13.4
*u*1223	C(148)...H(159)	396.0(14)	13.7(fixed)	—	–3.5	13.7
*u*1182	C(7)...H(47)	396.1(14)	13.4(fixed)	—	–3.8	13.4
*u*1206	C(54)...H(65)	396.2(14)	13.6(fixed)	—	–3.5	13.6
*u*1200	C(7)...H(18)	396.2(14)	13.8(fixed)	—	–3.7	13.8
*u*1198	C(8)...H(29)	396.2(22)	13.9(fixed)	—	–4.2	13.9
*u*1210	C(12)...H(40)	396.2(22)	14.0(fixed)	—	–4.2	14.0
*u*1213	Si(5)...C(10)	396.3(18)	15.6(tied to *u*1322)	—	–0.1	15.6
*u*1193	C(101)...H(112)	396.3(14)	13.6(fixed)	—	–3.5	13.6
*u*1227	C(103)...H(120)	396.4(23)	13.2(fixed)	—	–3.3	13.2
*u*1231	C(53)...H(69)	396.4(14)	13.3(fixed)	—	–3.3	13.3

*u*1225	C(9)...H(26)	396.5(22)	13.4(fixed)	—	–4.0	13.4
*u*2499	Cl(109)...H(127)	396.5(57)	34.6(fixed)	—	–1.3	34.6
*u*1209	C(57)...H(89)	396.5(14)	13.5(fixed)	—	–3.2	13.5
*u*1196	C(64)...H(70)	396.5(14)	13.5(fixed)	—	–3.2	13.5
*u*1237	C(104)...H(129)	396.6(14)	13.4(fixed)	—	–3.3	13.4
*u*1220	C(56)...H(73)	396.9(22)	13.2(fixed)	—	–3.5	13.2
*u*1205	C(111)...H(117)	396.9(14)	13.4(fixed)	—	–2.9	13.4
*u*1204	C(100)...H(116)	396.9(14)	13.2(fixed)	—	–3.0	13.2
*u*1194	C(55)...H(76)	397.0(22)	13.5(fixed)	—	–3.3	13.5
*u*1218	C(59)...H(87)	397.1(22)	13.5(fixed)	—	–3.3	13.5
*u*1216	C(150)...H(167)	397.1(22)	13.4(fixed)	—	–3.8	13.4
*u*1685	Si(146)...C(149)	397.1(13)	11.4(tied to *u*1322)	—	–0.7	11.3
*u*1222	C(13)...H(36)	397.3(22)	13.2(fixed)	—	–3.2	13.2
*u*1201	C(149)...H(170)	397.3(22)	13.6(fixed)	—	–3.6	13.6
*u*1106	C(55)...C(63)	397.3(38)	22.4(tied to *u*1322)	—	0.3	22.3
*u*1291	H(77)...H(94)	397.4(53)	45.3(fixed)	—	–2.5	45.3
*u*1470	C(158)...H(176)	397.6(77)	37.1(fixed)	—	–3.3	37.1
*u*1279	H(67)...H(85)	397.7(43)	43.8(fixed)	—	–3.8	43.8
*u*1265	Si(5)...C(9)	397.7(30)	15.9(tied to *u*1322)	—	–0.1	15.8
*u*953	Si(98)...C(102)	397.9(15)	16.7(tied to *u*1322)	—	0.2	16.6
*u*1260	Si(49)...Cl(62)	398.1(17)	17.4(tied to *u*1322)	—	–0.3	17.3
*u*2580	C(148)...H(165)	398.3(31)	22.3(fixed)	—	–2.3	22.3
*u*1746	Si(144)...Cl(155)	398.7(15)	11.6(tied to *u*1322)	—	–0.8	11.5
*u*1389	C(55)...H(80)	399.0(44)	36.2(fixed)	—	–2.8	36.2
*u*1246	Si(52)...C(57)	399.1(17)	15.5(tied to *u*1322)	—	–0.1	15.5
*u*1398	H(28)...H(34)	399.4(34)	50.2(fixed)	—	–4.6	50.2
*u*1212	C(16)...H(33)	399.9(28)	13.1(fixed)	—	–5.1	13.1
*u*1259	Si(5)...C(12)	400.1(16)	15.7(tied to *u*1322)	—	–0.2	15.6
*u*1195	Si(144)...C(147)	400.3(22)	15.7(tied to *u*1322)	—	–0.2	15.7
*u*1329	C(1)...H(43)	400.3(7)	15.2(fixed)	—	–8.2	15.2
*u*1189	C(157)...H(174)	400.4(28)	13.9(fixed)	—	–4.3	13.9
*u*1188	C(63)...H(80)	400.6(28)	13.9(fixed)	—	–4.2	13.9
*u*1405	C(60)...H(89)	400.6(48)	31.2(fixed)	—	–1.9	31.2
*u*1516	Cl(62)...H(66)	400.7(44)	33.2(fixed)	—	–2.7	33.2
*u*1207	C(158)...H(161)	401.0(28)	13.4(fixed)	—	–3.7	13.4
*u*1358	H(119)...H(123)	401.0(24)	27.1(fixed)	—	–5.3	27.1
*u*1190	C(53)...H(92)	401.1(28)	13.6(fixed)	—	–3.7	13.6
*u*1419	C(6)...H(37)	401.1(38)	32.0(fixed)	—	–2.1	32.0
*u*1211	C(6)...H(45)	401.1(28)	13.7(fixed)	—	–3.9	13.7
*u*1244	Si(145)...C(148)	401.3(13)	15.9(tied to *u*1322)	—	–0.2	15.9
*u*1233	C(17)...H(20)	401.4(28)	12.8(fixed)	—	–3.7	12.8
*u*1185	C(64)...H(67)	401.4(28)	13.2(fixed)	—	–3.4	13.2
*u*1308	H(38)...H(40)	401.5(23)	25.4(fixed)	—	–4.3	25.4
*u*1180	C(111)...H(114)	401.6(28)	13.2(fixed)	—	–3.5	13.2
*u*1197	C(58)...H(91)	401.6(28)	13.2(fixed)	—	–3.2	13.2
*u*1186	C(110)...H(127)	401.7(28)	13.5(fixed)	—	–3.3	13.5

*u*1270	Si(144)...C(152)	401.8(16)	15.0(tied to *u*1322)	—	–0.2	14.9
*u*1288	H(83)...H(88)	401.9(23)	25.8(fixed)	—	–4.9	25.8
*u*1258	Si(4)...C(7)	402.0(12)	16.2(tied to *u*1322)	—	–0.2	16.2
*u*1414	C(8)...H(18)	402.0(45)	33.6(fixed)	—	–2.4	33.6
*u*1277	H(25)...H(29)	402.2(23)	26.0(fixed)	—	–3.5	26.0
*u*2323	H(123)...H(131)	402.4(40)	34.3(fixed)	—	4.7	34.3
*u*2595	H(163)...H(166)	402.5(27)	53.1(fixed)	—	–2.1	53.1
*u*1274	H(26)...H(27)	402.6(23)	25.0(fixed)	—	–3.3	25.0
*u*2639	Cl(156)...H(159)	402.7(43)	25.0(fixed)	—	–3.9	25.0
*u*957	Si(96)...C(103)	402.7(18)	16.0(tied to *u*1322)	—	0.2	16.0
*u*1147	H(28)...H(42)	402.8(63)	41.6(fixed)	—	15.3	41.6
*u*1321	C(1)...H(30)	403.0(7)	14.2(fixed)	—	–5.6	14.2
*u*1391	C(12)...H(24)	403.1(39)	36.7(fixed)	—	–2.9	36.7
*u*1280	H(36)...H(41)	403.6(23)	24.6(fixed)	—	–2.3	24.6
*u*1285	H(72)...H(76)	403.7(23)	26.3(fixed)	—	–3.1	26.3
*u*1278	H(73)...H(74)	403.7(23)	24.8(fixed)	—	–3.2	24.8
*u*1303	C(142)...H(162)	403.8(7)	14.0(fixed)	—	–5.0	14.0
*u*3183	H(113)...H(122)	403.8(36)	27.6(fixed)	—	–8.9	27.6
*u*1325	C(1)...H(34)	403.9(7)	13.9(fixed)	—	–4.7	13.9
*u*1338	H(120)...H(121)	404.0(24)	26.9(fixed)	—	–2.3	26.9
*u*1294	H(167)...H(168)	404.1(23)	25.4(fixed)	—	–3.5	25.4
*u*1700	Si(145)...C(150)	404.1(16)	11.3(tied to *u*1322)	—	–0.7	11.3
*u*1383	H(115)...H(129)	404.2(46)	45.1(fixed)	—	–1.4	45.1
*u*1324	H(166)...H(170)	404.2(23)	26.7(fixed)	—	–3.3	26.7
*u*1301	H(85)...H(87)	404.3(23)	27.5(fixed)	—	–2.3	27.5
*u*1384	C(64)...H(79)	404.3(36)	35.8(fixed)	—	–2.7	35.8
*u*1276	Si(51)...Cl(61)	404.4(14)	16.9(tied to *u*1322)	—	–0.3	16.9
*u*1296	C(1)...H(21)	404.4(7)	13.7(fixed)	—	–4.2	13.7
*u*1352	H(30)...H(42)	404.4(17)	29.4(fixed)	—	–9.3	29.4
*u*1380	Cl(109)...H(122)	404.5(10)	14.1(fixed)	—	–5.5	14.1
*u*1264	Si(51)...C(54)	404.6(16)	16.2(tied to *u*1322)	—	–0.2	16.2
*u*1304	C(95)...H(121)	404.6(7)	13.5(fixed)	—	–4.6	13.5
*u*1349	C(142)...H(175)	404.7(7)	13.8(fixed)	—	–4.1	13.8
*u*1323	C(48)...H(81)	404.8(7)	13.6(fixed)	—	–4.0	13.6
*u*1328	Si(2)...C(17)	404.8(16)	15.1(tied to *u*1322)	—	–0.1	15.0
*u*1357	C(1)...H(46)	405.0(7)	13.6(fixed)	—	–3.6	13.6
*u*1297	C(48)...H(85)	405.0(7)	13.5(fixed)	—	–4.3	13.5
*u*1327	C(48)...H(77)	405.1(7)	13.4(fixed)	—	–3.6	13.4
*u*1343	C(1)...H(19)	405.2(7)	13.4(fixed)	—	–3.5	13.4
*u*2424	C(103)...H(112)	405.2(54)	32.3(fixed)	—	–1.1	32.3
*u*1337	C(48)...H(93)	405.2(7)	13.5(fixed)	—	–3.5	13.5
*u*1364	Cl(14)...H(39)	405.3(11)	13.8(fixed)	—	–4.7	13.8
*u*1376	Cl(15)...H(28)	405.4(11)	13.8(fixed)	—	–4.7	13.8
*u*1347	C(95)...H(113)	405.4(7)	13.5(fixed)	—	–3.2	13.5
*u*1322	Si(4)...Cl(15)	405.4(16)	17.7(5)	—	–0.3	17.6
*u*1125	H(74)...H(86)	405.4(40)	32.2(fixed)	—	4.4	32.2

*u*1354	C(48)...H(66)	405.4(7)	13.5(fixed)	—	–3.3	13.5
*u*1335	C(142)...H(160)	405.4(7)	13.4(fixed)	—	–3.4	13.4
*u*1317	C(95)...H(128)	405.5(7)	13.3(fixed)	—	–3.1	13.3
*u*1368	Cl(15)...H(24)	405.5(11)	13.7(fixed)	—	–4.5	13.7
*u*1313	C(48)...H(68)	405.6(7)	13.3(fixed)	—	–3.1	13.3
*u*1377	Cl(61)...H(84)	405.6(10)	13.9(fixed)	—	–5.1	13.9
*u*1400	C(7)...H(29)	405.7(55)	36.2(fixed)	—	–3.0	36.2
*u*1293	C(142)...H(166)	405.7(7)	13.4(fixed)	—	–3.5	13.4
*u*1319	C(48)...H(90)	405.9(7)	13.3(fixed)	—	–2.9	13.3
*u*1331	C(95)...H(115)	405.9(7)	13.2(fixed)	—	–2.8	13.2
*u*1326	C(142)...H(182)	405.9(7)	13.2(fixed)	—	–3.3	13.2
*u*1341	C(1)...H(41)	406.1(7)	13.5(fixed)	—	–4.0	13.5
*u*1286	C(95)...H(119)	406.1(7)	13.2(fixed)	—	–3.0	13.2
*u*1311	C(1)...H(27)	406.2(7)	13.3(fixed)	—	–3.9	13.3
*u*1371	Cl(62)...H(71)	406.2(10)	13.7(fixed)	—	–3.8	13.7
*u*1300	C(48)...H(72)	406.2(7)	13.3(fixed)	—	–3.2	13.3
*u*1307	C(48)...H(88)	406.2(7)	13.1(fixed)	—	–3.1	13.1
*u*1305	C(48)...H(74)	406.3(7)	13.1(fixed)	—	–3.0	13.1
*u*1365	Cl(156)...H(165)	406.4(10)	13.8(fixed)	—	–4.2	13.8
*u*1372	Cl(62)...H(75)	406.4(10)	13.4(fixed)	—	–3.6	13.4
*u*1306	C(1)...H(25)	406.4(7)	13.3(fixed)	—	–3.6	13.3
*u*1367	Cl(109)...H(118)	406.5(10)	13.5(fixed)	—	–3.6	13.5
*u*1369	Cl(14)...H(37)	406.6(11)	13.6(fixed)	—	–3.5	13.6
*u*1375	Cl(156)...H(169)	406.6(10)	13.5(fixed)	—	–4.0	13.5
*u*1257	Si(51)...C(56)	406.7(17)	15.3(tied to *u*1322)	—	–0.1	15.3
*u*1370	Cl(61)...H(86)	407.1(10)	13.3(fixed)	—	–3.7	13.3
*u*1295	C(1)...H(38)	407.2(7)	13.1(fixed)	—	–2.9	13.1
*u*1289	Si(49)...C(64)	407.2(20)	15.0(tied to *u*1322)	—	–0.2	14.9
*u*1192	Si(50)...C(60)	407.2(18)	15.4(tied to *u*1322)	—	–0.1	15.3
*u*1361	H(173)...H(175)	407.3(17)	29.8(fixed)	—	–5.7	29.8
*u*1334	H(160)...H(163)	407.4(17)	27.5(fixed)	—	–5.9	27.5
*u*1363	H(32)...H(34)	407.7(17)	28.0(fixed)	—	–6.2	28.0
*u*493	C(110)...H(118)	408.0(34)	30.8(fixed)	—	6.9	30.8
*u*976	Si(98)...Cl(108)	408.2(16)	17.8(tied to *u*1322)	—	0.1	17.7
*u*1348	Si(4)...Cl(14)	408.3(18)	17.9(tied to *u*1322)	—	–0.3	17.8
*u*1413	C(11)...H(23)	408.3(26)	36.4(fixed)	—	–3.2	36.4
*u*1310	H(34)...H(44)	408.6(31)	29.0(fixed)	—	–10.0	29.0
*u*1181	H(76)...H(87)	408.8(54)	40.2(fixed)	—	–1.1	40.2
*u*1393	C(152)...H(164)	409.3(32)	44.6(fixed)	—	–4.3	44.6
*u*1298	H(23)...H(46)	409.5(17)	27.8(fixed)	—	–4.4	27.8
*u*1401	H(86)...H(90)	409.6(32)	45.8(fixed)	—	–2.0	45.8
*u*1351	H(77)...H(82)	409.6(17)	26.5(fixed)	—	–4.1	26.5
*u*1359	H(30)...H(35)	409.7(17)	28.9(fixed)	—	–4.1	28.9
*u*1345	H(19)...H(22)	409.7(17)	25.9(fixed)	—	–4.5	25.9
*u*1366	H(79)...H(81)	409.7(17)	28.2(fixed)	—	–3.7	28.2
*u*1282	H(78)...H(90)	409.7(17)	25.4(fixed)	—	–4.1	25.4

*u*1340	H(31)...H(43)	409.8(17)	30.4(fixed)	—	–3.7	30.4
*u*1309	H(171)...H(176)	409.8(17)	27.9(fixed)	—	–3.4	27.9
*u*1299	H(68)...H(94)	410.0(17)	25.7(fixed)	—	–3.9	25.7
*u*1355	H(65)...H(68)	410.1(17)	26.8(fixed)	—	–3.5	26.8
*u*1360	H(20)...H(38)	410.3(38)	43.6(fixed)	—	–1.4	43.6
*u*1435	C(58)...H(94)	410.4(74)	33.4(fixed)	—	–2.5	33.4
*u*1316	H(112)...H(115)	410.5(17)	26.2(fixed)	—	–3.6	26.2
*u*1330	H(66)...H(69)	410.7(17)	26.1(fixed)	—	–3.1	26.1
*u*1497	Cl(62)...H(69)	410.7(45)	33.9(fixed)	—	–2.4	33.9
*u*1362	H(18)...H(21)	410.8(17)	28.0(fixed)	—	–3.2	28.0
*u*1350	H(70)...H(93)	410.8(17)	27.3(fixed)	—	–2.8	27.3
*u*1342	H(159)...H(162)	410.9(17)	29.3(fixed)	—	–2.2	29.3
*u*1271	H(21)...H(47)	411.0(17)	25.9(fixed)	—	–3.2	25.9
*u*1315	H(124)...H(129)	411.0(17)	25.0(fixed)	—	–3.3	25.0
*u*2961	Cl(109)...H(128)	411.0(34)	22.6(fixed)	—	–5.5	22.6
*u*1312	H(77)...H(89)	411.1(17)	27.0(fixed)	—	–2.5	27.0
*u*1411	H(21)...H(35)	411.3(49)	56.6(fixed)	—	–3.9	56.6
*u*1333	H(126)...H(128)	411.5(17)	26.0(fixed)	—	–2.6	26.0
*u*1275	H(113)...H(116)	411.7(17)	24.9(fixed)	—	–2.6	24.9
*u*1472	C(7)...H(27)	411.8(54)	34.4(fixed)	—	–3.6	34.4
*u*1418	Cl(14)...H(45)	411.9(47)	33.8(fixed)	—	–2.8	33.8
*u*1548	Cl(62)...H(68)	412.1(45)	34.5(fixed)	—	–3.0	34.5
*u*1483	C(13)...H(43)	412.3(31)	43.0(fixed)	—	–9.8	43.0
*u*1407	H(19)...H(26)	412.6(53)	49.8(fixed)	—	–2.4	49.8
*u*1466	C(64)...H(82)	412.7(72)	35.3(fixed)	—	–3.2	35.3
*u*1403	H(68)...H(82)	413.2(48)	51.3(fixed)	—	–1.8	51.3
*u*2598	H(161)...H(182)	413.5(37)	40.9(fixed)	—	–1.7	40.9
*u*1344	H(174)...H(184)	413.6(31)	28.2(fixed)	—	–4.3	28.2
*u*1353	H(80)...H(90)	414.0(31)	27.2(fixed)	—	–4.3	27.2
*u*1339	Si(3)...C(13)	414.4(20)	14.8(tied to *u*1322)	—	–0.1	14.7
*u*1554	C(152)...H(187)	414.7(59)	32.4(fixed)	—	–4.2	32.4
*u*1284	H(66)...H(92)	414.9(31)	26.8(fixed)	—	–3.5	26.8
*u*1290	H(175)...H(185)	415.0(31)	26.6(fixed)	—	–3.1	26.6
*u*1332	H(19)...H(45)	415.3(31)	26.2(fixed)	—	–3.6	26.2
*u*1272	H(128)...H(138)	415.5(31)	25.6(fixed)	—	–3.4	25.6
*u*1267	H(67)...H(93)	415.6(31)	25.3(fixed)	—	–3.0	25.3
*u*1318	H(127)...H(137)	415.6(31)	27.0(fixed)	—	–3.1	27.0
*u*1155	H(73)...H(89)	415.7(54)	36.9(fixed)	—	1.9	36.9
*u*1428	C(53)...H(85)	415.7(18)	35.3(fixed)	—	–4.2	35.3
*u*1787	H(114)...H(132)	415.7(44)	43.1(fixed)	—	–5.1	43.1
*u*1281	H(20)...H(46)	415.8(31)	25.1(fixed)	—	–3.2	25.1
*u*1461	C(8)...H(22)	415.8(40)	36.8(fixed)	—	–3.3	36.8
*u*1500	C(17)...H(30)	415.9(35)	34.5(fixed)	—	–6.3	34.5
*u*1292	H(81)...H(91)	415.9(31)	26.3(fixed)	—	–2.6	26.3
*u*1346	H(33)...H(43)	415.9(31)	31.4(fixed)	—	–2.3	31.4
*u*1158	H(71)...H(91)	416.5(54)	37.5(fixed)	—	2.7	37.5

*u*1492	H(32)...H(42)	416.6(25)	31.0(fixed)	—	–11.0	31.0
*u*1399	C(63)...H(76)	416.7(43)	33.2(fixed)	—	–2.0	33.2
*u*1433	C(58)...H(70)	417.1(38)	31.5(fixed)	—	–2.1	31.5
*u*2558	C(157)...H(170)	417.8(41)	22.5(fixed)	—	–1.9	22.5
*u*1581	C(55)...H(68)	418.2(52)	23.6(fixed)	—	–3.4	23.6
*u*1469	C(105)...H(115)	418.7(27)	31.2(fixed)	—	–2.1	31.2
*u*1503	C(8)...H(19)	419.3(44)	33.4(fixed)	—	–3.0	33.4
*u*1477	H(31)...H(44)	419.7(25)	36.9(fixed)	—	–7.0	36.9
*u*1487	C(11)...H(47)	420.0(67)	35.0(fixed)	—	–2.6	35.0
*u*1427	Cl(61)...H(92)	420.0(55)	33.1(fixed)	—	–2.6	33.1
*u*2548	Cl(156)...H(160)	421.0(27)	30.7(fixed)	—	–3.6	30.7
*u*1488	C(9)...H(34)	421.0(25)	34.8(fixed)	—	–4.9	34.8
*u*1432	H(32)...H(33)	421.0(25)	28.2(fixed)	—	–7.0	28.2
*u*1495	C(152)...H(162)	421.0(24)	36.0(fixed)	—	–5.3	36.0
*u*1506	H(172)...H(185)	421.1(25)	27.7(fixed)	—	–6.7	27.7
*u*1429	H(173)...H(174)	421.3(25)	28.6(fixed)	—	–6.4	28.6
*u*1519	C(17)...H(35)	421.3(68)	38.6(fixed)	—	–4.0	38.6
*u*1478	Cl(14)...H(20)	421.7(45)	36.2(fixed)	—	–2.9	36.2
*u*1456	C(64)...H(77)	422.0(33)	32.2(fixed)	—	–3.3	32.2
*u*1545	C(7)...H(25)	422.2(46)	32.3(fixed)	—	–3.8	32.3
*u*1434	H(172)...H(176)	422.6(25)	31.1(fixed)	—	–4.8	31.1
*u*1515	C(10)...H(39)	422.6(40)	34.4(fixed)	—	–3.5	34.4
*u*1430	H(31)...H(35)	422.6(25)	30.4(fixed)	—	–5.1	30.4
*u*1467	H(78)...H(82)	422.7(25)	28.4(fixed)	—	–5.0	28.4
*u*1356	H(25)...H(36)	422.9(34)	41.7(fixed)	—	–2.9	41.7
*u*1486	H(78)...H(91)	423.0(25)	26.7(fixed)	—	–4.9	26.7
*u*1423	H(23)...H(45)	423.0(25)	26.6(fixed)	—	–5.2	26.6
*u*1448	Cl(14)...H(46)	423.0(33)	34.6(fixed)	—	–2.9	34.6
*u*1444	H(79)...H(80)	423.2(25)	27.9(fixed)	—	–4.6	27.9
*u*1468	H(20)...H(22)	423.2(25)	26.1(fixed)	—	–5.1	26.1
*u*1491	H(159)...H(164)	423.6(25)	30.7(fixed)	—	–3.9	30.7
*u*1776	C(154)...H(169)	423.7(57)	29.6(fixed)	—	2.8	29.6
*u*2564	C(149)...H(174)	423.7(40)	26.3(fixed)	—	–4.1	26.3
*u*1462	H(69)...H(94)	423.8(25)	26.0(fixed)	—	–4.4	26.0
*u*1446	H(22)...H(47)	423.8(25)	27.9(fixed)	—	–4.3	27.9
*u*1422	H(112)...H(117)	424.0(25)	25.5(fixed)	—	–4.3	25.5
*u*1460	H(79)...H(89)	424.0(25)	28.3(fixed)	—	–3.7	28.3
*u*1436	H(65)...H(70)	424.0(25)	25.4(fixed)	—	–4.2	25.4
*u*1442	H(18)...H(23)	424.1(25)	27.6(fixed)	—	–4.0	27.6
*u*2411	C(148)...H(166)	424.3(18)	23.4(fixed)	—	–1.8	23.4
*u*1493	C(7)...H(26)	424.3(43)	35.5(fixed)	—	–3.0	35.5
*u*1459	H(67)...H(69)	424.3(25)	26.0(fixed)	—	–3.8	26.0
*u*1530	Si(2)...H(42)	424.4(31)	48.9(fixed)	—	–3.8	48.9
*u*1441	H(70)...H(92)	424.5(25)	26.8(fixed)	—	–3.6	26.8
*u*1499	H(125)...H(129)	424.5(25)	25.0(fixed)	—	–3.9	25.0
*u*1455	H(114)...H(116)	424.6(25)	26.8(fixed)	—	–3.5	26.8

*u*1465	H(126)...H(127)	424.9(25)	25.4(fixed)	—	–3.4	25.4
*u*1529	C(13)...H(31)	425.2(36)	42.4(fixed)	—	–5.7	42.4
*u*2857	C(103)...H(113)	425.3(31)	22.8(fixed)	—	–5.4	22.8
*u*1567	C(110)...H(119)	425.5(22)	30.5(fixed)	—	–3.0	30.5
*u*1542	C(64)...H(81)	426.1(58)	32.7(fixed)	—	–4.1	32.7
*u*1449	C(6)...H(38)	426.2(21)	31.7(fixed)	—	–2.2	31.7
*u*1463	H(35)...H(44)	426.3(47)	30.0(fixed)	—	–10.9	30.0
*u*1561	C(8)...H(21)	426.4(47)	33.8(fixed)	—	–4.5	33.8
*u*1390	H(73)...H(81)	426.7(40)	45.9(fixed)	—	–3.4	45.9
*u*1471	C(60)...H(90)	426.7(28)	31.1(fixed)	—	–2.4	31.1
*u*734	Cl(156)...H(163)	426.8(27)	57.1(fixed)	—	3.6	57.1
*u*2495	C(101)...H(122)	427.5(41)	22.3(fixed)	—	–1.8	22.3
*u*1458	C(111)...H(129)	427.8(83)	31.4(fixed)	—	–2.2	31.4
*u*1534	Cl(14)...H(19)	428.3(33)	35.5(fixed)	—	–3.5	35.5
*u*2213	C(103)...H(116)	428.8(40)	32.2(fixed)	—	–0.7	32.2
*u*1508	Cl(61)...H(67)	428.9(48)	34.7(fixed)	—	–2.6	34.7
*u*1412	Cl(15)...H(40)	428.9(39)	34.8(fixed)	—	–2.9	34.8
*u*1496	C(11)...H(21)	429.0(28)	37.0(fixed)	—	–4.0	37.0
*u*1556	C(58)...H(93)	429.0(57)	30.6(fixed)	—	–3.6	30.6
*u*1453	H(118)...H(123)	429.2(40)	26.2(fixed)	—	–6.2	26.2
*u*1587	Si(52)...H(71)	429.5(31)	27.7(fixed)	—	–1.8	27.7
*u*1532	Si(3)...H(33)	429.7(26)	35.4(fixed)	—	–2.3	35.4
*u*1593	Cl(156)...H(162)	430.2(20)	28.5(fixed)	—	–7.5	28.5
*u*3058	H(121)...H(130)	430.5(44)	25.0(fixed)	—	–9.1	25.0
*u*1457	H(33)...H(42)	430.9(47)	37.2(fixed)	—	–5.2	37.2
*u*1464	H(120)...H(122)	431.3(40)	29.1(fixed)	—	–3.8	29.1
*u*1494	H(83)...H(86)	431.6(39)	25.7(fixed)	—	–5.9	25.7
*u*2448	C(157)...H(168)	431.8(25)	23.3(fixed)	—	–1.8	23.3
*u*1845	C(106)...H(123)	431.9(39)	34.0(fixed)	—	6.2	34.0
*u*1544	Si(3)...H(21)	432.0(30)	20.0(fixed)	—	–5.6	20.0
*u*1557	C(17)...H(34)	432.1(54)	35.3(fixed)	—	–5.0	35.3
*u*1416	H(174)...H(183)	432.3(47)	26.7(fixed)	—	–5.0	26.7
*u*1424	H(80)...H(89)	432.3(47)	26.2(fixed)	—	–5.0	26.2
*u*1526	C(57)...H(86)	432.5(33)	32.9(fixed)	—	–2.6	32.9
*u*1476	C(55)...H(81)	432.5(24)	33.9(fixed)	—	–3.7	33.9
*u*1474	H(167)...H(169)	432.8(39)	27.2(fixed)	—	–4.7	27.2
*u*1601	Si(50)...H(68)	432.8(31)	18.8(fixed)	—	3.9	18.8
*u*1475	H(24)...H(29)	432.9(38)	27.2(fixed)	—	–5.3	27.2
*u*1426	H(65)...H(92)	433.0(47)	26.5(fixed)	—	–4.5	26.5
*u*1439	H(18)...H(45)	433.0(47)	26.0(fixed)	—	–4.7	26.0
*u*1511	C(58)...H(68)	433.0(31)	33.4(fixed)	—	–2.6	33.4
*u*1451	H(165)...H(170)	433.0(39)	27.4(fixed)	—	–4.4	27.4
*u*1445	H(176)...H(185)	433.0(47)	28.0(fixed)	—	–4.2	28.0
*u*1524	C(60)...H(78)	433.0(31)	35.6(fixed)	—	–3.2	35.6
*u*1447	H(37)...H(40)	433.0(38)	25.3(fixed)	—	–5.3	25.3
*u*1502	H(26)...H(28)	433.2(38)	27.4(fixed)	—	–5.0	27.4

*u*1480	H(20)...H(47)	433.2(47)	26.5(fixed)	—	–4.5	26.5
*u*1490	H(73)...H(75)	433.2(39)	26.0(fixed)	—	–4.2	26.0
*u*1394	C(56)...H(87)	433.2(41)	32.3(fixed)	—	–1.9	32.3
*u*1443	H(67)...H(94)	433.3(47)	27.3(fixed)	—	–4.1	27.3
*u*1479	H(84)...H(87)	433.3(39)	28.3(fixed)	—	–3.9	28.3
*u*1452	C(12)...H(25)	433.4(18)	32.9(fixed)	—	–3.5	32.9
*u*1450	H(71)...H(76)	433.4(39)	25.8(fixed)	—	–4.1	25.8
*u*1482	Cl(61)...H(93)	433.6(37)	34.4(fixed)	—	–2.9	34.4
*u*1437	H(129)...H(138)	433.6(47)	26.0(fixed)	—	–4.0	26.0
*u*1425	H(127)...H(136)	433.7(47)	26.6(fixed)	—	–3.8	26.6
*u*1454	H(82)...H(91)	433.7(47)	27.9(fixed)	—	–3.5	27.9
*u*2436	C(154)...H(168)	433.8(40)	28.0(fixed)	—	–3.4	28.0
*u*706	C(153)...H(161)	434.1(45)	40.9(fixed)	—	3.0	40.9
*u*1473	H(36)...H(39)	434.4(38)	26.8(fixed)	—	–3.8	26.8
*u*1547	Si(49)...H(89)	434.4(28)	26.1(fixed)	—	–1.5	26.1
*u*1538	Si(50)...H(80)	434.4(23)	29.9(fixed)	—	–2.1	29.9
*u*1553	Si(3)...H(18)	434.9(27)	28.2(fixed)	—	–1.9	28.2
*u*1536	C(13)...H(30)	435.0(28)	40.7(fixed)	—	–6.0	40.7
*u*2972	Cl(108)...H(113)	435.4(37)	19.1(fixed)	—	–5.8	19.1
*u*1528	C(9)...H(44)	435.8(51)	55.5(fixed)	—	–8.5	55.5
*u*1410	H(75)...H(88)	435.8(33)	46.3(fixed)	—	–2.3	46.3
*u*1558	Si(52)...H(84)	435.9(19)	33.1(fixed)	—	–2.3	33.1
*u*1578	C(11)...H(46)	436.0(55)	32.0(fixed)	—	–3.7	32.0
*u*1639	Si(97)...H(112)	436.1(31)	26.9(fixed)	—	–1.7	26.9
*u*1540	C(111)...H(128)	436.8(66)	30.1(fixed)	—	–3.0	30.1
*u*1533	Si(5)...H(32)	437.0(23)	39.1(fixed)	—	–2.4	39.1
*u*1512	Cl(15)...H(41)	437.0(29)	34.6(fixed)	—	–3.7	34.6
*u*1523	C(16)...H(28)	437.3(48)	36.9(fixed)	—	–3.5	36.9
*u*1549	Si(2)...H(24)	437.5(21)	30.9(fixed)	—	–2.3	30.9
*u*1509	Cl(15)...H(36)	437.8(36)	34.7(fixed)	—	–2.5	34.7
*u*2777	C(106)...H(121)	438.2(30)	21.9(fixed)	—	–8.0	21.9
*u*1546	Cl(61)...H(66)	438.3(30)	35.2(fixed)	—	–3.3	35.2
*u*1583	C(59)...H(66)	438.6(20)	23.8(fixed)	—	–3.9	23.8
*u*1629	Si(50)...H(65)	438.6(30)	27.1(fixed)	—	–1.7	27.1
*u*1586	Si(98)...H(117)	438.8(21)	25.4(fixed)	—	–1.5	25.4
*u*2801	C(103)...H(115)	439.1(29)	19.0(fixed)	—	–4.9	19.0
*u*2351	Cl(108)...H(114)	439.1(52)	35.2(fixed)	—	–0.7	35.2
*u*1552	Si(97)...H(127)	439.3(25)	27.6(fixed)	—	–1.8	27.6
*u*2768	C(149)...H(162)	439.7(22)	21.3(fixed)	—	–8.8	21.3
*u*1525	C(56)...H(83)	439.8(21)	39.0(fixed)	—	–3.9	39.0
*u*2072	H(167)...H(175)	440.0(38)	39.0(fixed)	—	2.5	39.0
*u*1527	C(59)...H(75)	440.6(24)	32.8(fixed)	—	–2.6	32.8
*u*1397	H(74)...H(91)	440.8(40)	43.3(fixed)	—	–2.1	43.3
*u*1440	C(157)...H(166)	441.0(33)	32.9(fixed)	—	–3.1	32.9
*u*1625	C(101)...H(128)	441.1(30)	24.9(fixed)	—	–3.8	24.9
*u*1604	C(9)...H(21)	441.2(56)	25.0(fixed)	—	–5.4	25.0

*u*2414	C(149)...H(175)	441.8(25)	29.8(fixed)	—	–4.0	29.8
*u*1564	C(9)...H(43)	441.9(36)	45.2(fixed)	—	–9.7	45.2
*u*1562	Cl(15)...H(38)	442.5(24)	33.9(fixed)	—	–3.0	33.9
*u*1560	Si(52)...H(79)	442.8(20)	30.1(fixed)	—	–1.7	30.1
*u*1555	C(10)...H(41)	443.1(26)	36.4(fixed)	—	–4.3	36.4
*u*1917	Si(146)...H(165)	443.2(18)	22.5(fixed)	—	–0.1	22.5
*u*1620	Cl(15)...H(43)	443.5(20)	27.5(fixed)	—	–13.9	27.5
*u*1595	C(10)...H(46)	443.5(36)	24.4(fixed)	—	–4.4	24.4
*u*1501	C(63)...H(74)	443.6(27)	30.5(fixed)	—	–2.6	30.5
*u*2445	C(101)...H(121)	444.1(29)	23.2(fixed)	—	–1.6	23.2
*u*1574	C(60)...H(77)	444.2(24)	32.8(fixed)	—	–3.8	32.8
*u*1598	Si(5)...H(37)	444.4(22)	26.8(fixed)	—	–1.8	26.8
*u*1649	C(6)...H(25)	444.9(43)	24.9(fixed)	—	–5.2	24.9
*u*1551	Si(144)...H(159)	445.0(27)	27.6(fixed)	—	–1.8	27.6
*u*1627	Si(146)...H(175)	445.2(16)	19.8(fixed)	—	–5.4	19.8
*u*1591	C(153)...H(160)	445.5(33)	24.3(fixed)	—	–4.1	24.3
*u*1607	C(16)...H(41)	445.7(39)	24.0(fixed)	—	–5.0	24.0
*u*1559	Si(145)...H(164)	446.0(17)	35.2(fixed)	—	–2.3	35.2
*u*1577	C(106)...H(113)	446.0(25)	30.7(fixed)	—	–3.3	30.7
*u*1588	Si(4)...H(23)	446.2(15)	30.4(fixed)	—	–2.2	30.4
*u*1635	Si(143)...H(160)	446.4(12)	19.2(fixed)	—	–4.5	19.2
*u*1634	Si(5)...H(25)	446.6(28)	19.6(fixed)	—	–4.9	19.6
*u*1597	Si(144)...H(162)	446.9(13)	20.7(fixed)	—	–6.9	20.7
*u*1596	Cl(61)...H(77)	446.9(12)	26.8(fixed)	—	–5.0	26.8
*u*1623	C(12)...H(19)	447.0(27)	25.2(fixed)	—	–4.4	25.2
*u*1566	C(57)...H(88)	447.0(22)	31.7(fixed)	—	–3.2	31.7
*u*1599	C(11)...H(27)	447.2(33)	24.5(fixed)	—	–5.1	24.5
*u*2872	C(106)...H(120)	448.0(61)	24.3(fixed)	—	–0.5	24.3
*u*768	Si(98)...H(118)	448.2(20)	30.8(fixed)	—	3.7	30.8
*u*1605	Si(144)...H(174)	448.3(21)	28.9(fixed)	—	–1.7	28.9
*u*1582	Si(5)...H(29)	448.3(30)	29.9(fixed)	—	–1.8	29.9
*u*1504	C(56)...H(88)	448.5(24)	31.6(fixed)	—	–2.7	31.6
*u*1592	C(57)...H(93)	448.7(33)	23.4(fixed)	—	–4.3	23.4
*u*1615	Si(49)...H(66)	448.8(12)	19.2(fixed)	—	–4.2	19.2
*u*1608	Cl(62)...H(85)	449.1(21)	27.7(fixed)	—	–6.3	27.7
*u*2981	Cl(155)...H(168)	449.3(18)	22.5(fixed)	—	–5.8	22.5
*u*1633	Si(2)...H(19)	449.4(10)	19.7(fixed)	—	–4.5	19.7
*u*1603	Si(51)...H(93)	449.7(18)	18.9(fixed)	—	–4.5	18.9
*u*1606	Si(99)...H(128)	450.0(17)	19.2(fixed)	—	–4.0	19.2
*u*384	C(157)...H(167)	450.1(42)	29.9(fixed)	—	10.1	29.9
*u*1565	Si(96)...H(113)	450.1(13)	18.7(fixed)	—	–4.2	18.7
*u*1616	C(63)...H(88)	450.3(35)	23.8(fixed)	—	–3.9	23.8
*u*1630	Si(3)...H(43)	450.3(15)	25.7(fixed)	—	–11.9	25.7
*u*1590	Si(51)...H(70)	450.4(21)	26.3(fixed)	—	–1.6	26.3
*u*1637	Si(4)...H(46)	450.5(17)	19.2(fixed)	—	–4.7	19.2
*u*1648	Si(2)...H(45)	450.7(20)	27.5(fixed)	—	–1.7	27.5

*u*1684	Si(143)...H(168)	451.3(10)	21.4(fixed)	—	–3.8	21.4
*u*1580	C(56)...H(85)	451.3(19)	34.5(fixed)	—	–4.7	34.5
*u*1621	C(148)...H(175)	451.6(26)	25.5(fixed)	—	–5.5	25.5
*u*1619	Si(2)...H(30)	451.7(13)	22.8(fixed)	—	–7.6	22.8
*u*1636	Si(52)...H(81)	451.8(17)	20.2(fixed)	—	–5.3	20.2
*u*1632	Si(5)...H(34)	451.8(17)	21.8(fixed)	—	–6.4	21.8
*u*2676	C(100)...H(121)	452.0(40)	27.6(fixed)	—	–3.8	27.6
*u*1645	Cl(14)...H(30)	452.3(25)	29.4(fixed)	—	–8.6	29.4
*u*1644	C(7)...H(34)	452.5(26)	26.3(fixed)	—	–6.9	26.3
*u*1642	Si(49)...H(77)	453.5(12)	19.8(fixed)	—	–4.8	19.8
*u*1575	Cl(109)...H(115)	453.5(20)	33.8(fixed)	—	–2.7	33.8
*u*1641	Si(97)...H(115)	453.8(13)	18.2(fixed)	—	–3.5	18.2
*u*3168	C(106)...H(119)	453.8(47)	16.1(fixed)	—	–4.6	16.1
*u*1646	Si(49)...H(92)	453.8(24)	27.0(fixed)	—	–1.7	27.0
*u*1568	Si(51)...H(76)	453.9(22)	26.9(fixed)	—	–1.5	26.9
*u*1612	Si(4)...H(41)	454.2(10)	20.8(fixed)	—	–5.3	20.8
*u*1610	C(58)...H(72)	454.3(29)	23.8(fixed)	—	–3.9	23.8
*u*1572	C(59)...H(74)	454.7(16)	31.6(fixed)	—	–3.1	31.6
*u*1874	Si(145)...H(170)	454.9(21)	21.4(fixed)	—	0.2	21.4
*u*1535	Si(50)...H(87)	455.1(22)	26.8(fixed)	—	–1.4	26.8
*u*2806	C(154)...H(160)	455.3(32)	20.1(fixed)	—	–6.1	20.1
*u*1624	Si(4)...H(27)	455.5(9)	20.3(fixed)	—	–5.2	20.3
*u*1571	C(16)...H(27)	455.8(38)	33.8(fixed)	—	–4.2	33.8
*u*2192	Si(96)...H(119)	456.1(12)	15.5(fixed)	—	–3.1	15.5
*u*2218	Si(99)...H(121)	456.2(10)	16.7(fixed)	—	–4.1	16.7
*u*1600	C(8)...H(38)	456.3(25)	23.3(fixed)	—	–3.4	23.3
*u*1640	Si(50)...H(85)	457.0(11)	19.8(fixed)	—	–5.8	19.8
*u*1563	Si(49)...H(74)	457.0(12)	19.2(fixed)	—	–4.0	19.2
*u*1622	Si(51)...H(88)	457.1(9)	19.6(fixed)	—	–4.1	19.6
*u*1715	Si(145)...H(166)	457.5(12)	23.0(fixed)	—	–4.1	23.0
*u*1569	Si(50)...H(90)	457.7(14)	18.5(fixed)	—	–3.8	18.5
*u*1782	H(176)...H(187)	458.1(76)	49.1(fixed)	—	–7.0	49.1
*u*1650	C(54)...H(81)	458.1(33)	26.1(fixed)	—	–5.5	26.1
*u*1628	Si(3)...H(38)	458.1(12)	18.6(fixed)	—	–3.7	18.6
*u*697	Si(96)...H(123)	458.7(22)	32.7(fixed)	—	7.4	32.7
*u*1517	C(55)...H(91)	461.8(44)	32.3(fixed)	—	–2.2	32.3
*u*1647	Si(51)...H(72)	462.2(13)	19.5(fixed)	—	–4.1	19.5
*u*1522	C(63)...H(73)	462.3(43)	32.7(fixed)	—	–2.4	32.7
*u*1618	Si(3)...H(40)	463.7(24)	27.8(fixed)	—	–1.5	27.8
*u*1693	H(67)...H(73)	464.6(57)	37.8(fixed)	—	4.7	37.8
*u*1613	C(56)...H(90)	464.7(34)	23.9(fixed)	—	–3.5	23.9
*u*1738	H(116)...H(125)	467.0(64)	36.7(fixed)	—	3.3	36.7
*u*1589	C(63)...H(72)	467.8(36)	31.7(fixed)	—	–3.3	31.7
*u*1594	C(55)...H(90)	468.5(36)	30.5(fixed)	—	–2.9	30.5
*u*2402	C(152)...H(166)	469.2(30)	29.3(fixed)	—	–3.6	29.3
*u*1810	H(176)...H(188)	469.2(81)	42.0(fixed)	—	–8.2	42.0

*u*1667	Si(50)...C(64)	469.3(17)	12.2(tied to *u*1752)	—	–0.6	11.5
*u*1655	Si(3)...C(17)	469.9(16)	12.4(tied to *u*1752)	—	–0.7	11.7
*u*1766	H(22)...H(25)	470.1(44)	46.2(fixed)	—	–6.4	46.2
*u*1716	Si(52)...H(72)	470.3(30)	22.5(fixed)	—	–3.7	22.5
*u*1756	H(81)...H(94)	470.4(75)	44.8(fixed)	—	–6.0	44.8
*u*2441	C(107)...H(119)	470.6(32)	23.2(fixed)	—	–1.7	23.2
*u*2506	H(161)...H(167)	471.3(50)	35.9(fixed)	—	–0.6	35.9
*u*1688	Si(2)...H(43)	471.9(20)	29.2(fixed)	—	–10.4	29.2
*u*1677	Si(3)...H(19)	473.2(25)	22.7(fixed)	—	–4.1	22.7
*u*1945	H(68)...H(71)	474.3(55)	35.8(fixed)	—	–7.0	35.8
*u*1698	Si(52)...C(56)	475.0(16)	12.0(tied to *u*1752)	—	–0.7	11.3
*u*1765	Si(50)...H(66)	475.6(26)	21.6(fixed)	—	–3.9	21.6
*u*1795	H(82)...H(93)	476.4(71)	45.2(fixed)	—	–6.4	45.2
*u*1617	C(60)...H(74)	476.4(30)	24.0(fixed)	—	–3.8	24.0
*u*1668	Si(143)...C(148)	476.4(7)	12.1(tied to *u*1752)	—	–0.7	11.4
*u*1846	C(56)...H(70)	476.7(41)	32.0(fixed)	—	2.2	32.0
*u*1662	Si(49)...C(54)	477.1(8)	12.3(tied to *u*1752)	—	–0.7	11.6
*u*1669	Si(143)...C(152)	477.7(10)	12.2(tied to *u*1752)	—	–0.7	11.4
*u*1695	Si(3)...H(34)	477.7(14)	23.8(fixed)	—	–5.9	23.8
*u*1666	Si(2)...C(7)	477.8(7)	12.1(tied to *u*1752)	—	–0.7	11.4
*u*1652	Si(96)...C(101)	478.0(7)	12.4(tied to *u*1752)	—	–0.7	11.6
*u*1779	C(53)...H(73)	478.2(45)	29.1(fixed)	—	2.7	29.1
*u*1777	H(30)...H(39)	478.6(43)	52.3(fixed)	—	–8.3	52.3
*u*1770	H(34)...H(47)	478.8(67)	48.4(fixed)	—	–6.7	48.4
*u*1729	H(31)...H(42)	478.9(13)	16.3(fixed)	—	–12.7	16.3
*u*317	H(120)...H(129)	479.0(59)	48.0(fixed)	—	10.5	48.0
*u*1659	H(75)...H(82)	479.0(52)	37.3(fixed)	—	5.9	37.3
*u*1672	Si(96)...C(105)	479.5(9)	12.2(tied to *u*1752)	—	–0.6	11.5
*u*1658	Si(2)...C(9)	479.6(8)	12.0(tied to *u*1752)	—	–0.8	11.3
*u*1676	Si(49)...C(58)	480.0(9)	11.9(tied to *u*1752)	—	–0.6	11.2
*u*876	Si(143)...C(149)	480.1(9)	17.8(tied to *u*1752)	—	0.2	16.8
*u*1250	Si(98)...C(103)	480.2(8)	16.7(tied to *u*1752)	—	–0.1	15.7
*u*1743	Si(5)...H(27)	480.4(30)	23.0(fixed)	—	–4.5	23.0
*u*1674	Si(2)...C(11)	480.4(9)	12.2(tied to *u*1752)	—	–0.7	11.4
*u*1680	Si(145)...C(147)	480.6(8)	12.2(tied to *u*1752)	—	–0.7	11.5
*u*1665	Si(50)...H(81)	481.1(13)	23.5(fixed)	—	–4.7	23.5
*u*1656	Si(50)...C(57)	481.1(8)	12.2(tied to *u*1752)	—	–0.7	11.5
*u*1671	Si(3)...C(10)	481.4(8)	11.9(tied to *u*1752)	—	–0.7	11.2
*u*1758	H(73)...H(92)	481.5(53)	40.8(fixed)	—	6.8	40.8
*u*1737	Si(5)...H(30)	481.7(16)	25.3(fixed)	—	–7.1	25.3
*u*1933	H(122)...H(133)	481.8(70)	45.1(fixed)	—	–10.7	45.1
*u*1689	Si(49)...H(90)	481.8(19)	21.3(fixed)	—	–3.4	21.3
*u*1704	Si(52)...H(85)	481.9(9)	24.5(fixed)	—	–5.2	24.5
*u*1660	Si(49)...C(55)	482.0(9)	11.8(tied to *u*1752)	—	–0.7	11.1
*u*1702	H(26)...H(29)	482.0(16)	16.1(fixed)	—	–7.2	16.1
*u*1681	Si(98)...C(100)	482.1(8)	12.4(tied to *u*1752)	—	–0.6	11.7

*u*1678	Si(51)...C(53)	482.1(9)	12.4(tied to *u*1752)	—	–0.7	11.7
*u*1805	C(55)...H(67)	482.1(47)	29.6(fixed)	—	2.3	29.6
*u*1718	H(120)...H(123)	482.1(17)	16.7(fixed)	—	–7.3	16.7
*u*1690	Si(5)...C(13)	482.1(8)	12.2(tied to *u*1752)	—	–0.7	11.5
*u*1732	H(32)...H(35)	482.3(13)	15.3(fixed)	—	–9.4	15.3
*u*1724	H(33)...H(44)	482.5(19)	16.0(fixed)	—	–12.2	16.0
*u*1703	H(83)...H(87)	482.5(17)	16.8(fixed)	—	–7.0	16.8
*u*1757	Si(97)...H(113)	482.6(20)	21.6(fixed)	—	–3.8	21.6
*u*2379	H(123)...H(129)	482.6(32)	32.9(fixed)	—	–3.3	32.9
*u*1675	Si(97)...H(128)	482.6(15)	21.8(fixed)	—	–3.7	21.8
*u*1682	Si(4)...C(6)	482.6(8)	12.3(tied to *u*1752)	—	–0.7	11.6
*u*1727	H(173)...H(176)	482.8(13)	16.9(fixed)	—	–8.5	16.9
*u*1708	H(36)...H(40)	482.8(16)	15.7(fixed)	—	–6.5	15.7
*u*949	Si(146)...C(150)	482.9(7)	17.2(tied to *u*1752)	—	0.2	16.2
*u*1710	H(159)...H(163)	483.1(13)	17.5(fixed)	—	–8.2	17.5
*u*1664	Si(2)...H(25)	483.1(11)	22.8(fixed)	—	–4.4	22.8
*u*1736	Si(98)...H(115)	483.2(14)	21.5(fixed)	—	–3.2	21.5
*u*1706	H(167)...H(170)	483.3(17)	16.6(fixed)	—	–6.6	16.6
*u*1796	H(82)...H(94)	483.4(76)	39.4(fixed)	—	–7.0	39.4
*u*1705	H(73)...H(76)	483.4(17)	16.5(fixed)	—	–6.1	16.5
*u*1694	Si(52)...C(60)	483.5(7)	12.0(tied to *u*1752)	—	–0.6	11.3
*u*1934	H(41)...H(42)	483.6(55)	63.2(fixed)	—	–16.2	63.2
*u*1691	Si(52)...C(63)	483.6(8)	12.2(tied to *u*1752)	—	–0.6	11.5
*u*1731	H(79)...H(82)	483.9(13)	16.6(fixed)	—	–7.4	16.6
*u*1692	Si(5)...C(16)	484.0(8)	12.4(tied to *u*1752)	—	–0.8	11.7
*u*1717	H(23)...H(47)	484.3(13)	15.4(fixed)	—	–7.4	15.4
*u*1242	Si(99)...C(102)	484.4(8)	16.1(tied to *u*1752)	—	–0.1	15.2
*u*1851	H(35)...H(46)	484.4(69)	49.6(fixed)	—	–7.5	49.6
*u*1679	Si(4)...C(12)	484.4(8)	12.0(tied to *u*1752)	—	–0.7	11.3
*u*1719	H(18)...H(22)	484.5(13)	15.4(fixed)	—	–7.2	15.4
*u*1958	H(68)...H(72)	484.6(58)	36.7(fixed)	—	–6.9	36.7
*u*1722	H(78)...H(89)	484.7(13)	16.5(fixed)	—	–6.6	16.5
*u*1631	Si(98)...H(119)	484.7(11)	19.1(fixed)	—	–4.0	19.1
*u*1686	Si(51)...C(59)	484.9(8)	11.9(tied to *u*1752)	—	–0.7	11.2
*u*2026	H(175)...H(187)	485.0(56)	41.4(fixed)	—	–9.8	41.4
*u*1699	Si(4)...C(8)	485.1(8)	11.9(tied to *u*1752)	—	–0.7	11.2
*u*1800	C(104)...H(116)	485.2(48)	29.0(fixed)	—	1.7	29.0
*u*1709	H(70)...H(94)	485.2(13)	16.2(fixed)	—	–6.2	16.2
*u*1721	H(65)...H(69)	485.4(13)	16.1(fixed)	—	–6.1	16.1
*u*1609	Si(96)...H(121)	485.4(15)	21.4(fixed)	—	–6.3	21.4
*u*1809	H(21)...H(26)	485.5(49)	46.5(fixed)	—	–7.0	46.5
*u*1734	Si(145)...H(162)	485.6(11)	25.1(fixed)	—	–6.1	25.1
*u*1730	H(112)...H(116)	485.7(13)	16.1(fixed)	—	–5.9	16.1
*u*1929	H(66)...H(84)	485.9(33)	43.3(fixed)	—	–9.2	43.3
*u*1714	H(126)...H(129)	486.0(13)	16.2(fixed)	—	–5.6	16.2
*u*1651	H(22)...H(31)	486.4(39)	37.6(fixed)	—	10.4	37.6

*u*2222	Si(146)...H(166)	486.5(10)	15.9(fixed)	—	–3.5	15.9
*u*1735	Si(52)...H(77)	486.8(15)	22.5(fixed)	—	–4.4	22.5
*u*1751	Si(144)...H(175)	486.9(13)	23.3(fixed)	—	–4.8	23.3
*u*1728	H(174)...H(185)	487.2(19)	16.4(fixed)	—	–7.1	16.4
*u*1663	H(83)...H(94)	487.4(55)	39.2(fixed)	—	7.0	39.2
*u*1723	H(80)...H(91)	487.7(19)	16.3(fixed)	—	–6.7	16.3
*u*1697	Si(144)...H(160)	487.7(18)	22.8(fixed)	—	–4.1	22.8
*u*2669	C(147)...H(167)	487.9(35)	24.4(fixed)	—	–3.2	24.4
*u*1820	C(64)...H(73)	488.0(43)	31.9(fixed)	—	3.7	31.9
*u*1720	H(20)...H(28)	488.0(57)	37.0(fixed)	—	5.9	37.0
*u*1725	H(20)...H(45)	488.0(19)	15.5(fixed)	—	–6.7	15.5
*u*1713	H(67)...H(92)	488.1(19)	16.2(fixed)	—	–6.4	16.2
*u*1711	Si(5)...H(38)	488.2(12)	22.0(fixed)	—	–3.4	22.0
*u*1775	Si(5)...Cl(15)	488.3(15)	12.4(tied to *u*1752)	—	–0.8	11.7
*u*1733	Si(4)...H(21)	488.3(11)	24.9(fixed)	—	–5.0	24.9
*u*1712	H(127)...H(138)	488.4(19)	16.1(fixed)	—	–6.1	16.1
*u*3105	H(115)...H(122)	488.6(42)	23.3(fixed)	—	–6.4	23.3
*u*2131	H(168)...H(180)	488.9(55)	37.8(fixed)	—	2.3	37.8
*u*1806	H(28)...H(43)	489.3(48)	55.8(fixed)	—	–11.1	55.8
*u*1772	H(129)...H(140)	489.4(83)	41.0(fixed)	—	–4.9	41.0
*u*1838	H(31)...H(41)	489.6(35)	56.1(fixed)	—	–9.6	56.1
*u*1752	Si(3)...Cl(14)	489.7(10)	12.3(3)	—	–0.8	11.6
*u*1827	H(67)...H(76)	489.8(36)	40.9(fixed)	—	5.8	40.9
*u*1320	H(161)...H(179)	490.3(47)	44.8(fixed)	—	–2.5	44.8
*u*2024	H(21)...H(25)	490.7(53)	42.0(fixed)	—	–9.5	42.0
*u*2235	Si(145)...H(168)	490.7(13)	16.3(fixed)	—	–3.3	16.3
*u*1726	H(36)...H(47)	490.8(51)	37.5(fixed)	—	4.4	37.5
*u*1762	Si(2)...H(46)	491.0(13)	22.7(fixed)	—	–4.1	22.7
*u*780	C(105)...H(120)	491.0(42)	42.0(fixed)	—	2.5	42.0
*u*1905	H(32)...H(46)	491.0(44)	51.7(fixed)	—	–10.9	51.7
*u*1833	Si(50)...H(92)	491.2(23)	22.0(fixed)	—	0.5	22.0
*u*1262	Si(97)...Cl(108)	491.4(9)	18.3(tied to *u*1752)	—	–0.3	17.2
*u*1741	Si(51)...H(68)	491.9(14)	22.5(fixed)	—	–3.6	22.5
*u*1854	H(35)...H(47)	492.6(69)	40.5(fixed)	—	–8.1	40.5
*u*1683	H(69)...H(78)	492.6(45)	37.0(fixed)	—	5.3	37.0
*u*1707	Si(50)...H(88)	492.6(15)	21.1(fixed)	—	–3.8	21.1
*u*1761	Si(50)...Cl(61)	492.8(9)	12.0(tied to *u*1752)	—	–0.8	11.3
*u*1811	Si(3)...H(45)	492.9(20)	22.4(fixed)	—	0.4	22.4
*u*1739	Si(51)...H(74)	493.0(14)	20.8(fixed)	—	–3.5	20.8
*u*1753	Si(49)...H(93)	493.1(16)	22.3(fixed)	—	–4.0	22.3
*u*1745	C(56)...H(82)	493.4(40)	29.0(fixed)	—	4.1	29.0
*u*1798	H(28)...H(45)	493.5(46)	43.8(fixed)	—	8.0	43.8
*u*1836	H(77)...H(86)	493.6(35)	43.6(fixed)	—	–5.9	43.6
*u*1916	H(31)...H(39)	494.0(41)	41.0(fixed)	—	–10.7	41.0
*u*2001	H(117)...H(128)	494.9(43)	34.2(fixed)	—	–6.9	34.2
*u*1931	H(27)...H(33)	495.0(50)	43.9(fixed)	—	–10.4	43.9

*u*2597	H(116)...H(121)	495.2(40)	38.0(fixed)	—	–1.7	38.0
*u*1896	C(149)...H(161)	495.3(40)	33.5(fixed)	—	3.6	33.5
*u*980	Si(146)...Cl(155)	495.6(8)	18.9(tied to *u*1752)	—	0.1	17.8
*u*1814	H(22)...H(26)	495.7(40)	40.2(fixed)	—	–7.5	40.2
*u*1785	C(9)...H(20)	495.8(46)	29.0(fixed)	—	2.9	29.0
*u*409	C(102)...H(129)	496.0(45)	30.1(fixed)	—	8.0	30.1
*u*3077	H(162)...H(165)	496.1(33)	27.7(fixed)	—	–9.2	27.7
*u*1781	Si(51)...Cl(62)	496.1(8)	12.2(tied to *u*1752)	—	–0.8	11.5
*u*1815	Cl(61)...H(91)	496.4(39)	29.1(fixed)	—	2.1	29.1
*u*1789	H(40)...H(47)	496.5(40)	43.2(fixed)	—	7.8	43.2
*u*1813	H(78)...H(88)	496.6(30)	45.5(fixed)	—	–6.0	45.5
*u*1687	H(26)...H(39)	496.7(32)	37.7(fixed)	—	6.4	37.7
*u*1771	Si(3)...H(41)	497.0(17)	22.1(fixed)	—	–4.6	22.1
*u*1804	Si(49)...H(70)	497.2(14)	22.9(fixed)	—	–0.1	22.9
*u*2041	H(70)...H(74)	497.2(49)	36.8(fixed)	—	3.2	36.8
*u*1924	C(56)...H(67)	497.3(33)	32.1(fixed)	—	3.1	32.1
*u*2974	H(174)...H(177)	497.4(41)	35.3(fixed)	—	2.8	35.3
*u*1740	H(70)...H(83)	498.2(32)	45.4(fixed)	—	8.0	45.4
*u*2575	H(169)...H(176)	498.2(46)	38.1(fixed)	—	–0.2	38.1
*u*1865	C(60)...H(65)	498.3(17)	32.8(fixed)	—	2.8	32.8
*u*1870	C(13)...H(18)	498.5(15)	33.4(fixed)	—	2.9	33.4
*u*1908	C(147)...H(174)	498.6(20)	32.3(fixed)	—	4.3	32.3
*u*2019	H(81)...H(93)	498.7(55)	41.5(fixed)	—	–8.8	41.5
*u*1873	Si(143)...H(174)	499.1(19)	21.7(fixed)	—	0.6	21.7
*u*1821	Cl(15)...H(35)	499.1(40)	30.6(fixed)	—	4.8	30.6
*u*1744	C(7)...H(31)	499.1(33)	30.3(fixed)	—	7.2	30.3
*u*1388	C(153)...H(170)	499.2(16)	35.0(fixed)	—	–2.0	35.0
*u*1763	C(103)...H(129)	499.2(25)	28.6(fixed)	—	2.3	28.6
*u*1760	C(58)...H(75)	499.3(38)	28.3(fixed)	—	2.3	28.3
*u*1754	C(64)...H(83)	499.3(38)	29.6(fixed)	—	5.0	29.6
*u*1750	C(10)...H(22)	499.7(28)	29.8(fixed)	—	4.0	29.8
*u*1839	Si(2)...H(23)	499.7(11)	22.8(fixed)	—	0.7	22.8
*u*1747	H(65)...H(78)	499.8(41)	42.8(fixed)	—	7.1	42.8
*u*2993	H(169)...H(173)	499.9(24)	37.1(fixed)	—	3.7	37.1
*u*1843	Si(143)...H(164)	499.9(12)	22.3(fixed)	—	1.6	22.3
*u*1951	H(72)...H(80)	500.7(46)	39.6(fixed)	—	–8.2	39.6
*u*1837	H(75)...H(85)	500.7(29)	45.7(fixed)	—	–6.5	45.7
*u*2003	H(19)...H(37)	500.7(40)	34.3(fixed)	—	–7.8	34.3
*u*1541	Si(98)...H(123)	500.8(14)	34.4(fixed)	—	–2.0	34.4
*u*1802	C(6)...H(28)	501.0(46)	29.9(fixed)	—	3.5	29.9
*u*1759	H(159)...H(172)	501.2(35)	47.8(fixed)	—	9.4	47.8
*u*625	C(107)...H(112)	501.2(20)	36.2(fixed)	—	3.9	36.2
*u*1840	H(27)...H(44)	501.3(52)	65.6(fixed)	—	–12.1	65.6
*u*1986	H(88)...H(89)	501.6(50)	34.2(fixed)	—	–7.1	34.2
*u*2013	H(21)...H(27)	501.9(60)	38.8(fixed)	—	–10.1	38.8
*u*1878	C(100)...H(127)	501.9(22)	31.5(fixed)	—	2.8	31.5

*u*2419	H(114)...H(118)	502.0(42)	32.2(fixed)	—	–1.8	32.2
*u*1673	H(169)...H(180)	502.0(61)	38.1(fixed)	—	5.3	38.1
*u*1872	Si(52)...H(76)	502.2(17)	21.2(fixed)	—	0.1	21.2
*u*1808	H(129)...H(141)	502.2(85)	35.3(fixed)	—	–5.6	35.3
*u*1531	C(107)...H(122)	502.3(52)	39.7(fixed)	—	–4.7	39.7
*u*1919	C(17)...H(24)	502.4(34)	33.0(fixed)	—	3.8	33.0
*u*1889	C(63)...H(92)	502.6(22)	31.6(fixed)	—	3.4	31.6
*u*1985	C(53)...C(55)	502.6(36)	19.1(fixed)	—	–0.9	19.1
*u*1793	Si(96)...H(117)	502.7(13)	22.1(fixed)	—	–0.3	22.1
*u*2005	H(18)...H(25)	502.9(47)	35.6(fixed)	—	–8.8	35.6
*u*1829	H(74)...H(83)	503.1(24)	49.2(fixed)	—	–6.7	49.2
*u*1855	Si(96)...H(127)	503.3(19)	22.4(fixed)	—	0.1	22.4
*u*1794	C(17)...H(36)	503.5(38)	28.9(fixed)	—	2.1	28.9
*u*1932	H(79)...H(93)	503.6(39)	40.1(fixed)	—	–8.5	40.1
*u*1859	Si(145)...H(159)	503.8(14)	22.3(fixed)	—	0.1	22.3
*u*1920	C(16)...H(45)	503.8(22)	31.8(fixed)	—	3.3	31.8
*u*2037	H(34)...H(46)	503.9(53)	42.4(fixed)	—	–9.9	42.4
*u*1992	Cl(15)...H(23)	504.1(38)	34.2(fixed)	—	4.0	34.2
*u*2878	C(152)...H(177)	504.2(25)	25.8(fixed)	—	–0.4	25.8
*u*1964	H(21)...H(29)	504.2(59)	39.2(fixed)	—	–10.1	39.2
*u*1898	C(17)...H(28)	504.2(40)	34.4(fixed)	—	4.6	34.4
*u*1774	C(54)...H(78)	504.2(34)	28.6(fixed)	—	3.5	28.6
*u*1841	Si(51)...H(65)	504.5(16)	22.7(fixed)	—	0.1	22.7
*u*263	H(161)...H(170)	504.6(29)	44.0(fixed)	—	11.8	44.0
*u*582	C(102)...H(117)	504.6(19)	33.7(fixed)	—	3.5	33.7
*u*1887	Si(49)...H(80)	504.9(17)	21.7(fixed)	—	0.3	21.7
*u*1653	H(163)...H(172)	504.9(45)	40.2(fixed)	—	10.6	40.2
*u*1784	C(59)...H(94)	504.9(42)	29.5(fixed)	—	2.7	29.5
*u*1904	H(28)...H(44)	505.0(51)	53.2(fixed)	—	–13.5	53.2
*u*1799	Si(2)...H(29)	505.2(14)	22.2(fixed)	—	0.6	22.2
*u*1944	H(24)...H(38)	505.2(41)	39.0(fixed)	—	–7.7	39.0
*u*1910	H(78)...H(86)	505.2(34)	38.9(fixed)	—	–6.9	38.9
*u*1792	H(18)...H(31)	505.3(33)	48.5(fixed)	—	9.6	48.5
*u*2427	H(116)...H(122)	505.8(43)	37.1(fixed)	—	0.8	37.1
*u*1797	C(54)...H(83)	505.8(22)	35.6(fixed)	—	5.8	35.6
*u*2891	H(112)...H(121)	505.8(56)	39.8(fixed)	—	–6.1	39.8
*u*1773	C(13)...H(26)	505.9(23)	28.9(fixed)	—	3.7	28.9
*u*1864	Si(4)...H(18)	506.2(13)	22.5(fixed)	—	0.1	22.5
*u*2002	H(23)...H(34)	506.3(29)	38.4(fixed)	—	–11.7	38.4
*u*2027	H(41)...H(43)	506.4(35)	47.7(fixed)	—	–16.5	47.7
*u*1791	C(57)...H(69)	506.4(35)	29.3(fixed)	—	2.1	29.3
*u*1906	C(53)...H(80)	506.5(22)	33.2(fixed)	—	4.0	33.2
*u*2709	H(120)...H(126)	506.5(30)	34.0(fixed)	—	–3.0	34.0
*u*1769	H(23)...H(36)	506.5(20)	38.0(fixed)	—	7.3	38.0
*u*1886	C(59)...H(79)	506.6(17)	32.1(fixed)	—	4.0	32.1
*u*1816	C(12)...H(47)	506.6(36)	29.3(fixed)	—	2.6	29.3

*u*1856	Si(5)...H(40)	506.7(15)	21.8(fixed)	—	0.8	21.8
*u*1880	Si(2)...H(33)	506.7(17)	23.3(fixed)	—	0.6	23.3
*u*1998	H(128)...H(140)	506.8(63)	38.6(fixed)	—	–6.9	38.6
*u*1953	H(164)...H(175)	507.4(34)	49.7(fixed)	—	–11.8	49.7
*u*1830	Cl(14)...H(44)	507.7(43)	34.7(fixed)	—	11.6	34.7
*u*1573	Si(99)...H(118)	507.8(14)	28.0(fixed)	—	–1.8	28.0
*u*2694	C(152)...H(169)	508.0(33)	24.6(fixed)	—	–3.3	24.6
*u*2043	H(30)...H(46)	508.1(38)	39.7(fixed)	—	–12.1	39.7
*u*1978	H(66)...H(85)	508.1(19)	40.7(fixed)	—	–9.2	40.7
*u*1819	Si(50)...H(79)	508.3(13)	21.2(fixed)	—	0.4	21.2
*u*1818	C(53)...H(78)	508.3(28)	33.5(fixed)	—	4.4	33.5
*u*1888	Si(98)...H(112)	508.4(15)	21.7(fixed)	—	0.1	21.7
*u*1903	Si(52)...H(89)	508.5(14)	21.2(fixed)	—	–0.1	21.2
*u*2858	H(168)...H(182)	508.7(36)	37.8(fixed)	—	–6.5	37.8
*u*1900	C(13)...H(47)	509.0(29)	34.1(fixed)	—	3.7	34.1
*u*3225	H(119)...H(130)	509.0(60)	24.7(fixed)	—	–4.9	24.7
*u*2925	C(151)...H(169)	509.0(20)	26.2(fixed)	—	–0.7	26.2
*u*2372	C(151)...H(165)	509.3(16)	35.0(fixed)	—	–1.2	35.0
*u*1975	C(101)...C(104)	509.3(36)	19.4(fixed)	—	–0.9	19.4
*u*1884	Si(4)...H(37)	509.3(15)	22.0(fixed)	—	–0.5	22.0
*u*1901	C(6)...H(33)	509.5(23)	36.3(fixed)	—	5.4	36.3
*u*467	C(150)...H(164)	509.6(17)	32.5(fixed)	—	13.1	32.5
*u*1768	C(102)...H(114)	509.6(35)	30.0(fixed)	—	2.3	30.0
*u*1982	H(30)...H(41)	509.6(25)	49.1(fixed)	—	–11.7	49.1
*u*1871	Si(52)...H(87)	509.8(12)	21.3(fixed)	—	0.2	21.3
*u*2893	C(111)...H(123)	510.0(15)	26.6(fixed)	—	0.5	26.6
*u*1783	H(112)...H(125)	510.1(37)	39.4(fixed)	—	5.7	39.4
*u*1081	H(113)...H(131)	510.2(36)	39.8(fixed)	—	4.4	39.8
*u*1911	C(9)...H(37)	510.2(18)	32.2(fixed)	—	2.1	32.2
*u*1807	H(87)...H(94)	510.2(33)	41.3(fixed)	—	6.5	41.3
*u*395	Cl(109)...H(114)	510.4(45)	29.6(fixed)	—	9.4	29.6
*u*684	Si(143)...H(165)	510.4(14)	32.4(fixed)	—	4.3	32.4
*u*1863	C(110)...H(116)	510.5(20)	31.0(fixed)	—	2.6	31.0
*u*696	Si(146)...H(170)	510.6(12)	29.9(fixed)	—	4.5	29.9
*u*1788	H(37)...H(44)	510.6(43)	53.4(fixed)	—	14.7	53.4
*u*2045	H(19)...H(25)	510.7(48)	37.3(fixed)	—	–9.1	37.3
*u*1876	Si(3)...H(32)	510.7(13)	22.7(fixed)	—	1.5	22.7
*u*1858	Si(49)...H(71)	510.8(15)	21.7(fixed)	—	–0.3	21.7
*u*1902	C(8)...H(35)	511.0(27)	34.7(fixed)	—	5.6	34.7
*u*1862	C(6)...H(31)	511.0(25)	39.1(fixed)	—	7.4	39.1
*u*2010	H(115)...H(128)	511.0(29)	35.6(fixed)	—	–6.7	35.6
*u*1918	Si(4)...H(24)	511.6(14)	21.9(fixed)	—	0.0	21.9
*u*1877	H(24)...H(35)	511.8(38)	43.9(fixed)	—	8.3	43.9
*u*1857	C(12)...H(32)	511.9(18)	36.4(fixed)	—	7.9	36.4
*u*1844	C(157)...H(163)	511.9(21)	37.9(fixed)	—	6.8	37.9
*u*1832	C(7)...H(36)	512.0(18)	30.1(fixed)	—	3.1	30.1

*u*1812	H(69)...H(89)	512.2(38)	40.3(fixed)	—	5.5	40.3
*u*2267	C(104)...H(120)	512.2(21)	33.9(fixed)	—	–0.6	33.9
*u*1907	H(75)...H(83)	512.3(24)	40.4(fixed)	—	–7.6	40.4
*u*1970	Cl(15)...H(20)	512.4(28)	33.0(fixed)	—	3.5	33.0
*u*1755	C(151)...H(163)	512.7(33)	30.1(fixed)	—	5.8	30.1
*u*1892	C(59)...H(91)	512.7(32)	30.6(fixed)	—	3.0	30.6
*u*1891	Si(5)...H(42)	513.0(14)	24.5(fixed)	—	3.1	24.5
*u*1913	Si(51)...H(84)	513.1(13)	21.6(fixed)	—	0.5	21.6
*u*2034	H(162)...H(175)	513.2(27)	42.0(fixed)	—	–11.9	42.0
*u*1881	C(11)...H(40)	513.3(14)	33.1(fixed)	—	4.5	33.1
*u*1850	C(12)...H(44)	513.5(36)	43.5(fixed)	—	13.2	43.5
*u*1989	H(160)...H(179)	513.6(31)	38.1(fixed)	—	–8.3	38.1
*u*3034	H(162)...H(166)	513.6(20)	28.5(fixed)	—	–10.2	28.5
*u*1890	C(58)...H(87)	513.8(14)	30.4(fixed)	—	3.0	30.4
*u*422	C(150)...H(161)	514.6(25)	30.9(fixed)	—	9.2	30.9
*u*1057	H(160)...H(177)	514.6(43)	32.4(fixed)	—	5.9	32.4
*u*1895	C(10)...H(29)	514.7(13)	33.4(fixed)	—	4.3	33.4
*u*1915	C(150)...H(176)	514.7(35)	35.8(fixed)	—	4.3	35.8
*u*1909	C(55)...H(84)	514.7(16)	34.0(fixed)	—	4.8	34.0
*u*934	C(102)...C(105)	515.1(31)	22.1(fixed)	—	0.8	22.1
*u*2023	H(27)...H(34)	515.4(28)	38.6(fixed)	—	–11.2	38.6
*u*1817	C(8)...H(39)	515.4(28)	29.1(fixed)	—	3.2	29.1
*u*2004	H(77)...H(93)	515.5(35)	37.0(fixed)	—	–8.7	37.0
*u*1947	Si(3)...H(47)	515.6(12)	21.9(fixed)	—	–1.3	21.9
*u*2028	H(27)...H(43)	515.7(34)	51.8(fixed)	—	–15.8	51.8
*u*1959	Si(50)...H(94)	515.8(13)	22.0(fixed)	—	–1.1	22.0
*u*1853	H(84)...H(91)	516.1(38)	39.5(fixed)	—	6.8	39.5
*u*1860	H(29)...H(39)	516.3(35)	45.5(fixed)	—	7.8	45.5
*u*2179	C(147)...C(149)	516.4(27)	16.2(tied to *u*2304)	—	–0.9	18.3
*u*3046	H(115)...H(121)	516.6(27)	26.2(fixed)	—	–5.9	26.2
*u*2031	H(70)...H(81)	516.7(40)	35.1(fixed)	—	–8.7	35.1
*u*1969	C(6)...C(9)	516.9(36)	17.0(tied to *u*2304)	—	–0.9	19.3
*u*1849	Cl(62)...H(86)	517.0(29)	29.3(fixed)	—	2.2	29.3
*u*2052	H(113)...H(132)	517.0(23)	38.2(fixed)	—	–7.3	38.2
*u*2032	H(77)...H(88)	517.6(22)	41.7(fixed)	—	–8.0	41.7
*u*1949	H(170)...H(179)	517.7(17)	38.7(fixed)	—	–7.9	38.7
*u*1928	C(7)...C(10)	518.0(24)	17.1(tied to *u*2304)	—	–0.9	19.3
*u*1930	C(56)...C(58)	518.3(28)	16.5(tied to *u*2304)	—	–0.8	18.7
*u*1955	H(76)...H(90)	518.4(46)	36.5(fixed)	—	–6.8	36.5
*u*1997	H(19)...H(38)	518.6(23)	36.2(fixed)	—	–7.5	36.2
*u*1899	C(63)...H(69)	518.7(26)	32.9(fixed)	—	2.9	32.9
*u*1927	C(57)...H(71)	518.8(15)	32.9(fixed)	—	2.7	32.9
*u*3070	H(160)...H(181)	519.0(44)	26.4(fixed)	—	–6.6	26.4
*u*1879	C(8)...H(42)	519.4(20)	44.4(fixed)	—	12.8	44.4
*u*2025	H(21)...H(34)	519.7(30)	41.3(fixed)	—	–11.7	41.3
*u*1938	Si(96)...H(116)	519.7(9)	20.6(fixed)	—	–1.2	20.6

*u*2077	C(54)...C(56)	519.7(33)	14.9(tied to *u*2304)	—	–0.9	16.9
*u*1914	C(60)...H(94)	519.7(28)	32.6(fixed)	—	3.7	32.6
*u*1963	Si(143)...H(163)	520.0(9)	24.2(fixed)	—	–1.0	24.2
*u*1966	Si(3)...H(31)	520.1(9)	23.6(fixed)	—	–0.7	23.6
*u*2196	H(71)...H(92)	520.5(48)	41.8(fixed)	—	3.8	41.8
*u*2087	C(55)...H(92)	520.5(44)	27.9(fixed)	—	2.4	27.9
*u*1941	Si(50)...H(78)	520.5(9)	21.4(fixed)	—	–1.0	21.4
*u*2000	Cl(61)...C(63)	520.6(23)	17.5(tied to *u*2304)	—	–1.0	19.8
*u*2007	C(11)...Cl(15)	520.9(28)	18.2(tied to *u*2304)	—	–1.1	20.5
*u*1885	C(16)...H(22)	520.9(25)	34.7(fixed)	—	4.6	34.7
*u*1971	Si(2)...H(35)	520.9(9)	22.2(fixed)	—	–0.8	22.2
*u*1956	Si(49)...H(69)	521.0(9)	21.7(fixed)	—	–1.1	21.7
*u*2015	Si(52)...H(75)	521.0(14)	20.4(fixed)	—	–1.2	20.4
*u*1954	Si(2)...H(22)	521.0(9)	23.0(fixed)	—	–1.0	23.0
*u*1961	Si(143)...H(176)	521.1(9)	23.2(fixed)	—	–1.2	23.2
*u*1968	Si(96)...H(129)	521.1(9)	21.0(fixed)	—	–1.0	21.0
*u*1957	Si(49)...H(82)	521.3(9)	22.2(fixed)	—	–0.7	22.2
*u*1962	C(59)...C(64)	521.4(28)	16.7(tied to *u*2304)	—	–0.9	18.9
*u*1059	Si(143)...H(167)	521.7(9)	35.1(fixed)	—	–0.1	35.1
*u*1102	H(112)...H(135)	521.8(24)	50.5(fixed)	—	1.2	50.5
*u*2009	H(88)...H(90)	521.9(31)	35.8(fixed)	—	–7.1	35.8
*u*2115	H(66)...H(73)	522.4(52)	37.6(fixed)	—	2.0	37.6
*u*3135	H(113)...H(121)	522.4(35)	32.8(fixed)	—	–7.9	32.8
*u*1940	Cl(14)...H(26)	522.8(22)	32.3(fixed)	—	4.4	32.3
*u*1987	Si(98)...H(114)	522.9(10)	21.5(fixed)	—	–1.2	21.5
*u*1967	Si(2)...H(28)	523.1(9)	21.9(fixed)	—	–1.5	21.9
*u*1935	Si(49)...H(73)	523.3(9)	20.6(fixed)	—	–0.9	20.6
*u*472	Cl(155)...H(159)	523.3(18)	35.5(fixed)	—	7.3	35.5
*u*1828	H(72)...H(91)	523.3(46)	42.0(fixed)	—	–5.1	42.0
*u*2020	Cl(14)...C(16)	523.4(27)	18.4(tied to *u*2304)	—	–1.1	20.8
*u*2048	H(65)...H(88)	523.5(19)	37.8(fixed)	—	3.7	37.8
*u*1993	Si(145)...H(161)	523.8(10)	22.0(fixed)	—	–1.0	22.0
*u*1824	H(22)...H(42)	524.0(40)	46.7(fixed)	—	14.0	46.7
*u*2046	H(18)...H(41)	524.0(17)	37.9(fixed)	—	4.2	37.9
*u*1972	Cl(62)...H(82)	524.2(18)	34.5(fixed)	—	4.5	34.5
*u*1996	Si(5)...H(44)	524.4(11)	25.7(fixed)	—	–0.4	25.7
*u*1965	C(54)...C(57)	524.5(26)	16.8(tied to *u*2304)	—	–0.9	18.9
*u*1995	C(12)...C(17)	524.7(26)	17.0(tied to *u*2304)	—	–1.0	19.2
*u*1990	Si(52)...H(91)	524.7(11)	20.8(fixed)	—	–1.0	20.8
*u*1991	Si(51)...H(67)	524.7(10)	21.4(fixed)	—	–1.2	21.4
*u*1994	Si(4)...H(20)	524.8(10)	21.4(fixed)	—	–0.9	21.4
*u*3048	H(160)...H(182)	524.9(28)	27.3(fixed)	—	–7.3	27.3
*u*2096	H(70)...H(84)	524.9(36)	48.9(fixed)	—	3.1	48.9
*u*1852	H(73)...H(90)	525.1(44)	41.6(fixed)	—	–5.0	41.6
*u*251	H(161)...H(177)	525.4(46)	45.4(fixed)	—	13.3	45.4
*u*2044	H(74)...H(85)	525.5(18)	42.5(fixed)	—	–8.9	42.5

*u*1159	Si(146)...H(169)	525.5(8)	34.3(fixed)	—	–0.3	34.3
*u*2047	H(68)...H(81)	525.8(33)	38.5(fixed)	—	–8.8	38.5
*u*2491	C(105)...H(123)	525.9(28)	29.6(fixed)	—	–4.7	29.6
*u*3007	H(120)...H(130)	525.9(64)	34.8(fixed)	—	0.5	34.8
*u*2138	C(55)...C(64)	525.9(34)	16.0(tied to *u*2304)	—	–0.6	18.1
*u*2021	H(72)...H(81)	525.9(26)	38.8(fixed)	—	–8.6	38.8
*u*2910	H(123)...H(127)	526.2(36)	32.6(fixed)	—	–5.9	32.6
*u*2016	Si(52)...H(86)	526.4(8)	21.4(fixed)	—	–1.3	21.4
*u*2022	Si(5)...H(39)	526.5(8)	22.4(fixed)	—	–1.6	22.4
*u*1942	C(9)...H(39)	526.9(26)	36.0(fixed)	—	4.0	36.0
*u*1936	C(148)...C(151)	527.0(25)	16.8(tied to *u*2304)	—	–0.9	19.0
*u*1973	Si(51)...H(83)	527.4(8)	22.2(fixed)	—	–0.7	22.2
*u*2088	H(160)...H(174)	527.5(21)	37.4(fixed)	—	5.3	37.4
*u*3252	H(119)...H(132)	527.5(43)	19.5(fixed)	—	–7.3	19.5
*u*2940	H(166)...H(174)	527.5(42)	34.6(fixed)	—	–7.4	34.6
*u*784	Cl(108)...H(122)	528.0(15)	54.5(fixed)	—	2.9	54.5
*u*945	C(100)...Cl(109)	528.0(28)	18.5(tied to *u*2304)	—	1.0	20.9
*u*3119	H(174)...H(178)	528.1(38)	33.6(fixed)	—	–1.7	33.6
*u*2006	H(25)...H(38)	528.5(20)	36.9(fixed)	—	–7.9	36.9
*u*984	H(117)...H(119)	528.5(22)	43.6(fixed)	—	2.3	43.6
*u*1988	Si(4)...H(26)	528.7(8)	20.4(fixed)	—	–0.8	20.4
*u*1974	Si(4)...H(36)	528.8(8)	20.1(fixed)	—	–1.0	20.1
*u*1981	C(8)...C(13)	529.1(18)	16.5(tied to *u*2304)	—	–0.9	18.6
*u*2198	Cl(108)...H(118)	529.1(18)	28.7(fixed)	—	1.4	28.7
*u*2145	H(67)...H(72)	529.2(54)	38.5(fixed)	—	1.6	38.5
*u*1921	C(57)...H(75)	530.3(23)	31.0(fixed)	—	3.0	31.0
*u*1090	C(103)...C(107)	530.3(39)	19.7(tied to *u*2304)	—	0.2	22.3
*u*2054	C(59)...H(70)	530.3(28)	29.0(fixed)	—	1.6	29.0
*u*1861	H(75)...H(79)	530.4(28)	40.2(fixed)	—	6.3	40.2
*u*2221	H(73)...H(93)	530.7(49)	38.2(fixed)	—	2.5	38.2
*u*2190	C(150)...C(152)	531.0(25)	16.1(tied to *u*2304)	—	–0.8	18.2
*u*2011	C(60)...Cl(62)	531.2(18)	17.8(tied to *u*2304)	—	–1.0	20.1
*u*2083	H(24)...H(46)	531.2(42)	37.6(fixed)	—	5.1	37.6
*u*970	H(164)...H(168)	531.3(20)	42.8(fixed)	—	10.9	42.8
*u*2184	Cl(62)...C(64)	531.3(31)	16.1(tied to *u*2304)	—	–0.9	18.1
*u*2030	Cl(62)...H(89)	531.4(20)	29.5(fixed)	—	2.2	29.5
*u*1068	Si(98)...H(122)	531.9(8)	29.8(fixed)	—	6.5	29.8
*u*995	Si(99)...H(120)	532.0(8)	26.4(fixed)	—	4.0	26.4
*u*2057	H(113)...H(127)	532.0(24)	36.1(fixed)	—	3.7	36.1
*u*2071	H(90)...H(92)	532.4(24)	36.3(fixed)	—	4.2	36.3
*u*2935	C(153)...H(174)	532.5(35)	25.4(fixed)	—	–0.1	25.4
*u*2956	Cl(155)...Cl(156)	533.1(21)	12.6(tied to *u*2304)	—	–1.7	14.3
*u*2252	H(70)...H(76)	533.4(39)	34.9(fixed)	—	1.2	34.9
*u*3157	H(160)...H(167)	533.6(36)	26.3(fixed)	—	–8.1	26.3
*u*2108	C(9)...H(45)	534.0(39)	28.9(fixed)	—	2.6	28.9
*u*2061	H(79)...H(85)	534.3(20)	37.1(fixed)	—	5.7	37.1

*u*2847	H(165)...H(171)	534.3(19)	41.6(fixed)	—	–6.6	41.6
*u*1897	H(71)...H(86)	534.4(43)	41.4(fixed)	—	5.5	41.4
*u*1925	C(55)...H(86)	534.4(36)	33.0(fixed)	—	3.1	33.0
*u*2150	H(37)...H(42)	534.4(49)	66.5(fixed)	—	4.1	66.5
*u*2159	C(53)...H(76)	534.5(30)	27.7(fixed)	—	1.7	27.7
*u*2112	C(147)...C(152)	534.6(19)	15.2(tied to *u*2304)	—	–0.8	17.2
*u*1999	Cl(61)...H(76)	534.7(16)	30.0(fixed)	—	2.8	30.0
*u*2155	H(116)...H(124)	535.0(50)	36.6(fixed)	—	1.1	36.6
*u*2106	H(65)...H(79)	535.1(40)	46.1(fixed)	—	3.6	46.1
*u*2189	C(56)...H(69)	535.6(38)	33.3(fixed)	—	–0.6	33.3
*u*1960	H(74)...H(87)	535.8(42)	35.4(fixed)	—	–7.1	35.4
*u*1866	H(73)...H(91)	535.8(44)	36.0(fixed)	—	–5.6	36.0
*u*2089	C(53)...C(60)	535.9(14)	15.0(tied to *u*2304)	—	–0.8	17.0
*u*3035	H(121)...H(132)	536.0(31)	28.9(fixed)	—	–9.3	28.9
*u*2080	H(18)...H(32)	536.1(34)	54.1(fixed)	—	4.7	54.1
*u*2035	H(74)...H(90)	536.3(30)	34.9(fixed)	—	–7.0	34.9
*u*2099	H(43)...H(45)	536.5(23)	36.4(fixed)	—	6.6	36.4
*u*2059	C(57)...H(65)	536.6(35)	29.1(fixed)	—	1.9	29.1
*u*2066	H(27)...H(37)	536.9(20)	37.0(fixed)	—	3.3	37.0
*u*1402	H(120)...H(128)	537.1(44)	47.0(fixed)	—	–2.2	47.0
*u*2100	C(6)...C(13)	537.1(12)	15.2(tied to *u*2304)	—	–0.9	17.2
*u*2199	C(53)...C(56)	537.2(25)	15.9(tied to *u*2304)	—	–0.8	17.9
*u*3206	H(128)...H(134)	537.2(19)	27.1(fixed)	—	–2.9	27.1
*u*2094	C(54)...C(59)	537.3(18)	16.5(tied to *u*2304)	—	–0.8	18.7
*u*2079	H(66)...H(80)	537.3(23)	38.0(fixed)	—	5.0	38.0
*u*2787	H(166)...H(175)	537.3(27)	41.0(fixed)	—	–7.2	41.0
*u*2085	C(63)...C(64)	537.6(22)	14.5(tied to *u*2304)	—	–0.7	16.4
*u*1249	H(159)...H(170)	537.6(32)	41.9(fixed)	—	–1.2	41.9
*u*1943	C(103)...C(105)	537.8(21)	16.7(tied to *u*2304)	—	–0.9	18.9
*u*2992	H(112)...H(118)	537.9(46)	30.1(fixed)	—	–5.4	30.1
*u*1045	C(148)...C(150)	538.0(13)	19.0(tied to *u*2304)	—	0.3	21.4
*u*392	Cl(155)...H(188)	538.0(18)	30.7(fixed)	—	11.9	30.7
*u*2090	C(100)...C(105)	538.2(21)	14.9(tied to *u*2304)	—	–0.8	16.8
*u*2116	C(16)...C(17)	538.3(22)	15.0(tied to *u*2304)	—	–0.9	17.0
*u*2073	C(151)...H(159)	538.5(28)	28.9(fixed)	—	1.9	28.9
*u*2913	C(154)...H(164)	538.7(22)	26.7(fixed)	—	0.8	26.7
*u*2067	H(72)...H(90)	538.8(34)	39.2(fixed)	—	–7.1	39.2
*u*2141	H(20)...H(27)	538.8(51)	37.1(fixed)	—	2.2	37.1
*u*2242	H(23)...H(37)	538.9(28)	40.7(fixed)	—	4.5	40.7
*u*2134	C(8)...C(17)	539.1(26)	15.0(tied to *u*2304)	—	–0.8	16.9
*u*2345	H(70)...H(75)	539.3(39)	35.0(fixed)	—	–0.3	35.0
*u*2074	C(10)...H(18)	539.3(28)	28.6(fixed)	—	1.9	28.6
*u*2123	C(17)...H(40)	539.4(33)	27.9(fixed)	—	3.1	27.9
*u*2102	C(12)...H(23)	539.7(19)	28.3(fixed)	—	3.1	28.3
*u*2050	H(32)...H(38)	539.8(22)	38.7(fixed)	—	9.6	38.7
*u*2070	H(74)...H(82)	539.9(42)	36.5(fixed)	—	3.9	36.5

*u*2819	C(101)...Cl(108)	539.9(20)	12.2(tied to *u*2304)	—	–1.5	13.8
*u*2212	Si(50)...H(93)	540.0(20)	16.1(fixed)	—	–3.6	16.1
*u*2635	Cl(108)...H(127)	540.1(37)	23.4(fixed)	—	–2.1	23.4
*u*2745	C(152)...C(153)	540.1(21)	12.1(tied to *u*2304)	—	–1.4	13.7
*u*2582	C(100)...H(118)	540.2(36)	26.0(fixed)	—	–3.7	26.0
*u*931	C(150)...C(153)	540.2(15)	19.7(tied to *u*2304)	—	1.0	22.3
*u*2165	C(9)...C(17)	540.3(32)	16.5(tied to *u*2304)	—	–0.7	18.7
*u*2143	H(159)...H(173)	540.5(30)	51.1(fixed)	—	4.0	51.1
*u*2164	Si(3)...H(46)	540.6(19)	16.4(fixed)	—	–3.6	16.4
*u*2093	C(16)...H(37)	540.6(38)	28.8(fixed)	—	1.2	28.8
*u*917	C(100)...C(107)	540.7(16)	19.3(tied to *u*2304)	—	0.9	21.8
*u*2039	H(123)...H(132)	540.8(41)	38.7(fixed)	—	7.8	38.7
*u*1130	H(119)...H(129)	540.8(48)	32.4(fixed)	—	3.7	32.4
*u*2129	C(7)...Cl(14)	540.9(22)	16.0(tied to *u*2304)	—	–1.0	18.1
*u*579	C(147)...H(170)	541.1(25)	37.6(fixed)	—	4.4	37.6
*u*2125	C(53)...C(58)	541.4(20)	15.0(tied to *u*2304)	—	–0.9	16.9
*u*2084	H(19)...H(33)	541.4(24)	39.3(fixed)	—	6.8	39.3
*u*3056	H(170)...H(173)	541.5(29)	34.6(fixed)	—	–0.9	34.6
*u*2111	C(57)...C(59)	541.7(13)	14.9(tied to *u*2304)	—	–0.8	16.8
*u*2223	C(7)...Cl(15)	541.8(28)	14.5(tied to *u*2304)	—	–1.1	16.4
*u*2133	C(12)...C(16)	541.9(29)	16.8(tied to *u*2304)	—	–0.8	19.0
*u*2230	Si(52)...H(74)	542.1(20)	16.2(fixed)	—	–3.1	16.2
*u*2322	H(67)...H(74)	542.2(41)	37.7(fixed)	—	2.2	37.7
*u*2270	H(65)...H(76)	542.4(38)	41.2(fixed)	—	3.0	41.2
*u*884	C(101)...C(102)	542.6(14)	17.9(tied to *u*2304)	—	1.0	20.2
*u*2110	C(53)...C(57)	542.7(23)	16.5(tied to *u*2304)	—	–0.8	18.7
*u*2064	H(72)...H(84)	542.8(18)	38.9(fixed)	—	6.2	38.9
*u*2135	C(6)...C(11)	542.8(21)	15.5(tied to *u*2304)	—	–0.9	17.5
*u*2113	C(11)...C(13)	542.9(11)	15.3(tied to *u*2304)	—	–0.8	17.3
*u*2124	C(6)...C(10)	542.9(21)	16.3(tied to *u*2304)	—	–0.8	18.4
*u*2202	H(29)...H(45)	543.0(45)	44.4(fixed)	—	4.2	44.4
*u*2740	C(103)...C(111)	543.8(11)	11.9(tied to *u*2304)	—	–1.3	13.5
*u*2114	C(9)...C(10)	543.9(10)	15.0(tied to *u*2304)	—	–0.8	16.9
*u*2119	C(10)...C(12)	544.2(14)	15.2(tied to *u*2304)	—	–0.9	17.2
*u*2148	C(7)...C(12)	544.2(15)	16.0(tied to *u*2304)	—	–0.8	18.1
*u*2175	Cl(61)...H(80)	544.4(32)	28.1(fixed)	—	2.7	28.1
*u*2240	H(24)...H(33)	544.5(39)	49.0(fixed)	—	4.3	49.0
*u*2065	H(34)...H(40)	544.5(18)	37.0(fixed)	—	6.0	37.0
*u*2132	H(121)...H(129)	544.5(30)	39.2(fixed)	—	1.0	39.2
*u*2038	H(74)...H(88)	544.7(27)	36.2(fixed)	—	–7.4	36.2
*u*2139	C(147)...C(151)	544.7(17)	16.7(tied to *u*2304)	—	–0.8	18.8
*u*2569	C(106)...H(117)	544.8(25)	22.6(fixed)	—	–1.8	22.6
*u*2254	H(40)...H(45)	544.9(38)	41.0(fixed)	—	4.8	41.0
*u*2076	H(81)...H(87)	545.0(18)	35.5(fixed)	—	4.1	35.5
*u*2367	C(64)...H(71)	545.1(36)	33.6(fixed)	—	–1.2	33.6
*u*2168	C(8)...C(11)	545.1(22)	16.0(tied to *u*2304)	—	–0.8	18.1

*u*2205	C(152)...Cl(155)	545.1(19)	17.6(tied to *u*2304)	—	–0.8	19.9
*u*1826	H(121)...H(133)	545.5(54)	54.3(fixed)	—	–8.9	54.3
*u*2127	C(58)...C(60)	545.5(10)	15.1(tied to *u*2304)	—	–0.8	17.0
*u*2291	H(161)...H(166)	545.6(45)	38.6(fixed)	—	2.7	38.6
*u*2188	C(13)...C(17)	545.7(23)	16.2(tied to *u*2304)	—	–0.8	18.3
*u*1950	C(100)...C(102)	545.7(28)	17.0(tied to *u*2304)	—	–0.9	19.2
*u*2162	C(100)...C(104)	545.8(16)	16.2(tied to *u*2304)	—	–0.7	18.3
*u*937	C(147)...C(150)	546.2(20)	19.2(tied to *u*2304)	—	0.8	21.7
*u*2097	C(9)...C(12)	546.2(17)	14.9(tied to *u*2304)	—	–0.9	16.9
*u*2121	C(104)...H(112)	546.2(29)	28.0(fixed)	—	2.0	28.0
*u*2248	H(112)...H(126)	546.3(31)	39.2(fixed)	—	3.1	39.2
*u*1742	Si(98)...H(121)	546.4(8)	23.3(fixed)	—	–5.6	23.3
*u*2120	C(55)...C(59)	546.4(14)	15.0(tied to *u*2304)	—	–0.9	17.0
*u*2736	C(150)...C(151)	546.4(17)	12.0(tied to *u*2304)	—	–1.3	13.6
*u*2172	C(11)...H(24)	546.7(32)	27.8(fixed)	—	2.1	27.8
*u*2069	H(83)...H(93)	546.8(40)	38.3(fixed)	—	4.9	38.3
*u*2078	H(29)...H(30)	546.9(17)	36.7(fixed)	—	6.4	36.7
*u*1570	Si(143)...H(166)	547.0(9)	19.5(fixed)	—	–4.6	19.5
*u*3232	H(175)...H(177)	547.3(26)	26.2(fixed)	—	–6.2	26.2
*u*1505	C(150)...H(163)	547.4(21)	42.6(fixed)	—	–4.8	42.6
*u*2122	C(8)...C(16)	547.4(16)	15.5(tied to *u*2304)	—	–0.9	17.6
*u*2229	Si(143)...H(162)	547.8(7)	16.3(fixed)	—	–4.5	16.3
*u*2180	C(59)...C(63)	548.0(26)	15.5(tied to *u*2304)	—	–0.8	17.5
*u*2260	C(147)...H(176)	548.1(32)	40.8(fixed)	—	–0.9	40.8
*u*2171	C(54)...Cl(61)	548.2(20)	16.0(tied to *u*2304)	—	–1.0	18.1
*u*2151	C(149)...C(151)	548.4(13)	16.0(tied to *u*2304)	—	–0.7	18.1
*u*2126	C(102)...C(104)	548.4(16)	15.2(tied to *u*2304)	—	–0.8	17.2
*u*2156	Si(2)...H(27)	548.6(9)	16.8(fixed)	—	–3.8	16.8
*u*2153	C(54)...H(89)	548.9(32)	27.4(fixed)	—	1.5	27.4
*u*2056	H(21)...H(31)	548.9(37)	39.1(fixed)	—	7.0	39.1
*u*2207	C(58)...Cl(61)	549.2(21)	16.9(tied to *u*2304)	—	–0.8	19.1
*u*2287	C(6)...Cl(15)	549.3(19)	16.9(tied to *u*2304)	—	–1.0	19.1
*u*2193	C(63)...H(94)	549.4(37)	35.6(fixed)	—	–0.3	35.6
*u*2330	H(118)...H(126)	549.4(30)	33.7(fixed)	—	1.6	33.7
*u*2211	C(60)...H(67)	549.4(26)	34.0(fixed)	—	–0.6	34.0
*u*2238	C(16)...H(47)	549.6(36)	37.0(fixed)	—	–0.6	37.0
*u*2104	H(26)...H(41)	549.7(26)	36.9(fixed)	—	3.1	36.9
*u*2185	Cl(14)...H(33)	550.0(35)	30.5(fixed)	—	3.5	30.5
*u*2033	Cl(155)...H(165)	550.0(21)	33.0(fixed)	—	3.2	33.0
*u*2149	C(64)...H(87)	550.1(27)	27.3(fixed)	—	1.9	27.3
*u*2163	H(19)...H(28)	550.1(52)	38.4(fixed)	—	3.0	38.4
*u*1239	H(112)...H(134)	550.2(28)	45.2(fixed)	—	–3.7	45.2
*u*2140	H(22)...H(30)	550.2(28)	41.6(fixed)	—	2.1	41.6
*u*2226	Si(2)...H(21)	550.3(7)	16.3(fixed)	—	–4.2	16.3
*u*2201	Si(143)...H(175)	550.4(10)	16.1(fixed)	—	–3.9	16.1
*u*2208	Si(49)...H(68)	550.5(8)	16.0(fixed)	—	–3.4	16.0

*u*2053	H(25)...H(42)	550.5(25)	45.3(fixed)	—	16.1	45.3
*u*2178	C(105)...Cl(108)	550.6(24)	16.1(tied to *u*2304)	—	–0.9	18.2
*u*2277	C(149)...Cl(155)	550.8(15)	15.1(tied to *u*2304)	—	–1.0	17.1
*u*2166	Si(96)...H(115)	550.8(7)	16.0(fixed)	—	–3.0	16.0
*u*1614	Si(146)...H(168)	550.9(8)	19.8(fixed)	—	–4.3	19.8
*u*2200	Si(5)...H(41)	550.9(9)	17.1(fixed)	—	–3.9	17.1
*u*2136	C(55)...C(57)	551.0(13)	15.4(tied to *u*2304)	—	–0.7	17.4
*u*2333	C(54)...H(84)	551.0(27)	40.3(fixed)	—	–1.2	40.3
*u*2271	H(18)...H(40)	551.2(23)	35.0(fixed)	—	2.1	35.0
*u*2276	H(70)...H(89)	551.3(38)	39.8(fixed)	—	2.5	39.8
*u*2161	Si(49)...H(72)	551.4(10)	15.8(fixed)	—	–3.3	15.8
*u*2303	H(159)...H(174)	551.5(26)	33.9(fixed)	—	3.4	33.9
*u*2130	H(71)...H(77)	551.9(19)	37.7(fixed)	—	3.8	37.7
*u*2181	C(63)...H(84)	551.9(33)	26.9(fixed)	—	2.9	26.9
*u*2299	H(84)...H(89)	552.1(42)	39.3(fixed)	—	4.8	39.3
*u*2091	H(75)...H(81)	552.1(40)	38.9(fixed)	—	1.4	38.9
*u*2137	H(36)...H(46)	552.3(41)	37.3(fixed)	—	1.4	37.3
*u*2183	C(54)...C(63)	552.3(21)	16.4(tied to *u*2304)	—	–0.8	18.5
*u*2219	Si(49)...H(81)	552.4(9)	15.9(fixed)	—	–3.8	15.9
*u*2209	Si(2)...H(34)	552.4(9)	16.1(fixed)	—	–4.3	16.1
*u*2191	H(68)...H(83)	552.5(24)	40.0(fixed)	—	5.2	40.0
*u*2243	Si(145)...H(160)	552.5(8)	16.2(fixed)	—	–3.5	16.2
*u*2177	C(7)...C(16)	552.6(20)	16.8(tied to *u*2304)	—	–1.0	19.0
*u*2232	Si(96)...H(128)	552.6(9)	15.7(fixed)	—	–3.3	15.7
*u*2210	Si(3)...H(30)	552.7(8)	16.3(fixed)	—	–4.8	16.3
*u*2258	C(8)...Cl(14)	552.8(20)	16.5(tied to *u*2304)	—	–0.9	18.6
*u*1701	Si(99)...H(119)	552.8(9)	21.8(fixed)	—	–3.6	21.8
*u*2295	H(28)...H(46)	552.8(48)	39.8(fixed)	—	3.6	39.8
*u*2245	C(100)...H(129)	552.9(33)	33.4(fixed)	—	–0.6	33.4
*u*2215	Si(52)...H(88)	552.9(8)	16.3(fixed)	—	–3.2	16.3
*u*2086	H(114)...H(119)	553.3(41)	37.8(fixed)	—	1.9	37.8
*u*2274	H(25)...H(35)	553.4(30)	37.4(fixed)	—	5.5	37.4
*u*2227	Si(51)...H(85)	553.4(9)	16.0(fixed)	—	–3.9	16.0
*u*2236	C(11)...Cl(14)	553.5(24)	18.3(tied to *u*2304)	—	–1.0	20.6
*u*2214	Si(4)...H(38)	553.6(9)	15.8(fixed)	—	–3.1	15.8
*u*2250	Si(5)...H(43)	553.6(8)	17.4(fixed)	—	–6.3	17.4
*u*2174	Si(50)...H(77)	553.6(8)	16.1(fixed)	—	–3.5	16.1
*u*2268	H(65)...H(87)	553.7(24)	35.2(fixed)	—	1.9	35.2
*u*2194	C(60)...C(64)	553.7(21)	15.6(tied to *u*2304)	—	–0.8	17.7
*u*2228	Si(4)...H(25)	553.7(9)	15.8(fixed)	—	–3.4	15.8
*u*3178	H(169)...H(175)	553.8(35)	27.3(fixed)	—	–9.2	27.3
*u*2105	H(68)...H(78)	554.1(36)	37.0(fixed)	—	3.1	37.0
*u*2233	Si(98)...H(113)	554.2(8)	16.2(fixed)	—	–3.3	16.2
*u*2340	C(12)...H(42)	554.2(40)	58.1(fixed)	—	–1.1	58.1
*u*3248	H(169)...H(171)	554.2(24)	26.9(fixed)	—	–7.6	26.9
*u*2275	H(85)...H(91)	554.3(38)	37.5(fixed)	—	1.8	37.5

*u*2249	C(13)...H(20)	554.4(23)	34.8(fixed)	—	–0.7	34.8
*u*2280	C(11)...H(39)	554.4(23)	39.6(fixed)	—	–0.9	39.6
*u*2264	C(10)...H(28)	554.7(19)	39.0(fixed)	—	–0.6	39.0
*u*2217	Si(51)...H(66)	554.9(9)	16.3(fixed)	—	–3.4	16.3
*u*1095	C(147)...Cl(155)	554.9(13)	23.2(tied to *u*2304)	—	0.2	26.2
*u*2247	Si(4)...H(19)	555.3(9)	16.1(fixed)	—	–3.6	16.1
*u*2335	Cl(61)...Cl(62)	555.3(27)	18.2(tied to *u*2304)	—	–1.0	20.6
*u*2346	H(114)...H(127)	555.3(25)	35.6(fixed)	—	0.2	35.6
*u*2157	C(13)...H(29)	555.5(28)	28.9(fixed)	—	2.9	28.9
*u*2559	C(103)...H(127)	555.9(29)	25.1(fixed)	—	–3.5	25.1
*u*2237	C(10)...Cl(15)	556.4(22)	17.8(tied to *u*2304)	—	–0.9	20.2
*u*2259	C(59)...H(78)	556.4(18)	37.6(fixed)	—	–0.6	37.6
*u*2251	Si(52)...H(90)	556.5(8)	16.0(fixed)	—	–3.0	16.0
*u*2278	H(113)...H(125)	556.6(18)	37.0(fixed)	—	1.4	37.0
*u*2290	C(58)...Cl(62)	556.7(14)	16.3(tied to *u*2304)	—	–0.9	18.5
*u*2284	H(87)...H(92)	556.7(34)	41.0(fixed)	—	3.2	41.0
*u*2334	Cl(15)...H(22)	556.9(31)	38.9(fixed)	—	–0.6	38.9
*u*2396	C(54)...H(74)	557.1(41)	23.1(fixed)	—	–1.6	23.1
*u*2142	H(85)...H(94)	557.2(47)	40.2(fixed)	—	1.7	40.2
*u*2360	H(44)...H(45)	557.4(27)	36.8(fixed)	—	–0.9	36.8
*u*2283	C(53)...H(82)	557.6(33)	38.3(fixed)	—	–0.7	38.3
*u*2203	H(66)...H(78)	557.7(28)	38.7(fixed)	—	3.6	38.7
*u*2314	H(89)...H(92)	557.8(24)	33.4(fixed)	—	2.5	33.4
*u*2316	C(6)...H(32)	557.8(28)	46.6(fixed)	—	–0.7	46.6
*u*2332	H(24)...H(45)	557.9(35)	34.2(fixed)	—	2.8	34.2
*u*2152	H(38)...H(47)	557.9(38)	36.6(fixed)	—	2.2	36.6
*u*2970	C(158)...H(165)	557.9(26)	26.0(fixed)	—	–0.9	26.0
*u*2324	H(79)...H(83)	558.0(16)	37.5(fixed)	—	1.2	37.5
*u*2244	H(38)...H(44)	558.1(41)	40.8(fixed)	—	14.4	40.8
*u*1203	H(170)...H(178)	558.2(18)	44.2(fixed)	—	–1.2	44.2
*u*2353	H(65)...H(86)	558.2(19)	35.9(fixed)	—	0.1	35.9
*u*2154	C(7)...H(42)	558.3(33)	31.5(fixed)	—	8.3	31.5
*u*2170	H(69)...H(77)	558.3(38)	38.5(fixed)	—	1.1	38.5
*u*2315	C(6)...H(35)	558.4(34)	41.5(fixed)	—	–0.8	41.5
*u*2627	H(120)...H(124)	558.5(25)	39.8(fixed)	—	–1.9	39.8
*u*2195	Cl(15)...H(32)	558.8(30)	29.8(fixed)	—	5.0	29.8
*u*1241	H(117)...H(118)	558.8(25)	39.3(fixed)	—	–1.9	39.3
*u*2261	H(21)...H(36)	558.9(23)	37.6(fixed)	—	1.4	37.6
*u*2265	H(41)...H(47)	559.1(31)	40.5(fixed)	—	2.4	40.5
*u*2204	C(9)...C(13)	559.4(21)	16.1(tied to *u*2304)	—	–0.8	18.1
*u*1136	H(161)...H(168)	559.4(31)	33.1(fixed)	—	4.7	33.1
*u*2341	C(53)...H(79)	559.5(29)	37.2(fixed)	—	–0.9	37.2
*u*695	C(102)...H(116)	559.5(21)	37.4(fixed)	—	2.8	37.4
*u*2326	C(12)...H(31)	559.6(21)	47.9(fixed)	—	–1.4	47.9
*u*2362	H(185)...H(186)	559.9(21)	36.3(fixed)	—	1.5	36.3
*u*2354	H(18)...H(39)	560.1(18)	36.4(fixed)	—	–0.3	36.4

*u*2255	H(19)...H(31)	560.2(27)	40.9(fixed)	—	7.4	40.9
*u*2343	H(42)...H(45)	560.3(21)	35.6(fixed)	—	1.3	35.6
*u*1034	H(170)...H(177)	560.3(17)	55.2(fixed)	—	2.8	55.2
*u*2311	H(65)...H(80)	560.4(24)	34.4(fixed)	—	3.0	34.4
*u*2176	C(56)...C(57)	560.4(18)	15.7(tied to *u*2304)	—	–0.7	17.8
*u*2357	H(91)...H(92)	560.7(25)	35.5(fixed)	—	0.7	35.5
*u*2304	Cl(14)...Cl(15)	560.8(22)	16.2(5)	18.3(15)	–1.2	18.3
*u*2363	H(24)...H(47)	561.1(32)	37.4(fixed)	—	0.8	37.4
*u*2365	C(8)...H(33)	561.2(31)	41.7(fixed)	—	–1.2	41.7
*u*2293	C(58)...H(86)	561.4(19)	35.6(fixed)	—	–0.8	35.6
*u*2927	C(111)...H(122)	561.4(21)	27.7(fixed)	—	–0.2	27.7
*u*2377	C(7)...H(37)	561.5(24)	32.6(fixed)	—	–1.4	32.6
*u*2256	C(55)...H(83)	561.5(19)	42.0(fixed)	—	–0.5	42.0
*u*3062	H(127)...H(134)	561.6(24)	35.0(fixed)	—	–1.2	35.0
*u*2307	H(112)...H(127)	561.7(29)	33.7(fixed)	—	1.8	33.7
*u*2273	H(23)...H(42)	562.1(39)	45.2(fixed)	—	12.0	45.2
*u*722	C(107)...H(114)	562.1(26)	42.4(fixed)	—	3.0	42.4
*u*2583	C(102)...H(112)	562.4(38)	25.1(fixed)	—	–3.6	25.1
*u*2404	C(56)...H(65)	562.4(32)	33.1(fixed)	—	–1.2	33.1
*u*2098	H(163)...H(171)	562.4(35)	41.4(fixed)	—	5.0	41.4
*u*2158	C(56)...H(79)	562.6(24)	27.1(fixed)	—	2.5	27.1
*u*2262	H(160)...H(172)	562.9(19)	42.4(fixed)	—	6.3	42.4
*u*2285	C(8)...H(44)	562.9(25)	58.2(fixed)	—	–0.3	58.2
*u*2216	C(102)...Cl(108)	563.0(13)	17.4(tied to *u*2304)	—	–0.9	19.7
*u*2413	H(65)...H(73)	563.1(39)	30.8(fixed)	—	–1.3	30.8
*u*2308	H(29)...H(37)	563.2(21)	34.6(fixed)	—	1.0	34.6
*u*418	C(153)...H(169)	563.4(25)	31.4(fixed)	—	9.2	31.4
*u*1417	C(150)...H(159)	563.4(28)	32.6(fixed)	—	–2.3	32.6
*u*2279	H(168)...H(176)	563.5(39)	40.4(fixed)	—	3.8	40.4
*u*2476	C(55)...H(66)	563.9(40)	28.5(fixed)	—	–3.5	28.5
*u*2348	C(157)...H(164)	564.1(21)	42.6(fixed)	—	–1.0	42.6
*u*935	C(152)...Cl(156)	564.5(14)	18.2(tied to *u*2304)	—	1.1	20.6
*u*2266	Cl(62)...C(63)	564.5(14)	14.4(tied to *u*2304)	—	–1.0	16.2
*u*2428	Cl(14)...H(24)	564.5(32)	38.5(fixed)	—	–1.3	38.5
*u*2187	C(55)...C(60)	564.8(28)	16.0(tied to *u*2304)	—	–0.7	18.0
*u*2378	C(110)...H(117)	564.8(21)	30.7(fixed)	—	–1.2	30.7
*u*2312	H(32)...H(36)	564.9(18)	40.9(fixed)	—	4.6	40.9
*u*2350	H(20)...H(33)	564.9(26)	40.1(fixed)	—	2.5	40.1
*u*2358	H(67)...H(80)	565.0(25)	37.4(fixed)	—	1.2	37.4
*u*2289	C(17)...H(26)	565.0(28)	36.0(fixed)	—	–0.5	36.0
*u*2337	H(73)...H(84)	565.2(18)	39.1(fixed)	—	2.0	39.1
*u*2493	H(67)...H(71)	565.2(41)	31.6(fixed)	—	–1.9	31.6
*u*2269	C(56)...Cl(61)	565.2(14)	14.6(tied to *u*2304)	—	–1.0	16.6
*u*2756	H(165)...H(172)	565.4(13)	44.0(fixed)	—	–4.4	44.0
*u*919	C(103)...Cl(108)	565.7(11)	21.3(tied to *u*2304)	—	0.9	24.1
*u*2320	H(26)...H(42)	565.9(18)	50.1(fixed)	—	7.9	50.1

*u*2321	H(18)...H(33)	566.1(24)	35.5(fixed)	—	4.3	35.5
*u*1521	Cl(155)...H(161)	566.1(21)	36.7(fixed)	—	–3.0	36.7
*u*2370	C(17)...H(29)	566.2(36)	36.1(fixed)	—	–1.0	36.1
*u*2388	C(59)...H(89)	566.5(35)	31.1(fixed)	—	–1.1	31.1
*u*1131	H(164)...H(169)	566.6(20)	39.8(fixed)	—	7.2	39.8
*u*2451	C(53)...H(72)	566.6(40)	29.0(fixed)	—	–3.4	29.0
*u*2206	C(9)...H(36)	566.7(29)	31.4(fixed)	—	–0.4	31.4
*u*2318	H(33)...H(40)	566.8(23)	33.7(fixed)	—	3.1	33.7
*u*2400	C(13)...H(45)	567.2(28)	33.4(fixed)	—	–1.1	33.4
*u*2246	H(29)...H(40)	567.6(31)	42.1(fixed)	—	5.1	42.1
*u*2344	H(79)...H(84)	567.6(22)	33.1(fixed)	—	2.2	33.1
*u*2364	H(71)...H(78)	567.8(13)	36.7(fixed)	—	0.1	36.7
*u*2456	H(117)...H(125)	567.8(44)	30.1(fixed)	—	–1.6	30.1
*u*2186	C(60)...H(71)	568.0(37)	27.8(fixed)	—	1.5	27.8
*u*2327	H(80)...H(87)	568.1(21)	32.7(fixed)	—	1.7	32.7
*u*2331	H(29)...H(31)	568.4(13)	37.6(fixed)	—	1.1	37.6
*u*2239	H(76)...H(79)	568.4(31)	40.2(fixed)	—	4.4	40.2
*u*2484	Cl(15)...H(18)	568.5(24)	35.8(fixed)	—	–1.4	35.8
*u*2282	H(22)...H(43)	568.7(23)	44.7(fixed)	—	2.8	44.7
*u*250	H(117)...H(120)	569.1(17)	40.4(fixed)	—	10.8	40.4
*u*2167	H(25)...H(39)	569.3(34)	38.0(fixed)	—	2.7	38.0
*u*2257	C(57)...H(73)	569.3(21)	34.3(fixed)	—	–0.4	34.3
*u*2325	H(69)...H(90)	569.4(27)	38.0(fixed)	—	1.9	38.0
*u*2488	Cl(62)...H(80)	569.5(23)	37.3(fixed)	—	–1.2	37.3
*u*2366	H(28)...H(37)	569.9(19)	35.2(fixed)	—	–1.0	35.2
*u*2294	H(88)...H(94)	570.2(34)	38.4(fixed)	—	2.8	38.4
*u*2895	C(151)...H(170)	570.6(24)	24.5(fixed)	—	–0.5	24.5
*u*2485	C(54)...H(75)	570.7(33)	22.2(fixed)	—	–1.7	22.2
*u*2425	H(69)...H(75)	570.8(40)	37.8(fixed)	—	0.4	37.8
*u*2342	H(82)...H(87)	571.0(14)	34.6(fixed)	—	0.5	34.6
*u*2546	H(69)...H(74)	571.3(46)	38.3(fixed)	—	–1.5	38.3
*u*2313	H(32)...H(37)	571.4(23)	34.0(fixed)	—	6.5	34.0
*u*2225	H(165)...H(173)	571.6(22)	43.5(fixed)	—	6.9	43.5
*u*2417	H(73)...H(94)	571.7(37)	34.7(fixed)	—	–0.5	34.7
*u*2387	C(16)...H(23)	571.8(27)	37.0(fixed)	—	–1.5	37.0
*u*2347	H(35)...H(40)	571.9(14)	36.4(fixed)	—	1.5	36.4
*u*2339	H(29)...H(32)	572.2(20)	34.0(fixed)	—	2.5	34.0
*u*2551	Cl(62)...H(93)	572.2(39)	24.2(fixed)	—	–1.9	24.2
*u*2758	H(159)...H(167)	572.5(31)	38.6(fixed)	—	–3.1	38.6
*u*2384	C(63)...H(70)	572.6(28)	31.9(fixed)	—	–1.2	31.9
*u*2609	C(53)...H(71)	572.7(31)	25.4(fixed)	—	–3.7	25.4
*u*1923	C(104)...H(118)	572.9(23)	31.6(fixed)	—	2.7	31.6
*u*2501	C(54)...H(76)	573.2(29)	22.4(fixed)	—	–1.9	22.4
*u*271	H(112)...H(133)	573.3(20)	43.7(fixed)	—	15.8	43.7
*u*2951	H(129)...H(134)	573.8(14)	36.3(fixed)	—	3.3	36.3
*u*232	H(164)...H(170)	574.1(20)	40.5(fixed)	—	23.9	40.5

*u*2602	C(55)...H(65)	575.0(32)	24.9(fixed)	—	–3.6	24.9
*u*1083	H(120)...H(127)	575.4(38)	51.2(fixed)	—	2.2	51.2
*u*2461	C(104)...H(115)	575.8(36)	27.6(fixed)	—	–3.1	27.6
*u*2453	C(6)...H(27)	576.2(39)	29.2(fixed)	—	–3.8	29.2
*u*2373	H(22)...H(32)	576.2(26)	34.6(fixed)	—	–2.9	34.6
*u*2375	H(76)...H(82)	576.3(35)	30.7(fixed)	—	–0.1	30.7
*u*2349	H(71)...H(84)	576.4(26)	34.3(fixed)	—	3.4	34.3
*u*1537	C(148)...H(168)	576.6(17)	32.1(fixed)	—	–3.3	32.1
*u*1848	C(151)...H(167)	576.6(20)	32.6(fixed)	—	4.0	32.6
*u*1875	H(163)...H(169)	576.6(27)	44.3(fixed)	—	–9.0	44.3
*u*2426	C(60)...H(92)	576.7(28)	32.9(fixed)	—	–1.1	32.9
*u*2272	H(71)...H(87)	577.0(46)	41.0(fixed)	—	3.1	41.0
*u*2416	C(53)...H(88)	577.3(18)	23.4(fixed)	—	–1.7	23.4
*u*1510	C(110)...H(121)	577.6(21)	34.7(fixed)	—	–4.8	34.7
*u*1626	C(154)...H(166)	577.7(16)	25.4(fixed)	—	–4.5	25.4
*u*1643	C(105)...H(119)	577.7(32)	24.8(fixed)	—	–4.0	24.8
*u*2399	H(75)...H(80)	577.9(35)	31.0(fixed)	—	–2.5	31.0
*u*2594	C(104)...H(117)	578.3(34)	23.7(fixed)	—	–3.2	23.7
*u*2420	C(6)...H(41)	578.4(15)	23.8(fixed)	—	–1.9	23.8
*u*2418	H(20)...H(29)	578.4(40)	30.5(fixed)	—	–1.8	30.5
*u*2380	H(23)...H(31)	578.6(30)	30.5(fixed)	—	1.4	30.5
*u*2336	H(27)...H(39)	578.7(30)	41.3(fixed)	—	3.0	41.3
*u*2468	H(114)...H(129)	578.7(40)	38.3(fixed)	—	0.4	38.3
*u*2500	C(152)...H(160)	579.2(20)	23.4(fixed)	—	–1.9	23.4
*u*2431	H(44)...H(47)	579.2(46)	43.3(fixed)	—	2.9	43.3
*u*1409	Cl(156)...H(174)	579.3(22)	35.9(fixed)	—	–2.9	35.9
*u*2359	H(71)...H(79)	579.3(21)	34.9(fixed)	—	1.3	34.9
*u*2310	H(75)...H(77)	579.5(27)	37.2(fixed)	—	2.1	37.2
*u*2592	H(67)...H(75)	579.5(28)	34.6(fixed)	—	–0.8	34.6
*u*2826	C(149)...H(160)	579.6(26)	23.5(fixed)	—	–5.8	23.5
*u*1498	C(102)...H(128)	580.1(31)	31.9(fixed)	—	–2.7	31.9
*u*2409	H(91)...H(94)	580.2(43)	39.6(fixed)	—	1.0	39.6
*u*2480	C(105)...H(114)	580.4(26)	23.1(fixed)	—	–1.6	23.1
*u*2391	H(83)...H(92)	580.8(33)	31.3(fixed)	—	0.5	31.3
*u*2392	C(58)...H(74)	580.9(29)	27.0(fixed)	—	–3.1	27.0
*u*2319	H(72)...H(86)	581.2(40)	37.8(fixed)	—	2.2	37.8
*u*3200	Cl(108)...H(115)	581.3(24)	16.3(fixed)	—	–4.7	16.3
*u*2457	C(7)...H(32)	581.3(24)	33.4(fixed)	—	–5.5	33.4
*u*2460	C(9)...H(19)	581.6(40)	29.5(fixed)	—	–3.6	29.5
*u*2591	Cl(62)...H(94)	581.8(33)	23.8(fixed)	—	–1.7	23.8
*u*2469	H(18)...H(28)	581.8(40)	30.6(fixed)	—	–1.0	30.6
*u*2497	C(17)...H(44)	581.9(30)	23.5(fixed)	—	–1.3	23.5
*u*2702	Cl(108)...H(120)	582.0(19)	24.4(fixed)	—	–3.0	24.4
*u*1831	H(161)...H(165)	582.1(35)	42.6(fixed)	—	6.6	42.6
*u*2423	H(84)...H(94)	582.1(37)	33.5(fixed)	—	–2.9	33.5
*u*2474	H(67)...H(86)	582.2(27)	38.2(fixed)	—	0.4	38.2

*u*2385	C(10)...H(21)	582.5(26)	31.3(fixed)	—	–4.1	31.3
*u*2412	H(78)...H(83)	582.6(20)	42.1(fixed)	—	2.0	42.1
*u*1404	C(102)...H(127)	582.6(29)	33.4(fixed)	—	–2.1	33.4
*u*2338	H(24)...H(42)	582.7(25)	38.3(fixed)	—	11.0	38.3
*u*1431	C(101)...H(119)	582.8(18)	31.0(fixed)	—	–2.5	31.0
*u*2355	Cl(62)...H(91)	582.8(21)	33.1(fixed)	—	–0.7	33.1
*u*2672	C(147)...H(166)	582.8(30)	25.2(fixed)	—	–3.5	25.2
*u*2537	C(56)...H(80)	582.9(27)	26.6(fixed)	—	–4.1	26.6
*u*2435	H(28)...H(31)	583.0(22)	43.1(fixed)	—	2.5	43.1
*u*2631	Cl(62)...H(92)	583.2(26)	23.2(fixed)	—	–1.9	23.2
*u*2454	C(7)...H(30)	583.2(22)	33.2(fixed)	—	–5.7	33.2
*u*2521	H(161)...H(176)	583.5(37)	44.3(fixed)	—	0.9	44.3
*u*2439	C(64)...H(90)	583.5(24)	22.4(fixed)	—	–1.5	22.4
*u*2477	C(64)...H(91)	583.5(28)	22.4(fixed)	—	–1.4	22.4
*u*262	H(118)...H(129)	583.6(39)	41.7(fixed)	—	10.7	41.7
*u*2374	C(57)...H(76)	583.6(25)	32.3(fixed)	—	–0.9	32.3
*u*2649	C(55)...H(93)	583.7(39)	26.0(fixed)	—	–3.4	26.0
*u*2369	Cl(61)...H(75)	583.7(22)	34.2(fixed)	—	–0.9	34.2
*u*2437	C(57)...H(83)	583.8(14)	23.3(fixed)	—	–1.2	23.3
*u*2517	C(53)...H(86)	583.8(17)	22.3(fixed)	—	–1.7	22.3
*u*2555	C(152)...H(159)	583.8(21)	22.4(fixed)	—	–1.8	22.4
*u*1514	C(148)...H(169)	583.9(18)	33.5(fixed)	—	–2.9	33.5
*u*2534	C(152)...H(161)	584.0(23)	23.1(fixed)	—	–1.5	23.1
*u*2494	C(8)...H(46)	584.1(33)	23.2(fixed)	—	–1.9	23.2
*u*2622	Cl(14)...H(42)	584.1(27)	39.1(fixed)	—	–8.7	39.1
*u*2444	H(36)...H(45)	584.3(33)	30.5(fixed)	—	–2.0	30.5
*u*2406	H(70)...H(78)	584.4(31)	30.0(fixed)	—	–0.3	30.0
*u*1780	H(163)...H(168)	584.5(24)	52.8(fixed)	—	–7.6	52.8
*u*2410	C(59)...H(93)	584.5(28)	28.7(fixed)	—	–3.5	28.7
*u*2532	H(28)...H(47)	584.6(35)	36.8(fixed)	—	0.1	36.8
*u*2422	H(69)...H(79)	584.6(32)	32.1(fixed)	—	–2.3	32.1
*u*2440	C(105)...H(113)	584.7(23)	22.7(fixed)	—	–1.7	22.7
*u*2482	Cl(14)...H(21)	584.8(27)	24.4(fixed)	—	–1.9	24.4
*u*2550	C(10)...H(23)	584.9(22)	26.4(fixed)	—	–4.3	26.4
*u*2566	C(64)...H(84)	585.0(25)	29.1(fixed)	—	–4.7	29.1
*u*2507	C(17)...H(43)	585.1(23)	23.0(fixed)	—	–1.4	23.0
*u*2584	C(9)...H(18)	585.2(32)	25.4(fixed)	—	–3.7	25.4
*u*2475	C(57)...H(85)	585.3(16)	23.3(fixed)	—	–1.8	23.3
*u*2539	Cl(15)...H(34)	585.5(25)	32.9(fixed)	—	–4.7	32.9
*u*3003	Cl(108)...H(116)	585.5(21)	25.3(fixed)	—	–1.0	25.3
*u*779	C(154)...H(167)	585.7(18)	44.9(fixed)	—	2.8	44.9
*u*2573	Cl(14)...H(43)	585.8(26)	39.0(fixed)	—	–7.2	39.0
*u*2386	C(149)...H(159)	586.0(26)	33.4(fixed)	—	–1.4	33.4
*u*2479	Cl(61)...H(90)	586.0(21)	28.8(fixed)	—	–3.1	28.8
*u*2511	H(37)...H(47)	586.1(31)	30.0(fixed)	—	–1.4	30.0
*u*1374	C(110)...H(123)	586.1(20)	43.0(fixed)	—	–3.6	43.0

*u*2471	C(9)...H(31)	586.4(13)	23.2(fixed)	—	–1.0	23.2
*u*2421	H(73)...H(83)	586.4(24)	45.3(fixed)	—	1.7	45.3
*u*2540	C(6)...H(40)	586.4(17)	22.8(fixed)	—	–1.6	22.8
*u*2390	C(9)...H(40)	586.4(25)	34.0(fixed)	—	–0.7	34.0
*u*2393	C(56)...H(81)	586.5(28)	30.2(fixed)	—	–3.9	30.2
*u*2621	Cl(15)...H(33)	586.9(28)	30.3(fixed)	—	–5.2	30.3
*u*2522	H(35)...H(39)	586.9(27)	44.1(fixed)	—	1.3	44.1
*u*2394	H(69)...H(83)	587.0(20)	37.5(fixed)	—	1.7	37.5
*u*2464	C(59)...H(73)	587.0(17)	23.1(fixed)	—	–1.3	23.1
*u*2687	Cl(155)...H(175)	587.1(23)	28.4(fixed)	—	–3.8	28.4
*u*2561	H(39)...H(47)	587.2(26)	36.4(fixed)	—	–1.4	36.4
*u*2544	C(6)...H(39)	587.4(17)	22.5(fixed)	—	–2.1	22.5
*u*2478	C(10)...H(38)	587.6(18)	23.7(fixed)	—	–1.9	23.7
*u*2429	H(67)...H(78)	587.8(27)	35.8(fixed)	—	0.4	35.8
*u*2527	C(11)...H(20)	587.9(26)	23.0(fixed)	—	–1.3	23.0
*u*2574	C(6)...H(29)	587.9(32)	26.5(fixed)	—	–4.0	26.5
*u*2530	C(53)...H(87)	588.0(17)	22.5(fixed)	—	–1.7	22.5
*u*2504	C(58)...H(66)	588.0(21)	23.1(fixed)	—	–2.0	23.1
*u*2541	C(8)...H(47)	588.1(24)	22.6(fixed)	—	–1.7	22.6
*u*2467	C(16)...H(26)	588.2(16)	23.3(fixed)	—	–1.2	23.3
*u*1661	H(122)...H(129)	588.3(22)	38.0(fixed)	—	6.8	38.0
*u*2395	H(26)...H(40)	588.3(21)	29.8(fixed)	—	–0.9	29.8
*u*3018	H(176)...H(177)	588.3(24)	40.0(fixed)	—	0.5	40.0
*u*2589	C(8)...H(45)	588.3(26)	22.6(fixed)	—	–1.7	22.6
*u*2481	C(10)...H(36)	588.5(16)	23.2(fixed)	—	–1.4	23.2
*u*3188	C(107)...H(128)	588.5(16)	16.2(fixed)	—	–4.8	16.2
*u*2173	C(147)...H(165)	588.5(24)	28.9(fixed)	—	1.8	28.9
*u*2514	C(58)...H(76)	588.5(25)	24.4(fixed)	—	–3.4	24.4
*u*2472	C(8)...H(41)	588.6(17)	28.7(fixed)	—	–3.9	28.7
*u*2531	C(58)...H(67)	588.7(26)	22.9(fixed)	—	–1.6	22.9
*u*2443	C(64)...H(85)	588.7(30)	31.1(fixed)	—	–4.3	31.1
*u*2433	C(12)...H(27)	588.7(19)	23.5(fixed)	—	–1.8	23.5
*u*2556	H(20)...H(35)	588.7(40)	44.1(fixed)	—	1.4	44.1
*u*2381	H(164)...H(172)	588.8(30)	34.6(fixed)	—	–0.8	34.6
*u*2576	H(67)...H(88)	588.8(32)	39.1(fixed)	—	–1.7	39.1
*u*2549	H(31)...H(36)	588.9(25)	50.7(fixed)	—	1.3	50.7
*u*616	C(105)...H(118)	589.0(28)	36.7(fixed)	—	3.8	36.7
*u*2557	C(64)...H(89)	589.1(20)	21.7(fixed)	—	–1.6	21.7
*u*2490	C(13)...H(34)	589.1(16)	23.7(fixed)	—	–1.8	23.7
*u*2486	C(12)...H(46)	589.3(27)	29.0(fixed)	—	–3.6	29.0
*u*2512	C(13)...H(35)	589.3(14)	23.3(fixed)	—	–1.3	23.3
*u*2533	Cl(14)...H(22)	589.4(21)	23.6(fixed)	—	–1.7	23.6
*u*2554	C(54)...H(79)	589.4(25)	26.6(fixed)	—	–3.9	26.6
*u*2629	Cl(61)...H(89)	589.6(24)	24.3(fixed)	—	–3.5	24.3
*u*2473	H(114)...H(125)	589.7(19)	33.7(fixed)	—	–1.1	33.7
*u*2498	C(55)...H(78)	589.8(13)	23.0(fixed)	—	–1.3	23.0

*u*2780	H(169)...H(174)	590.0(29)	39.5(fixed)	—	–2.8	39.5
*u*2434	C(57)...H(68)	590.1(27)	28.1(fixed)	—	–3.3	28.1
*u*2463	H(26)...H(44)	590.1(25)	59.1(fixed)	—	4.2	59.1
*u*2535	C(11)...H(19)	590.1(23)	23.7(fixed)	—	–2.1	23.7
*u*2536	H(67)...H(82)	590.2(41)	42.3(fixed)	—	0.9	42.3
*u*2492	H(20)...H(31)	590.2(23)	39.4(fixed)	—	2.7	39.4
*u*2458	H(161)...H(172)	590.3(21)	40.3(fixed)	—	2.0	40.3
*u*2599	C(59)...H(92)	590.3(26)	24.8(fixed)	—	–3.7	24.8
*u*2459	C(59)...H(72)	590.5(16)	23.7(fixed)	—	–1.9	23.7
*u*2624	H(160)...H(176)	590.5(35)	46.2(fixed)	—	–2.1	46.2
*u*2560	C(58)...H(65)	590.5(19)	22.4(fixed)	—	–1.8	22.4
*u*2520	H(20)...H(39)	590.5(28)	38.3(fixed)	—	0.5	38.3
*u*2513	Cl(62)...H(88)	590.6(18)	29.2(fixed)	—	–3.4	29.2
*u*2508	C(9)...H(30)	590.6(15)	23.2(fixed)	—	–1.8	23.2
*u*2618	C(17)...H(37)	590.8(24)	24.3(fixed)	—	–3.6	24.3
*u*1550	C(107)...H(121)	590.8(39)	37.3(fixed)	—	–5.0	37.3
*u*2376	C(55)...H(87)	590.9(36)	32.3(fixed)	—	–0.9	32.3
*u*2705	Cl(155)...H(176)	591.0(23)	27.5(fixed)	—	–3.9	27.5
*u*2596	C(17)...H(42)	591.0(18)	22.2(fixed)	—	–2.5	22.2
*u*494	Cl(108)...H(123)	591.0(15)	44.7(fixed)	—	6.5	44.7
*u*2496	C(60)...H(82)	591.2(13)	23.1(fixed)	—	–1.2	23.1
*u*2432	C(151)...H(162)	591.3(25)	31.4(fixed)	—	–4.8	31.4
*u*2430	H(22)...H(36)	591.4(17)	32.7(fixed)	—	–1.4	32.7
*u*2523	C(151)...H(164)	591.5(24)	30.1(fixed)	—	–5.0	30.1
*u*326	H(169)...H(177)	591.5(28)	51.5(fixed)	—	11.7	51.5
*u*2462	C(17)...H(38)	591.6(26)	27.9(fixed)	—	–3.2	27.9
*u*2608	Cl(14)...H(23)	591.6(19)	23.5(fixed)	—	–2.1	23.5
*u*2542	H(26)...H(35)	591.7(24)	35.6(fixed)	—	1.0	35.6
*u*2487	C(54)...H(77)	591.8(27)	29.2(fixed)	—	–3.9	29.2
*u*2442	H(73)...H(78)	591.8(21)	38.8(fixed)	—	1.3	38.8
*u*2581	C(57)...H(70)	591.8(25)	23.9(fixed)	—	–3.3	23.9
*u*2899	C(107)...H(129)	591.9(14)	25.1(fixed)	—	–0.6	25.1
*u*2664	C(153)...H(163)	592.0(12)	28.1(fixed)	—	–4.4	28.1
*u*2516	H(24)...H(39)	592.0(24)	31.5(fixed)	—	–2.1	31.5
*u*2505	H(83)...H(91)	592.0(29)	34.1(fixed)	—	–1.9	34.1
*u*3028	H(169)...H(172)	592.0(19)	42.1(fixed)	—	0.9	42.1
*u*2604	C(13)...H(24)	592.1(18)	27.7(fixed)	—	–4.4	27.7
*u*1481	Cl(109)...H(113)	592.2(26)	32.8(fixed)	—	–2.7	32.8
*u*2509	H(82)...H(86)	592.2(24)	40.2(fixed)	—	1.0	40.2
*u*2613	C(12)...H(45)	592.2(23)	25.5(fixed)	—	–3.8	25.5
*u*2563	C(105)...H(112)	592.3(23)	22.1(fixed)	—	–1.7	22.1
*u*2470	C(16)...H(25)	592.3(21)	23.9(fixed)	—	–1.6	23.9
*u*3032	H(129)...H(133)	592.5(26)	39.3(fixed)	—	0.6	39.3
*u*2515	C(60)...H(81)	592.5(15)	23.2(fixed)	—	–1.9	23.2
*u*2524	H(22)...H(44)	592.9(23)	40.6(fixed)	—	–4.4	40.6
*u*1387	C(101)...H(118)	593.1(18)	33.1(fixed)	—	–2.1	33.1

*u*2552	Cl(61)...H(68)	593.1(24)	24.4(fixed)	—	–2.1	24.4
*u*2565	H(90)...H(94)	593.1(42)	40.9(fixed)	—	–1.3	40.9
*u*2593	C(13)...H(33)	593.3(16)	22.7(fixed)	—	–2.1	22.7
*u*2655	C(153)...H(162)	593.5(16)	27.4(fixed)	—	–4.1	27.4
*u*2585	C(11)...H(18)	593.5(19)	22.8(fixed)	—	–2.0	22.8
*u*2601	H(20)...H(41)	593.6(27)	39.9(fixed)	—	–1.9	39.9
*u*2848	C(150)...H(175)	593.8(25)	24.6(fixed)	—	–6.8	24.6
*u*2931	C(107)...H(127)	594.1(17)	25.4(fixed)	—	–0.7	25.4
*u*1420	Cl(109)...H(112)	594.5(28)	33.5(fixed)	—	–2.4	33.5
*u*2446	H(36)...H(44)	594.6(32)	42.2(fixed)	—	7.8	42.2
*u*2526	C(12)...H(28)	594.6(20)	22.5(fixed)	—	–1.9	22.5
*u*2616	H(43)...H(47)	594.8(39)	42.5(fixed)	—	–1.3	42.5
*u*2683	C(53)...H(74)	595.1(31)	25.2(fixed)	—	–3.1	25.2
*u*2668	C(152)...H(168)	595.4(26)	25.7(fixed)	—	–3.2	25.7
*u*382	C(101)...H(120)	595.4(15)	28.5(fixed)	—	9.1	28.5
*u*246	H(116)...H(120)	595.5(23)	42.9(fixed)	—	11.9	42.9
*u*2605	C(60)...H(80)	595.7(14)	22.0(fixed)	—	–1.9	22.0
*u*1657	H(114)...H(120)	595.7(31)	39.2(fixed)	—	4.5	39.2
*u*1164	H(123)...H(133)	595.8(46)	43.9(fixed)	—	4.3	43.9
*u*2547	C(12)...H(29)	595.8(16)	22.9(fixed)	—	–1.8	22.9
*u*3012	Cl(108)...H(117)	595.9(18)	25.0(fixed)	—	–1.2	25.0
*u*2588	Cl(61)...H(69)	596.0(22)	23.6(fixed)	—	–1.7	23.6
*u*455	C(148)...H(170)	596.0(14)	30.2(fixed)	—	7.8	30.2
*u*2452	C(105)...H(121)	596.1(24)	30.2(fixed)	—	–4.6	30.2
*u*2503	H(120)...H(125)	596.3(19)	38.1(fixed)	—	0.5	38.1
*u*2519	H(69)...H(91)	596.7(24)	35.1(fixed)	—	–0.5	35.1
*u*2650	C(55)...H(94)	596.8(27)	24.8(fixed)	—	–3.0	24.8
*u*2600	C(10)...H(37)	596.8(17)	22.3(fixed)	—	–2.2	22.3
*u*2610	C(57)...H(84)	597.0(16)	21.5(fixed)	—	–2.3	21.5
*u*599	C(154)...H(165)	597.3(15)	38.6(fixed)	—	4.6	38.6
*u*2603	C(9)...H(32)	597.6(13)	22.0(fixed)	—	–2.0	22.0
*u*2568	H(86)...H(94)	597.6(24)	35.3(fixed)	—	–0.4	35.3
*u*2466	C(13)...H(25)	597.7(21)	29.5(fixed)	—	–3.8	29.5
*u*2619	Cl(61)...H(70)	598.0(18)	23.5(fixed)	—	–2.0	23.5
*u*2630	H(34)...H(39)	598.1(29)	44.5(fixed)	—	–2.1	44.5
*u*1385	H(114)...H(135)	598.2(33)	47.1(fixed)	—	–4.4	47.1
*u*2640	C(59)...H(68)	598.3(19)	25.9(fixed)	—	–3.3	25.9
*u*2645	C(16)...H(38)	598.4(33)	24.7(fixed)	—	–3.1	24.7
*u*2389	C(150)...H(174)	598.7(23)	34.9(fixed)	—	–1.0	34.9
*u*2607	H(113)...H(129)	598.9(38)	38.8(fixed)	—	–1.7	38.8
*u*1287	H(116)...H(119)	599.0(25)	42.7(fixed)	—	–2.0	42.7
*u*327	H(161)...H(169)	599.2(23)	48.4(fixed)	—	12.1	48.4
*u*2543	H(26)...H(47)	599.2(28)	39.4(fixed)	—	1.0	39.4
*u*2633	H(28)...H(30)	599.3(25)	45.0(fixed)	—	–2.1	45.0
*u*2586	C(8)...H(40)	599.3(19)	25.3(fixed)	—	–3.8	25.3
*u*2160	Cl(155)...H(174)	599.7(17)	29.5(fixed)	—	3.0	29.5

*u*2620	H(78)...H(85)	600.0(21)	44.0(fixed)	—	–1.9	44.0
*u*2528	C(55)...H(77)	600.1(16)	23.5(fixed)	—	–1.8	23.5
*u*1823	H(170)...H(176)	600.1(30)	45.8(fixed)	—	7.0	45.8
*u*3187	C(153)...H(175)	600.4(20)	16.6(fixed)	—	–5.8	16.6
*u*2455	H(28)...H(36)	600.7(32)	35.7(fixed)	—	0.7	35.7
*u*2465	H(167)...H(172)	601.1(19)	37.0(fixed)	—	–2.1	37.0
*u*407	C(110)...H(122)	601.1(18)	32.6(fixed)	—	13.4	32.6
*u*1132	H(169)...H(179)	601.1(28)	33.9(fixed)	—	4.4	33.9
*u*2653	C(11)...H(25)	601.2(24)	25.0(fixed)	—	–3.2	25.0
*u*2665	C(9)...H(46)	601.6(37)	26.4(fixed)	—	–3.5	26.4
*u*2615	C(16)...H(24)	601.8(18)	22.1(fixed)	—	–2.4	22.1
*u*2614	C(59)...H(71)	602.2(20)	21.8(fixed)	—	–2.2	21.8
*u*2128	C(153)...H(164)	602.2(16)	28.6(fixed)	—	4.5	28.6
*u*2634	H(66)...H(82)	602.6(37)	44.1(fixed)	—	–2.2	44.1
*u*2623	Cl(62)...H(87)	602.7(17)	24.6(fixed)	—	–3.6	24.6
*u*2641	H(31)...H(38)	602.8(25)	54.6(fixed)	—	–3.0	54.6
*u*2617	H(28)...H(39)	603.1(24)	37.9(fixed)	—	–1.1	37.9
*u*2685	H(69)...H(76)	603.3(32)	33.8(fixed)	—	–3.1	33.8
*u*3249	H(128)...H(133)	603.3(27)	27.4(fixed)	—	–5.1	27.4
*u*2403	C(100)...H(119)	603.5(32)	28.2(fixed)	—	–3.2	28.2
*u*2147	C(152)...H(170)	603.6(22)	28.3(fixed)	—	2.0	28.3
*u*2663	C(63)...H(85)	604.1(30)	25.6(fixed)	—	–3.7	25.6
*u*2977	Cl(155)...H(166)	604.4(16)	19.7(fixed)	—	–6.3	19.7
*u*2644	H(19)...H(35)	604.5(38)	47.7(fixed)	—	–2.5	47.7
*u*2646	C(10)...H(19)	604.6(22)	25.9(fixed)	—	–3.5	25.9
*u*2606	C(55)...H(79)	605.0(16)	22.2(fixed)	—	–1.9	22.2
*u*1638	C(147)...H(168)	605.0(24)	24.7(fixed)	—	–4.2	24.7
*u*2611	H(72)...H(83)	605.2(22)	48.8(fixed)	—	–2.0	48.8
*u*2666	C(12)...H(21)	605.4(18)	27.1(fixed)	—	–4.1	27.1
*u*2642	C(57)...H(66)	605.5(23)	25.9(fixed)	—	–3.3	25.9
*u*2643	C(59)...H(69)	605.6(16)	24.1(fixed)	—	–2.8	24.1
*u*286	H(114)...H(133)	606.1(28)	49.7(fixed)	—	16.4	49.7
*u*2571	H(75)...H(78)	606.2(21)	33.9(fixed)	—	–1.3	33.9
*u*2699	C(53)...H(75)	606.3(20)	23.8(fixed)	—	–3.0	23.8
*u*2667	C(104)...H(113)	606.4(15)	25.4(fixed)	—	–3.3	25.4
*u*2638	H(81)...H(86)	606.9(24)	41.2(fixed)	—	–2.1	41.2
*u*2577	H(27)...H(36)	607.5(33)	36.9(fixed)	—	–1.5	36.9
*u*2673	C(9)...H(47)	607.6(26)	25.5(fixed)	—	–3.1	25.5
*u*2662	C(17)...H(41)	607.7(24)	27.7(fixed)	—	–3.8	27.7
*u*3194	C(154)...H(162)	607.8(19)	16.7(fixed)	—	–6.6	16.7
*u*2625	H(25)...H(44)	607.8(32)	66.3(fixed)	—	–2.3	66.3
*u*2659	C(151)...H(160)	607.9(15)	26.4(fixed)	—	–3.6	26.4
*u*2648	C(57)...H(67)	608.8(21)	24.5(fixed)	—	–2.9	24.5
*u*2651	C(10)...H(20)	609.2(19)	24.4(fixed)	—	–2.9	24.4
*u*2690	Cl(61)...H(81)	609.6(20)	27.7(fixed)	—	–3.7	27.7
*u*2632	H(26)...H(46)	609.8(34)	42.3(fixed)	—	–1.9	42.3

*u*2909	C(153)...H(176)	609.9(19)	28.3(fixed)	—	–0.6	28.3
*u*2654	C(151)...H(161)	610.2(17)	25.3(fixed)	—	–3.1	25.3
*u*2657	C(12)...H(22)	610.3(12)	25.9(fixed)	—	–3.4	25.9
*u*2695	C(17)...H(39)	610.7(19)	25.4(fixed)	—	–3.8	25.4
*u*2851	H(71)...H(93)	610.9(41)	38.5(fixed)	—	–5.3	38.5
*u*2518	C(106)...H(115)	610.9(19)	23.2(fixed)	—	–1.9	23.2
*u*2660	C(104)...H(114)	611.6(16)	24.4(fixed)	—	–3.0	24.4
*u*2708	H(159)...H(176)	611.7(28)	40.2(fixed)	—	–3.6	40.2
*u*2647	C(16)...H(36)	611.7(24)	23.1(fixed)	—	–2.7	23.1
*u*2572	H(73)...H(86)	611.9(31)	35.1(fixed)	—	–0.6	35.1
*u*485	C(107)...H(123)	612.2(35)	32.8(fixed)	—	12.0	32.8
*u*2677	C(7)...H(43)	612.4(18)	31.1(fixed)	—	–6.0	31.1
*u*2682	C(7)...H(44)	612.5(19)	32.9(fixed)	—	–6.3	32.9
*u*2746	H(71)...H(94)	612.7(34)	39.1(fixed)	—	–3.0	39.1
*u*2707	H(42)...H(47)	613.6(29)	37.3(fixed)	—	–5.7	37.3
*u*2675	C(11)...H(26)	613.6(18)	23.9(fixed)	—	–3.1	23.9
*u*1767	C(105)...H(122)	613.8(17)	29.5(fixed)	—	5.0	29.5
*u*2553	Cl(108)...H(128)	614.5(24)	24.3(fixed)	—	–1.9	24.3
*u*2696	H(89)...H(94)	614.7(31)	35.7(fixed)	—	–2.8	35.7
*u*802	C(147)...H(169)	614.8(16)	42.6(fixed)	—	2.5	42.6
*u*2674	C(63)...H(83)	614.9(21)	25.5(fixed)	—	–3.5	25.5
*u*2887	C(154)...H(163)	615.0(15)	29.5(fixed)	—	0.2	29.5
*u*2692	Cl(14)...H(34)	615.3(25)	29.2(fixed)	—	–4.1	29.2
*u*2693	H(67)...H(87)	615.6(24)	34.4(fixed)	—	–3.0	34.4
*u*2529	C(106)...H(116)	615.9(13)	22.8(fixed)	—	–1.5	22.8
*u*2688	Cl(15)...H(30)	616.1(24)	30.5(fixed)	—	–4.4	30.5
*u*2706	Cl(61)...H(82)	616.2(18)	26.0(fixed)	—	–3.5	26.0
*u*2680	C(64)...H(88)	616.3(25)	25.4(fixed)	—	–3.2	25.4
*u*2689	C(54)...H(90)	616.3(21)	25.1(fixed)	—	–3.1	25.1
*u*2678	C(54)...H(91)	616.4(19)	24.1(fixed)	—	–2.7	24.1
*u*2766	H(38)...H(42)	616.9(44)	61.6(fixed)	—	–6.5	61.6
*u*2727	H(69)...H(84)	617.2(26)	42.7(fixed)	—	–2.4	42.7
*u*2704	H(20)...H(40)	617.7(20)	34.7(fixed)	—	–3.2	34.7
*u*2697	C(64)...H(86)	618.1(16)	24.3(fixed)	—	–3.1	24.3
*u*2711	Cl(14)...H(35)	618.2(20)	27.9(fixed)	—	–4.1	27.9
*u*2770	C(56)...H(68)	618.3(32)	19.8(fixed)	—	–5.4	19.8
*u*2721	H(33)...H(39)	618.4(19)	39.0(fixed)	—	–4.3	39.0
*u*2626	H(73)...H(77)	618.7(25)	39.9(fixed)	—	–1.7	39.9
*u*1748	C(100)...H(120)	618.9(23)	29.3(fixed)	—	2.6	29.3
*u*1111	H(163)...H(170)	619.1(18)	44.7(fixed)	—	0.2	44.7
*u*2769	H(68)...H(84)	619.1(28)	45.0(fixed)	—	–5.5	45.0
*u*2579	Cl(108)...H(129)	619.3(21)	23.5(fixed)	—	–1.6	23.5
*u*2710	H(112)...H(129)	619.4(30)	33.8(fixed)	—	–3.1	33.8
*u*2714	Cl(15)...H(31)	619.8(19)	29.1(fixed)	—	–5.0	29.1
*u*2713	H(65)...H(82)	620.2(28)	37.8(fixed)	—	–3.4	37.8
*u*2716	H(28)...H(32)	620.5(17)	38.2(fixed)	—	–4.5	38.2

*u*2361	Cl(155)...H(167)	621.6(15)	36.6(fixed)	—	–0.7	36.6
*u*2724	H(18)...H(35)	622.0(29)	39.9(fixed)	—	–3.8	39.9
*u*2729	H(67)...H(79)	622.1(30)	40.7(fixed)	—	–2.4	40.7
*u*2684	C(13)...H(27)	622.2(23)	27.1(fixed)	—	–3.7	27.1
*u*2701	C(13)...H(28)	622.3(18)	25.8(fixed)	—	–3.7	25.8
*u*2775	H(72)...H(92)	622.3(45)	30.8(fixed)	—	–3.0	30.8
*u*2717	H(20)...H(32)	622.5(27)	47.7(fixed)	—	–1.7	47.7
*u*2681	C(56)...H(78)	622.8(15)	24.7(fixed)	—	–3.2	24.7
*u*2670	C(56)...H(77)	622.9(21)	25.4(fixed)	—	–3.3	25.4
*u*2720	H(78)...H(84)	623.0(17)	37.3(fixed)	—	–4.0	37.3
*u*2763	C(64)...H(72)	623.2(33)	23.0(fixed)	—	–5.3	23.0
*u*974	H(114)...H(134)	623.7(24)	62.6(fixed)	—	1.3	62.6
*u*2241	H(167)...H(171)	623.9(24)	40.3(fixed)	—	2.8	40.3
*u*2751	H(22)...H(37)	624.1(22)	39.4(fixed)	—	–3.5	39.4
*u*2971	H(121)...H(127)	624.3(34)	33.5(fixed)	—	–7.5	33.5
*u*2811	H(25)...H(33)	624.4(35)	45.6(fixed)	—	–5.7	45.6
*u*2732	H(31)...H(37)	624.6(19)	44.9(fixed)	—	–4.6	44.9
*u*2726	H(80)...H(86)	624.6(16)	35.7(fixed)	—	–3.7	35.7
*u*2671	C(60)...H(72)	624.7(31)	24.6(fixed)	—	–3.2	24.6
*u*2723	H(36)...H(42)	625.3(35)	55.8(fixed)	—	–1.0	55.8
*u*2408	H(122)...H(127)	625.5(26)	31.2(fixed)	—	0.5	31.2
*u*3013	H(176)...H(178)	625.7(28)	37.2(fixed)	—	1.9	37.2
*u*2730	H(161)...H(173)	625.7(25)	45.3(fixed)	—	–2.1	45.3
*u*996	H(116)...H(118)	625.8(20)	48.5(fixed)	—	2.0	48.5
*u*2757	H(19)...H(32)	626.3(29)	51.0(fixed)	—	–5.6	51.0
*u*2794	H(39)...H(45)	626.5(27)	39.2(fixed)	—	–3.4	39.2
*u*2840	H(66)...H(72)	626.5(44)	39.2(fixed)	—	–6.3	39.2
*u*2718	H(26)...H(45)	626.6(25)	35.7(fixed)	—	–3.2	35.7
*u*2778	H(65)...H(75)	627.1(27)	37.8(fixed)	—	–2.8	37.8
*u*3226	H(175)...H(178)	627.3(27)	27.5(fixed)	—	–5.2	27.5
*u*2728	H(24)...H(44)	627.8(22)	54.3(fixed)	—	–4.7	54.3
*u*2762	H(23)...H(44)	628.2(28)	50.8(fixed)	—	–6.2	50.8
*u*2749	H(114)...H(126)	628.5(24)	36.4(fixed)	—	–2.9	36.4
*u*3004	H(127)...H(133)	628.6(18)	36.1(fixed)	—	2.6	36.1
*u*2747	H(29)...H(47)	628.8(32)	41.1(fixed)	—	–2.5	41.1
*u*2679	C(60)...H(73)	628.8(23)	23.7(fixed)	—	–2.7	23.7
*u*2884	H(123)...H(128)	628.9(27)	37.6(fixed)	—	–7.9	37.6
*u*2719	H(71)...H(83)	629.0(20)	40.8(fixed)	—	–3.6	40.8
*u*2953	H(112)...H(119)	629.1(43)	32.4(fixed)	—	–6.5	32.4
*u*2748	H(26)...H(33)	629.3(28)	44.0(fixed)	—	–2.7	44.0
*u*1154	H(159)...H(169)	629.4(24)	52.2(fixed)	—	2.0	52.2
*u*2691	H(29)...H(36)	629.6(24)	32.1(fixed)	—	–3.2	32.1
*u*2906	H(65)...H(74)	629.9(37)	37.5(fixed)	—	–5.0	37.5
*u*2873	H(85)...H(89)	630.1(39)	36.8(fixed)	—	–5.8	36.8
*u*2767	H(66)...H(79)	630.1(29)	41.9(fixed)	—	–5.1	41.9
*u*2882	H(21)...H(37)	630.4(29)	37.9(fixed)	—	–6.2	37.9

*u*2743	C(56)...C(64)	630.5(9)	14.2(tied to *u*2835)	—	–1.3	13.4
*u*2755	H(70)...H(85)	631.0(28)	32.5(fixed)	—	–6.0	32.5
*u*2735	C(6)...C(16)	631.2(15)	14.7(tied to *u*2835)	—	–1.5	13.8
*u*2792	C(12)...H(43)	631.2(26)	29.0(fixed)	—	–13.8	29.0
*u*2734	C(147)...C(157)	631.4(14)	14.4(tied to *u*2835)	—	–1.4	13.6
*u*2742	C(53)...C(63)	631.5(15)	14.4(tied to *u*2835)	—	–1.3	13.6
*u*2807	C(147)...H(175)	631.9(16)	20.4(fixed)	—	–7.0	20.4
*u*2012	H(159)...H(168)	632.0(33)	35.5(fixed)	—	–7.9	35.5
*u*2864	C(56)...H(66)	632.0(25)	22.5(fixed)	—	–5.5	22.5
*u*2383	H(112)...H(120)	632.0(33)	31.1(fixed)	—	–1.5	31.1
*u*2761	H(83)...H(89)	632.0(31)	38.8(fixed)	—	–3.5	38.8
*u*2752	H(70)...H(91)	632.8(28)	36.9(fixed)	—	–2.6	36.9
*u*2820	H(27)...H(45)	632.8(39)	30.8(fixed)	—	–4.2	30.8
*u*2144	C(103)...C(104)	632.9(6)	20.3(tied to *u*2835)	—	–0.7	19.1
*u*2817	C(17)...H(25)	633.0(27)	19.3(fixed)	—	–6.4	19.3
*u*2876	H(113)...H(126)	633.1(20)	35.4(fixed)	—	–5.0	35.4
*u*2733	C(54)...C(60)	633.1(7)	14.5(tied to *u*2835)	—	–1.4	13.6
*u*2813	C(17)...H(27)	633.6(31)	22.8(fixed)	—	–6.5	22.8
*u*2118	C(152)...C(154)	633.6(7)	17.8(tied to *u*2835)	—	–0.8	16.8
*u*2810	H(37)...H(43)	633.6(37)	31.9(fixed)	—	–13.6	31.9
*u*2759	C(54)...H(85)	633.9(16)	24.8(fixed)	—	–7.3	24.8
*u*2146	C(105)...C(106)	633.9(8)	18.8(tied to *u*2835)	—	–0.7	17.8
*u*2744	C(7)...C(13)	633.9(7)	14.3(tied to *u*2835)	—	–1.4	13.5
*u*2737	C(58)...C(59)	633.9(7)	14.3(tied to *u*2835)	—	–1.3	13.5
*u*1543	C(150)...H(162)	634.3(12)	35.7(fixed)	—	–5.5	35.7
*u*2715	H(73)...H(79)	634.3(20)	34.5(fixed)	—	–3.2	34.5
*u*2861	H(66)...H(76)	634.3(30)	30.5(fixed)	—	–3.8	30.5
*u*2738	C(11)...C(12)	634.6(7)	14.3(tied to *u*2835)	—	–1.4	13.5
*u*2795	C(13)...H(19)	634.6(11)	20.8(fixed)	—	–6.2	20.8
*u*260	H(169)...H(178)	634.7(21)	43.9(fixed)	—	12.7	43.9
*u*2741	C(8)...C(10)	634.8(7)	14.2(tied to *u*2835)	—	–1.3	13.4
*u*2782	C(60)...H(66)	634.9(12)	20.2(fixed)	—	–5.7	20.2
*u*2996	H(66)...H(71)	635.0(37)	32.7(fixed)	—	–6.8	32.7
*u*2804	H(160)...H(173)	635.1(19)	47.5(fixed)	—	–5.8	47.5
*u*2808	C(8)...H(43)	635.8(14)	26.3(fixed)	—	–14.1	26.3
*u*2368	H(118)...H(125)	635.9(22)	35.2(fixed)	—	0.4	35.2
*u*2812	H(86)...H(92)	636.0(24)	38.1(fixed)	—	–2.8	38.1
*u*2862	H(29)...H(46)	636.1(40)	40.5(fixed)	—	–5.5	40.5
*u*2950	H(170)...H(172)	636.2(23)	36.5(fixed)	—	3.6	36.5
*u*1098	C(149)...C(153)	636.5(14)	23.4(tied to *u*2835)	—	0.3	22.1
*u*2771	H(159)...H(171)	636.5(28)	33.1(fixed)	—	–6.8	33.1
*u*2407	C(103)...H(128)	636.8(18)	28.1(fixed)	—	–3.3	28.1
*u*2783	C(63)...H(93)	636.8(19)	19.5(fixed)	—	–5.9	19.5
*u*2798	C(6)...H(30)	636.9(19)	25.0(fixed)	—	–9.5	25.0
*u*3210	H(174)...H(179)	636.9(35)	27.2(fixed)	—	–3.7	27.2
*u*2781	C(100)...H(128)	637.1(18)	19.8(fixed)	—	–5.4	19.8

*u*2823	C(16)...H(46)	637.4(18)	18.7(fixed)	—	–6.3	18.7
*u*1611	C(107)...H(113)	637.4(14)	24.7(fixed)	—	–3.9	24.7
*u*2786	H(18)...H(30)	637.4(28)	30.2(fixed)	—	–8.0	30.2
*u*2788	C(12)...H(30)	637.7(13)	23.5(fixed)	—	–9.6	23.5
*u*2881	H(23)...H(43)	637.8(24)	44.6(fixed)	—	–9.6	44.6
*u*2760	H(65)...H(77)	638.0(35)	31.7(fixed)	—	–4.3	31.7
*u*2877	H(41)...H(45)	638.3(30)	39.7(fixed)	—	–6.0	39.7
*u*2814	C(53)...H(81)	638.3(17)	20.9(fixed)	—	–6.9	20.9
*u*2789	C(157)...H(162)	638.4(16)	25.4(fixed)	—	–8.3	25.4
*u*2818	C(6)...H(34)	638.4(18)	22.3(fixed)	—	–8.1	22.3
*u*2938	Cl(15)...H(21)	638.6(28)	20.4(fixed)	—	–7.4	20.4
*u*2999	H(65)...H(71)	639.1(25)	30.0(fixed)	—	–5.4	30.0
*u*2842	H(19)...H(27)	639.2(44)	40.1(fixed)	—	–7.1	40.1
*u*2825	H(40)...H(46)	639.2(33)	31.2(fixed)	—	–3.1	31.2
*u*2835	Cl(15)...C(17)	639.2(8)	14.9(9)	—	–1.5	14.1
*u*3174	C(158)...H(166)	639.2(20)	16.6(fixed)	—	–5.2	16.6
*u*1513	C(153)...H(168)	639.4(13)	32.1(fixed)	—	–2.8	32.1
*u*2805	C(59)...H(77)	639.6(13)	20.2(fixed)	—	–6.4	20.2
*u*2772	C(53)...H(77)	639.8(22)	23.2(fixed)	—	–6.2	23.2
*u*2976	H(65)...H(72)	640.2(38)	32.5(fixed)	—	–6.6	32.5
*u*2836	C(8)...H(34)	640.4(20)	24.0(fixed)	—	–7.8	24.0
*u*2793	C(11)...H(41)	640.7(10)	21.4(fixed)	—	–7.0	21.4
*u*2839	H(115)...H(124)	641.2(36)	36.9(fixed)	—	–5.4	36.9
*u*2841	C(13)...H(46)	641.4(21)	24.3(fixed)	—	–6.0	24.3
*u*2964	H(117)...H(126)	641.5(29)	27.9(fixed)	—	–4.7	27.9
*u*3211	H(170)...H(171)	641.5(27)	26.6(fixed)	—	–5.8	26.6
*u*2824	C(57)...Cl(62)	641.7(8)	14.8(tied to *u*2835)	—	–1.5	14.0
*u*1584	C(102)...H(115)	641.8(14)	23.0(fixed)	—	–3.0	23.0
*u*3209	H(168)...H(173)	641.9(21)	27.0(fixed)	—	–2.8	27.0
*u*3173	C(111)...H(121)	642.0(10)	16.7(fixed)	—	–6.1	16.7
*u*2800	C(10)...H(27)	642.2(9)	20.7(fixed)	—	–6.8	20.7
*u*2042	H(119)...H(128)	642.2(31)	36.2(fixed)	—	–7.5	36.2
*u*2774	C(7)...H(38)	642.3(12)	22.3(fixed)	—	–4.9	22.3
*u*2791	H(23)...H(38)	642.6(18)	29.5(fixed)	—	–1.9	29.5
*u*2182	C(148)...Cl(155)	642.6(8)	19.3(tied to *u*2835)	—	–0.9	18.2
*u*2809	C(55)...H(85)	642.7(14)	20.3(fixed)	—	–7.6	20.3
*u*1485	C(150)...H(160)	643.3(18)	33.8(fixed)	—	–2.9	33.8
*u*2896	H(23)...H(32)	643.4(22)	35.1(fixed)	—	–7.2	35.1
*u*2753	H(76)...H(78)	643.5(22)	38.0(fixed)	—	–2.9	38.0
*u*2784	C(151)...H(166)	643.5(11)	23.3(fixed)	—	–5.8	23.3
*u*1801	H(167)...H(173)	643.6(20)	43.5(fixed)	—	9.1	43.5
*u*3169	C(151)...H(168)	643.6(15)	16.3(fixed)	—	–4.9	16.3
*u*2796	C(9)...H(38)	643.6(14)	19.5(fixed)	—	–5.2	19.5
*u*2816	C(9)...Cl(14)	643.7(13)	14.7(tied to *u*2835)	—	–1.5	13.9
*u*2765	H(28)...H(40)	643.7(24)	40.0(fixed)	—	–2.8	40.0
*u*2802	C(58)...H(88)	643.8(9)	20.0(fixed)	—	–5.5	20.0

*u*2797	C(110)...H(115)	643.9(16)	22.3(fixed)	—	–4.6	22.3
*u*2830	C(55)...Cl(61)	644.3(14)	14.6(tied to *u*2835)	—	–1.5	13.8
*u*2944	H(113)...H(118)	644.5(36)	32.9(fixed)	—	–6.5	32.9
*u*2919	H(70)...H(90)	645.0(28)	35.7(fixed)	—	–4.8	35.7
*u*2401	C(102)...H(113)	645.2(25)	28.0(fixed)	—	–3.2	28.0
*u*2815	C(104)...H(119)	645.2(14)	19.6(fixed)	—	–5.4	19.6
*u*2923	H(74)...H(80)	645.2(32)	33.5(fixed)	—	–7.0	33.5
*u*2984	H(117)...H(124)	645.4(36)	30.2(fixed)	—	–5.8	30.2
*u*1980	H(119)...H(127)	645.4(34)	36.6(fixed)	—	–7.3	36.6
*u*2949	Cl(15)...H(19)	645.9(20)	23.2(fixed)	—	–6.1	23.2
*u*992	H(160)...H(170)	645.9(25)	48.3(fixed)	—	3.4	48.3
*u*2828	C(59)...H(90)	646.0(23)	22.0(fixed)	—	–4.9	22.0
*u*2863	H(21)...H(32)	646.1(28)	42.1(fixed)	—	–9.5	42.1
*u*2109	H(118)...H(124)	646.1(26)	36.2(fixed)	—	3.4	36.2
*u*2879	H(24)...H(34)	646.2(31)	29.6(fixed)	—	–6.2	29.6
*u*2968	H(18)...H(27)	646.3(37)	32.2(fixed)	—	–7.2	32.2
*u*2838	H(21)...H(30)	646.4(25)	44.7(fixed)	—	–9.6	44.7
*u*3133	H(160)...H(166)	646.6(28)	31.7(fixed)	—	–8.0	31.7
*u*3057	H(119)...H(126)	647.8(25)	26.0(fixed)	—	–5.9	26.0
*u*2901	C(16)...H(18)	647.8(19)	26.0(fixed)	—	–0.8	26.0
*u*1253	H(118)...H(127)	647.8(22)	41.6(fixed)	—	–1.4	41.6
*u*2926	H(76)...H(80)	647.9(22)	30.2(fixed)	—	–5.5	30.2
*u*2827	C(16)...H(21)	648.0(19)	24.1(fixed)	—	–7.0	24.1
*u*2928	H(84)...H(93)	648.2(28)	36.9(fixed)	—	–8.0	36.9
*u*2980	H(84)...H(92)	648.3(20)	32.3(fixed)	—	–6.1	32.3
*u*2904	C(63)...H(65)	648.4(19)	25.8(fixed)	—	–0.6	25.8
*u*2829	C(57)...H(72)	648.5(12)	19.9(fixed)	—	–5.5	19.9
*u*2785	H(74)...H(81)	648.5(27)	39.4(fixed)	—	–6.7	39.4
*u*2922	H(88)...H(92)	648.6(33)	37.8(fixed)	—	–5.1	37.8
*u*2942	C(56)...H(92)	649.0(19)	24.8(fixed)	—	–0.3	24.8
*u*2846	C(60)...H(93)	649.0(19)	23.2(fixed)	—	–5.7	23.2
*u*2821	H(112)...H(124)	649.1(30)	30.5(fixed)	—	–2.6	30.5
*u*2892	C(60)...H(70)	649.2(16)	25.6(fixed)	—	–0.8	25.6
*u*2832	C(63)...H(68)	649.3(19)	22.9(fixed)	—	–5.1	22.9
*u*2948	H(18)...H(29)	649.6(26)	30.5(fixed)	—	–5.6	30.5
*u*2905	H(164)...H(173)	649.9(22)	35.2(fixed)	—	–7.3	35.2
*u*2845	H(87)...H(93)	650.1(27)	30.7(fixed)	—	–3.9	30.7
*u*2943	H(70)...H(79)	650.2(23)	30.1(fixed)	—	–5.2	30.1
*u*1977	H(121)...H(135)	650.5(39)	49.1(fixed)	—	–11.4	49.1
*u*2966	C(110)...H(112)	650.5(18)	24.4(fixed)	—	–0.7	24.4
*u*2590	C(154)...H(174)	650.5(17)	22.0(fixed)	—	–1.7	22.0
*u*2328	C(104)...H(123)	650.6(10)	42.0(fixed)	—	–0.7	42.0
*u*2916	C(157)...H(159)	650.8(17)	25.5(fixed)	—	–0.8	25.5
*u*2854	H(68)...H(89)	650.9(31)	30.2(fixed)	—	–3.5	30.2
*u*2920	Cl(14)...H(25)	651.0(18)	23.2(fixed)	—	–6.5	23.2
*u*2883	C(53)...H(91)	651.1(20)	25.0(fixed)	—	–0.6	25.0

*u*2803	H(85)...H(93)	651.3(29)	41.9(fixed)	—	–7.4	41.9
*u*2986	H(23)...H(30)	651.6(21)	36.1(fixed)	—	–9.5	36.1
*u*2930	C(59)...H(80)	651.7(13)	26.0(fixed)	—	–0.3	26.0
*u*2888	H(159)...H(166)	651.8(32)	37.5(fixed)	—	–5.5	37.5
*u*2978	H(24)...H(41)	651.9(21)	34.7(fixed)	—	–7.8	34.7
*u*2868	H(160)...H(165)	651.9(26)	31.9(fixed)	—	–4.0	31.9
*u*2912	C(110)...H(114)	652.0(19)	25.7(fixed)	—	–0.8	25.7
*u*2867	C(9)...H(41)	652.0(19)	23.7(fixed)	—	–6.6	23.7
*u*3006	H(37)...H(45)	652.0(18)	29.3(fixed)	—	–5.4	29.3
*u*2967	C(53)...H(89)	652.3(18)	23.8(fixed)	—	–0.9	23.8
*u*2658	C(107)...H(116)	652.3(11)	24.1(fixed)	—	–2.7	24.1
*u*2750	H(73)...H(87)	652.3(31)	36.6(fixed)	—	–2.4	36.6
*u*2889	C(6)...H(44)	652.4(21)	32.1(fixed)	—	2.2	32.1
*u*3033	H(68)...H(74)	653.0(42)	26.8(fixed)	—	–6.4	26.8
*u*2957	H(65)...H(91)	653.1(28)	35.1(fixed)	—	1.6	35.1
*u*2898	C(16)...H(20)	653.2(19)	25.8(fixed)	—	–0.5	25.8
*u*2296	H(159)...H(165)	653.3(21)	42.5(fixed)	—	3.2	42.5
*u*2947	C(10)...H(24)	653.4(14)	26.2(fixed)	—	–0.7	26.2
*u*2865	H(29)...H(41)	653.6(28)	30.7(fixed)	—	–4.0	30.7
*u*2921	C(63)...H(67)	653.6(20)	25.7(fixed)	—	–0.7	25.7
*u*2117	C(106)...H(127)	653.6(14)	27.6(fixed)	—	1.8	27.6
*u*2856	H(76)...H(77)	653.7(28)	37.8(fixed)	—	–5.1	37.8
*u*2937	C(11)...H(37)	653.7(13)	25.2(fixed)	—	–1.2	25.2
*u*2954	C(13)...H(23)	653.7(14)	26.2(fixed)	—	–0.3	26.2
*u*2890	C(157)...H(161)	653.8(19)	26.7(fixed)	—	–0.5	26.7
*u*2371	C(111)...H(118)	653.9(12)	33.3(fixed)	—	–1.1	33.3
*u*1576	Cl(155)...H(160)	653.9(11)	35.8(fixed)	—	–3.6	35.8
*u*2661	C(106)...H(129)	654.0(11)	23.5(fixed)	—	–2.7	23.5
*u*2068	Cl(108)...Cl(109)	654.0(24)	22.7(tied to *u*2835)	—	–1.1	21.4
*u*2850	H(162)...H(171)	654.1(26)	43.5(fixed)	—	–9.3	43.5
*u*2924	C(6)...H(42)	654.2(18)	32.3(fixed)	—	2.0	32.3
*u*2875	H(84)...H(90)	654.4(32)	29.5(fixed)	—	–2.2	29.5
*u*2955	Cl(62)...H(81)	654.4(13)	23.8(fixed)	—	–6.8	23.8
*u*2915	C(54)...H(86)	654.7(14)	26.2(fixed)	—	–0.8	26.2
*u*2301	C(158)...H(169)	654.7(14)	35.7(fixed)	—	–0.9	35.7
*u*2725	H(174)...H(180)	654.9(25)	35.7(fixed)	—	–3.7	35.7
*u*2933	C(12)...H(33)	655.0(13)	28.2(fixed)	—	–0.2	28.2
*u*2965	H(19)...H(29)	655.1(37)	33.8(fixed)	—	–7.5	33.8
*u*2917	C(8)...H(31)	655.3(14)	29.5(fixed)	—	0.5	29.5
*u*2722	H(123)...H(125)	655.4(18)	43.5(fixed)	—	–1.6	43.5
*u*3011	H(114)...H(136)	655.8(25)	34.2(fixed)	—	1.5	34.2
*u*2831	H(38)...H(46)	655.8(26)	38.6(fixed)	—	–6.2	38.6
*u*2939	H(68)...H(79)	656.0(27)	34.0(fixed)	—	–6.9	34.0
*u*2837	C(57)...H(74)	656.1(16)	21.4(fixed)	—	–5.1	21.4
*u*2958	H(18)...H(44)	656.2(29)	37.8(fixed)	—	6.5	37.8
*u*2907	C(12)...H(35)	656.2(12)	27.0(fixed)	—	0.0	27.0

*u*2075	C(107)...H(117)	656.3(13)	29.5(fixed)	—	1.2	29.5
*u*2502	C(154)...H(176)	656.4(9)	22.9(fixed)	—	–1.7	22.9
*u*2929	C(64)...H(75)	656.4(15)	24.6(fixed)	—	–0.7	24.6
*u*2853	H(68)...H(77)	656.4(28)	39.3(fixed)	—	–6.7	39.3
*u*2982	H(24)...H(40)	656.6(18)	31.1(fixed)	—	–5.9	31.1
*u*3001	H(37)...H(46)	656.6(29)	31.6(fixed)	—	–6.8	31.6
*u*2941	C(58)...H(84)	656.6(11)	26.4(fixed)	—	–0.2	26.4
*u*2985	H(70)...H(86)	656.6(24)	35.4(fixed)	—	1.2	35.4
*u*2871	C(58)...H(83)	656.7(11)	27.4(fixed)	—	0.2	27.4
*u*2932	C(64)...H(76)	656.8(9)	23.9(fixed)	—	–0.7	23.9
*u*2885	C(59)...H(82)	656.8(11)	27.1(fixed)	—	–0.1	27.1
*u*2911	C(7)...H(40)	656.9(10)	25.1(fixed)	—	0.1	25.1
*u*2852	H(25)...H(41)	657.0(18)	39.9(fixed)	—	–7.4	39.9
*u*2908	C(8)...H(32)	657.0(10)	28.5(fixed)	—	1.0	28.5
*u*1520	C(153)...H(167)	657.1(15)	34.9(fixed)	—	–2.9	34.9
*u*3025	Cl(15)...H(45)	657.5(11)	25.7(fixed)	—	–0.6	25.7
*u*2936	H(164)...H(171)	657.6(25)	40.4(fixed)	—	–9.5	40.4
*u*1053	H(118)...H(128)	657.6(31)	45.3(fixed)	—	2.9	45.3
*u*2900	C(60)...H(69)	657.7(10)	26.2(fixed)	—	–0.8	26.2
*u*2897	C(13)...H(22)	657.7(10)	27.7(fixed)	—	–0.2	27.7
*u*2945	C(7)...H(39)	657.7(13)	27.6(fixed)	—	–0.9	27.6
*u*2860	H(21)...H(42)	657.8(32)	31.8(fixed)	—	0.3	31.8
*u*2918	H(76)...H(81)	657.9(28)	33.2(fixed)	—	–6.9	33.2
*u*2636	Cl(155)...H(164)	657.9(10)	23.4(fixed)	—	–2.2	23.4
*u*3138	H(168)...H(175)	658.0(25)	33.3(fixed)	—	–8.8	33.3
*u*2914	C(54)...H(87)	658.1(9)	24.2(fixed)	—	–0.6	24.2
*u*3002	Cl(62)...H(78)	658.2(12)	26.7(fixed)	—	–0.3	26.7
*u*2880	H(27)...H(40)	658.3(29)	39.2(fixed)	—	–5.5	39.2
*u*2754	H(129)...H(131)	658.3(20)	37.4(fixed)	—	–2.7	37.4
*u*2989	H(85)...H(92)	658.8(31)	34.0(fixed)	—	–7.6	34.0
*u*2844	C(55)...H(88)	659.0(25)	21.9(fixed)	—	–5.3	21.9
*u*2987	H(161)...H(183)	659.1(25)	36.0(fixed)	—	1.7	36.0
*u*1602	Cl(108)...H(121)	659.1(10)	27.6(fixed)	—	–6.8	27.6
*u*2903	C(56)...H(94)	659.2(9)	26.3(fixed)	—	–0.5	26.3
*u*2859	H(72)...H(87)	659.3(38)	36.7(fixed)	—	–4.8	36.7
*u*2874	C(11)...H(36)	659.3(11)	24.3(fixed)	—	–0.6	24.3
*u*3019	H(67)...H(89)	659.7(27)	33.8(fixed)	—	1.2	33.8
*u*2960	H(80)...H(83)	659.8(18)	36.8(fixed)	—	3.6	36.8
*u*3005	H(24)...H(31)	659.8(22)	37.4(fixed)	—	4.1	37.4
*u*1834	C(111)...H(120)	659.9(11)	30.6(fixed)	—	3.5	30.6
*u*1867	C(158)...H(170)	660.0(9)	30.6(fixed)	—	3.4	30.6
*u*2886	C(10)...H(26)	660.0(9)	24.9(fixed)	—	–0.1	24.9
*u*2991	H(38)...H(45)	660.0(26)	32.1(fixed)	—	–6.7	32.1
*u*1484	Cl(156)...H(175)	660.5(12)	35.6(fixed)	—	–3.8	35.6
*u*2998	H(70)...H(77)	660.9(27)	31.5(fixed)	—	–6.7	31.5
*u*3010	H(75)...H(92)	660.9(27)	33.9(fixed)	—	1.8	33.9

*u*3000	H(35)...H(37)	661.1(21)	34.8(fixed)	—	2.3	34.8
*u*2686	Cl(108)...H(119)	662.0(12)	26.0(fixed)	—	–3.1	26.0
*u*3016	Cl(62)...H(79)	662.0(10)	25.7(fixed)	—	–0.4	25.7
*u*2997	Cl(61)...H(73)	662.4(21)	25.8(fixed)	—	–0.5	25.8
*u*2979	Cl(62)...H(90)	662.4(13)	18.7(fixed)	—	–5.3	18.7
*u*2567	Cl(155)...H(163)	662.5(10)	23.7(fixed)	—	–1.7	23.7
*u*2962	Cl(61)...H(74)	662.5(12)	19.5(fixed)	—	–5.6	19.5
*u*2983	H(20)...H(42)	662.8(26)	42.0(fixed)	—	6.3	42.0
*u*3008	Cl(15)...H(47)	662.9(12)	27.1(fixed)	—	–0.8	27.1
*u*1790	H(127)...H(130)	663.1(19)	39.6(fixed)	—	5.9	39.6
*u*1883	C(104)...H(122)	663.4(12)	36.9(fixed)	—	5.7	36.9
*u*3009	Cl(14)...H(28)	663.6(16)	27.8(fixed)	—	–0.6	27.8
*u*2869	H(168)...H(174)	663.7(27)	40.1(fixed)	—	–5.1	40.1
*u*2866	H(74)...H(79)	663.8(24)	29.4(fixed)	—	–2.8	29.4
*u*526	C(153)...H(165)	664.4(15)	31.7(fixed)	—	7.9	31.7
*u*3022	H(23)...H(39)	664.5(24)	36.7(fixed)	—	2.4	36.7
*u*2253	H(181)...H(186)	664.9(19)	43.0(fixed)	—	3.9	43.0
*u*2975	H(33)...H(36)	665.0(20)	36.8(fixed)	—	2.6	36.8
*u*2988	H(82)...H(84)	665.2(18)	37.2(fixed)	—	3.4	37.2
*u*2329	H(176)...H(181)	665.8(16)	34.9(fixed)	—	0.5	34.9
*u*3039	H(68)...H(76)	666.1(29)	26.2(fixed)	—	–5.9	26.2
*u*1160	H(165)...H(177)	666.3(18)	40.0(fixed)	—	2.7	40.0
*u*3015	Cl(14)...H(29)	667.7(17)	26.2(fixed)	—	–0.4	26.2
*u*2946	H(26)...H(32)	667.8(16)	37.0(fixed)	—	4.9	37.0
*u*2855	H(170)...H(175)	667.9(25)	32.4(fixed)	—	–5.0	32.4
*u*3030	Cl(61)...H(71)	667.9(13)	25.9(fixed)	—	–1.1	25.9
*u*2969	H(22)...H(40)	668.1(16)	35.6(fixed)	—	3.4	35.6
*u*2894	H(71)...H(88)	668.2(35)	30.0(fixed)	—	–3.9	30.0
*u*3021	H(67)...H(91)	668.7(24)	36.2(fixed)	—	0.3	36.2
*u*2990	H(69)...H(87)	669.1(17)	34.6(fixed)	—	1.5	34.6
*u*2963	H(25)...H(40)	669.3(24)	33.2(fixed)	—	–7.2	33.2
*u*3023	H(114)...H(138)	670.1(24)	36.9(fixed)	—	0.1	36.9
*u*3024	H(20)...H(44)	670.3(24)	45.4(fixed)	—	3.3	45.4
*u*1786	H(122)...H(126)	670.5(21)	47.0(fixed)	—	7.6	47.0
*u*1983	H(162)...H(168)	670.5(16)	44.7(fixed)	—	–10.1	44.7
*u*3017	H(161)...H(185)	671.1(24)	38.7(fixed)	—	0.7	38.7
*u*2049	H(113)...H(135)	672.1(18)	39.4(fixed)	—	–9.9	39.4
*u*2994	H(76)...H(94)	672.2(18)	34.3(fixed)	—	1.7	34.3
*u*3096	H(68)...H(75)	673.4(31)	23.3(fixed)	—	–6.7	23.3
*u*3027	H(69)...H(86)	673.7(16)	37.6(fixed)	—	0.0	37.6
*u*2545	H(176)...H(180)	673.9(16)	40.1(fixed)	—	0.6	40.1
*u*3036	H(19)...H(41)	674.1(14)	27.5(fixed)	—	–7.5	27.5
*u*3037	H(66)...H(88)	674.6(16)	27.5(fixed)	—	–6.9	27.5
*u*3075	H(160)...H(175)	674.7(18)	27.4(fixed)	—	–8.5	27.4
*u*2450	H(129)...H(130)	674.8(16)	33.0(fixed)	—	–0.2	33.0
*u*3031	H(22)...H(39)	675.2(15)	41.0(fixed)	—	0.7	41.0

*u*3073	H(25)...H(45)	675.5(29)	26.0(fixed)	—	–6.4	26.0
*u*2051	H(166)...H(182)	675.5(14)	36.7(fixed)	—	–8.4	36.7
*u*1926	H(113)...H(134)	675.5(20)	47.2(fixed)	—	–9.3	47.2
*u*3053	H(159)...H(175)	675.5(20)	26.6(fixed)	—	–7.3	26.6
*u*1868	H(167)...H(177)	675.8(19)	39.0(fixed)	—	–6.8	39.0
*u*3061	H(25)...H(46)	676.0(35)	26.4(fixed)	—	–8.0	26.4
*u*981	H(121)...H(134)	676.1(38)	47.9(fixed)	—	8.5	47.9
*u*3123	H(72)...H(93)	676.2(40)	31.8(fixed)	—	–7.6	31.8
*u*2525	H(122)...H(125)	676.2(15)	38.6(fixed)	—	1.7	38.6
*u*3014	H(82)...H(83)	676.4(16)	41.0(fixed)	—	1.6	41.0
*u*3020	H(35)...H(36)	677.6(16)	37.3(fixed)	—	1.0	37.3
*u*3042	H(25)...H(43)	677.8(19)	30.1(fixed)	—	–15.8	30.1
*u*3029	H(26)...H(31)	677.9(16)	41.5(fixed)	—	1.5	41.5
*u*3045	H(19)...H(40)	678.0(19)	26.2(fixed)	—	–6.1	26.2
*u*3066	H(18)...H(42)	678.6(24)	41.2(fixed)	—	–1.1	41.2
*u*3038	H(30)...H(38)	678.7(17)	28.6(fixed)	—	–11.2	28.6
*u*3121	H(112)...H(136)	679.3(24)	31.3(fixed)	—	–1.7	31.3
*u*3026	H(75)...H(94)	679.7(17)	36.8(fixed)	—	0.3	36.8
*u*3109	H(65)...H(89)	680.0(23)	31.8(fixed)	—	–1.9	31.8
*u*1979	H(115)...H(119)	680.1(18)	35.3(fixed)	—	–6.5	35.3
*u*3052	H(77)...H(85)	680.9(16)	27.4(fixed)	—	–7.6	27.4
*u*3083	H(26)...H(43)	681.1(15)	23.8(fixed)	—	–15.5	23.8
*u*3049	H(90)...H(93)	681.1(21)	26.0(fixed)	—	–7.1	26.0
*u*3088	H(159)...H(183)	681.3(22)	32.6(fixed)	—	–2.0	32.6
*u*3043	H(66)...H(87)	681.5(17)	26.5(fixed)	—	–6.1	26.5
*u*3055	H(65)...H(81)	681.6(19)	27.3(fixed)	—	–7.1	27.3
*u*3040	H(113)...H(128)	681.6(20)	26.5(fixed)	—	–6.6	26.5
*u*3085	H(43)...H(46)	682.7(20)	25.6(fixed)	—	–7.1	25.6
*u*3068	H(89)...H(93)	682.9(18)	25.7(fixed)	—	–6.3	25.7
*u*3089	H(114)...H(128)	683.1(24)	24.2(fixed)	—	–6.7	24.2
*u*3067	H(66)...H(81)	683.2(19)	27.9(fixed)	—	–8.4	27.9
*u*3101	H(80)...H(84)	683.3(13)	35.5(fixed)	—	–1.5	35.5
*u*3128	H(38)...H(43)	683.4(30)	34.9(fixed)	—	–15.7	34.9
*u*3102	H(44)...H(46)	683.5(28)	23.4(fixed)	—	–7.8	23.4
*u*3084	H(24)...H(32)	683.5(14)	38.0(fixed)	—	–1.1	38.0
*u*3103	H(33)...H(37)	683.8(13)	35.2(fixed)	—	–2.1	35.2
*u*3147	H(66)...H(74)	683.9(32)	30.8(fixed)	—	–7.5	30.8
*u*3064	H(18)...H(34)	683.9(17)	27.1(fixed)	—	–8.2	27.1
*u*3079	H(19)...H(34)	683.9(20)	27.6(fixed)	—	–9.7	27.6
*u*3117	H(161)...H(175)	684.6(21)	24.6(fixed)	—	–8.2	24.6
*u*3044	H(72)...H(85)	685.0(15)	27.7(fixed)	—	–9.1	27.7
*u*1803	H(162)...H(169)	685.1(17)	47.1(fixed)	—	–7.6	47.1
*u*3041	H(27)...H(38)	685.2(16)	26.1(fixed)	—	–6.5	26.1
*u*3069	H(77)...H(83)	685.3(13)	24.6(fixed)	—	–7.4	24.6
*u*3095	H(42)...H(46)	685.4(17)	25.3(fixed)	—	–7.0	25.3
*u*3063	H(30)...H(37)	685.5(19)	28.1(fixed)	—	–9.8	28.1

*u*3072	H(33)...H(41)	685.6(18)	26.7(fixed)	—	–7.5	26.7
*u*3218	H(127)...H(135)	685.6(20)	27.0(fixed)	—	–5.6	27.0
*u*3090	H(91)...H(93)	685.7(26)	23.8(fixed)	—	–7.0	23.8
*u*3065	H(70)...H(87)	685.8(14)	31.7(fixed)	—	–1.7	31.7
*u*3112	H(66)...H(86)	686.1(16)	23.7(fixed)	—	–7.1	23.7
*u*3059	H(112)...H(128)	686.1(22)	26.1(fixed)	—	–5.8	26.1
*u*1939	H(115)...H(118)	686.2(20)	36.4(fixed)	—	–6.5	36.4
*u*3082	H(30)...H(36)	686.2(15)	23.4(fixed)	—	–10.8	23.4
*u*3108	H(24)...H(43)	686.3(18)	28.7(fixed)	—	–14.0	28.7
*u*3054	H(34)...H(41)	686.5(15)	27.1(fixed)	—	–8.2	27.1
*u*3050	H(29)...H(38)	686.7(17)	25.5(fixed)	—	–5.5	25.5
*u*3104	H(76)...H(92)	686.8(13)	31.3(fixed)	—	–1.5	31.3
*u*3115	H(25)...H(47)	686.8(23)	22.8(fixed)	—	–7.8	22.8
*u*3258	H(128)...H(135)	687.0(15)	20.2(fixed)	—	–8.8	20.2
*u*3078	H(73)...H(85)	687.0(16)	24.4(fixed)	—	–8.5	24.4
*u*3080	H(27)...H(31)	687.0(13)	23.1(fixed)	—	–7.9	23.1
*u*3111	H(20)...H(34)	687.2(24)	23.3(fixed)	—	–9.2	23.3
*u*975	H(162)...H(170)	687.3(15)	44.9(fixed)	—	3.4	44.9
*u*2224	H(127)...H(131)	687.3(13)	41.4(fixed)	—	3.1	41.4
*u*1408	H(168)...H(177)	687.8(17)	49.5(fixed)	—	–2.4	49.5
*u*3086	H(80)...H(88)	687.9(18)	25.8(fixed)	—	–5.9	25.8
*u*3099	H(23)...H(40)	688.1(13)	33.0(fixed)	—	–1.2	33.0
*u*3126	H(166)...H(171)	688.1(14)	33.2(fixed)	—	–8.6	33.2
*u*3074	H(27)...H(30)	688.2(14)	26.2(fixed)	—	–8.2	26.2
*u*2095	H(123)...H(126)	688.4(13)	50.7(fixed)	—	3.3	50.7
*u*3118	H(19)...H(39)	688.6(16)	22.9(fixed)	—	–7.9	22.9
*u*2833	H(166)...H(173)	688.8(17)	31.7(fixed)	—	–1.9	31.7
*u*2843	H(121)...H(128)	688.8(21)	40.3(fixed)	—	–7.6	40.3
*u*3116	H(67)...H(81)	689.1(24)	24.5(fixed)	—	–8.1	24.5
*u*239	H(123)...H(134)	689.4(29)	41.7(fixed)	—	26.7	41.7
*u*3100	H(35)...H(41)	689.6(13)	23.2(fixed)	—	–8.3	23.2
*u*3134	H(27)...H(46)	689.6(38)	32.1(fixed)	—	–8.9	32.1
*u*3071	H(81)...H(88)	689.9(14)	26.8(fixed)	—	–6.9	26.8
*u*3106	H(77)...H(84)	690.1(17)	25.6(fixed)	—	–7.0	25.6
*u*2302	H(174)...H(181)	690.2(14)	32.9(fixed)	—	2.3	32.9
*u*3092	H(27)...H(32)	691.0(15)	25.4(fixed)	—	–7.1	25.4
*u*3122	H(68)...H(85)	691.1(17)	33.5(fixed)	—	–9.6	33.5
*u*3097	H(72)...H(78)	691.1(13)	24.0(fixed)	—	–6.6	24.0
*u*3153	H(166)...H(172)	692.1(12)	29.1(fixed)	—	–9.4	29.1
*u*3132	H(25)...H(34)	692.2(21)	31.0(fixed)	—	–9.9	31.0
*u*3235	H(129)...H(135)	692.2(13)	26.0(fixed)	—	–6.9	26.0
*u*3093	H(82)...H(88)	692.5(12)	24.1(fixed)	—	–6.5	24.1
*u*1075	H(168)...H(178)	693.2(16)	47.0(fixed)	—	3.6	47.0
*u*3107	H(71)...H(85)	693.3(22)	26.2(fixed)	—	–8.1	26.2
*u*3145	H(72)...H(94)	694.4(26)	26.5(fixed)	—	–7.7	26.5
*u*3137	H(19)...H(30)	694.4(21)	32.2(fixed)	—	–11.9	32.2

*u*3114	H(28)...H(38)	695.8(18)	22.7(fixed)	—	–6.7	22.7
*u*3256	H(175)...H(179)	696.2(19)	20.2(fixed)	—	–8.8	20.2
*u*3091	H(72)...H(77)	696.3(15)	26.7(fixed)	—	–6.9	26.7
*u*2017	H(160)...H(168)	696.8(22)	38.8(fixed)	—	–8.0	38.8
*u*3098	H(72)...H(79)	696.8(17)	25.5(fixed)	—	–6.0	25.5
*u*3136	H(160)...H(171)	696.9(15)	34.5(fixed)	—	–10.8	34.5
*u*2773	H(113)...H(119)	697.7(29)	38.1(fixed)	—	–6.0	38.1
*u*3130	H(85)...H(90)	698.0(27)	30.8(fixed)	—	–7.3	30.8
*u*3129	H(41)...H(46)	698.3(23)	33.7(fixed)	—	–8.5	33.7
*u*3124	H(66)...H(77)	698.4(22)	31.8(fixed)	—	–8.5	31.8
*u*1043	H(115)...H(120)	699.4(14)	30.7(fixed)	—	5.5	30.7
*u*3127	H(21)...H(38)	700.1(15)	31.3(fixed)	—	–7.7	31.3
*u*3131	H(113)...H(124)	700.4(14)	30.4(fixed)	—	–6.8	30.4
*u*3260	H(168)...H(171)	701.0(17)	20.3(fixed)	—	–9.3	20.3
*u*3149	H(36)...H(43)	701.6(21)	25.6(fixed)	—	–15.2	25.6
*u*3160	H(27)...H(47)	701.8(24)	25.9(fixed)	—	–8.9	25.9
*u*3143	H(69)...H(85)	702.1(14)	26.9(fixed)	—	–9.3	26.9
*u*3186	H(66)...H(75)	702.1(19)	25.5(fixed)	—	–7.8	25.5
*u*3081	H(119)...H(124)	703.1(17)	26.2(fixed)	—	–6.8	26.2
*u*3158	H(20)...H(30)	703.5(18)	25.4(fixed)	—	–11.4	25.4
*u*1115	H(113)...H(133)	703.6(16)	34.9(fixed)	—	9.4	34.9
*u*3139	H(21)...H(43)	704.6(18)	36.4(fixed)	—	–10.9	36.4
*u*3154	H(161)...H(171)	704.7(16)	28.1(fixed)	—	–10.5	28.1
*u*3152	H(67)...H(77)	706.2(19)	26.2(fixed)	—	–8.4	26.2
*u*3140	H(88)...H(93)	706.5(23)	32.2(fixed)	—	–7.8	32.2
*u*242	H(165)...H(178)	706.7(18)	38.0(fixed)	—	18.8	38.0
*u*3171	C(64)...H(74)	707.0(14)	16.3(fixed)	—	–4.5	16.3
*u*3239	H(176)...H(179)	707.4(17)	28.2(fixed)	—	–5.8	28.2
*u*3177	H(39)...H(46)	707.7(17)	26.8(fixed)	—	–9.0	26.8
*u*3164	H(21)...H(44)	708.0(17)	31.1(fixed)	—	–12.4	31.1
*u*3146	H(22)...H(38)	708.2(11)	26.0(fixed)	—	–7.6	26.0
*u*3162	H(26)...H(34)	708.7(16)	24.9(fixed)	—	–10.0	24.9
*u*3148	H(68)...H(90)	709.0(19)	30.8(fixed)	—	–7.1	30.8
*u*3155	H(114)...H(124)	709.3(15)	25.8(fixed)	—	–7.0	25.8
*u*2799	C(104)...H(121)	709.3(6)	23.9(fixed)	—	–7.8	23.9
*u*3150	H(27)...H(41)	709.8(22)	32.7(fixed)	—	–9.2	32.7
*u*3190	C(56)...H(93)	709.9(12)	16.3(fixed)	—	–5.1	16.3
*u*3184	C(6)...H(43)	710.0(13)	18.1(fixed)	—	–9.7	18.1
*u*3230	H(168)...H(172)	711.1(14)	29.0(fixed)	—	–5.0	29.0
*u*3110	H(119)...H(125)	711.4(12)	23.8(fixed)	—	–6.5	23.8
*u*1406	H(160)...H(169)	711.6(15)	48.0(fixed)	—	–2.6	48.0
*u*2790	C(158)...H(168)	711.8(9)	20.4(fixed)	—	–5.8	20.4
*u*3159	H(83)...H(90)	712.2(19)	26.6(fixed)	—	–7.7	26.6
*u*3167	C(7)...H(41)	712.4(7)	16.7(fixed)	—	–5.8	16.7
*u*3166	C(54)...H(88)	712.6(8)	16.4(fixed)	—	–4.8	16.4
*u*3161	H(68)...H(91)	713.4(17)	25.7(fixed)	—	–7.1	25.7

*u*2776	C(111)...H(119)	713.4(9)	22.4(fixed)	—	–5.1	22.4
*u*3175	C(58)...H(85)	713.4(9)	16.5(fixed)	—	–5.9	16.5
*u*3179	C(157)...H(160)	713.5(12)	16.5(fixed)	—	–5.3	16.5
*u*3176	H(86)...H(93)	714.0(15)	26.4(fixed)	—	–8.1	26.4
*u*3142	H(72)...H(88)	714.4(28)	29.7(fixed)	—	–7.5	29.7
*u*3191	C(110)...H(113)	714.6(13)	16.5(fixed)	—	–4.8	16.5
*u*3144	H(74)...H(77)	714.8(19)	29.8(fixed)	—	–7.3	29.8
*u*3195	C(13)...H(21)	714.9(6)	16.7(fixed)	—	–6.0	16.7
*u*3192	C(16)...H(19)	715.0(13)	15.8(fixed)	—	–5.4	15.8
*u*3181	C(53)...H(90)	715.1(13)	16.5(fixed)	—	–4.5	16.5
*u*1585	C(153)...H(166)	715.2(14)	31.5(fixed)	—	–3.6	31.5
*u*3172	C(10)...H(25)	715.2(8)	16.4(fixed)	—	–5.3	16.4
*u*3185	C(63)...H(66)	715.2(13)	16.3(fixed)	—	–5.0	16.3
*u*3170	C(11)...H(38)	715.2(8)	16.4(fixed)	—	–4.7	16.4
*u*3196	C(8)...H(30)	715.6(7)	16.8(fixed)	—	–7.2	16.8
*u*2656	C(107)...H(115)	715.6(6)	25.3(fixed)	—	–3.0	25.3
*u*2092	H(122)...H(128)	715.7(14)	38.3(fixed)	—	5.0	38.3
*u*3193	H(28)...H(41)	715.8(17)	26.0(fixed)	—	–9.5	26.0
*u*3182	C(60)...H(68)	716.0(6)	16.2(fixed)	—	–4.9	16.2
*u*3180	C(12)...H(34)	716.1(7)	16.7(fixed)	—	–6.4	16.7
*u*3189	C(59)...H(81)	716.5(7)	16.4(fixed)	—	–5.6	16.4
*u*3165	H(74)...H(78)	717.4(14)	25.7(fixed)	—	–7.5	25.7
*u*2652	C(106)...H(128)	718.1(7)	24.6(fixed)	—	–3.0	24.6
*u*2489	C(154)...H(175)	718.3(6)	23.2(fixed)	—	–1.9	23.2
*u*2063	H(113)...H(120)	719.9(20)	37.0(fixed)	—	2.2	37.0
*u*3199	Cl(15)...H(46)	721.2(11)	15.9(fixed)	—	–5.6	15.9
*u*3163	H(73)...H(88)	722.0(20)	25.1(fixed)	—	–7.3	25.1
*u*3197	Cl(14)...H(27)	723.4(12)	16.7(fixed)	—	–5.9	16.7
*u*3212	H(74)...H(92)	725.1(25)	26.3(fixed)	—	–3.4	26.3
*u*3198	Cl(61)...H(72)	725.9(13)	16.5(fixed)	—	–5.1	16.5
*u*3201	Cl(62)...H(77)	726.2(9)	16.4(fixed)	—	–5.5	16.4
*u*3208	H(18)...H(43)	727.4(17)	27.7(fixed)	—	–8.9	27.7
*u*3202	H(70)...H(88)	728.0(18)	27.2(fixed)	—	–4.1	27.2
*u*3060	H(174)...H(182)	728.5(21)	26.6(fixed)	—	–5.9	26.6
*u*2570	Cl(156)...H(171)	729.4(9)	24.5(fixed)	—	–1.7	24.5
*u*2764	H(123)...H(124)	731.3(13)	46.2(fixed)	—	–4.8	46.2
*u*3217	H(23)...H(41)	731.6(14)	26.5(fixed)	—	–4.4	26.5
*u*2779	H(121)...H(126)	732.1(15)	32.4(fixed)	—	–6.8	32.4
*u*3203	H(65)...H(90)	732.3(19)	27.6(fixed)	—	–3.6	27.6
*u*3216	H(80)...H(85)	732.4(17)	27.5(fixed)	—	–4.8	27.5
*u*2822	H(127)...H(132)	733.1(19)	30.3(fixed)	—	–3.5	30.3
*u*3207	H(160)...H(183)	733.2(16)	27.3(fixed)	—	–4.4	27.3
*u*3222	H(113)...H(136)	735.5(16)	26.3(fixed)	—	–3.9	26.3
*u*3227	H(24)...H(30)	735.5(16)	26.6(fixed)	—	–6.7	26.6
*u*3220	H(34)...H(37)	735.9(16)	26.5(fixed)	—	–6.1	26.5
*u*3215	H(76)...H(93)	736.3(13)	25.8(fixed)	—	–4.4	25.8

*u*3224	H(66)...H(89)	736.6(17)	25.6(fixed)	—	–4.5	25.6
*u*3213	H(33)...H(38)	737.2(17)	28.1(fixed)	—	–3.2	28.1
*u*3205	H(21)...H(40)	737.3(15)	26.2(fixed)	—	–4.3	26.2
*u*2849	H(128)...H(131)	737.4(15)	38.0(fixed)	—	–4.8	38.0
*u*3156	H(121)...H(125)	737.9(11)	26.1(fixed)	—	–9.6	26.1
*u*3244	H(20)...H(43)	738.1(18)	25.4(fixed)	—	–11.2	25.4
*u*3219	H(19)...H(42)	739.8(17)	29.6(fixed)	—	–1.7	29.6
*u*3204	H(25)...H(32)	739.8(13)	27.7(fixed)	—	–2.9	27.7
*u*3223	H(81)...H(84)	740.5(13)	27.3(fixed)	—	–4.4	27.3
*u*3214	H(68)...H(87)	740.9(12)	25.8(fixed)	—	–4.0	25.8
*u*3237	H(66)...H(91)	742.0(19)	25.4(fixed)	—	–5.4	25.4
*u*3242	H(19)...H(44)	742.2(19)	30.0(fixed)	—	–4.1	30.0
*u*3241	H(25)...H(31)	742.3(13)	28.0(fixed)	—	–5.2	28.0
*u*3245	H(114)...H(137)	742.3(18)	26.1(fixed)	—	–5.4	26.1
*u*3151	H(129)...H(132)	742.4(11)	25.4(fixed)	—	–7.1	25.4
*u*3094	H(176)...H(182)	743.4(10)	24.3(fixed)	—	–7.2	24.3
*u*3233	H(82)...H(85)	743.5(11)	27.2(fixed)	—	–6.2	27.2
*u*3243	H(161)...H(184)	743.6(18)	26.9(fixed)	—	–5.6	26.9
*u*3250	H(75)...H(93)	743.7(14)	25.1(fixed)	—	–5.8	25.1
*u*3240	H(35)...H(38)	744.4(12)	26.2(fixed)	—	–4.6	26.2
*u*3228	H(22)...H(41)	744.4(11)	26.8(fixed)	—	–6.0	26.8
*u*1835	H(166)...H(177)	744.5(15)	44.7(fixed)	—	–6.0	44.7
*u*3236	H(74)...H(94)	744.5(10)	26.5(fixed)	—	–5.0	26.5
*u*3246	H(67)...H(90)	744.8(18)	26.1(fixed)	—	–4.9	26.1
*u*3247	H(68)...H(86)	745.1(13)	26.2(fixed)	—	–5.4	26.2
*u*3234	H(69)...H(88)	745.6(11)	26.3(fixed)	—	–5.3	26.3
*u*3229	H(81)...H(83)	745.7(10)	27.5(fixed)	—	–5.6	27.5
*u*1101	H(166)...H(178)	745.7(17)	41.2(fixed)	—	5.3	41.2
*u*2055	H(170)...H(187)	746.3(12)	35.9(fixed)	—	4.7	35.9
*u*3251	H(21)...H(39)	746.3(12)	26.7(fixed)	—	–6.9	26.7
*u*3238	H(26)...H(30)	746.9(10)	24.4(fixed)	—	–7.7	24.4
*u*3231	H(34)...H(36)	747.6(11)	24.0(fixed)	—	–7.0	24.0
*u*2637	H(169)...H(187)	747.8(13)	41.5(fixed)	—	–2.2	41.5
*u*2234	H(128)...H(130)	753.7(11)	35.9(fixed)	—	2.6	35.9
*u*2286	H(122)...H(124)	757.1(11)	40.3(fixed)	—	5.6	40.3
*u*3255	H(74)...H(93)	779.4(20)	20.1(fixed)	—	–7.8	20.1
*u*3141	H(121)...H(124)	785.1(9)	31.8(fixed)	—	–9.8	31.8
*u*2058	H(166)...H(179)	785.3(16)	40.0(fixed)	—	–8.3	40.0
*u*3253	H(21)...H(41)	787.5(9)	19.6(fixed)	—	–9.6	19.6
*u*3265	H(19)...H(43)	788.9(13)	19.0(fixed)	—	–12.2	19.0
*u*3254	H(68)...H(88)	789.2(10)	20.0(fixed)	—	–7.9	20.0
*u*3047	H(175)...H(182)	789.4(10)	27.5(fixed)	—	–7.2	27.5
*u*3264	H(160)...H(184)	789.7(13)	20.1(fixed)	—	–8.6	20.1
*u*3261	H(81)...H(85)	789.8(11)	20.0(fixed)	—	–9.4	20.0
*u*3259	H(25)...H(30)	790.1(10)	19.0(fixed)	—	–10.0	19.0
*u*3257	H(34)...H(38)	790.5(11)	19.0(fixed)	—	–8.9	19.0

*u*3125	H(128)...H(132)	790.9(11)	30.2(fixed)	—	–7.2	30.2
*u*3262	H(113)...H(137)	791.9(13)	20.0(fixed)	—	–7.7	20.0
*u*3263	H(66)...H(90)	792.9(13)	19.9(fixed)	—	–7.7	19.9

Table S13. Interatomic distances (r_a / pm), refined and calculated amplitudes of vibration (u_{hl} / pm) and perpendicular corrections (k_{hl} / pm) for the SARACEN-restrained GED structure of **3**

	Atom Pair	r_a	u_{hl} (GED)	Restraint	k_{hl}	u_{hl} (Calc.)
*u*38	C(16)–H(42)	107.9(4)	8.9(tied to *u*88)	—	0.4	7.8
*u*18	C(16)–H(44)	107.9(4)	8.9(tied to *u*88)	—	0.4	7.8
*u*86	C(16)–H(43)	107.9(4)	8.8(tied to *u*88)	—	0.4	7.8
*u*24	C(10)–H(32)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*15	C(10)–H(31)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*26	C(101)–H(117)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*34	C(13)–H(39)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*19	C(53)–H(67)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*12	C(9)–H(29)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*7	C(106)–H(130)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*4	C(17)–H(47)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*11	C(103)–H(123)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*6	C(102)–H(120)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*9	C(12)–H(36)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*8	C(150)–H(170)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*10	C(13)–H(40)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*88	C(10)–H(30)	107.9(4)	8.7(4)	—	0.4	7.7
*u*67	C(9)–H(27)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*70	C(13)–H(41)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*65	C(103)–H(121)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*68	C(56)–H(74)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*71	C(59)–H(85)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*72	C(150)–H(168)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*64	C(8)–H(25)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*2	C(59)–H(83)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*5	C(8)–H(26)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*1	C(55)–H(73)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*3	C(149)–H(167)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*69	C(60)–H(88)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*60	C(102)–H(118)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*59	C(12)–H(37)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*53	C(8)–H(24)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*33	C(11)–H(33)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*66	C(149)–H(166)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*55	C(63)–H(89)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*62	C(12)–H(38)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*45	C(7)–H(23)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*56	C(59)–H(84)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*61	C(102)–H(119)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*58	C(149)–H(165)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*57	C(55)–H(71)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*63	C(55)–H(72)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7

*u*49	C(147)–H(159)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*89	C(57)–H(77)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*75	C(11)–H(34)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*35	C(64)–H(92)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*39	C(100)–H(114)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*44	C(54)–H(70)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*42	C(17)–H(45)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*22	C(11)–H(35)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*51	C(60)–H(86)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*52	C(103)–H(122)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*54	C(56)–H(75)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*46	C(53)–H(65)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*48	C(100)–H(112)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*47	C(148)–H(164)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*43	C(54)–H(69)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.7
*u*80	C(58)–H(81)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*81	C(152)–H(175)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*74	C(7)–H(21)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*84	C(64)–H(93)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*83	C(53)–H(66)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*90	C(101)–H(115)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*78	C(6)–H(19)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*85	C(147)–H(160)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*82	C(17)–H(46)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*87	C(105)–H(128)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*41	C(9)–H(28)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*40	C(152)–H(176)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*32	C(6)–H(18)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*30	C(63)–H(91)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*21	C(58)–H(82)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*31	C(105)–H(127)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*25	C(148)–H(163)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*28	C(57)–H(79)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*29	C(58)–H(80)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*50	C(154)–H(180)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*37	C(6)–H(20)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*36	C(7)–H(22)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*27	C(152)–H(174)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*73	C(63)–H(90)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*79	C(54)–H(68)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*76	C(100)–H(113)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*77	C(148)–H(162)	107.9(4)	8.7(tied to *u*88)	—	0.4	7.7
*u*17	C(64)–H(94)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*23	C(101)–H(116)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*20	C(56)–H(76)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*13	C(57)–H(78)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6

*u*14	C(147)–H(161)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*16	C(60)–H(87)	107.9(4)	8.6(tied to *u*88)	—	0.4	7.6
*u*96	H(42)...H(44)	171.4(16)	12.9(fixed)	—	–0.4	12.9
*u*99	H(31)...H(32)	171.5(16)	12.7(fixed)	—	–0.3	12.7
*u*150	H(33)...H(35)	171.6(16)	12.6(fixed)	—	–0.3	12.6
*u*157	H(22)...H(23)	171.6(16)	12.7(fixed)	—	–0.3	12.7
*u*168	H(45)...H(47)	171.6(16)	12.6(fixed)	—	–0.2	12.6
*u*171	H(18)...H(20)	171.6(16)	12.6(fixed)	—	–0.2	12.6
*u*148	H(174)...H(176)	171.7(16)	12.6(fixed)	—	–0.2	12.6
*u*167	H(159)...H(161)	171.7(16)	12.6(fixed)	—	–0.2	12.6
*u*103	H(116)...H(117)	171.7(16)	12.7(fixed)	—	–0.2	12.7
*u*177	H(163)...H(164)	171.7(16)	12.6(fixed)	—	–0.2	12.6
*u*162	H(127)...H(129)	171.7(16)	12.6(fixed)	—	–0.2	12.6
*u*175	H(112)...H(114)	171.7(16)	12.6(fixed)	—	–0.2	12.6
*u*144	H(80)...H(82)	171.8(16)	12.6(fixed)	—	–0.2	12.6
*u*105	H(78)...H(79)	171.8(16)	12.7(fixed)	—	–0.2	12.7
*u*164	H(92)...H(94)	171.8(16)	12.6(fixed)	—	–0.2	12.6
*u*153	H(89)...H(91)	171.8(16)	12.6(fixed)	—	–0.2	12.6
*u*176	H(69)...H(70)	171.9(16)	12.6(fixed)	—	–0.2	12.6
*u*179	H(65)...H(67)	171.9(16)	12.6(fixed)	—	–0.2	12.6
*u*127	H(83)...H(84)	173.3(16)	12.7(fixed)	—	–0.2	12.7
*u*169	H(71)...H(73)	173.3(16)	12.6(fixed)	—	–0.2	12.6
*u*165	H(86)...H(87)	173.3(16)	12.6(fixed)	—	–0.2	12.6
*u*174	H(75)...H(76)	173.3(16)	12.6(fixed)	—	–0.2	12.6
*u*166	H(118)...H(120)	173.3(16)	12.6(fixed)	—	–0.2	12.6
*u*161	H(122)...H(123)	173.3(16)	12.6(fixed)	—	–0.2	12.6
*u*129	H(169)...H(170)	173.5(16)	12.7(fixed)	—	–0.2	12.7
*u*170	H(165)...H(167)	173.6(16)	12.6(fixed)	—	–0.2	12.6
*u*173	H(28)...H(29)	173.6(16)	12.6(fixed)	—	–0.2	12.6
*u*178	H(39)...H(40)	173.6(16)	12.7(fixed)	—	–0.2	12.7
*u*160	H(24)...H(26)	173.6(16)	12.6(fixed)	—	–0.2	12.6
*u*180	H(36)...H(37)	173.6(16)	12.6(fixed)	—	–0.2	12.6
*u*124	H(42)...H(43)	173.9(8)	12.9(fixed)	—	–0.4	12.9
*u*133	H(43)...H(44)	173.9(8)	12.9(fixed)	—	–0.4	12.9
*u*122	H(30)...H(32)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*95	H(127)...H(128)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*119	H(115)...H(117)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*132	H(128)...H(129)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*140	H(30)...H(31)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*139	H(115)...H(116)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*114	H(113)...H(114)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*94	H(33)...H(34)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*107	H(112)...H(113)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*131	H(118)...H(119)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*102	H(34)...H(35)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*138	H(119)...H(120)	174.1(8)	12.7(fixed)	—	–0.2	12.7

*u*91	H(21)...H(23)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*108	H(21)...H(22)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*123	H(121)...H(123)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*116	H(81)...H(82)	174.1(8)	12.7(fixed)	—	–0.3	12.7
*u*156	H(121)...H(122)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*101	H(80)...H(81)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*112	H(68)...H(69)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*92	H(89)...H(90)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*97	H(92)...H(93)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*111	H(65)...H(66)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*126	H(77)...H(79)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*134	H(66)...H(67)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*104	H(45)...H(46)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*93	H(159)...H(160)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*109	H(90)...H(91)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*121	H(40)...H(41)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*113	H(18)...H(19)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*106	H(68)...H(70)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*128	H(93)...H(94)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*159	H(84)...H(85)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*115	H(19)...H(20)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*110	H(175)...H(176)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*145	H(71)...H(72)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*147	H(24)...H(25)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*98	H(174)...H(175)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*146	H(77)...H(78)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*152	H(86)...H(88)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*120	H(27)...H(29)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*149	H(168)...H(170)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*154	H(83)...H(85)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*117	H(87)...H(88)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*130	H(25)...H(26)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*142	H(72)...H(73)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*141	H(46)...H(47)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*136	H(160)...H(161)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*118	H(162)...H(164)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*158	H(27)...H(28)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*125	H(162)...H(163)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*100	H(74)...H(76)	174.1(8)	12.7(fixed)	—	–0.2	12.7
*u*135	H(36)...H(38)	174.2(8)	12.7(fixed)	—	–0.2	12.7
*u*163	H(39)...H(41)	174.2(8)	12.7(fixed)	—	–0.2	12.7
*u*151	H(37)...H(38)	174.2(8)	12.7(fixed)	—	–0.2	12.7
*u*143	H(165)...H(166)	174.2(8)	12.7(fixed)	—	–0.2	12.7
*u*172	H(168)...H(169)	174.2(8)	12.7(fixed)	—	–0.2	12.7
*u*155	H(74)...H(75)	174.2(8)	12.7(fixed)	—	–0.2	12.7
*u*137	H(166)...H(167)	174.2(8)	12.7(fixed)	—	–0.2	12.7

*u*183	Si(2)–C(13)	187.5(2)	5.9(tied to *u*189)	—	0.2	5.9
*u*191	Si(96)–C(106)	187.5(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*192	Si(50)–C(56)	187.5(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*190	Si(49)–C(60)	187.5(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*186	Si(50)–C(55)	187.5(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*188	Si(143)–C(153)	187.5(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*187	Si(96)–C(107)	187.5(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*189	Si(3)–C(8)	187.5(2)	6.0(2)	—	0.2	5.9
*u*185	Si(3)–C(9)	187.5(2)	5.9(tied to *u*189)	—	0.2	5.9
*u*182	Si(49)–C(59)	187.5(2)	5.9(tied to *u*189)	—	0.2	5.9
*u*184	Si(2)–C(12)	187.5(2)	5.9(tied to *u*189)	—	0.2	5.9
*u*181	Si(143)–C(154)	187.5(2)	5.9(tied to *u*189)	—	0.2	5.9
*u*205	Si(145)–C(157)	188.7(2)	6.0(tied to *u*189)	—	0.2	6.0
*u*193	Si(52)–C(53)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*210	Si(5)–C(7)	188.7(2)	6.1(tied to *u*189)	—	0.2	6.0
*u*209	Si(51)–C(63)	188.7(2)	6.1(tied to *u*189)	—	0.2	6.0
*u*208	Si(145)–C(152)	188.7(2)	6.1(tied to *u*189)	—	0.2	6.0
*u*207	Si(4)–C(11)	188.7(2)	6.0(tied to *u*189)	—	0.2	6.0
*u*206	Si(51)–C(58)	188.7(2)	6.0(tied to *u*189)	—	0.2	6.0
*u*203	Si(52)–C(54)	188.7(2)	6.0(tied to *u*189)	—	0.2	6.0
*u*202	Si(52)–C(64)	188.7(2)	6.0(tied to *u*189)	—	0.2	6.0
*u*200	Si(4)–C(16)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*204	Si(98)–C(110)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*201	Si(98)–C(104)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*197	Si(5)–C(17)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*195	Si(4)–C(10)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*199	Si(5)–C(6)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*198	Si(98)–C(105)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*196	Si(145)–C(151)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*194	Si(51)–C(57)	188.7(2)	6.0(tied to *u*189)	—	0.2	5.9
*u*216	C(1)–Si(2)	189.6(13)	6.5(tied to *u*189)	—	0.2	6.5
*u*212	C(1)–Si(3)	189.6(13)	6.5(tied to *u*189)	—	0.3	6.5
*u*213	C(48)–Si(49)	189.6(13)	6.5(tied to *u*189)	—	0.3	6.4
*u*211	C(142)–Si(143)	189.6(13)	6.5(tied to *u*189)	—	0.3	6.4
*u*215	C(95)–Si(96)	189.6(13)	6.6(tied to *u*189)	—	0.3	6.5
*u*214	C(48)–Si(50)	189.6(13)	6.6(tied to *u*189)	—	0.3	6.5
*u*222	C(48)–Si(52)	195.1(13)	6.9(tied to *u*189)	—	0.3	6.9
*u*220	C(95)–Si(98)	195.1(13)	6.8(tied to *u*189)	—	0.3	6.8
*u*218	C(1)–Si(4)	195.1(13)	6.8(tied to *u*189)	—	0.3	6.7
*u*217	C(48)–Si(51)	195.1(13)	6.8(tied to *u*189)	—	0.3	6.7
*u*221	C(1)–Si(5)	195.1(13)	6.9(tied to *u*189)	—	0.3	6.8
*u*219	C(142)–Si(145)	195.1(13)	6.8(tied to *u*189)	—	0.3	6.8
*u*225	H(174)...H(186)	196.5(140)	34.6(fixed)	—	18.0	34.6
*u*261	H(70)...H(73)	212.0(96)	43.0(fixed)	—	10.3	43.0
*u*309	H(116)...H(127)	218.7(88)	47.8(fixed)	—	14.2	47.8
*u*269	H(65)...H(83)	219.6(82)	44.3(fixed)	—	13.0	44.3

*u*258	H(112)...H(130)	221.7(72)	44.6(fixed)	—	11.4	44.6
*u*265	H(31)...H(45)	222.9(65)	53.2(fixed)	—	21.3	53.2
*u*224	H(80)...H(92)	224.0(145)	36.6(fixed)	—	22.3	36.6
*u*242	H(170)...H(181)	224.4(114)	42.0(fixed)	—	20.7	42.0
*u*310	H(18)...H(36)	225.0(77)	46.0(fixed)	—	9.2	46.0
*u*251	H(164)...H(167)	226.0(60)	40.3(fixed)	—	10.7	40.3
*u*243	H(71)...H(82)	226.0(64)	41.1(fixed)	—	14.6	41.1
*u*244	H(69)...H(73)	226.1(100)	43.5(fixed)	—	12.1	43.5
*u*236	Si(50)–Br(62)	226.8(2)	7.1(tied to *u*239)	—	0.3	6.8
*u*234	Si(96)–Br(108)	226.8(2)	7.0(tied to *u*239)	—	0.3	6.7
*u*249	H(87)...H(91)	227.0(62)	39.6(fixed)	—	10.2	39.6
*u*235	Si(49)–Br(61)	227.8(2)	7.0(tied to *u*239)	—	0.3	6.7
*u*239	Si(3)–Br(15)	227.8(2)	7.2(2)	—	0.3	6.9
*u*240	Si(2)–Br(14)	227.8(2)	7.2(tied to *u*239)	—	0.3	6.9
*u*238	Si(143)–Br(155)	227.8(2)	7.1(tied to *u*239)	—	0.3	6.8
*u*227	H(23)...H(24)	228.8(99)	38.3(fixed)	—	21.1	38.3
*u*245	H(29)...H(35)	231.1(73)	47.5(fixed)	—	16.9	47.5
*u*264	H(75)...H(89)	231.4(71)	40.8(fixed)	—	9.5	40.8
*u*259	H(22)...H(33)	232.6(59)	50.7(fixed)	—	14.4	50.7
*u*228	H(126)...H(134)	233.2(88)	37.8(fixed)	—	19.6	37.8
*u*230	H(159)...H(178)	233.4(81)	36.9(fixed)	—	16.9	36.9
*u*287	H(78)...H(92)	233.4(68)	44.5(fixed)	—	11.1	44.5
*u*257	H(20)...H(24)	234.8(82)	44.8(fixed)	—	12.8	44.8
*u*253	H(26)...H(37)	235.1(96)	42.3(fixed)	—	12.2	42.3
*u*248	H(78)...H(94)	235.7(84)	46.3(fixed)	—	13.0	46.3
*u*263	H(114)...H(123)	236.1(88)	42.5(fixed)	—	11.9	42.5
*u*250	H(67)...H(83)	239.4(85)	45.2(fixed)	—	14.7	45.2
*u*262	H(40)...H(44)	240.4(84)	53.6(fixed)	—	28.8	53.6
*u*271	H(28)...H(35)	240.4(58)	50.5(fixed)	—	16.7	50.5
*u*246	H(163)...H(167)	241.5(46)	42.8(fixed)	—	11.6	42.8
*u*241	H(118)...H(131)	241.7(131)	36.9(fixed)	—	16.8	36.9
*u*285	Si(49)...H(85)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*278	Si(50)...H(72)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*298	Si(96)...H(132)	241.8(5)	13.2(fixed)	—	–0.4	13.2
*u*288	Si(49)...H(88)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*282	Si(143)...H(182)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*281	Si(3)...H(27)	241.8(5)	13.2(fixed)	—	–0.4	13.2
*u*291	Si(50)...H(74)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*280	Si(143)...H(179)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*299	Si(97)...H(121)	241.8(5)	13.1(fixed)	—	–0.4	13.1
*u*273	Si(2)...H(41)	241.8(5)	13.2(fixed)	—	–0.4	13.2
*u*290	Si(3)...H(25)	241.8(5)	13.2(fixed)	—	–0.4	13.2
*u*286	Si(2)...H(38)	241.9(5)	13.1(fixed)	—	–0.4	13.1
*u*255	H(31)...H(47)	241.9(71)	55.0(fixed)	—	23.5	55.0
*u*267	H(23)...H(28)	242.1(82)	48.1(fixed)	—	12.7	48.1
*u*283	Si(145)...H(184)	242.9(5)	13.4(fixed)	—	–0.4	13.4

*u*297	Si(52)...H(68)	242.9(5)	13.5(fixed)	—	–0.4	13.5
*u*279	Si(52)...H(66)	242.9(5)	13.3(fixed)	—	–0.4	13.3
*u*294	Si(51)...H(77)	242.9(5)	13.3(fixed)	—	–0.4	13.3
*u*293	Si(145)...H(171)	242.9(5)	13.3(fixed)	—	–0.4	13.3
*u*306	Si(98)...H(137)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*292	Si(145)...H(175)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*308	Si(51)...H(90)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*274	Si(52)...H(93)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*303	Si(51)...H(81)	242.9(5)	13.5(fixed)	—	–0.4	13.5
*u*289	Si(98)...H(124)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*277	Si(98)...H(128)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*304	Si(5)...H(19)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*275	Si(5)...H(46)	242.9(5)	13.4(fixed)	—	–0.4	13.4
*u*301	Si(5)...H(21)	243.0(5)	13.6(fixed)	—	–0.4	13.6
*u*300	Si(4)...H(34)	243.0(5)	13.6(fixed)	—	–0.3	13.6
*u*296	Si(4)...H(30)	243.0(5)	13.5(fixed)	—	–0.3	13.5
*u*305	Si(4)...H(43)	243.0(5)	13.7(fixed)	—	–0.3	13.7
*u*276	H(163)...H(176)	243.7(61)	46.5(fixed)	—	10.2	46.5
*u*314	H(69)...H(80)	243.8(106)	48.0(fixed)	—	10.7	48.0
*u*295	H(159)...H(180)	244.6(79)	44.1(fixed)	—	13.2	44.1
*u*232	H(79)...H(87)	244.9(62)	36.3(fixed)	—	16.6	36.3
*u*226	H(33)...H(45)	246.3(120)	40.9(fixed)	—	25.8	40.9
*u*315	H(114)...H(122)	246.6(59)	46.2(fixed)	—	12.5	46.2
*u*318	Si(2)...H(39)	247.7(5)	13.3(fixed)	—	–0.4	13.3
*u*321	Si(3)...H(28)	247.7(5)	13.4(fixed)	—	–0.4	13.4
*u*320	Si(2)...H(37)	247.8(5)	13.2(fixed)	—	–0.4	13.2
*u*326	Si(3)...H(24)	247.8(5)	13.3(fixed)	—	–0.4	13.3
*u*319	Si(143)...H(180)	247.8(5)	13.3(fixed)	—	–0.4	13.3
*u*327	Si(143)...H(178)	247.9(5)	13.2(fixed)	—	–0.4	13.2
*u*270	H(20)...H(36)	247.9(62)	45.4(fixed)	—	10.8	45.4
*u*307	H(116)...H(129)	248.0(72)	52.5(fixed)	—	15.5	52.5
*u*331	Si(96)...H(131)	248.2(5)	13.5(fixed)	—	–0.4	13.5
*u*237	H(76)...H(84)	248.2(62)	37.9(fixed)	—	17.1	37.9
*u*323	Si(96)...H(133)	248.2(5)	13.2(fixed)	—	–0.4	13.2
*u*322	Si(50)...H(71)	248.3(5)	13.2(fixed)	—	–0.4	13.2
*u*328	Si(49)...H(86)	248.3(5)	13.2(fixed)	—	–0.3	13.2
*u*325	Si(49)...H(84)	248.3(5)	13.1(fixed)	—	–0.4	13.1
*u*329	Si(50)...H(75)	248.3(5)	13.0(fixed)	—	–0.3	13.0
*u*247	H(118)...H(133)	248.4(83)	40.9(fixed)	—	11.4	40.9
*u*223	H(127)...H(139)	248.5(157)	37.0(fixed)	—	23.8	37.0
*u*229	H(32)...H(40)	248.7(77)	45.0(fixed)	—	30.2	45.0
*u*272	H(39)...H(44)	249.4(54)	58.4(fixed)	—	31.8	58.4
*u*335	Si(50)...H(73)	249.9(5)	13.1(fixed)	—	–0.4	13.1
*u*330	Si(49)...H(83)	249.9(5)	13.0(fixed)	—	–0.4	13.0
*u*341	Si(49)...H(87)	249.9(5)	12.9(fixed)	—	–0.4	12.9
*u*256	H(22)...H(28)	249.9(76)	49.4(fixed)	—	14.4	49.4

*u*353	Si(50)...H(76)	250.0(5)	12.8(fixed)	—	–0.4	12.8
*u*334	Si(3)...H(29)	250.0(5)	13.1(fixed)	—	–0.4	13.1
*u*338	Si(96)...H(130)	250.0(5)	13.1(fixed)	—	–0.4	13.1
*u*339	Si(143)...H(177)	250.0(5)	12.9(fixed)	—	–0.4	12.9
*u*340	Si(2)...H(40)	250.0(5)	13.0(fixed)	—	–0.4	13.0
*u*346	Si(143)...H(181)	250.0(5)	13.0(fixed)	—	–0.4	13.0
*u*337	Si(96)...H(134)	250.0(5)	13.0(fixed)	—	–0.4	13.0
*u*342	Si(3)...H(26)	250.0(5)	12.9(fixed)	—	–0.4	12.9
*u*333	Si(2)...H(36)	250.0(5)	12.9(fixed)	—	–0.4	12.9
*u*312	H(86)...H(91)	250.1(51)	44.9(fixed)	—	10.4	44.9
*u*252	H(76)...H(86)	251.0(79)	39.2(fixed)	—	10.3	39.2
*u*357	Si(52)...H(70)	251.0(5)	13.2(fixed)	—	–0.4	13.2
*u*364	Si(52)...H(69)	251.0(5)	13.3(fixed)	—	–0.4	13.3
*u*351	Si(51)...H(78)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*347	Si(52)...H(94)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*349	Si(52)...H(65)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*343	Si(52)...H(67)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*366	Si(51)...H(80)	251.1(5)	13.2(fixed)	—	–0.4	13.2
*u*367	Si(51)...H(82)	251.1(5)	13.2(fixed)	—	–0.3	13.2
*u*377	Si(51)...H(89)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*361	Si(51)...H(79)	251.1(5)	13.0(fixed)	—	–0.4	13.0
*u*376	Si(52)...H(92)	251.1(5)	13.2(fixed)	—	–0.3	13.2
*u*373	Si(51)...H(91)	251.1(5)	13.2(fixed)	—	–0.3	13.2
*u*355	Si(5)...H(47)	251.1(5)	13.3(fixed)	—	–0.4	13.3
*u*375	Si(145)...H(183)	251.1(5)	13.3(fixed)	—	–0.4	13.3
*u*352	Si(145)...H(185)	251.1(5)	13.2(fixed)	—	–0.4	13.2
*u*359	Si(5)...H(45)	251.1(5)	13.3(fixed)	—	–0.4	13.3
*u*380	Si(5)...H(23)	251.1(5)	13.4(fixed)	—	–0.4	13.4
*u*336	Si(145)...H(173)	251.1(5)	13.0(fixed)	—	–0.4	13.0
*u*378	Si(145)...H(174)	251.1(5)	13.3(fixed)	—	–0.4	13.3
*u*348	Si(98)...H(136)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*365	Si(5)...H(22)	251.1(5)	13.3(fixed)	—	–0.4	13.3
*u*345	Si(5)...H(18)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*369	Si(145)...H(176)	251.1(5)	13.1(fixed)	—	–0.4	13.1
*u*350	Si(98)...H(125)	251.2(5)	13.2(fixed)	—	–0.4	13.2
*u*362	Si(98)...H(127)	251.2(5)	13.2(fixed)	—	–0.4	13.2
*u*370	Si(4)...H(33)	251.2(5)	13.5(fixed)	—	–0.3	13.5
*u*379	Si(98)...H(126)	251.2(5)	13.2(fixed)	—	–0.4	13.2
*u*363	Si(5)...H(20)	251.2(5)	13.0(fixed)	—	–0.4	13.0
*u*360	Si(145)...H(172)	251.2(5)	13.0(fixed)	—	–0.3	13.0
*u*372	Si(98)...H(138)	251.2(5)	13.2(fixed)	—	–0.3	13.2
*u*371	Si(4)...H(32)	251.2(5)	13.4(fixed)	—	–0.3	13.4
*u*354	Si(4)...H(31)	251.2(5)	13.3(fixed)	—	–0.3	13.3
*u*374	Si(4)...H(35)	251.2(5)	13.2(fixed)	—	–0.3	13.2
*u*356	Si(98)...H(129)	251.2(5)	13.1(fixed)	—	–0.4	13.1
*u*368	Si(4)...H(42)	251.2(5)	13.9(fixed)	—	–0.2	13.9

*u*358	Si(4)...H(44)	251.3(5)	13.8(fixed)	—	–0.2	13.8
*u*268	H(161)...H(180)	251.4(49)	48.4(fixed)	—	14.7	48.4
*u*254	H(165)...H(176)	252.8(80)	41.2(fixed)	—	11.4	41.2
*u*284	H(163)...H(174)	252.8(83)	42.5(fixed)	—	9.0	42.5
*u*344	H(20)...H(26)	257.0(87)	50.4(fixed)	—	12.0	50.4
*u*316	H(69)...H(82)	258.4(86)	53.0(fixed)	—	11.7	53.0
*u*260	H(114)...H(130)	259.7(67)	46.3(fixed)	—	12.4	46.3
*u*332	H(22)...H(35)	260.8(82)	58.5(fixed)	—	13.5	58.5
*u*382	C(54)...H(73)	261.6(73)	29.3(fixed)	—	8.6	29.3
*u*231	H(29)...H(42)	264.7(95)	51.7(fixed)	—	38.0	51.7
*u*302	H(73)...H(82)	265.4(49)	47.1(fixed)	—	14.3	47.1
*u*266	H(26)...H(36)	267.3(70)	42.5(fixed)	—	12.7	42.5
*u*233	H(71)...H(89)	267.5(73)	36.1(fixed)	—	15.2	36.1
*u*317	H(120)...H(133)	267.6(66)	49.7(fixed)	—	10.7	49.7
*u*434	Br(62)...H(67)	267.7(101)	29.8(fixed)	—	9.1	29.8
*u*429	Br(108)...H(141)	268.5(60)	30.0(fixed)	—	12.4	30.0
*u*313	H(75)...H(86)	268.5(67)	43.3(fixed)	—	10.3	43.3
*u*386	C(53)...H(83)	272.4(47)	30.9(fixed)	—	11.4	30.9
*u*311	H(75)...H(91)	273.5(43)	44.8(fixed)	—	9.8	44.8
*u*324	H(167)...H(176)	274.1(50)	47.7(fixed)	—	10.7	47.7
*u*400	H(72)...H(74)	274.4(60)	34.6(fixed)	—	5.7	34.6
*u*413	H(119)...H(121)	274.9(61)	35.4(fixed)	—	6.3	35.4
*u*410	H(38)...H(41)	275.0(59)	35.1(fixed)	—	7.2	35.1
*u*404	H(85)...H(88)	275.6(60)	35.9(fixed)	—	7.2	35.9
*u*395	H(25)...H(27)	275.9(59)	36.1(fixed)	—	8.4	36.1
*u*381	C(148)...H(167)	276.0(42)	28.4(fixed)	—	8.9	28.4
*u*437	C(152)...H(186)	276.0(109)	29.4(fixed)	—	7.5	29.4
*u*421	H(166)...H(168)	276.9(60)	35.3(fixed)	—	7.2	35.3
*u*411	C(105)...H(116)	276.9(53)	32.1(fixed)	—	11.8	32.1
*u*385	C(9)...H(35)	276.9(48)	31.2(fixed)	—	14.0	31.2
*u*387	C(17)...H(31)	277.0(51)	36.0(fixed)	—	19.1	36.0
*u*389	C(64)...H(78)	277.4(37)	29.4(fixed)	—	9.4	29.4
*u*393	C(60)...H(91)	278.1(42)	28.8(fixed)	—	7.9	28.8
*u*430	Br(14)...H(47)	278.4(61)	30.2(fixed)	—	10.8	30.2
*u*431	Br(155)...H(185)	279.0(63)	28.3(fixed)	—	9.5	28.3
*u*407	C(6)...H(36)	279.9(53)	29.6(fixed)	—	7.4	29.6
*u*415	C(103)...H(114)	281.4(60)	30.7(fixed)	—	9.6	30.7
*u*384	C(110)...H(120)	283.2(52)	30.0(fixed)	—	9.3	30.0
*u*383	C(55)...H(82)	285.1(34)	30.4(fixed)	—	11.9	30.4
*u*566	C(55)...H(70)	285.2(74)	37.5(fixed)	—	3.4	37.5
*u*396	C(13)...H(44)	286.1(54)	42.5(fixed)	—	27.3	42.5
*u*422	C(8)...H(20)	286.3(72)	30.3(fixed)	—	9.6	30.3
*u*419	H(162)...H(187)	286.8(28)	35.4(fixed)	—	5.8	35.4
*u*402	H(160)...H(162)	286.9(28)	34.9(fixed)	—	5.8	34.9
*u*423	H(66)...H(68)	287.6(28)	36.4(fixed)	—	6.4	36.4
*u*399	H(77)...H(90)	287.7(28)	35.8(fixed)	—	6.3	35.8

*u*416	H(68)...H(93)	287.8(28)	37.1(fixed)	—	6.7	37.1
*u*424	H(77)...H(81)	288.5(28)	38.1(fixed)	—	7.7	38.1
*u*427	H(113)...H(115)	288.8(28)	39.0(fixed)	—	8.0	39.0
*u*426	H(19)...H(21)	288.8(28)	39.2(fixed)	—	7.9	39.2
*u*482	Br(62)...H(70)	288.9(102)	34.7(fixed)	—	7.2	34.7
*u*432	Br(61)...H(94)	289.2(94)	28.5(fixed)	—	9.9	28.5
*u*390	H(21)...H(46)	289.6(28)	37.7(fixed)	—	8.3	37.7
*u*391	C(7)...H(28)	289.7(70)	31.1(fixed)	—	10.6	31.1
*u*398	H(124)...H(128)	290.2(28)	39.0(fixed)	—	9.4	39.0
*u*403	C(157)...H(169)	290.5(46)	31.7(fixed)	—	11.2	31.7
*u*406	C(152)...H(163)	290.5(54)	29.9(fixed)	—	7.0	29.9
*u*394	H(160)...H(187)	290.7(66)	36.3(fixed)	—	6.5	36.3
*u*388	C(12)...H(26)	291.0(69)	28.8(fixed)	—	10.2	28.8
*u*420	C(11)...H(22)	291.3(54)	31.8(fixed)	—	10.5	31.8
*u*392	H(66)...H(93)	291.9(66)	36.6(fixed)	—	7.2	36.6
*u*412	H(81)...H(90)	292.2(66)	36.9(fixed)	—	7.5	36.9
*u*417	H(128)...H(137)	292.7(66)	38.7(fixed)	—	8.3	38.7
*u*593	C(10)...H(45)	292.9(48)	41.5(fixed)	—	4.3	41.5
*u*405	H(19)...H(46)	293.1(66)	37.2(fixed)	—	8.1	37.2
*u*433	Br(15)...H(39)	293.4(50)	31.4(fixed)	—	11.5	31.4
*u*602	C(59)...H(65)	293.4(53)	37.5(fixed)	—	3.4	37.5
*u*408	C(63)...H(75)	293.5(43)	29.3(fixed)	—	7.2	29.3
*u*418	H(30)...H(34)	294.1(28)	42.2(fixed)	—	14.0	42.2
*u*620	C(101)...H(127)	294.4(60)	41.3(fixed)	—	4.7	41.3
*u*428	C(58)...H(69)	294.5(84)	31.8(fixed)	—	8.1	31.8
*u*438	C(58)...H(92)	294.6(113)	30.0(fixed)	—	8.5	30.0
*u*576	C(106)...H(112)	297.6(50)	38.8(fixed)	—	3.7	38.8
*u*401	C(102)...H(133)	298.0(61)	30.0(fixed)	—	8.3	30.0
*u*425	H(30)...H(43)	298.1(28)	47.2(fixed)	—	19.6	47.2
*u*440	C(64)...H(80)	298.2(110)	30.1(fixed)	—	9.9	30.1
*u*451	C(8)...H(23)	298.2(82)	31.4(fixed)	—	9.4	31.4
*u*414	H(34)...H(43)	298.6(67)	48.1(fixed)	—	16.8	48.1
*u*458	C(102)...C(103)	299.0(42)	13.6(tied to *u*513)	—	–0.2	11.7
*u*397	C(56)...H(86)	299.0(57)	28.6(fixed)	—	8.0	28.6
*u*567	C(149)...H(164)	299.5(41)	33.5(fixed)	—	3.3	33.5
*u*473	Br(14)...H(18)	299.6(71)	34.0(fixed)	—	8.7	34.0
*u*528	Br(155)...H(173)	299.8(51)	33.8(fixed)	—	5.8	33.8
*u*518	C(150)...H(181)	299.9(89)	33.2(fixed)	—	9.2	33.2
*u*455	C(55)...C(56)	300.1(41)	13.4(tied to *u*513)	—	–0.1	11.5
*u*465	C(59)...C(60)	300.1(41)	13.4(tied to *u*513)	—	–0.1	11.5
*u*626	C(12)...H(18)	300.2(54)	41.2(fixed)	—	3.7	41.2
*u*446	C(147)...C(148)	300.4(13)	13.7(tied to *u*513)	—	–0.2	11.8
*u*463	C(7)...H(24)	300.4(83)	30.6(fixed)	—	8.4	30.6
*u*454	C(148)...C(158)	300.4(13)	13.6(tied to *u*513)	—	–0.1	11.8
*u*453	C(53)...C(54)	300.6(13)	14.0(tied to *u*513)	—	–0.2	12.0
*u*447	C(54)...C(64)	300.6(13)	13.7(tied to *u*513)	—	–0.1	11.8

*u*452	C(57)...C(58)	300.6(13)	13.6(tied to *u*513)	—	–0.1	11.7
*u*449	C(57)...C(63)	300.6(13)	13.5(tied to *u*513)	—	–0.1	11.6
*u*456	C(10)...C(16)	300.7(13)	14.1(tied to *u*513)	—	–0.2	12.1
*u*459	C(100)...C(101)	300.7(13)	13.8(tied to *u*513)	—	–0.1	11.9
*u*450	C(6)...C(7)	300.7(13)	13.9(tied to *u*513)	—	–0.2	12.0
*u*435	C(7)...C(17)	300.7(13)	13.8(tied to *u*513)	—	–0.2	11.9
*u*439	C(101)...C(111)	300.7(13)	13.5(tied to *u*513)	—	–0.1	11.6
*u*444	C(10)...C(11)	300.8(13)	13.5(tied to *u*513)	—	–0.1	11.7
*u*461	C(149)...C(150)	300.8(40)	13.4(tied to *u*513)	—	–0.1	11.6
*u*466	C(12)...C(13)	301.1(39)	13.7(tied to *u*513)	—	–0.2	11.8
*u*464	C(8)...C(9)	301.1(39)	13.5(tied to *u*513)	—	–0.1	11.7
*u*617	Br(61)...H(79)	301.7(41)	39.1(fixed)	—	4.3	39.1
*u*532	C(58)...H(71)	302.3(49)	35.2(fixed)	—	3.9	35.2
*u*409	C(149)...H(176)	303.0(51)	29.7(fixed)	—	8.5	29.7
*u*535	C(11)...H(29)	303.2(55)	40.6(fixed)	—	4.7	40.6
*u*573	C(16)...H(40)	303.4(56)	39.2(fixed)	—	4.7	39.2
*u*436	C(147)...C(158)	304.0(48)	13.5(tied to *u*513)	—	–0.1	11.6
*u*590	C(57)...H(92)	304.1(44)	39.4(fixed)	—	3.8	39.4
*u*548	C(63)...H(87)	304.2(43)	34.5(fixed)	—	3.7	34.5
*u*445	C(100)...C(111)	304.2(48)	13.9(tied to *u*513)	—	–0.2	11.9
*u*460	C(104)...H(134)	304.2(68)	30.0(fixed)	—	6.8	30.0
*u*442	C(53)...C(64)	304.2(48)	13.6(tied to *u*513)	—	–0.2	11.7
*u*441	C(58)...C(63)	304.2(48)	13.6(tied to *u*513)	—	–0.2	11.7
*u*448	C(11)...C(16)	304.3(48)	14.1(tied to *u*513)	—	–0.2	12.1
*u*457	C(6)...C(17)	304.3(48)	13.9(tied to *u*513)	—	–0.2	12.0
*u*544	C(103)...H(119)	304.5(48)	25.6(fixed)	—	0.7	25.6
*u*534	C(56)...H(72)	304.9(47)	25.0(fixed)	—	0.6	25.0
*u*550	C(13)...H(38)	305.0(46)	24.2(fixed)	—	0.5	24.2
*u*499	C(102)...H(121)	305.0(48)	24.0(fixed)	—	1.0	24.0
*u*475	C(149)...H(183)	305.2(59)	30.9(fixed)	—	7.4	30.9
*u*537	C(60)...H(85)	305.3(47)	26.3(fixed)	—	1.2	26.3
*u*486	C(55)...H(74)	305.4(47)	23.6(fixed)	—	0.8	23.6
*u*531	C(9)...H(25)	305.4(46)	25.3(fixed)	—	1.1	25.3
*u*500	C(59)...H(88)	305.5(47)	23.7(fixed)	—	1.0	23.7
*u*541	C(150)...H(166)	305.9(46)	24.7(fixed)	—	0.7	24.7
*u*497	C(12)...H(41)	306.0(46)	25.5(fixed)	—	1.6	25.5
*u*487	C(8)...H(27)	306.0(46)	25.4(fixed)	—	1.7	25.4
*u*563	C(6)...H(24)	306.3(66)	39.2(fixed)	—	4.6	39.2
*u*507	C(149)...H(168)	306.6(46)	25.2(fixed)	—	1.4	25.2
*u*501	Br(61)...H(65)	306.7(99)	33.1(fixed)	—	7.3	33.1
*u*652	C(55)...H(69)	306.9(83)	38.7(fixed)	—	3.1	38.7
*u*470	C(107)...H(126)	307.0(64)	31.1(fixed)	—	10.1	31.1
*u*701	Si(50)...H(70)	307.1(48)	31.7(fixed)	—	3.3	31.7
*u*568	C(7)...H(33)	307.1(46)	45.3(fixed)	—	6.1	45.3
*u*476	C(147)...H(178)	307.4(61)	30.8(fixed)	—	6.8	30.8
*u*560	C(9)...H(23)	307.9(68)	41.8(fixed)	—	4.4	41.8

*u*644	Br(15)...H(42)	308.0(52)	59.9(fixed)	—	11.4	59.9
*u*562	C(100)...H(123)	308.6(60)	36.0(fixed)	—	3.8	36.0
*u*472	Si(96)...Si(97)	308.6(21)	11.4(tied to *u*513)	—	0.0	9.8
*u*553	Si(143)...Si(144)	308.7(21)	10.9(tied to *u*513)	—	0.0	9.4
*u*513	Si(3)...Si(5)	308.7(19)	11.7(3)	10.1(1)	0.0	10.1
*u*598	Si(50)...Si(52)	308.8(19)	11.2(tied to *u*513)	—	0.1	9.7
*u*578	C(56)...H(89)	308.9(51)	35.5(fixed)	—	3.5	35.5
*u*571	C(8)...H(37)	309.1(72)	35.6(fixed)	—	3.4	35.6
*u*467	C(11)...H(45)	309.5(91)	31.5(fixed)	—	9.0	31.5
*u*582	Si(3)...H(23)	309.7(44)	33.2(fixed)	—	4.9	33.2
*u*503	Si(49)...Si(50)	310.1(22)	11.2(tied to *u*513)	—	0.0	9.6
*u*527	Si(2)...Si(3)	310.1(22)	11.0(tied to *u*513)	—	0.0	9.5
*u*542	C(147)...H(162)	310.8(17)	24.7(fixed)	—	0.3	24.7
*u*662	Br(14)...H(32)	311.0(51)	53.0(fixed)	—	7.8	53.0
*u*554	C(148)...H(187)	311.0(17)	25.7(fixed)	—	0.6	25.7
*u*580	Br(62)...H(84)	311.0(50)	40.1(fixed)	—	5.3	40.1
*u*561	C(53)...H(68)	311.1(17)	26.0(fixed)	—	0.5	26.0
*u*520	Br(15)...H(37)	311.2(58)	34.3(fixed)	—	6.2	34.3
*u*547	C(54)...H(93)	311.3(17)	26.6(fixed)	—	0.7	26.6
*u*559	C(57)...H(81)	311.3(17)	28.0(fixed)	—	1.0	28.0
*u*565	C(100)...H(115)	311.4(17)	28.3(fixed)	—	0.9	28.3
*u*524	C(101)...H(140)	311.4(17)	28.5(fixed)	—	1.0	28.5
*u*491	C(152)...H(171)	311.4(17)	23.9(fixed)	—	0.8	23.9
*u*536	C(63)...H(77)	311.5(17)	25.8(fixed)	—	0.7	25.8
*u*557	C(6)...H(21)	311.5(17)	27.6(fixed)	—	0.8	27.6
*u*523	C(7)...H(46)	311.6(17)	26.7(fixed)	—	0.7	26.7
*u*478	C(148)...H(160)	311.6(17)	24.8(fixed)	—	1.1	24.8
*u*469	C(10)...H(40)	311.7(60)	33.2(fixed)	—	9.4	33.2
*u*483	C(64)...H(68)	311.7(17)	25.3(fixed)	—	0.9	25.3
*u*495	C(54)...H(66)	311.8(17)	25.3(fixed)	—	1.0	25.3
*u*529	C(10)...H(34)	311.9(17)	29.4(fixed)	—	1.5	29.4
*u*481	C(57)...H(90)	311.9(17)	24.3(fixed)	—	1.0	24.3
*u*545	C(16)...H(30)	311.9(17)	32.0(fixed)	—	2.1	32.0
*u*493	C(58)...H(77)	311.9(17)	25.1(fixed)	—	1.1	25.1
*u*496	C(7)...H(19)	312.1(17)	26.7(fixed)	—	1.3	26.7
*u*504	C(101)...H(113)	312.2(17)	25.6(fixed)	—	1.3	25.6
*u*468	C(17)...H(21)	312.4(17)	26.6(fixed)	—	1.6	26.6
*u*604	C(150)...H(183)	312.4(56)	36.8(fixed)	—	4.0	36.8
*u*480	C(105)...H(124)	312.5(17)	26.3(fixed)	—	1.7	26.3
*u*498	C(11)...H(30)	313.0(17)	30.4(fixed)	—	2.9	30.4
*u*607	Si(96)...Si(99)	313.2(4)	11.1(tied to *u*513)	—	0.1	9.6
*u*516	Si(143)...Si(146)	313.2(4)	10.0(fixed)	—	0.0	10.0
*u*519	H(161)...H(164)	313.5(41)	38.7(fixed)	—	3.7	38.7
*u*443	C(105)...H(139)	313.5(121)	30.1(fixed)	—	10.1	30.1
*u*569	H(79)...H(91)	313.6(41)	40.3(fixed)	—	4.4	40.3
*u*510	C(102)...H(131)	313.9(99)	30.9(fixed)	—	7.2	30.9

*u*546	H(67)...H(70)	313.9(41)	39.1(fixed)	—	4.4	39.1
*u*512	C(10)...H(43)	314.0(17)	33.8(fixed)	—	4.6	33.8
*u*634	Br(108)...H(126)	314.1(51)	42.5(fixed)	—	4.9	42.5
*u*525	C(152)...H(184)	314.2(53)	25.8(fixed)	—	0.5	25.8
*u*589	H(163)...H(186)	314.2(41)	37.8(fixed)	—	4.2	37.8
*u*558	H(78)...H(80)	314.4(41)	42.5(fixed)	—	5.8	42.5
*u*549	C(105)...H(137)	314.5(53)	27.3(fixed)	—	0.6	27.3
*u*538	H(69)...H(92)	314.5(41)	40.1(fixed)	—	5.2	40.1
*u*551	C(58)...H(90)	314.5(53)	25.3(fixed)	—	0.4	25.3
*u*530	C(64)...H(66)	314.5(53)	26.2(fixed)	—	0.5	26.2
*u*517	Si(50)...Si(51)	314.6(5)	11.6(tied to *u*513)	—	0.0	10.0
*u*575	Si(49)...Si(51)	314.6(5)	11.4(tied to *u*513)	—	0.0	9.8
*u*572	Si(2)...Si(4)	314.6(5)	11.5(tied to *u*513)	—	0.0	9.9
*u*601	Si(49)...Si(52)	314.6(5)	11.2(tied to *u*513)	—	0.1	9.7
*u*570	Si(96)...Si(98)	314.6(5)	11.4(tied to *u*513)	—	0.0	9.8
*u*574	Si(3)...Si(4)	314.6(5)	11.4(tied to *u*513)	—	0.0	9.8
*u*603	Si(2)...Si(5)	314.6(5)	11.3(tied to *u*513)	—	0.1	9.7
*u*606	Si(143)...Si(145)	314.7(5)	11.1(tied to *u*513)	—	0.1	9.6
*u*471	C(147)...H(187)	314.7(53)	25.5(fixed)	—	1.0	25.5
*u*637	C(54)...H(80)	314.7(75)	42.5(fixed)	—	4.6	42.5
*u*489	H(22)...H(45)	314.9(41)	43.4(fixed)	—	6.1	43.4
*u*608	H(126)...H(138)	315.0(41)	42.7(fixed)	—	6.0	42.7
*u*490	C(57)...H(87)	315.0(52)	30.2(fixed)	—	6.3	30.2
*u*552	C(17)...H(19)	315.0(53)	26.6(fixed)	—	0.9	26.6
*u*556	H(20)...H(23)	315.1(41)	42.4(fixed)	—	6.0	42.4
*u*738	C(16)...H(39)	315.2(48)	47.8(fixed)	—	3.3	47.8
*u*678	C(59)...H(67)	315.2(66)	40.2(fixed)	—	2.9	40.2
*u*690	C(10)...H(47)	315.4(60)	43.2(fixed)	—	3.7	43.2
*u*474	C(53)...H(93)	315.4(53)	25.7(fixed)	—	1.3	25.7
*u*508	C(60)...H(79)	315.4(42)	30.3(fixed)	—	7.8	30.3
*u*462	C(17)...H(33)	315.5(94)	33.2(fixed)	—	12.5	33.2
*u*492	C(16)...H(34)	315.6(53)	29.3(fixed)	—	1.9	29.3
*u*484	C(100)...H(140)	315.7(53)	26.7(fixed)	—	1.7	26.7
*u*539	Br(108)...H(112)	315.7(78)	34.2(fixed)	—	7.8	34.2
*u*479	C(63)...H(81)	315.7(53)	26.6(fixed)	—	1.8	26.6
*u*533	C(11)...H(43)	315.7(54)	36.2(fixed)	—	3.4	36.2
*u*515	H(116)...H(139)	315.7(41)	43.1(fixed)	—	6.9	43.1
*u*485	C(6)...H(46)	315.8(53)	25.6(fixed)	—	1.5	25.6
*u*687	Si(145)...H(186)	316.1(29)	31.6(fixed)	—	3.9	31.6
*u*588	Br(155)...H(170)	316.3(48)	40.5(fixed)	—	5.6	40.5
*u*651	Si(143)...H(159)	316.5(21)	30.2(fixed)	—	4.0	30.2
*u*753	Si(49)...H(65)	317.0(24)	30.8(fixed)	—	3.5	30.8
*u*674	C(57)...H(94)	317.2(68)	41.7(fixed)	—	3.1	41.7
*u*586	Si(145)...Si(146)	317.6(22)	11.9(tied to *u*513)	—	0.1	10.3
*u*579	C(148)...H(174)	317.6(57)	37.7(fixed)	—	3.7	37.7
*u*594	Si(98)...Si(99)	317.7(22)	11.7(tied to *u*513)	—	0.1	10.1

*u*600	C(1)...C(7)	317.8(12)	12.9(tied to *u*513)	—	–0.1	11.1
*u*611	C(1)...C(16)	317.8(12)	13.2(tied to *u*513)	—	–0.1	11.3
*u*614	C(1)...C(11)	317.8(12)	13.0(tied to *u*513)	—	–0.1	11.2
*u*752	Si(143)...H(173)	317.8(22)	28.2(fixed)	—	2.9	28.2
*u*599	C(1)...C(10)	317.8(12)	13.0(tied to *u*513)	—	–0.1	11.2
*u*647	C(1)...C(17)	317.8(12)	12.9(tied to *u*513)	—	0.0	11.2
*u*630	C(1)...C(6)	317.8(12)	12.9(tied to *u*513)	—	0.0	11.1
*u*640	C(95)...C(105)	317.8(12)	13.1(tied to *u*513)	—	–0.1	11.3
*u*595	C(95)...C(101)	317.9(12)	12.8(tied to *u*513)	—	–0.1	11.1
*u*596	C(48)...C(54)	317.9(12)	13.1(tied to *u*513)	—	–0.1	11.3
*u*613	C(95)...C(100)	317.9(12)	12.7(tied to *u*513)	—	0.0	10.9
*u*632	C(48)...C(64)	317.9(12)	12.8(tied to *u*513)	—	–0.1	11.0
*u*616	C(48)...C(58)	317.9(12)	12.8(tied to *u*513)	—	–0.1	11.1
*u*721	C(11)...H(28)	317.9(54)	44.7(fixed)	—	3.1	44.7
*u*642	C(48)...C(53)	317.9(12)	12.9(tied to *u*513)	—	0.0	11.1
*u*612	C(48)...C(57)	318.0(12)	12.8(tied to *u*513)	—	0.0	11.0
*u*619	C(48)...C(63)	318.0(12)	12.6(tied to *u*513)	—	0.0	10.9
*u*618	C(142)...C(152)	318.1(12)	12.9(tied to *u*513)	—	–0.1	11.1
*u*643	C(142)...C(147)	318.1(12)	12.9(tied to *u*513)	—	0.0	11.1
*u*639	C(95)...C(103)	318.1(15)	12.6(tied to *u*513)	—	0.0	10.9
*u*628	C(95)...C(102)	318.1(15)	12.6(tied to *u*513)	—	0.0	10.9
*u*610	C(142)...C(148)	318.2(12)	12.5(tied to *u*513)	—	0.0	10.7
*u*521	H(31)...H(33)	318.2(41)	47.8(fixed)	—	10.7	47.8
*u*494	C(59)...H(76)	318.3(51)	30.7(fixed)	—	6.0	30.7
*u*697	Si(51)...H(92)	318.3(32)	32.2(fixed)	—	4.4	32.2
*u*583	H(32)...H(44)	318.3(42)	57.9(fixed)	—	14.2	57.9
*u*629	C(142)...C(150)	318.4(15)	12.5(tied to *u*513)	—	0.0	10.7
*u*615	C(142)...C(149)	318.5(15)	12.4(tied to *u*513)	—	0.0	10.7
*u*749	Si(2)...H(18)	318.6(17)	33.5(fixed)	—	4.1	33.5
*u*638	C(48)...C(55)	318.7(15)	12.7(tied to *u*513)	—	0.0	11.0
*u*623	C(48)...C(59)	318.7(15)	12.5(tied to *u*513)	—	0.0	10.7
*u*636	C(48)...C(56)	318.7(15)	12.4(tied to *u*513)	—	0.0	10.7
*u*625	C(48)...C(60)	318.7(15)	12.6(tied to *u*513)	—	0.0	10.8
*u*592	H(118)...H(122)	318.7(84)	39.9(fixed)	—	4.1	39.9
*u*488	C(16)...H(29)	319.1(71)	33.5(fixed)	—	9.1	33.5
*u*591	Si(51)...Si(52)	319.1(21)	11.9(tied to *u*513)	—	0.1	10.3
*u*597	Si(4)...Si(5)	319.1(21)	11.8(tied to *u*513)	—	0.1	10.2
*u*477	C(13)...H(32)	319.4(54)	35.7(fixed)	—	16.5	35.7
*u*543	C(103)...H(131)	319.5(61)	35.7(fixed)	—	4.4	35.7
*u*649	C(1)...C(13)	319.5(15)	12.9(tied to *u*513)	—	–0.1	11.2
*u*633	C(1)...C(9)	319.5(15)	12.7(tied to *u*513)	—	0.0	10.9
*u*641	C(1)...C(8)	319.6(15)	12.4(tied to *u*513)	—	0.0	10.7
*u*621	C(1)...C(12)	319.6(15)	12.4(tied to *u*513)	—	0.0	10.7
*u*736	Si(4)...H(45)	320.2(26)	32.1(fixed)	—	4.8	32.1
*u*666	C(149)...H(163)	320.5(38)	37.0(fixed)	—	2.8	37.0
*u*522	C(56)...H(84)	320.9(51)	31.9(fixed)	—	8.9	31.9

*u*751	Si(97)...H(136)	321.1(23)	31.5(fixed)	—	3.8	31.5
*u*577	H(18)...H(47)	321.8(89)	43.5(fixed)	—	4.9	43.5
*u*564	C(152)...H(165)	322.0(59)	35.9(fixed)	—	4.1	35.9
*u*540	C(60)...H(76)	322.2(57)	33.8(fixed)	—	3.6	33.8
*u*514	H(65)...H(94)	322.2(89)	39.8(fixed)	—	4.8	39.8
*u*509	H(159)...H(188)	322.4(90)	39.7(fixed)	—	4.8	39.7
*u*526	H(82)...H(89)	322.4(89)	41.4(fixed)	—	5.3	41.4
*u*720	C(10)...H(44)	322.4(24)	41.9(fixed)	—	1.3	41.9
*u*723	Si(98)...H(139)	322.5(33)	32.1(fixed)	—	5.6	32.1
*u*718	Si(5)...H(24)	322.6(46)	31.6(fixed)	—	4.7	31.6
*u*581	H(165)...H(169)	322.7(82)	41.2(fixed)	—	4.5	41.2
*u*794	Br(155)...H(169)	322.8(45)	51.2(fixed)	—	3.0	51.2
*u*511	H(112)...H(141)	322.9(89)	41.8(fixed)	—	5.8	41.8
*u*584	H(71)...H(75)	322.9(82)	37.4(fixed)	—	3.7	37.4
*u*653	H(84)...H(86)	323.3(82)	39.7(fixed)	—	4.6	39.7
*u*680	C(11)...H(31)	323.7(23)	34.9(fixed)	—	0.9	34.9
*u*725	C(58)...H(78)	323.8(23)	28.1(fixed)	—	–0.1	28.1
*u*710	C(148)...H(161)	323.8(23)	27.3(fixed)	—	–0.2	27.3
*u*686	C(105)...H(125)	323.9(23)	29.9(fixed)	—	0.2	29.9
*u*673	C(17)...H(22)	324.0(23)	29.4(fixed)	—	0.1	29.4
*u*677	C(8)...Br(15)	324.0(14)	14.5(tied to *u*513)	—	–0.2	12.5
*u*696	C(12)...Br(14)	324.0(14)	14.5(tied to *u*513)	—	–0.2	12.5
*u*670	C(13)...Br(14)	324.0(14)	14.5(tied to *u*513)	—	–0.2	12.5
*u*684	C(9)...Br(15)	324.0(14)	14.5(tied to *u*513)	—	–0.1	12.5
*u*729	C(57)...H(91)	324.1(23)	26.1(fixed)	—	–0.1	26.1
*u*719	C(54)...H(67)	324.1(23)	26.6(fixed)	—	0.0	26.6
*u*728	Si(52)...H(80)	324.2(29)	33.2(fixed)	—	5.3	33.2
*u*712	C(64)...H(69)	324.2(23)	26.2(fixed)	—	0.0	26.2
*u*658	C(63)...H(79)	324.2(23)	28.1(fixed)	—	0.4	28.1
*u*693	C(16)...H(32)	324.2(23)	34.9(fixed)	—	1.4	34.9
*u*743	C(152)...H(172)	324.3(23)	25.0(fixed)	—	–0.1	25.0
*u*694	C(55)...Br(62)	324.3(14)	14.5(tied to *u*513)	—	–0.2	12.5
*u*1015	H(39)...H(42)	324.3(69)	87.3(fixed)	—	–2.0	87.3
*u*676	C(56)...Br(62)	324.3(14)	14.3(tied to *u*513)	—	–0.1	12.3
*u*675	C(102)...Br(109)	324.4(14)	14.4(tied to *u*513)	—	–0.2	12.4
*u*717	C(7)...H(20)	324.4(23)	27.8(fixed)	—	0.2	27.8
*u*688	C(103)...Br(109)	324.4(14)	14.4(tied to *u*513)	—	–0.1	12.4
*u*754	C(101)...H(114)	324.4(23)	27.1(fixed)	—	0.2	27.1
*u*655	C(53)...H(70)	324.4(23)	26.5(fixed)	—	0.3	26.5
*u*656	C(57)...H(80)	324.4(23)	29.2(fixed)	—	0.8	29.2
*u*645	C(54)...H(92)	324.5(23)	28.3(fixed)	—	0.6	28.3
*u*622	C(147)...H(164)	324.5(23)	25.2(fixed)	—	0.2	25.2
*u*691	C(100)...H(117)	324.5(23)	29.8(fixed)	—	0.8	29.8
*u*669	C(148)...H(186)	324.6(23)	26.5(fixed)	—	0.5	26.5
*u*765	C(101)...H(129)	324.6(58)	48.1(fixed)	—	3.0	48.1
*u*646	Si(96)...H(118)	324.6(30)	30.5(fixed)	—	4.0	30.5

*u*660	C(6)...H(23)	324.6(23)	29.3(fixed)	—	0.7	29.3
*u*585	C(7)...H(45)	324.6(23)	29.1(fixed)	—	0.7	29.1
*u*635	C(101)...H(139)	324.7(23)	29.1(fixed)	—	0.8	29.1
*u*650	C(10)...H(33)	324.8(23)	30.7(fixed)	—	1.1	30.7
*u*708	Si(96)...H(126)	324.8(24)	31.2(fixed)	—	5.8	31.2
*u*757	Si(49)...H(79)	325.0(20)	29.7(fixed)	—	4.5	29.7
*u*698	C(59)...Br(61)	325.1(14)	14.3(tied to *u*513)	—	–0.1	12.3
*u*679	C(149)...Br(156)	325.1(14)	14.3(tied to *u*513)	—	–0.1	12.3
*u*671	C(60)...Br(61)	325.1(14)	14.1(tied to *u*513)	—	–0.1	12.2
*u*700	C(150)...Br(156)	325.1(14)	14.3(tied to *u*513)	—	–0.1	12.4
*u*685	Si(98)...H(134)	325.3(31)	29.3(fixed)	—	3.8	29.3
*u*722	Si(143)...H(170)	325.4(32)	30.0(fixed)	—	5.7	30.0
*u*740	C(102)...H(122)	325.5(58)	26.5(fixed)	—	–0.2	26.5
*u*587	H(37)...H(39)	325.8(80)	40.5(fixed)	—	4.1	40.5
*u*681	C(103)...H(118)	325.8(58)	27.3(fixed)	—	0.2	27.3
*u*654	Si(50)...H(89)	326.0(17)	29.1(fixed)	—	3.3	29.1
*u*648	H(24)...H(28)	326.1(80)	42.3(fixed)	—	4.9	42.3
*u*756	C(12)...H(20)	326.3(53)	42.0(fixed)	—	3.0	42.0
*u*779	Br(61)...H(78)	326.4(35)	45.1(fixed)	—	2.9	45.1
*u*555	H(35)...H(42)	326.6(90)	55.3(fixed)	—	13.3	55.3
*u*774	C(100)...H(122)	326.6(53)	40.3(fixed)	—	2.4	40.3
*u*605	Si(49)...H(76)	326.9(32)	28.3(fixed)	—	3.3	28.3
*u*702	Si(4)...H(40)	327.0(30)	32.3(fixed)	—	5.3	32.3
*u*707	Si(4)...H(29)	327.1(29)	33.2(fixed)	—	5.1	33.2
*u*760	C(148)...H(176)	327.2(53)	41.5(fixed)	—	2.6	41.5
*u*732	Br(108)...H(135)	327.4(15)	27.3(fixed)	—	0.7	27.3
*u*758	Si(3)...H(37)	327.6(29)	29.8(fixed)	—	3.1	29.8
*u*731	C(149)...H(169)	327.8(56)	29.3(fixed)	—	–0.1	29.3
*u*705	Si(51)...H(87)	327.9(31)	29.1(fixed)	—	3.6	29.1
*u*724	C(60)...H(84)	328.0(56)	28.5(fixed)	—	0.3	28.5
*u*762	C(59)...H(86)	328.1(56)	25.4(fixed)	—	–0.2	25.4
*u*745	C(55)...H(75)	328.1(56)	25.2(fixed)	—	–0.2	25.2
*u*713	Si(5)...H(33)	328.1(31)	35.9(fixed)	—	7.0	35.9
*u*657	Br(108)...H(132)	328.2(15)	26.9(fixed)	—	1.4	26.9
*u*726	Si(145)...H(165)	328.3(27)	30.3(fixed)	—	3.8	30.3
*u*668	C(56)...H(71)	328.4(56)	25.9(fixed)	—	0.2	25.9
*u*689	C(150)...H(165)	328.6(56)	26.1(fixed)	—	0.2	26.1
*u*727	Br(62)...H(74)	328.6(15)	26.3(fixed)	—	0.6	26.3
*u*737	Br(15)...H(27)	328.9(15)	30.4(fixed)	—	1.0	30.4
*u*715	Br(14)...H(41)	328.9(15)	30.7(fixed)	—	1.1	30.7
*u*741	C(6)...H(47)	329.0(64)	29.6(fixed)	—	–0.3	29.6
*u*733	Br(61)...H(88)	329.0(15)	27.4(fixed)	—	0.5	27.4
*u*663	C(11)...H(42)	329.1(64)	41.6(fixed)	—	2.4	41.6
*u*661	Br(62)...H(72)	329.2(15)	26.4(fixed)	—	1.2	26.4
*u*672	C(9)...H(22)	329.2(66)	43.6(fixed)	—	3.3	43.6
*u*695	C(53)...H(94)	329.3(64)	28.0(fixed)	—	–0.1	28.0

*u*711	C(63)...H(82)	329.3(64)	29.4(fixed)	—	0.2	29.4
*u*699	C(100)...H(141)	329.3(64)	29.6(fixed)	—	0.2	29.6
*u*704	C(16)...H(35)	329.4(64)	31.7(fixed)	—	0.5	31.7
*u*682	C(147)...H(188)	329.5(64)	26.6(fixed)	—	0.0	26.6
*u*747	C(12)...H(39)	329.6(55)	28.5(fixed)	—	–0.1	28.5
*u*763	C(8)...H(28)	329.6(55)	28.4(fixed)	—	–0.1	28.4
*u*667	Br(14)...H(38)	329.6(15)	25.8(fixed)	—	1.0	25.8
*u*665	Br(15)...H(25)	329.7(15)	28.2(fixed)	—	1.4	28.2
*u*609	C(152)...H(183)	329.8(64)	27.6(fixed)	—	0.4	27.6
*u*730	Br(155)...H(182)	329.8(15)	28.7(fixed)	—	1.3	28.7
*u*880	H(30)...H(44)	329.9(23)	68.0(fixed)	—	–4.5	68.0
*u*716	C(150)...H(185)	329.9(41)	42.6(fixed)	—	3.0	42.6
*u*709	C(9)...H(24)	330.0(55)	28.2(fixed)	—	0.2	28.2
*u*664	C(17)...H(18)	330.0(64)	28.2(fixed)	—	0.4	28.2
*u*631	C(64)...H(65)	330.0(64)	26.3(fixed)	—	0.4	26.3
*u*624	C(105)...H(136)	330.1(64)	26.9(fixed)	—	0.4	26.9
*u*692	Br(61)...H(85)	330.1(15)	28.2(fixed)	—	1.7	28.2
*u*683	C(13)...H(37)	330.1(55)	26.0(fixed)	—	–0.1	26.0
*u*627	C(58)...H(89)	330.1(64)	26.0(fixed)	—	0.4	26.0
*u*769	C(63)...H(86)	330.1(44)	40.0(fixed)	—	2.3	40.0
*u*659	Br(155)...H(179)	330.1(15)	26.3(fixed)	—	1.2	26.3
*u*735	Si(51)...H(71)	330.9(26)	30.9(fixed)	—	3.6	30.9
*u*742	Si(50)...H(84)	331.3(29)	31.0(fixed)	—	5.3	31.0
*u*734	Si(2)...H(32)	331.9(23)	36.5(fixed)	—	9.7	36.5
*u*876	C(54)...C(55)	331.9(63)	24.1(tied to *u*513)	—	1.0	20.7
*u*502	C(55)...H(89)	333.0(52)	30.2(fixed)	—	6.3	30.2
*u*505	C(63)...H(71)	333.2(56)	31.3(fixed)	—	6.5	31.3
*u*959	H(32)...H(47)	333.5(65)	66.5(fixed)	—	0.5	66.5
*u*767	Br(108)...H(125)	333.6(49)	49.9(fixed)	—	3.6	49.9
*u*506	C(9)...H(42)	333.6(69)	41.6(fixed)	—	23.5	41.6
*u*807	Br(15)...H(44)	334.3(57)	76.4(fixed)	—	5.4	76.4
*u*796	Br(62)...H(83)	334.5(45)	50.4(fixed)	—	2.8	50.4
*u*805	H(32)...H(43)	334.6(23)	64.6(fixed)	—	–1.0	64.6
*u*852	H(31)...H(34)	334.8(22)	58.0(fixed)	—	–3.2	58.0
*u*954	H(174)...H(187)	334.9(98)	39.6(fixed)	—	5.0	39.6
*u*703	C(102)...H(138)	335.5(55)	41.8(fixed)	—	3.0	41.8
*u*821	Br(14)...H(31)	335.7(48)	62.1(fixed)	—	4.1	62.1
*u*904	H(119)...H(122)	337.1(60)	40.1(fixed)	—	–1.8	40.1
*u*746	Si(3)...H(42)	337.2(21)	42.5(fixed)	—	14.2	42.5
*u*827	Br(15)...H(26)	337.3(27)	31.2(fixed)	—	0.1	31.2
*u*842	Br(14)...H(36)	337.6(27)	28.2(fixed)	—	–0.1	28.2
*u*782	H(30)...H(33)	337.6(22)	56.2(fixed)	—	–0.9	56.2
*u*792	Br(14)...H(40)	337.9(27)	31.4(fixed)	—	0.8	31.4
*u*783	C(6)...H(26)	338.0(73)	43.9(fixed)	—	2.5	43.9
*u*789	H(34)...H(42)	338.0(67)	65.5(fixed)	—	–2.3	65.5
*u*787	H(118)...H(121)	338.0(60)	40.5(fixed)	—	–0.7	40.5

*u*871	H(116)...H(140)	338.1(22)	48.6(fixed)	—	–2.6	48.6
*u*889	H(166)...H(169)	338.1(58)	43.0(fixed)	—	–2.1	43.0
*u*791	Br(15)...H(29)	338.1(27)	30.7(fixed)	—	0.9	30.7
*u*964	H(69)...H(71)	338.5(81)	49.1(fixed)	—	2.7	49.1
*u*909	H(25)...H(28)	338.7(57)	42.8(fixed)	—	–2.0	42.8
*u*899	H(85)...H(86)	338.7(58)	40.9(fixed)	—	–1.5	40.9
*u*902	H(38)...H(39)	338.8(57)	41.4(fixed)	—	–2.2	41.4
*u*803	H(84)...H(88)	338.8(59)	42.4(fixed)	—	–1.1	42.4
*u*851	Br(62)...H(73)	339.1(26)	28.8(fixed)	—	0.0	28.8
*u*901	H(72)...H(75)	339.2(58)	38.2(fixed)	—	–1.6	38.2
*u*773	C(54)...H(82)	339.3(76)	48.0(fixed)	—	3.1	48.0
*u*974	H(70)...H(72)	339.3(72)	46.6(fixed)	—	2.6	46.6
*u*784	C(7)...H(35)	339.3(69)	52.7(fixed)	—	3.0	52.7
*u*913	H(78)...H(81)	339.4(22)	44.6(fixed)	—	–2.2	44.6
*u*958	H(67)...H(84)	339.4(66)	56.9(fixed)	—	1.8	56.9
*u*863	H(35)...H(43)	339.4(67)	60.6(fixed)	—	–2.7	60.6
*u*835	Br(61)...H(83)	339.5(27)	32.1(fixed)	—	0.3	32.1
*u*793	Br(62)...H(76)	339.5(26)	28.0(fixed)	—	0.2	28.0
*u*877	H(22)...H(46)	339.5(22)	44.7(fixed)	—	–2.4	44.7
*u*832	Br(155)...H(177)	339.7(27)	29.1(fixed)	—	0.0	29.1
*u*790	H(24)...H(27)	339.7(57)	44.0(fixed)	—	–0.7	44.0
*u*824	Br(155)...H(181)	339.8(27)	31.8(fixed)	—	0.6	31.8
*u*971	H(28)...H(33)	339.9(70)	64.2(fixed)	—	1.8	64.2
*u*795	H(165)...H(168)	339.9(58)	41.4(fixed)	—	–0.7	41.4
*u*781	H(71)...H(74)	340.0(58)	38.9(fixed)	—	–0.7	38.9
*u*924	H(114)...H(115)	340.0(22)	43.6(fixed)	—	–2.0	43.6
*u*908	H(20)...H(21)	340.1(22)	43.7(fixed)	—	–2.1	43.7
*u*748	C(58)...H(73)	340.2(41)	40.5(fixed)	—	2.5	40.5
*u*896	C(10)...C(17)	340.2(43)	22.9(tied to *u*1009)	—	1.0	21.7
*u*836	Br(108)...H(130)	340.3(27)	30.2(fixed)	—	0.0	30.2
*u*766	H(124)...H(127)	340.3(22)	47.7(fixed)	—	–0.7	47.7
*u*906	C(53)...C(59)	340.3(37)	21.5(fixed)	—	0.9	21.5
*u*788	Br(61)...H(87)	340.4(27)	27.7(fixed)	—	0.4	27.7
*u*785	H(37)...H(41)	340.5(57)	41.4(fixed)	—	–0.5	41.4
*u*898	H(69)...H(93)	340.5(22)	40.9(fixed)	—	–1.9	40.9
*u*894	H(161)...H(162)	340.6(22)	39.6(fixed)	—	–2.0	39.6
*u*900	H(67)...H(68)	340.7(22)	40.5(fixed)	—	–1.9	40.5
*u*777	H(77)...H(80)	340.7(22)	45.0(fixed)	—	–0.7	45.0
*u*912	Si(50)...C(54)	340.8(45)	17.3(tied to *u*1009)	—	0.2	16.4
*u*801	Br(108)...H(134)	340.9(27)	28.7(fixed)	—	0.3	28.7
*u*786	H(113)...H(117)	340.9(22)	45.6(fixed)	—	–0.7	45.6
*u*778	H(19)...H(23)	340.9(22)	46.2(fixed)	—	–0.6	46.2
*u*714	H(21)...H(45)	340.9(22)	46.8(fixed)	—	–0.4	46.8
*u*907	H(77)...H(91)	341.0(22)	39.5(fixed)	—	–1.7	39.5
*u*920	H(163)...H(187)	341.2(22)	38.8(fixed)	—	–1.6	38.8
*u*770	H(68)...H(92)	341.2(22)	43.7(fixed)	—	–0.6	43.7

*u*771	H(79)...H(90)	341.5(22)	41.8(fixed)	—	–0.7	41.8
*u*776	H(66)...H(70)	341.8(22)	41.3(fixed)	—	–0.6	41.3
*u*780	H(162)...H(186)	342.0(22)	39.8(fixed)	—	–0.5	39.8
*u*706	C(8)...H(36)	342.2(63)	36.6(fixed)	—	2.7	36.6
*u*755	H(160)...H(164)	342.2(22)	39.3(fixed)	—	–0.4	39.3
*u*844	C(48)...H(70)	342.4(14)	23.4(fixed)	—	0.3	23.4
*u*822	Si(3)...C(7)	342.4(38)	18.7(tied to *u*513)	—	0.1	16.1
*u*857	C(1)...H(18)	342.5(14)	24.2(fixed)	—	0.6	24.2
*u*870	C(48)...H(65)	342.6(14)	22.8(fixed)	—	0.4	22.8
*u*891	C(1)...H(45)	342.6(14)	23.9(fixed)	—	0.7	23.9
*u*872	C(1)...H(23)	342.6(14)	24.4(fixed)	—	0.8	24.4
*u*885	C(48)...H(89)	342.6(14)	22.0(fixed)	—	0.4	22.0
*u*799	C(48)...H(69)	342.6(14)	24.3(fixed)	—	0.7	24.3
*u*818	C(48)...H(67)	342.7(14)	24.2(fixed)	—	0.7	24.2
*u*854	C(95)...H(112)	342.7(14)	23.3(fixed)	—	0.5	23.3
*u*846	C(1)...Br(14)	342.7(8)	12.4(tied to *u*1009)	—	–0.1	11.7
*u*884	C(48)...H(92)	342.7(14)	23.6(fixed)	—	0.7	23.6
*u*859	C(1)...Br(15)	342.7(8)	12.5(tied to *u*1009)	—	–0.1	11.8
*u*826	C(95)...H(129)	342.8(14)	26.2(fixed)	—	1.1	26.2
*u*869	C(142)...H(174)	342.8(14)	23.8(fixed)	—	0.5	23.8
*u*847	C(1)...H(33)	342.8(14)	26.9(fixed)	—	1.3	26.9
*u*868	C(48)...H(80)	342.8(14)	24.4(fixed)	—	0.9	24.4
*u*1057	H(174)...H(188)	342.8(130)	36.2(fixed)	—	3.0	36.2
*u*809	C(48)...H(91)	342.8(14)	22.9(fixed)	—	0.7	22.9
*u*850	C(142)...H(164)	342.8(14)	21.6(fixed)	—	0.2	21.6
*u*800	C(1)...H(22)	342.9(14)	25.0(fixed)	—	1.1	25.0
*u*810	C(95)...H(114)	342.9(14)	24.7(fixed)	—	1.0	24.7
*u*914	C(13)...C(16)	342.9(42)	24.4(tied to *u*1009)	—	1.0	23.0
*u*849	C(48)...H(79)	342.9(14)	22.7(fixed)	—	0.8	22.7
*u*797	C(95)...H(116)	343.0(14)	26.4(fixed)	—	1.3	26.4
*u*895	C(142)...H(159)	343.0(14)	22.7(fixed)	—	0.5	22.7
*u*828	C(1)...H(47)	343.0(14)	23.8(fixed)	—	1.0	23.8
*u*813	C(48)...H(78)	343.0(14)	23.5(fixed)	—	0.9	23.5
*u*806	C(142)...H(163)	343.0(14)	22.4(fixed)	—	0.5	22.4
*u*815	C(48)...H(94)	343.0(14)	23.6(fixed)	—	1.0	23.6
*u*816	C(1)...H(20)	343.0(14)	24.1(fixed)	—	1.1	24.1
*u*820	C(142)...H(161)	343.1(14)	23.5(fixed)	—	0.7	23.5
*u*814	C(48)...H(82)	343.1(14)	25.7(fixed)	—	1.3	25.7
*u*874	C(95)...H(127)	343.1(14)	23.8(fixed)	—	1.1	23.8
*u*819	C(142)...H(176)	343.2(14)	23.3(fixed)	—	0.8	23.3
*u*855	C(95)...H(117)	343.2(14)	23.7(fixed)	—	1.2	23.7
*u*825	C(1)...H(35)	343.3(14)	26.1(fixed)	—	1.7	26.1
*u*811	C(1)...H(31)	343.3(14)	29.8(fixed)	—	2.4	29.8
*u*875	C(142)...H(165)	343.5(17)	22.5(fixed)	—	0.3	22.5
*u*883	C(95)...H(118)	343.5(17)	22.9(fixed)	—	0.4	22.9
*u*834	C(95)...H(122)	343.5(17)	23.4(fixed)	—	0.5	23.4

*u*838	C(1)...H(32)	343.6(14)	27.6(fixed)	—	2.2	27.6
*u*864	C(48)...Br(62)	343.6(8)	12.4(tied to *u*1009)	—	–0.1	11.7
*u*831	C(142)...H(169)	343.7(17)	24.5(fixed)	—	0.8	24.5
*u*999	Br(108)...C(111)	343.7(49)	21.3(tied to *u*1009)	—	1.0	20.2
*u*1045	C(53)...Br(62)	343.8(78)	22.7(tied to *u*1009)	—	1.0	21.4
*u*890	H(113)...H(141)	343.9(66)	45.9(fixed)	—	–2.4	45.9
*u*887	C(48)...H(71)	344.0(17)	22.8(fixed)	—	0.3	22.8
*u*843	C(1)...H(42)	344.1(14)	31.8(fixed)	—	3.5	31.8
*u*888	C(9)...C(11)	344.1(41)	22.1(tied to *u*1009)	—	1.0	20.9
*u*830	C(48)...H(86)	344.2(17)	23.4(fixed)	—	0.5	23.4
*u*833	C(48)...H(75)	344.2(17)	22.2(fixed)	—	0.4	22.2
*u*817	C(1)...H(44)	344.3(14)	33.4(fixed)	—	3.9	33.4
*u*860	C(142)...Br(155)	344.3(8)	12.4(tied to *u*1009)	—	–0.1	11.7
*u*858	C(48)...H(84)	344.4(17)	23.8(fixed)	—	0.8	23.8
*u*856	C(48)...Br(61)	344.4(8)	12.4(tied to *u*1009)	—	–0.1	11.7
*u*917	H(82)...H(90)	344.5(66)	43.2(fixed)	—	–2.4	43.2
*u*915	H(19)...H(47)	344.6(66)	44.3(fixed)	—	–2.3	44.3
*u*839	C(1)...H(39)	344.6(17)	26.0(fixed)	—	0.7	26.0
*u*873	C(1)...H(37)	344.7(17)	22.0(fixed)	—	0.2	22.0
*u*882	H(66)...H(94)	344.7(66)	42.8(fixed)	—	–2.2	42.8
*u*879	C(1)...H(24)	344.8(17)	23.6(fixed)	—	0.6	23.6
*u*829	C(1)...H(28)	344.9(17)	25.2(fixed)	—	0.9	25.2
*u*927	C(101)...C(105)	345.2(44)	23.6(tied to *u*1009)	—	0.8	22.3
*u*841	C(95)...H(123)	345.3(17)	21.8(fixed)	—	0.6	21.8
*u*878	H(160)...H(188)	345.3(66)	40.6(fixed)	—	–2.0	40.6
*u*886	C(148)...C(149)	345.3(32)	20.1(fixed)	—	1.0	20.1
*u*804	C(95)...H(120)	345.3(17)	23.5(fixed)	—	0.9	23.5
*u*1058	H(30)...H(45)	345.7(44)	57.1(fixed)	—	0.5	57.1
*u*802	C(142)...H(167)	345.7(17)	22.2(fixed)	—	0.8	22.2
*u*840	C(48)...H(87)	345.7(17)	21.7(fixed)	—	0.5	21.7
*u*812	C(48)...H(73)	345.8(17)	23.5(fixed)	—	0.8	23.5
*u*848	C(48)...H(76)	345.8(17)	21.1(fixed)	—	0.5	21.1
*u*866	C(95)...Br(108)	345.8(7)	12.3(tied to *u*1009)	—	–0.1	11.6
*u*744	H(159)...H(187)	346.0(66)	43.2(fixed)	—	–0.7	43.2
*u*837	C(142)...H(170)	346.0(17)	23.2(fixed)	—	1.1	23.2
*u*768	H(112)...H(140)	346.1(66)	44.5(fixed)	—	–0.5	44.5
*u*808	C(48)...H(83)	346.2(17)	24.1(fixed)	—	1.3	24.1
*u*982	C(152)...C(158)	346.3(89)	20.3(fixed)	—	0.4	20.3
*u*759	H(65)...H(93)	346.5(66)	42.8(fixed)	—	–0.5	42.8
*u*775	H(18)...H(46)	346.5(66)	43.7(fixed)	—	–0.6	43.7
*u*893	C(57)...C(64)	346.5(33)	22.1(tied to *u*1009)	—	0.8	20.9
*u*750	H(81)...H(89)	346.7(66)	43.2(fixed)	—	–0.1	43.2
*u*845	C(1)...H(29)	347.0(17)	24.1(fixed)	—	0.9	24.1
*u*798	C(1)...H(36)	347.0(17)	21.9(fixed)	—	0.7	21.9
*u*761	C(60)...H(75)	347.1(58)	38.0(fixed)	—	2.3	38.0
*u*764	C(107)...H(120)	347.2(58)	43.6(fixed)	—	2.6	43.6

*u*861	C(1)...H(40)	347.3(17)	23.1(fixed)	—	1.1	23.1
*u*823	C(1)...H(26)	347.4(17)	22.7(fixed)	—	1.1	22.7
*u*1085	H(117)...H(129)	348.2(63)	63.1(fixed)	—	2.2	63.1
*u*853	Si(143)...C(147)	348.6(18)	17.3(tied to *u*1009)	—	0.2	16.3
*u*962	H(81)...H(92)	348.9(105)	42.8(fixed)	—	4.8	42.8
*u*1037	H(40)...H(43)	349.2(45)	66.9(fixed)	—	–1.4	66.9
*u*929	C(6)...C(12)	349.2(41)	22.1(fixed)	—	0.7	22.1
*u*932	Si(49)...C(53)	349.4(26)	17.2(tied to *u*1009)	—	0.2	16.2
*u*988	H(79)...H(94)	349.5(49)	54.5(fixed)	—	2.6	54.5
*u*918	C(60)...C(63)	349.7(34)	22.0(tied to *u*1009)	—	0.8	20.8
*u*922	Si(145)...C(158)	349.8(27)	17.3(tied to *u*1009)	—	0.2	16.3
*u*1061	H(65)...H(85)	349.9(36)	49.4(fixed)	—	1.6	49.4
*u*956	H(163)...H(165)	350.1(54)	48.1(fixed)	—	2.1	48.1
*u*957	H(23)...H(25)	350.3(82)	41.7(fixed)	—	6.7	41.7
*u*938	Si(143)...C(151)	350.4(18)	16.5(tied to *u*1009)	—	0.2	15.5
*u*739	C(56)...H(91)	350.4(36)	39.5(fixed)	—	2.5	39.5
*u*925	C(100)...C(103)	350.5(47)	22.7(tied to *u*1009)	—	0.8	21.5
*u*1053	H(115)...H(127)	350.8(49)	54.6(fixed)	—	3.4	54.6
*u*945	Si(2)...C(6)	351.3(15)	17.5(tied to *u*1009)	—	0.2	16.5
*u*905	C(100)...C(106)	351.3(41)	21.1(fixed)	—	0.8	21.1
*u*984	Br(14)...C(17)	351.5(51)	22.0(tied to *u*1009)	—	1.0	20.8
*u*911	Si(51)...C(64)	351.5(33)	17.1(tied to *u*1009)	—	0.2	16.1
*u*1032	H(68)...H(73)	352.1(78)	31.7(fixed)	—	4.7	31.7
*u*960	C(57)...Br(61)	353.1(34)	24.6(tied to *u*1009)	—	0.7	23.2
*u*892	C(55)...C(58)	353.2(31)	21.9(tied to *u*1009)	—	0.9	20.6
*u*951	Si(143)...C(150)	353.3(28)	17.3(tied to *u*1009)	—	0.1	16.4
*u*772	C(152)...H(167)	353.4(46)	41.6(fixed)	—	2.3	41.6
*u*934	Si(4)...C(17)	353.5(24)	17.2(tied to *u*1009)	—	0.3	16.2
*u*1017	C(147)...Br(156)	354.0(48)	21.4(tied to *u*1009)	—	1.0	20.2
*u*928	C(6)...C(8)	354.4(61)	22.7(tied to *u*1009)	—	0.8	21.5
*u*881	C(7)...C(9)	354.4(60)	22.2(tied to *u*1009)	—	0.9	20.9
*u*943	Si(96)...C(100)	354.5(20)	17.0(tied to *u*1009)	—	0.2	16.0
*u*998	H(21)...H(24)	355.1(87)	42.1(fixed)	—	5.2	42.1
*u*935	Si(4)...C(13)	355.6(27)	18.1(tied to *u*1009)	—	0.2	17.1
*u*936	Si(98)...C(111)	355.6(30)	17.6(tied to *u*1009)	—	0.2	16.7
*u*1084	H(86)...H(89)	355.7(54)	49.2(fixed)	—	1.9	49.2
*u*1122	H(112)...H(122)	355.8(73)	51.5(fixed)	—	1.6	51.5
*u*926	Si(96)...C(104)	355.9(21)	16.8(tied to *u*1009)	—	0.2	15.9
*u*980	H(80)...H(93)	355.9(98)	41.4(fixed)	—	6.8	41.4
*u*937	Si(5)...C(8)	356.0(40)	17.3(tied to *u*1009)	—	0.2	16.4
*u*940	Si(98)...C(107)	356.0(27)	17.4(tied to *u*1009)	—	0.2	16.4
*u*865	Si(96)...C(102)	356.1(29)	17.4(tied to *u*1009)	—	0.2	16.4
*u*916	C(147)...C(154)	356.1(36)	23.5(tied to *u*1009)	—	1.0	22.2
*u*1004	H(164)...H(166)	356.3(32)	42.7(fixed)	—	2.1	42.7
*u*942	Si(4)...C(9)	356.3(25)	17.5(tied to *u*1009)	—	0.2	16.5
*u*1018	H(112)...H(132)	356.3(39)	49.2(fixed)	—	2.7	49.2

*u*867	Si(49)...C(56)	356.6(30)	17.2(tied to *u*1009)	—	0.1	16.3
*u*966	C(150)...Br(155)	357.0(32)	25.6(tied to *u*1009)	—	0.9	24.2
*u*1249	H(32)...H(45)	357.0(60)	55.2(fixed)	—	–6.3	55.2
*u*976	H(23)...H(27)	357.1(70)	53.4(fixed)	—	3.4	53.4
*u*1007	H(29)...H(34)	357.1(44)	54.4(fixed)	—	2.0	54.4
*u*950	Si(49)...C(57)	357.2(15)	17.1(tied to *u*1009)	—	0.1	16.1
*u*1095	H(20)...H(37)	357.4(70)	50.8(fixed)	—	3.0	50.8
*u*941	Si(52)...C(58)	357.6(25)	17.6(tied to *u*1009)	—	0.2	16.6
*u*897	C(8)...C(12)	357.6(58)	21.4(tied to *u*1009)	—	0.9	20.2
*u*921	C(148)...C(152)	357.6(43)	23.3(tied to *u*1009)	—	0.7	22.0
*u*1023	H(77)...H(92)	358.2(36)	49.8(fixed)	—	3.0	49.8
*u*1050	H(168)...H(181)	358.3(81)	42.8(fixed)	—	6.5	42.8
*u*930	C(7)...C(11)	358.5(46)	23.8(tied to *u*1009)	—	0.8	22.5
*u*1029	H(18)...H(38)	358.9(40)	49.1(fixed)	—	3.4	49.1
*u*1031	H(73)...H(80)	358.9(53)	56.1(fixed)	—	1.3	56.1
*u*986	H(124)...H(134)	359.1(61)	42.1(fixed)	—	3.2	42.1
*u*946	Si(51)...C(60)	359.1(26)	17.4(tied to *u*1009)	—	0.2	16.4
*u*931	Si(3)...C(12)	359.3(28)	16.9(tied to *u*1009)	—	0.3	15.9
*u*862	Si(50)...C(63)	359.3(14)	17.0(tied to *u*1009)	—	0.1	16.0
*u*965	C(59)...Br(62)	359.6(36)	25.3(tied to *u*1009)	—	0.8	23.9
*u*1019	H(159)...H(179)	359.7(52)	39.6(fixed)	—	5.2	39.6
*u*949	Si(2)...C(10)	360.3(18)	17.6(tied to *u*1009)	—	0.2	16.6
*u*1145	C(54)...Br(62)	360.4(79)	26.9(tied to *u*1009)	—	0.3	25.4
*u*1124	Si(52)...Br(62)	360.4(29)	18.6(tied to *u*1009)	—	0.1	17.6
*u*978	H(34)...H(45)	360.6(84)	45.2(fixed)	—	4.6	45.2
*u*947	Si(5)...C(11)	360.6(27)	17.9(tied to *u*1009)	—	0.2	16.9
*u*989	H(19)...H(24)	360.7(68)	50.1(fixed)	—	3.6	50.1
*u*1042	Si(50)...H(69)	361.1(59)	33.1(fixed)	—	0.2	33.1
*u*948	Si(50)...C(59)	361.3(28)	17.2(tied to *u*1009)	—	0.2	16.3
*u*975	H(30)...H(40)	361.4(54)	49.6(fixed)	—	3.5	49.6
*u*963	H(71)...H(81)	361.6(36)	48.8(fixed)	—	1.9	48.8
*u*994	C(58)...C(64)	361.6(90)	21.7(tied to *u*1009)	—	0.4	20.5
*u*933	Si(145)...C(149)	361.9(22)	17.6(tied to *u*1009)	—	0.2	16.7
*u*944	C(54)...C(58)	362.0(67)	24.2(tied to *u*1009)	—	0.7	22.9
*u*1028	Br(61)...C(64)	362.1(74)	21.8(tied to *u*1009)	—	0.9	20.6
*u*1250	H(70)...H(71)	362.2(86)	41.5(fixed)	—	–1.8	41.5
*u*1009	Si(2)...Br(15)	362.4(19)	18.8(5)	—	0.0	17.8
*u*973	H(87)...H(90)	362.5(35)	44.2(fixed)	—	2.6	44.2
*u*952	Si(3)...C(16)	362.5(18)	18.4(tied to *u*1009)	—	0.2	17.4
*u*993	H(114)...H(131)	362.9(67)	53.6(fixed)	—	2.7	53.6
*u*919	C(56)...C(63)	362.9(35)	22.6(tied to *u*1009)	—	0.8	21.3
*u*1008	C(7)...C(8)	363.0(70)	25.0(tied to *u*513)	—	0.3	21.5
*u*1003	Br(15)...C(16)	363.0(43)	27.1(tied to *u*1009)	—	1.0	25.6
*u*1030	H(29)...H(43)	363.0(63)	55.9(fixed)	—	0.4	55.9
*u*1073	H(66)...H(83)	363.3(49)	33.3(fixed)	—	7.3	33.3
*u*1025	Si(52)...H(73)	363.3(49)	28.0(fixed)	—	3.8	28.0

*u*955	C(101)...Br(109)	363.3(39)	24.5(tied to *u*1009)	—	0.8	23.1
*u*1123	C(150)...C(154)	363.4(72)	25.2(tied to *u*1009)	—	0.1	23.7
*u*1014	C(13)...Br(15)	363.5(39)	22.7(tied to *u*1009)	—	1.0	21.4
*u*968	Si(3)...H(35)	363.6(26)	29.4(fixed)	—	7.0	29.4
*u*1264	H(117)...H(127)	363.6(83)	46.3(fixed)	—	–2.5	46.3
*u*1024	C(10)...Br(14)	363.6(41)	26.5(tied to *u*1009)	—	0.8	25.1
*u*1072	Si(5)...Br(14)	363.7(27)	18.4(tied to *u*1009)	—	0.1	17.4
*u*1041	H(82)...H(92)	363.7(130)	40.7(fixed)	—	2.5	40.7
*u*981	H(113)...H(123)	363.8(47)	47.5(fixed)	—	2.4	47.5
*u*967	Si(3)...H(22)	363.8(42)	36.2(fixed)	—	–0.1	36.2
*u*939	Si(51)...C(55)	364.1(21)	17.8(tied to *u*1009)	—	0.2	16.8
*u*1080	H(159)...H(182)	364.1(42)	47.5(fixed)	—	2.3	47.5
*u*1236	H(40)...H(42)	364.3(76)	53.6(fixed)	—	–9.3	53.6
*u*1256	H(65)...H(84)	364.5(79)	44.0(fixed)	—	–3.1	44.0
*u*977	Si(49)...H(91)	364.9(35)	27.2(fixed)	—	3.5	27.2
*u*983	H(161)...H(181)	365.2(55)	59.0(fixed)	—	1.9	59.0
*u*1027	H(80)...H(94)	365.4(134)	38.4(fixed)	—	4.5	38.4
*u*910	C(102)...C(107)	365.5(51)	21.4(fixed)	—	0.9	21.4
*u*995	H(21)...H(33)	365.6(46)	55.3(fixed)	—	5.6	55.3
*u*979	H(126)...H(135)	365.8(56)	40.4(fixed)	—	8.0	40.4
*u*1049	H(160)...H(178)	366.0(54)	39.9(fixed)	—	4.3	39.9
*u*970	H(127)...H(140)	366.1(111)	42.0(fixed)	—	6.5	42.0
*u*903	C(56)...C(60)	366.3(48)	21.6(tied to *u*1009)	—	0.8	20.4
*u*1121	H(116)...H(128)	366.7(58)	34.9(fixed)	—	6.2	34.9
*u*1128	Si(98)...Br(109)	366.8(21)	18.5(tied to *u*1009)	—	0.2	17.5
*u*1079	H(31)...H(46)	367.2(55)	37.8(fixed)	—	13.5	37.8
*u*1175	H(71)...H(80)	367.3(69)	41.6(fixed)	—	–2.6	41.6
*u*1167	H(169)...H(181)	367.4(104)	43.8(fixed)	—	3.1	43.8
*u*953	Si(50)...H(82)	367.6(19)	28.7(fixed)	—	5.8	28.7
*u*972	H(24)...H(36)	367.7(83)	51.0(fixed)	—	1.7	51.0
*u*996	Si(96)...H(138)	367.8(43)	28.8(fixed)	—	4.5	28.8
*u*1035	H(162)...H(167)	368.0(44)	30.6(fixed)	—	5.3	30.6
*u*1127	C(6)...Br(14)	368.0(57)	26.1(tied to *u*1009)	—	0.3	24.6
*u*1136	H(23)...H(35)	368.2(70)	62.7(fixed)	—	3.1	62.7
*u*1021	H(25)...H(37)	368.3(62)	46.3(fixed)	—	1.8	46.3
*u*1082	Si(49)...H(67)	368.5(48)	33.6(fixed)	—	0.2	33.6
*u*1125	Si(145)...Br(155)	368.7(20)	18.6(tied to *u*1009)	—	0.2	17.5
*u*987	Si(3)...H(20)	368.8(49)	27.6(fixed)	—	4.6	27.6
*u*1012	Si(143)...H(161)	368.8(29)	33.7(fixed)	—	0.0	33.7
*u*1245	H(112)...H(131)	368.8(69)	43.2(fixed)	—	–2.0	43.2
*u*1111	Si(145)...H(188)	368.8(41)	32.9(fixed)	—	0.0	32.9
*u*1081	H(78)...H(93)	369.0(40)	32.1(fixed)	—	4.9	32.1
*u*1047	C(101)...C(103)	369.1(52)	22.8(tied to *u*1009)	—	0.3	21.6
*u*923	C(149)...C(152)	369.2(42)	22.8(tied to *u*1009)	—	0.8	21.5
*u*1044	H(74)...H(89)	369.3(37)	43.3(fixed)	—	2.7	43.3
*u*961	Si(2)...H(44)	369.3(40)	36.6(fixed)	—	14.6	36.6

*u*985	H(162)...H(174)	369.5(48)	45.1(fixed)	—	3.4	45.1
*u*1068	H(27)...H(35)	369.7(54)	33.7(fixed)	—	8.9	33.7
*u*1141	Si(96)...H(141)	369.7(31)	28.8(fixed)	—	5.2	28.8
*u*1001	Si(52)...H(83)	369.8(37)	28.1(fixed)	—	5.5	28.1
*u*1069	Si(51)...H(94)	369.9(56)	34.2(fixed)	—	0.2	34.2
*u*1092	H(22)...H(24)	369.9(85)	40.5(fixed)	—	2.5	40.5
*u*1109	H(164)...H(176)	370.0(59)	49.1(fixed)	—	2.4	49.1
*u*1010	H(22)...H(29)	370.1(74)	56.0(fixed)	—	2.5	56.0
*u*1090	Si(143)...H(172)	370.1(28)	30.8(fixed)	—	0.2	30.8
*u*1026	Si(98)...H(116)	370.3(33)	29.8(fixed)	—	5.8	29.8
*u*1055	H(77)...H(87)	370.3(49)	39.9(fixed)	—	3.7	39.9
*u*1113	H(19)...H(36)	370.4(57)	32.5(fixed)	—	2.6	32.5
*u*1133	H(18)...H(26)	370.5(80)	53.6(fixed)	—	2.0	53.6
*u*1075	H(118)...H(132)	370.5(87)	40.6(fixed)	—	4.9	40.6
*u*1052	H(68)...H(80)	370.6(65)	51.0(fixed)	—	4.3	51.0
*u*990	Si(5)...H(31)	370.7(29)	32.7(fixed)	—	9.8	32.7
*u*1172	H(29)...H(33)	371.1(70)	49.0(fixed)	—	–3.5	49.0
*u*1048	C(147)...C(153)	371.4(48)	22.0(fixed)	—	0.3	22.0
*u*1022	Si(52)...H(78)	371.5(20)	27.3(fixed)	—	4.5	27.3
*u*992	Si(145)...H(177)	371.6(35)	26.4(fixed)	—	3.9	26.4
*u*1118	Si(52)...Br(61)	371.6(24)	18.7(tied to *u*1009)	—	0.1	17.6
*u*1164	C(148)...Br(156)	371.7(40)	27.0(tied to *u*1009)	—	0.2	25.5
*u*1154	Si(50)...H(67)	371.7(63)	28.1(fixed)	—	3.5	28.1
*u*1110	Si(2)...H(20)	371.9(28)	34.7(fixed)	—	0.3	34.7
*u*1094	H(88)...H(91)	371.9(45)	30.9(fixed)	—	4.1	30.9
*u*1020	H(33)...H(46)	372.2(89)	41.7(fixed)	—	9.5	41.7
*u*1064	H(79)...H(88)	372.7(34)	39.4(fixed)	—	5.7	39.4
*u*1093	H(125)...H(134)	372.9(80)	41.4(fixed)	—	0.8	41.4
*u*1033	H(76)...H(85)	372.9(53)	42.6(fixed)	—	2.9	42.6
*u*1040	C(11)...C(17)	373.1(74)	23.5(tied to *u*1009)	—	0.4	22.2
*u*969	Si(2)...H(26)	373.2(40)	26.4(fixed)	—	4.7	26.4
*u*1105	H(23)...H(26)	373.3(86)	39.7(fixed)	—	3.9	39.7
*u*1237	H(164)...H(165)	373.3(56)	39.6(fixed)	—	–1.9	39.6
*u*1108	Si(4)...H(47)	373.5(36)	35.5(fixed)	—	0.3	35.5
*u*1011	C(105)...C(111)	373.9(96)	21.8(tied to *u*1009)	—	0.4	20.6
*u*1063	H(120)...H(137)	373.9(55)	32.5(fixed)	—	4.8	32.5
*u*1134	Si(4)...H(39)	373.9(41)	38.3(fixed)	—	–0.3	38.3
*u*1065	C(10)...C(13)	374.1(45)	24.5(tied to *u*1009)	—	0.3	23.1
*u*1013	Si(98)...H(120)	374.7(40)	27.8(fixed)	—	4.2	27.8
*u*1269	H(18)...H(37)	374.8(72)	44.0(fixed)	—	–1.2	44.0
*u*1211	H(87)...H(89)	375.0(59)	38.5(fixed)	—	–1.2	38.5
*u*1170	Si(143)...H(169)	375.0(37)	38.4(fixed)	—	–0.7	38.4
*u*1034	Si(5)...H(36)	375.1(38)	26.6(fixed)	—	3.3	26.6
*u*1120	H(114)...H(121)	375.4(63)	32.8(fixed)	—	5.6	32.8
*u*1138	Si(4)...H(28)	375.5(39)	37.0(fixed)	—	–0.2	37.0
*u*1006	H(118)...H(135)	375.6(53)	43.9(fixed)	—	3.6	43.9

*u*1131	H(70)...H(82)	375.8(101)	55.4(fixed)	—	3.3	55.4
*u*1102	H(161)...H(178)	376.3(74)	38.2(fixed)	—	2.2	38.2
*u*1241	H(23)...H(33)	376.4(55)	50.5(fixed)	—	–1.2	50.5
*u*1155	C(53)...Br(61)	376.7(75)	26.0(tied to *u*1009)	—	0.3	24.5
*u*1002	Si(96)...H(122)	377.3(38)	27.5(fixed)	—	3.5	27.5
*u*1114	H(31)...H(40)	377.4(69)	51.0(fixed)	—	0.3	51.0
*u*1126	H(126)...H(133)	377.5(79)	37.9(fixed)	—	5.2	37.9
*u*1149	Si(98)...H(133)	377.5(41)	32.9(fixed)	—	–0.2	32.9
*u*1089	C(102)...C(106)	377.7(80)	22.6(tied to *u*1425)	—	0.3	21.8
*u*997	H(76)...H(88)	377.7(50)	43.2(fixed)	—	2.6	43.2
*u*1103	C(57)...C(60)	377.7(37)	23.3(tied to *u*1009)	—	0.2	22.0
*u*1000	Si(50)...H(86)	378.0(35)	27.2(fixed)	—	3.4	27.2
*u*1005	H(165)...H(175)	378.0(46)	45.4(fixed)	—	2.9	45.4
*u*1132	Si(98)...H(141)	378.1(45)	39.7(fixed)	—	–0.3	39.7
*u*1148	Si(143)...H(185)	378.2(42)	26.9(fixed)	—	3.7	26.9
*u*1070	H(72)...H(82)	378.4(41)	32.3(fixed)	—	8.1	32.3
*u*1016	H(32)...H(41)	378.4(47)	47.5(fixed)	—	13.5	47.5
*u*1129	Si(96)...H(125)	378.6(32)	39.5(fixed)	—	–0.3	39.5
*u*1226	H(24)...H(37)	378.7(91)	42.3(fixed)	—	–2.5	42.3
*u*1051	Si(4)...H(22)	378.7(29)	29.4(fixed)	—	5.1	29.4
*u*1038	H(76)...H(91)	379.2(55)	48.1(fixed)	—	2.3	48.1
*u*1054	Si(145)...H(163)	379.2(30)	27.1(fixed)	—	3.0	27.1
*u*1046	Si(145)...H(169)	379.2(28)	28.4(fixed)	—	5.1	28.4
*u*1101	Si(97)...H(138)	379.3(33)	35.2(fixed)	—	0.1	35.2
*u*1261	H(79)...H(92)	379.5(61)	43.5(fixed)	—	–2.0	43.5
*u*1156	C(12)...Br(15)	379.5(42)	27.1(tied to *u*1009)	—	0.3	25.6
*u*1130	H(20)...H(25)	379.6(76)	32.7(fixed)	—	4.6	32.7
*u*991	Si(143)...H(188)	379.7(28)	27.1(fixed)	—	3.8	27.1
*u*1160	Si(2)...H(47)	379.8(29)	27.5(fixed)	—	4.5	27.5
*u*1066	Si(5)...H(28)	379.8(41)	29.3(fixed)	—	5.0	29.3
*u*1097	H(35)...H(45)	379.8(105)	45.7(fixed)	—	1.9	45.7
*u*1243	H(76)...H(89)	379.8(71)	39.7(fixed)	—	–1.1	39.7
*u*1137	Si(52)...H(82)	379.9(37)	38.7(fixed)	—	–0.1	38.7
*u*1373	C(13)...H(42)	379.9(63)	60.3(fixed)	—	–8.5	60.3
*u*1116	H(159)...H(177)	379.9(70)	38.0(fixed)	—	3.0	38.0
*u*1074	Si(51)...H(75)	379.9(29)	26.6(fixed)	—	3.1	26.6
*u*1239	H(18)...H(24)	380.1(73)	44.0(fixed)	—	–1.4	44.0
*u*1099	H(41)...H(44)	380.2(56)	44.8(fixed)	—	22.9	44.8
*u*1067	H(74)...H(84)	380.3(50)	40.5(fixed)	—	7.3	40.5
*u*1098	C(9)...C(16)	380.3(54)	25.1(tied to *u*1009)	—	0.3	23.7
*u*1119	H(22)...H(34)	380.5(58)	34.6(fixed)	—	3.2	34.6
*u*1083	Si(49)...H(75)	380.6(41)	31.0(fixed)	—	–0.3	31.0
*u*1166	Br(109)...C(110)	381.1(59)	26.8(tied to *u*1009)	—	0.2	25.3
*u*1076	H(21)...H(28)	381.3(75)	33.6(fixed)	—	5.6	33.6
*u*1059	Si(51)...H(69)	381.3(50)	29.2(fixed)	—	3.7	29.2
*u*1144	H(29)...H(44)	381.4(84)	58.4(fixed)	—	–3.3	58.4

*u*1104	C(56)...C(59)	381.6(43)	24.1(tied to *u*1009)	—	0.2	22.7
*u*1060	Si(96)...H(120)	381.7(39)	34.1(fixed)	—	–0.2	34.1
*u*1247	H(112)...H(123)	381.7(79)	40.8(fixed)	—	–1.7	40.8
*u*1161	Si(49)...H(78)	381.9(19)	34.3(fixed)	—	–0.2	34.3
*u*1056	H(75)...H(87)	382.1(64)	47.7(fixed)	—	1.8	47.7
*u*1039	H(120)...H(134)	382.7(70)	52.6(fixed)	—	2.5	52.6
*u*1150	Si(51)...H(86)	382.7(39)	32.9(fixed)	—	–0.2	32.9
*u*1363	C(17)...H(32)	382.9(52)	48.9(fixed)	—	–5.6	48.9
*u*1106	H(160)...H(180)	383.2(50)	34.3(fixed)	—	7.0	34.3
*u*1112	H(163)...H(175)	383.4(58)	32.5(fixed)	—	2.7	32.5
*u*1168	Si(2)...H(31)	383.5(27)	48.5(fixed)	—	–0.8	48.5
*u*1152	Si(49)...H(94)	383.5(50)	26.6(fixed)	—	4.2	26.6
*u*1151	Si(5)...H(26)	383.9(46)	34.4(fixed)	—	–0.1	34.4
*u*1062	H(33)...H(47)	384.3(106)	43.8(fixed)	—	6.5	43.8
*u*1158	Si(5)...H(35)	384.4(41)	41.6(fixed)	—	–0.3	41.6
*u*1169	Si(3)...H(44)	384.6(29)	58.2(fixed)	—	–0.9	58.2
*u*1087	Si(3)...H(36)	384.8(37)	30.5(fixed)	—	0.3	30.5
*u*1078	H(26)...H(38)	385.0(76)	31.0(fixed)	—	6.6	31.0
*u*1036	H(127)...H(141)	385.6(137)	41.5(fixed)	—	4.1	41.5
*u*1107	H(75)...H(90)	385.7(49)	31.7(fixed)	—	3.4	31.7
*u*1159	H(118)...H(130)	386.0(118)	37.8(fixed)	—	2.3	37.8
*u*1143	H(69)...H(81)	386.0(91)	34.5(fixed)	—	2.3	34.5
*u*1043	Si(50)...H(91)	386.1(21)	31.8(fixed)	—	–0.1	31.8
*u*1117	H(32)...H(39)	386.2(68)	43.9(fixed)	—	9.4	43.9
*u*1077	H(72)...H(89)	386.9(46)	39.7(fixed)	—	4.1	39.7
*u*1244	H(23)...H(29)	387.2(72)	46.2(fixed)	—	–2.4	46.2
*u*1139	H(78)...H(87)	387.2(56)	38.7(fixed)	—	1.6	38.7
*u*1374	C(54)...H(71)	387.3(69)	32.4(fixed)	—	–2.0	32.4
*u*1165	Si(50)...H(83)	387.8(37)	36.9(fixed)	—	–0.3	36.9
*u*1091	H(167)...H(174)	387.8(64)	51.5(fixed)	—	1.8	51.5
*u*1088	H(71)...H(90)	388.1(51)	39.9(fixed)	—	4.4	39.9
*u*1174	Si(2)...C(16)	388.2(31)	17.3(tied to *u*1009)	—	–0.2	16.3
*u*1255	H(159)...H(181)	388.4(71)	44.2(fixed)	—	–2.7	44.2
*u*1366	H(39)...H(43)	388.4(50)	52.1(fixed)	—	–10.8	52.1
*u*1162	Si(3)...H(39)	388.7(36)	29.7(fixed)	—	4.5	29.7
*u*1153	H(79)...H(86)	388.7(54)	36.8(fixed)	—	3.4	36.8
*u*1173	Si(3)...C(11)	388.7(20)	16.2(tied to *u*1425)	—	–0.2	15.6
*u*1367	C(53)...H(84)	388.9(54)	39.1(fixed)	—	–3.0	39.1
*u*1266	H(69)...H(72)	389.0(95)	42.9(fixed)	—	–1.5	42.9
*u*1231	C(10)...H(42)	389.2(12)	16.3(fixed)	—	–9.3	16.3
*u*1140	Si(145)...H(167)	389.8(30)	32.8(fixed)	—	–0.1	32.8
*u*1358	C(9)...H(33)	389.9(58)	42.9(fixed)	—	–3.9	42.9
*u*1157	H(76)...H(83)	389.9(54)	39.8(fixed)	—	0.4	39.8
*u*1257	Si(52)...C(55)	390.0(39)	16.6(tied to *u*1009)	—	–0.1	15.7
*u*1270	H(70)...H(80)	390.3(92)	46.0(fixed)	—	–1.0	46.0
*u*1346	H(30)...H(47)	391.5(66)	52.9(fixed)	—	–6.5	52.9

*u*1135	Si(51)...H(73)	391.6(31)	32.8(fixed)	—	0.0	32.8
*u*1224	C(16)...H(31)	391.8(12)	14.9(fixed)	—	–6.8	14.9
*u*1206	C(11)...H(32)	391.9(12)	14.9(fixed)	—	–6.7	14.9
*u*1207	C(11)...H(44)	391.9(38)	16.0(fixed)	—	–9.5	16.0
*u*1100	H(119)...H(133)	392.2(66)	32.3(fixed)	—	3.9	32.3
*u*1192	Si(49)...C(63)	392.3(26)	16.2(tied to *u*1009)	—	–0.2	15.3
*u*1163	H(75)...H(84)	392.6(55)	37.0(fixed)	—	4.5	37.0
*u*1221	C(107)...H(130)	392.7(33)	13.4(fixed)	—	–3.6	13.4
*u*1228	C(60)...H(83)	392.8(32)	13.6(fixed)	—	–4.3	13.6
*u*1071	H(27)...H(42)	392.8(61)	51.0(fixed)	—	21.0	51.0
*u*1171	Si(50)...C(58)	392.8(13)	15.3(fixed)	—	–0.2	15.3
*u*1205	C(102)...H(123)	393.1(33)	13.5(fixed)	—	–3.3	13.5
*u*1179	Si(3)...C(6)	393.1(38)	16.4(tied to *u*1009)	—	–0.2	15.5
*u*1086	C(55)...C(63)	393.1(42)	23.0(tied to *u*1425)	—	0.3	22.1
*u*1393	C(105)...H(117)	393.2(60)	38.6(fixed)	—	–3.4	38.6
*u*1222	C(12)...H(40)	393.5(31)	14.1(fixed)	—	–4.2	14.1
*u*1229	C(149)...H(170)	393.5(32)	13.7(fixed)	—	–4.2	13.7
*u*1208	C(8)...H(29)	393.5(31)	13.9(fixed)	—	–4.1	13.9
*u*1209	C(10)...H(35)	393.6(12)	13.9(fixed)	—	–5.1	13.9
*u*1217	C(56)...H(73)	393.7(32)	13.2(fixed)	—	–3.3	13.2
*u*1230	C(9)...H(26)	393.8(31)	13.5(fixed)	—	–3.8	13.5
*u*1200	Si(96)...C(110)	393.9(32)	15.6(fixed)	—	–0.2	15.6
*u*1219	C(59)...H(87)	393.9(32)	13.5(fixed)	—	–3.1	13.5
*u*1203	C(55)...H(76)	394.0(32)	13.5(fixed)	—	–3.0	13.5
*u*1233	C(100)...H(116)	394.0(12)	13.8(fixed)	—	–4.7	13.8
*u*1227	C(57)...H(82)	394.0(12)	13.7(fixed)	—	–4.5	13.7
*u*1193	C(105)...H(126)	394.2(12)	14.0(fixed)	—	–4.5	14.0
*u*1223	Si(5)...C(10)	394.2(25)	16.7(tied to *u*1425)	—	–0.2	16.1
*u*1187	C(101)...H(141)	394.2(12)	13.6(fixed)	—	–4.5	13.6
*u*1225	C(150)...H(167)	394.4(32)	13.3(fixed)	—	–3.3	13.3
*u*1183	C(17)...H(23)	394.4(12)	14.0(fixed)	—	–4.3	14.0
*u*1176	H(118)...H(134)	394.5(75)	40.7(fixed)	—	–0.8	40.7
*u*1096	H(74)...H(86)	394.5(60)	30.6(fixed)	—	4.5	30.6
*u*1216	C(6)...H(22)	394.5(12)	13.6(fixed)	—	–4.2	13.6
*u*1292	Si(96)...C(111)	394.6(23)	15.4(tied to *u*1425)	—	–0.2	14.8
*u*1234	C(13)...H(36)	394.6(31)	13.2(fixed)	—	–3.1	13.2
*u*1246	Si(52)...C(59)	394.6(27)	16.5(tied to *u*1009)	—	–0.2	15.6
*u*1181	C(7)...H(47)	394.7(12)	13.5(fixed)	—	–4.0	13.5
*u*1195	C(54)...H(94)	394.7(12)	13.5(fixed)	—	–3.8	13.5
*u*1197	C(7)...H(18)	394.8(12)	13.9(fixed)	—	–3.9	13.9
*u*1196	C(148)...H(159)	394.8(12)	13.7(fixed)	—	–3.6	13.7
*u*1218	C(58)...H(79)	394.8(12)	13.7(fixed)	—	–3.7	13.7
*u*1204	C(63)...H(78)	394.8(12)	13.3(fixed)	—	–3.7	13.3
*u*1235	C(148)...H(188)	395.0(12)	13.4(fixed)	—	–3.5	13.4
*u*1214	C(101)...H(112)	395.1(12)	13.8(fixed)	—	–3.6	13.8
*u*1212	C(54)...H(65)	395.1(12)	13.6(fixed)	—	–3.5	13.6

*u*1232	C(53)...H(69)	395.1(12)	13.4(fixed)	—	–3.5	13.4
*u*1190	C(64)...H(70)	395.2(12)	13.6(fixed)	—	–3.3	13.6
*u*1198	C(57)...H(89)	395.4(12)	13.5(fixed)	—	–3.2	13.5
*u*1483	Br(108)...H(139)	395.4(70)	36.8(fixed)	—	–3.3	36.8
*u*1210	C(147)...H(163)	395.5(12)	13.2(fixed)	—	–2.9	13.2
*u*1201	C(152)...H(173)	395.6(12)	13.3(fixed)	—	–2.9	13.3
*u*1178	Si(2)...C(8)	395.9(33)	15.7(tied to *u*1425)	—	–0.2	15.1
*u*1220	H(165)...H(174)	396.0(75)	41.1(fixed)	—	–1.4	41.1
*u*1202	C(16)...H(33)	396.2(38)	14.4(fixed)	—	–5.4	14.4
*u*1251	Si(98)...C(101)	396.4(27)	16.0(fixed)	—	–0.2	16.0
*u*1349	Si(50)...C(53)	396.4(48)	15.2(fixed)	—	–0.2	15.2
*u*1194	C(100)...H(139)	397.0(38)	14.0(fixed)	—	–4.5	14.0
*u*1188	C(63)...H(80)	397.0(38)	14.0(fixed)	—	–4.4	14.0
*u*1285	H(77)...H(94)	397.2(83)	45.6(fixed)	—	–2.1	45.6
*u*1240	Si(145)...C(153)	397.2(26)	15.3(fixed)	—	–0.1	15.3
*u*1365	H(28)...H(34)	397.3(54)	49.1(fixed)	—	–4.8	49.1
*u*1371	C(55)...H(80)	397.4(47)	37.1(fixed)	—	–3.1	37.1
*u*1215	C(6)...H(45)	397.4(38)	13.9(fixed)	—	–4.1	13.9
*u*1191	C(53)...H(92)	397.5(38)	13.9(fixed)	—	–3.9	13.9
*u*1238	C(17)...H(20)	397.6(38)	13.7(fixed)	—	–4.0	13.7
*u*1364	C(148)...H(165)	397.6(47)	33.4(fixed)	—	–2.0	33.4
*u*1213	C(105)...H(138)	397.6(38)	13.5(fixed)	—	–3.9	13.5
*u*1184	H(76)...H(87)	397.7(72)	37.9(fixed)	—	–1.1	37.9
*u*1186	C(147)...H(186)	397.7(39)	13.6(fixed)	—	–3.6	13.6
*u*1182	C(152)...H(185)	397.8(39)	13.2(fixed)	—	–3.5	13.2
*u*1115	H(166)...H(176)	397.9(58)	31.9(fixed)	—	4.3	31.9
*u*1313	H(38)...H(40)	397.9(42)	26.4(fixed)	—	–4.3	26.4
*u*1189	C(64)...H(67)	398.0(38)	13.2(fixed)	—	–3.4	13.2
*u*1199	C(58)...H(91)	398.2(38)	13.2(fixed)	—	–3.2	13.2
*u*1327	H(67)...H(85)	398.4(78)	44.0(fixed)	—	–3.0	44.0
*u*1248	Si(52)...C(57)	398.4(18)	16.3(tied to *u*1425)	—	–0.1	15.6
*u*1263	H(164)...H(174)	398.5(70)	41.1(fixed)	—	–0.9	41.1
*u*1280	H(83)...H(88)	398.5(43)	25.5(fixed)	—	–4.3	25.5
*u*1275	H(25)...H(29)	398.6(42)	26.9(fixed)	—	–3.6	26.9
*u*1271	H(26)...H(27)	399.1(42)	26.2(fixed)	—	–3.1	26.2
*u*1253	Si(98)...C(102)	399.2(29)	15.5(fixed)	—	–0.1	15.5
*u*1387	C(60)...H(89)	399.3(48)	31.2(fixed)	—	–2.0	31.2
*u*1333	H(166)...H(170)	399.4(42)	26.2(fixed)	—	–4.1	26.2
*u*1288	H(120)...H(121)	399.4(43)	25.1(fixed)	—	–3.5	25.1
*u*1276	H(73)...H(74)	399.7(43)	24.6(fixed)	—	–3.2	24.6
*u*1300	H(119)...H(123)	399.8(43)	26.4(fixed)	—	–2.9	26.4
*u*1281	H(72)...H(76)	400.0(43)	26.1(fixed)	—	–2.7	26.1
*u*1262	Si(5)...C(12)	400.1(28)	16.7(tied to *u*1009)	—	–0.2	15.8
*u*1335	C(1)...H(43)	400.1(12)	15.7(fixed)	—	–8.5	15.7
*u*1381	C(64)...H(79)	400.2(35)	34.8(fixed)	—	–2.5	34.8
*u*1283	H(36)...H(41)	400.2(42)	25.4(fixed)	—	–2.2	25.4

*u*1286	H(85)...H(87)	400.4(43)	26.6(fixed)	—	–2.3	26.6
*u*1147	H(28)...H(42)	400.8(83)	49.1(fixed)	—	15.4	49.1
*u*1298	H(167)...H(168)	401.0(42)	25.6(fixed)	—	–2.6	25.6
*u*1177	Si(96)...C(103)	401.3(32)	16.0(tied to *u*1425)	—	–0.1	15.4
*u*1354	H(30)...H(42)	401.4(20)	33.6(fixed)	—	–9.3	33.6
*u*1515	Br(62)...H(65)	401.9(103)	32.5(fixed)	—	–2.4	32.5
*u*1443	C(152)...H(188)	402.1(105)	31.7(fixed)	—	–2.3	31.7
*u*1185	Si(50)...C(60)	402.1(31)	15.6(tied to *u*1425)	—	–0.1	15.0
*u*1341	Si(143)...C(157)	402.2(31)	15.3(tied to *u*1425)	—	–0.2	14.7
*u*1379	C(100)...H(131)	402.3(57)	34.1(fixed)	—	–2.4	34.1
*u*1396	C(103)...H(112)	402.4(67)	33.5(fixed)	—	–2.4	33.5
*u*1316	C(1)...H(30)	402.5(12)	14.5(fixed)	—	–6.1	14.5
*u*1401	C(6)...H(37)	402.5(59)	32.0(fixed)	—	–2.0	32.0
*u*1180	Si(143)...C(158)	402.8(20)	16.1(tied to *u*1425)	—	–0.2	15.5
*u*1357	Si(2)...C(17)	402.8(21)	15.7(tied to *u*1425)	—	–0.1	15.1
*u*1293	H(34)...H(44)	403.3(47)	32.1(fixed)	—	–10.3	32.1
*u*1259	Si(4)...C(7)	403.4(24)	16.9(tied to *u*1425)	—	–0.2	16.3
*u*1254	Si(5)...C(9)	403.4(33)	16.4(tied to *u*1425)	—	–0.1	15.8
*u*1291	H(163)...H(166)	403.6(41)	42.1(fixed)	—	–1.9	42.1
*u*1311	C(142)...H(168)	403.6(14)	13.3(fixed)	—	–3.7	13.3
*u*1242	Si(145)...C(150)	403.7(20)	16.5(tied to *u*1425)	—	–0.1	15.9
*u*1303	C(48)...H(85)	403.7(14)	13.4(fixed)	—	–3.7	13.4
*u*1322	C(1)...H(34)	403.8(12)	13.9(fixed)	—	–4.9	13.9
*u*1304	C(95)...H(119)	403.9(14)	13.3(fixed)	—	–3.2	13.3
*u*1331	C(95)...H(121)	404.1(14)	13.1(fixed)	—	–3.0	13.1
*u*1340	C(1)...H(41)	404.2(14)	13.5(fixed)	—	–3.9	13.5
*u*1314	C(1)...H(27)	404.3(14)	13.4(fixed)	—	–3.8	13.4
*u*1289	C(142)...H(166)	404.3(14)	13.2(fixed)	—	–3.0	13.2
*u*1309	C(48)...H(72)	404.5(14)	13.2(fixed)	—	–3.0	13.2
*u*1338	H(32)...H(34)	404.5(20)	30.3(fixed)	—	–6.7	30.3
*u*1343	C(95)...H(128)	404.5(12)	13.8(fixed)	—	–4.2	13.8
*u*1310	C(48)...H(88)	404.6(14)	13.1(fixed)	—	–2.9	13.1
*u*1302	C(95)...H(115)	404.6(12)	13.8(fixed)	—	–4.2	13.8
*u*1326	C(48)...H(81)	404.6(12)	13.7(fixed)	—	–4.1	13.7
*u*1321	C(1)...H(25)	404.6(14)	13.3(fixed)	—	–3.4	13.3
*u*1318	C(48)...H(74)	404.7(14)	13.0(fixed)	—	–2.7	13.0
*u*1305	C(1)...H(21)	404.8(12)	13.7(fixed)	—	–4.0	13.7
*u*1258	Si(145)...C(148)	404.8(25)	16.5(tied to *u*1425)	—	–0.2	15.8
*u*1361	H(162)...H(176)	404.9(60)	45.9(fixed)	—	–1.4	45.9
*u*1345	C(1)...H(19)	405.0(12)	13.6(fixed)	—	–3.7	13.6
*u*1353	C(1)...H(46)	405.1(12)	13.7(fixed)	—	–3.6	13.7
*u*1337	C(48)...H(93)	405.2(12)	13.6(fixed)	—	–3.6	13.6
*u*1334	C(95)...H(113)	405.2(12)	13.5(fixed)	—	–3.6	13.5
*u*1296	C(1)...H(38)	405.4(14)	13.0(fixed)	—	–2.7	13.0
*u*1325	C(48)...H(77)	405.4(12)	13.4(fixed)	—	–3.4	13.4
*u*1252	Si(51)...C(56)	405.5(21)	16.0(tied to *u*1425)	—	–0.1	15.4

*u*1351	C(48)...H(66)	405.5(12)	13.5(fixed)	—	–3.3	13.5
*u*1308	C(48)...H(68)	405.5(12)	13.5(fixed)	—	–3.3	13.5
*u*1324	C(142)...H(175)	405.6(12)	13.5(fixed)	—	–3.3	13.5
*u*1350	C(142)...H(160)	405.7(12)	13.5(fixed)	—	–3.2	13.5
*u*1342	Si(49)...C(64)	405.7(36)	15.1(tied to *u*1425)	—	–0.2	14.5
*u*1328	C(48)...H(90)	405.8(12)	13.4(fixed)	—	–3.0	13.4
*u*1299	H(22)...H(27)	406.1(70)	48.7(fixed)	—	–2.8	48.7
*u*1323	C(142)...H(162)	406.2(12)	13.2(fixed)	—	–2.7	13.2
*u*1336	H(31)...H(43)	406.3(20)	32.6(fixed)	—	–4.6	32.6
*u*1260	Si(51)...C(54)	406.4(38)	17.0(tied to *u*1425)	—	–0.2	16.4
*u*1368	C(12)...H(24)	406.5(76)	36.1(fixed)	—	–2.6	36.1
*u*1409	C(54)...H(72)	406.7(67)	31.0(fixed)	—	–2.4	31.0
*u*1370	H(115)...H(129)	406.8(68)	51.5(fixed)	—	–3.5	51.5
*u*1317	H(77)...H(82)	406.9(20)	26.1(fixed)	—	–4.6	26.1
*u*1332	H(113)...H(116)	407.0(20)	26.8(fixed)	—	–4.6	26.8
*u*1297	H(117)...H(140)	407.1(20)	29.1(fixed)	—	–4.2	29.1
*u*1301	H(30)...H(35)	407.3(20)	29.6(fixed)	—	–4.0	29.6
*u*1307	H(159)...H(162)	407.4(20)	26.3(fixed)	—	–3.7	26.3
*u*1279	H(23)...H(46)	407.5(19)	28.2(fixed)	—	–4.0	28.2
*u*1272	H(115)...H(141)	407.5(20)	26.8(fixed)	—	–4.0	26.8
*u*1282	H(68)...H(94)	407.6(19)	25.9(fixed)	—	–3.9	25.9
*u*1385	H(113)...H(122)	407.6(55)	45.8(fixed)	—	–2.8	45.8
*u*1320	H(19)...H(22)	407.6(19)	27.1(fixed)	—	–4.0	27.1
*u*1295	H(162)...H(188)	407.8(20)	25.0(fixed)	—	–3.5	25.0
*u*1274	H(78)...H(90)	407.9(19)	25.4(fixed)	—	–3.7	25.4
*u*1344	H(18)...H(21)	408.0(19)	28.6(fixed)	—	–3.5	28.6
*u*1356	H(79)...H(81)	408.0(20)	28.4(fixed)	—	–3.2	28.4
*u*1506	Br(14)...H(45)	408.0(62)	35.7(fixed)	—	–3.3	35.7
*u*1348	H(65)...H(68)	408.0(20)	26.8(fixed)	—	–3.3	26.8
*u*1265	H(21)...H(47)	408.1(19)	26.7(fixed)	—	–3.6	26.7
*u*1312	H(66)...H(69)	408.3(19)	25.6(fixed)	—	–3.2	25.6
*u*1347	H(112)...H(115)	408.3(20)	28.7(fixed)	—	–3.0	28.7
*u*1315	H(70)...H(93)	408.5(20)	27.2(fixed)	—	–2.9	27.2
*u*1395	C(8)...H(18)	408.5(67)	33.6(fixed)	—	–2.6	33.6
*u*1362	H(161)...H(182)	408.6(46)	46.4(fixed)	—	–3.0	46.4
*u*1306	H(164)...H(187)	408.6(20)	26.1(fixed)	—	–2.5	26.1
*u*1294	H(77)...H(89)	408.6(20)	26.8(fixed)	—	–2.7	26.8
*u*1273	H(160)...H(163)	408.8(20)	25.1(fixed)	—	–2.5	25.1
*u*1398	C(11)...H(23)	408.8(51)	36.2(fixed)	—	–3.0	36.2
*u*1142	H(71)...H(91)	408.8(63)	37.0(fixed)	—	2.4	37.0
*u*1505	Br(155)...H(183)	408.9(65)	33.9(fixed)	—	–2.5	33.9
*u*1330	H(80)...H(90)	409.4(47)	27.5(fixed)	—	–4.6	27.5
*u*1339	H(113)...H(139)	409.4(47)	28.5(fixed)	—	–4.5	28.5
*u*1478	C(13)...H(43)	409.5(35)	45.1(fixed)	—	–10.1	45.1
*u*1355	Si(3)...C(13)	409.8(32)	15.8(tied to *u*1425)	—	–0.2	15.2
*u*1146	H(73)...H(89)	409.8(61)	36.3(fixed)	—	2.1	36.3

*u*1290	H(66)...H(92)	410.1(47)	27.5(fixed)	—	–3.8	27.5
*u*1287	H(160)...H(186)	410.3(47)	27.0(fixed)	—	–3.3	27.0
*u*1268	H(161)...H(187)	410.4(47)	25.7(fixed)	—	–3.4	25.7
*u*1319	H(19)...H(45)	410.6(47)	27.6(fixed)	—	–3.7	27.6
*u*1329	H(33)...H(43)	410.6(47)	34.1(fixed)	—	–2.7	34.1
*u*1278	H(20)...H(46)	410.9(47)	26.3(fixed)	—	–3.5	26.3
*u*1284	H(114)...H(140)	411.0(47)	26.9(fixed)	—	–3.1	26.9
*u*1360	H(20)...H(38)	411.0(56)	45.1(fixed)	—	–1.2	45.1
*u*1466	C(17)...H(30)	411.2(43)	39.9(fixed)	—	–6.8	39.9
*u*1267	H(67)...H(93)	411.2(47)	25.8(fixed)	—	–3.0	25.8
*u*1523	Br(62)...H(66)	411.3(71)	34.2(fixed)	—	–2.6	34.2
*u*1277	H(81)...H(91)	411.7(47)	26.4(fixed)	—	–2.4	26.4
*u*1519	Br(108)...H(140)	411.7(43)	36.4(fixed)	—	–4.0	36.4
*u*1386	Si(49)...Br(62)	412.3(19)	18.0(tied to *u*1425)	—	–0.3	17.3
*u*1372	C(147)...H(181)	412.3(51)	39.7(fixed)	—	–2.9	39.7
*u*1389	Si(143)...Br(156)	412.4(16)	18.1(tied to *u*1425)	—	–0.2	17.4
*u*1378	H(86)...H(90)	414.0(48)	44.5(fixed)	—	–2.1	44.5
*u*1380	C(7)...H(29)	414.6(63)	35.2(fixed)	—	–3.0	35.2
*u*1467	H(32)...H(42)	414.9(24)	35.2(fixed)	—	–11.2	35.2
*u*1384	C(63)...H(76)	415.1(52)	31.3(fixed)	—	–1.7	31.3
*u*1464	C(53)...H(85)	416.1(36)	32.8(fixed)	—	–3.7	32.8
*u*1399	Si(51)...Br(61)	416.2(22)	17.9(tied to *u*1425)	—	–0.3	17.2
*u*1416	C(58)...H(94)	416.9(112)	33.7(fixed)	—	–2.6	33.7
*u*1465	C(9)...H(34)	417.3(36)	35.2(fixed)	—	–5.2	35.2
*u*1473	H(31)...H(44)	417.7(24)	38.9(fixed)	—	–7.7	38.9
*u*1394	H(19)...H(26)	417.7(81)	50.0(fixed)	—	–3.1	50.0
*u*1510	Br(61)...H(92)	418.0(100)	34.1(fixed)	—	–2.9	34.1
*u*1407	C(58)...H(70)	418.1(86)	32.6(fixed)	—	–2.2	32.6
*u*1397	C(152)...H(164)	418.5(54)	30.8(fixed)	—	–1.8	30.8
*u*1507	Br(14)...H(46)	418.8(48)	34.6(fixed)	—	–3.0	34.6
*u*1423	H(32)...H(33)	418.9(24)	30.8(fixed)	—	–7.9	30.8
*u*1531	C(152)...H(187)	419.2(82)	30.7(fixed)	—	–3.2	30.7
*u*1412	Si(4)...Br(15)	419.9(28)	18.6(tied to *u*1425)	—	–0.3	17.9
*u*1383	H(68)...H(82)	420.0(75)	52.5(fixed)	—	–1.9	52.5
*u*1481	C(105)...H(115)	420.0(42)	35.4(fixed)	—	–4.0	35.4
*u*1411	Br(14)...H(39)	420.1(12)	14.2(fixed)	—	–4.8	14.2
*u*1352	H(114)...H(132)	420.1(61)	45.5(fixed)	—	–2.2	45.5
*u*1426	Br(15)...H(28)	420.2(12)	14.2(fixed)	—	–4.7	14.2
*u*1457	H(35)...H(44)	420.2(58)	33.5(fixed)	—	–11.3	33.5
*u*1444	C(64)...H(82)	420.2(100)	37.1(fixed)	—	–3.4	37.1
*u*1436	C(64)...H(77)	420.2(40)	31.8(fixed)	—	–2.9	31.8
*u*1524	C(150)...H(180)	420.3(84)	39.2(fixed)	—	–3.9	39.2
*u*1415	Br(15)...H(24)	420.4(12)	14.2(fixed)	—	–4.4	14.2
*u*1446	C(8)...H(22)	420.6(70)	36.0(fixed)	—	–3.1	36.0
*u*1438	H(31)...H(35)	420.8(24)	32.8(fixed)	—	–5.7	32.8
*u*1425	Si(4)...Br(14)	421.0(23)	18.6(11)	17.8(18)	–0.3	17.8

*u*1413	Br(109)...H(118)	421.0(12)	14.1(fixed)	—	–4.1	14.1
*u*1431	Br(155)...H(180)	421.1(12)	14.2(fixed)	—	–4.7	14.2
*u*1392	H(21)...H(35)	421.1(75)	58.1(fixed)	—	–3.4	58.1
*u*1428	Br(61)...H(84)	421.2(12)	14.3(fixed)	—	–4.7	14.3
*u*1427	Br(108)...H(133)	421.4(12)	13.8(fixed)	—	–3.7	13.8
*u*1434	C(148)...H(166)	421.4(27)	30.3(fixed)	—	–2.5	30.3
*u*1421	Br(62)...H(71)	421.4(12)	14.0(fixed)	—	–3.7	14.0
*u*1468	H(78)...H(82)	421.4(24)	28.4(fixed)	—	–5.4	28.4
*u*1375	C(102)...H(134)	421.4(63)	32.6(fixed)	—	–1.8	32.6
*u*1418	Br(14)...H(37)	421.5(12)	13.9(fixed)	—	–3.4	13.9
*u*1433	H(116)...H(141)	421.8(24)	29.2(fixed)	—	–5.2	29.2
*u*1419	Br(62)...H(75)	421.8(12)	13.6(fixed)	—	–3.3	13.6
*u*1492	H(114)...H(116)	421.8(24)	27.5(fixed)	—	–5.4	27.5
*u*1410	H(117)...H(139)	421.9(24)	28.8(fixed)	—	–5.2	28.8
*u*1400	H(23)...H(45)	422.0(24)	28.9(fixed)	—	–5.0	28.9
*u*1414	Br(155)...H(178)	422.1(12)	13.9(fixed)	—	–3.7	13.9
*u*1460	H(20)...H(22)	422.4(24)	27.8(fixed)	—	–4.8	27.8
*u*1417	Br(61)...H(86)	422.4(12)	13.6(fixed)	—	–3.6	13.6
*u*1422	H(22)...H(47)	422.4(24)	29.1(fixed)	—	–4.6	29.1
*u*1376	C(56)...H(87)	422.5(59)	31.0(fixed)	—	–1.8	31.0
*u*1435	H(18)...H(23)	422.6(24)	28.6(fixed)	—	–4.5	28.6
*u*1449	H(69)...H(94)	422.6(24)	26.6(fixed)	—	–4.5	26.6
*u*1475	H(78)...H(91)	422.6(24)	26.5(fixed)	—	–4.5	26.5
*u*1432	H(79)...H(80)	422.7(24)	28.5(fixed)	—	–4.2	28.5
*u*1526	Si(2)...H(42)	422.7(41)	47.9(fixed)	—	–4.0	47.9
*u*1404	H(159)...H(164)	422.8(24)	25.4(fixed)	—	–4.4	25.4
*u*1503	Br(15)...H(40)	422.9(51)	36.8(fixed)	—	–3.2	36.8
*u*1469	H(112)...H(117)	422.9(24)	28.8(fixed)	—	–4.1	28.8
*u*1430	H(65)...H(70)	423.0(24)	26.1(fixed)	—	–4.2	26.1
*u*1463	H(67)...H(69)	423.0(24)	26.4(fixed)	—	–4.1	26.4
*u*1440	H(79)...H(89)	423.1(24)	27.5(fixed)	—	–3.8	27.5
*u*1491	H(163)...H(188)	423.1(24)	25.3(fixed)	—	–4.1	25.3
*u*1405	Si(98)...Br(108)	423.1(24)	17.5(tied to *u*1425)	—	–0.2	16.8
*u*1420	C(7)...H(27)	423.2(61)	34.2(fixed)	—	–3.5	34.2
*u*1424	H(70)...H(92)	423.2(24)	27.6(fixed)	—	–3.8	27.6
*u*1454	H(161)...H(163)	423.5(24)	26.9(fixed)	—	–3.5	26.9
*u*1518	Br(155)...H(184)	423.8(43)	32.2(fixed)	—	–2.6	32.2
*u*1369	H(73)...H(81)	423.8(45)	45.8(fixed)	—	–3.8	45.8
*u*1452	H(164)...H(186)	423.9(24)	25.9(fixed)	—	–3.3	25.9
*u*1390	C(149)...H(174)	424.1(57)	33.4(fixed)	—	–2.2	33.4
*u*1599	Br(62)...H(68)	424.7(74)	35.2(fixed)	—	–3.1	35.2
*u*1484	H(120)...H(122)	425.0(53)	26.3(fixed)	—	–4.5	26.3
*u*1474	C(103)...H(113)	425.2(39)	33.7(fixed)	—	–3.2	33.7
*u*1437	H(33)...H(42)	425.3(58)	38.7(fixed)	—	–5.4	38.7
*u*1455	H(118)...H(123)	425.4(53)	26.8(fixed)	—	–4.0	26.8
*u*1528	Br(62)...H(69)	425.7(95)	35.1(fixed)	—	–2.7	35.1

*u*1470	C(6)...H(38)	426.2(35)	31.1(fixed)	—	–2.2	31.1
*u*1359	H(25)...H(36)	426.4(65)	41.6(fixed)	—	–2.7	41.6
*u*1497	H(83)...H(86)	426.5(51)	25.5(fixed)	—	–5.3	25.5
*u*1459	H(165)...H(170)	426.8(51)	26.2(fixed)	—	–5.2	26.2
*u*1494	C(103)...H(116)	426.9(61)	38.5(fixed)	—	–3.7	38.5
*u*1461	C(60)...H(90)	427.0(30)	31.3(fixed)	—	–2.5	31.3
*u*1403	H(112)...H(139)	427.0(58)	27.0(fixed)	—	–5.4	27.0
*u*1406	H(80)...H(89)	427.0(58)	26.3(fixed)	—	–5.3	26.3
*u*1493	H(20)...H(47)	427.1(58)	29.1(fixed)	—	–5.1	29.1
*u*1527	Si(3)...H(33)	427.3(27)	36.0(fixed)	—	–2.4	36.0
*u*1486	C(8)...H(19)	427.3(63)	34.4(fixed)	—	–3.3	34.4
*u*1442	H(18)...H(45)	427.3(58)	27.8(fixed)	—	–5.0	27.8
*u*1472	C(149)...H(185)	427.4(59)	33.6(fixed)	—	–2.5	33.6
*u*1489	C(147)...H(182)	427.5(30)	32.4(fixed)	—	–3.5	32.4
*u*1476	H(167)...H(169)	427.6(51)	28.2(fixed)	—	–4.1	28.2
*u*1408	H(65)...H(92)	427.6(58)	26.3(fixed)	—	–4.7	26.3
*u*1448	H(114)...H(141)	427.7(58)	28.8(fixed)	—	–4.4	28.8
*u*1496	C(7)...H(26)	427.7(74)	34.3(fixed)	—	–3.0	34.3
*u*1453	C(100)...H(132)	427.8(37)	32.2(fixed)	—	–2.9	32.2
*u*1485	H(73)...H(75)	427.8(51)	25.1(fixed)	—	–4.1	25.1
*u*1490	H(84)...H(87)	427.8(51)	27.3(fixed)	—	–3.8	27.3
*u*1502	C(101)...H(122)	427.8(66)	32.4(fixed)	—	–2.5	32.4
*u*1402	H(159)...H(186)	428.0(59)	27.3(fixed)	—	–4.2	27.3
*u*1439	H(67)...H(94)	428.1(58)	27.4(fixed)	—	–4.1	27.4
*u*1447	H(71)...H(76)	428.1(51)	25.5(fixed)	—	–3.7	25.5
*u*1429	H(161)...H(188)	428.2(59)	26.6(fixed)	—	–4.0	26.6
*u*1477	H(24)...H(29)	428.2(50)	27.6(fixed)	—	–5.2	27.6
*u*1458	H(37)...H(40)	428.3(50)	26.0(fixed)	—	–5.4	26.0
*u*1450	H(82)...H(91)	428.5(58)	28.6(fixed)	—	–3.5	28.6
*u*1500	H(26)...H(28)	428.6(50)	27.7(fixed)	—	–4.8	27.7
*u*1388	H(120)...H(135)	429.2(61)	48.1(fixed)	—	–2.1	48.1
*u*1445	C(152)...H(162)	429.2(40)	31.0(fixed)	—	–2.1	31.0
*u*1498	C(10)...H(39)	429.2(59)	36.7(fixed)	—	–3.3	36.7
*u*1382	H(75)...H(88)	429.5(64)	42.4(fixed)	—	–2.0	42.4
*u*1488	H(36)...H(39)	429.6(50)	27.4(fixed)	—	–3.8	27.4
*u*1522	Br(15)...H(41)	429.7(36)	35.4(fixed)	—	–3.5	35.4
*u*1456	C(11)...H(47)	429.9(84)	37.3(fixed)	—	–2.7	37.3
*u*1441	C(55)...H(81)	430.2(27)	34.4(fixed)	—	–3.9	34.4
*u*1509	C(13)...H(31)	430.3(51)	48.2(fixed)	—	–6.2	48.2
*u*1576	C(55)...H(68)	430.3(66)	24.0(fixed)	—	–3.7	24.0
*u*1530	C(7)...H(25)	430.6(70)	31.9(fixed)	—	–3.5	31.9
*u*1533	C(64)...H(81)	430.7(86)	33.0(fixed)	—	–4.4	33.0
*u*1520	Br(61)...H(93)	430.9(63)	34.1(fixed)	—	–3.0	34.1
*u*1573	Br(14)...H(19)	431.7(53)	37.4(fixed)	—	–3.8	37.4
*u*1525	Br(14)...H(20)	432.4(67)	35.4(fixed)	—	–3.2	35.4
*u*1501	C(17)...H(35)	432.8(85)	41.4(fixed)	—	–4.3	41.4

*u*1538	Si(5)...H(32)	432.8(30)	39.5(fixed)	—	–2.9	39.5
*u*1487	C(11)...H(21)	433.2(48)	35.8(fixed)	—	–3.6	35.8
*u*1451	C(105)...H(141)	433.6(110)	37.9(fixed)	—	–3.4	37.9
*u*1517	C(9)...H(44)	433.6(64)	57.3(fixed)	—	–8.7	57.3
*u*1536	Si(50)...H(80)	433.7(19)	30.7(fixed)	—	–2.2	30.7
*u*1546	C(8)...H(21)	433.9(73)	33.0(fixed)	—	–4.2	33.0
*u*1550	Si(49)...H(89)	434.3(35)	26.4(fixed)	—	–1.5	26.4
*u*1391	H(167)...H(175)	434.4(46)	46.8(fixed)	—	–2.6	46.8
*u*1543	C(58)...H(93)	434.6(80)	31.5(fixed)	—	–3.7	31.5
*u*1462	C(12)...H(25)	434.8(53)	31.5(fixed)	—	–3.2	31.5
*u*1578	Si(52)...H(71)	435.3(43)	27.4(fixed)	—	–1.6	27.4
*u*1499	C(147)...H(177)	435.4(56)	32.8(fixed)	—	–2.5	32.8
*u*1539	Br(155)...H(172)	435.5(48)	34.8(fixed)	—	–2.3	34.8
*u*1577	C(150)...H(182)	435.6(67)	33.5(fixed)	—	–4.1	33.5
*u*1495	C(58)...H(68)	435.8(59)	33.5(fixed)	—	–2.7	33.5
*u*1548	Si(96)...H(136)	435.9(43)	28.3(fixed)	—	–1.8	28.3
*u*1511	C(16)...H(28)	436.1(67)	37.6(fixed)	—	–3.3	37.6
*u*1377	H(74)...H(91)	436.2(39)	43.7(fixed)	—	–1.6	43.7
*u*1553	Si(52)...H(84)	436.3(37)	32.0(fixed)	—	–2.0	32.0
*u*1613	Si(96)...H(139)	437.5(30)	29.6(fixed)	—	–1.8	29.6
*u*1595	C(10)...H(46)	437.6(46)	24.9(fixed)	—	–4.8	24.9
*u*1513	C(60)...H(78)	438.2(38)	34.7(fixed)	—	–2.8	34.7
*u*1597	C(59)...H(66)	438.5(38)	24.6(fixed)	—	–4.0	24.6
*u*1512	C(102)...H(130)	438.5(93)	33.2(fixed)	—	–2.7	33.2
*u*1552	Si(3)...H(18)	438.6(43)	28.6(fixed)	—	–2.0	28.6
*u*1549	C(13)...H(30)	438.7(42)	39.4(fixed)	—	–7.0	39.4
*u*1514	C(57)...H(86)	438.7(50)	32.4(fixed)	—	–2.4	32.4
*u*1540	Si(2)...H(24)	438.8(40)	29.9(fixed)	—	–2.0	29.9
*u*1638	Br(155)...H(171)	438.8(37)	32.7(fixed)	—	–2.6	32.7
*u*1555	C(103)...H(115)	438.9(48)	33.3(fixed)	—	–4.5	33.3
*u*1567	Si(98)...H(117)	438.9(32)	31.0(fixed)	—	–2.0	31.0
*u*1600	Si(50)...H(68)	439.2(41)	19.0(fixed)	—	–4.1	19.0
*u*1537	Si(3)...H(21)	439.2(38)	19.8(fixed)	—	–5.3	19.8
*u*1529	Br(61)...H(67)	439.6(96)	34.8(fixed)	—	–2.7	34.8
*u*1544	C(17)...H(34)	439.7(68)	35.8(fixed)	—	–5.2	35.8
*u*1479	C(102)...H(135)	439.8(47)	30.9(fixed)	—	–2.4	30.9
*u*1569	C(9)...H(43)	439.9(50)	45.0(fixed)	—	–10.1	45.0
*u*1551	C(147)...H(179)	440.2(44)	30.6(fixed)	—	–3.0	30.6
*u*1561	Si(145)...H(178)	440.5(34)	27.9(fixed)	—	–1.6	27.9
*u*1482	C(63)...H(74)	440.5(28)	30.1(fixed)	—	–2.2	30.1
*u*1471	C(56)...H(88)	440.9(46)	30.3(fixed)	—	–2.4	30.3
*u*1558	Si(52)...H(79)	441.1(20)	28.9(fixed)	—	–1.6	28.9
*u*1631	C(101)...H(128)	441.4(47)	25.7(fixed)	—	–5.9	25.7
*u*1516	C(59)...H(75)	441.5(48)	31.6(fixed)	—	–2.2	31.6
*u*1604	C(16)...H(41)	441.7(44)	26.1(fixed)	—	–5.0	26.1
*u*1521	C(56)...H(83)	442.3(46)	36.6(fixed)	—	–3.6	36.6

*u*1542	C(104)...H(135)	442.5(46)	30.8(fixed)	—	–3.0	30.8
*u*1541	C(105)...H(140)	442.5(90)	32.3(fixed)	—	–4.4	32.3
*u*1585	C(11)...H(27)	442.8(45)	24.3(fixed)	—	–5.0	24.3
*u*1639	Br(108)...H(113)	443.0(55)	35.7(fixed)	—	–3.7	35.7
*u*1612	Br(61)...H(66)	443.1(64)	34.4(fixed)	—	–3.2	34.4
*u*1641	Si(50)...H(65)	443.1(57)	26.4(fixed)	—	–1.6	26.4
*u*1480	C(149)...H(175)	443.3(35)	32.2(fixed)	—	–2.8	32.2
*u*1610	Br(15)...H(38)	444.0(37)	33.6(fixed)	—	–2.6	33.6
*u*1572	Si(98)...H(118)	444.2(38)	28.0(fixed)	—	–1.7	28.0
*u*1587	Si(5)...H(37)	444.5(37)	26.4(fixed)	—	–1.7	26.4
*u*1584	C(149)...H(162)	444.6(34)	22.9(fixed)	—	–3.0	22.9
*u*1590	C(57)...H(93)	444.8(35)	24.1(fixed)	—	–4.6	24.1
*u*1563	C(149)...H(184)	445.0(43)	30.9(fixed)	—	–3.3	30.9
*u*1562	C(11)...H(46)	445.4(70)	31.1(fixed)	—	–3.8	31.1
*u*1627	C(12)...H(19)	446.7(44)	25.6(fixed)	—	–4.9	25.6
*u*1559	Si(143)...H(160)	446.7(16)	18.9(fixed)	—	–4.2	18.9
*u*1643	Si(143)...H(183)	446.8(40)	27.0(fixed)	—	–1.7	27.0
*u*1644	Si(2)...H(45)	447.1(26)	29.1(fixed)	—	–1.9	29.1
*u*1589	Si(4)...H(23)	447.2(28)	30.2(fixed)	—	–2.1	30.2
*u*1557	C(10)...H(41)	447.5(38)	35.2(fixed)	—	–4.2	35.2
*u*1535	Br(15)...H(36)	447.7(53)	34.2(fixed)	—	–2.5	34.2
*u*1629	Si(49)...H(66)	447.8(21)	18.8(fixed)	—	–4.2	18.8
*u*1596	Si(145)...H(187)	448.1(24)	19.6(fixed)	—	–4.2	19.6
*u*1649	Br(15)...H(43)	448.2(45)	32.4(fixed)	—	–14.5	32.4
*u*1554	Si(143)...H(186)	448.2(26)	27.9(fixed)	—	–1.8	27.9
*u*1635	Si(2)...H(19)	448.4(13)	20.1(fixed)	—	–5.0	20.1
*u*1579	C(60)...H(77)	448.5(37)	31.5(fixed)	—	–3.5	31.5
*u*1534	Si(96)...H(123)	448.5(37)	26.3(fixed)	—	–1.5	26.3
*u*1593	C(102)...H(137)	448.6(42)	24.5(fixed)	—	–4.5	24.5
*u*1532	Si(50)...H(87)	448.6(35)	26.0(fixed)	—	–1.4	26.0
*u*1547	Br(109)...H(138)	448.7(70)	37.0(fixed)	—	–3.2	37.0
*u*1570	C(102)...H(132)	448.7(73)	31.2(fixed)	—	–3.3	31.2
*u*1646	Br(61)...H(77)	448.9(37)	26.5(fixed)	—	–4.5	26.5
*u*1636	Si(3)...H(43)	448.9(15)	25.6(fixed)	—	–12.3	25.6
*u*1591	Si(51)...H(93)	449.4(27)	19.5(fixed)	—	–4.8	19.5
*u*1633	Si(143)...H(171)	449.4(17)	17.8(fixed)	—	–3.4	17.8
*u*1624	Si(143)...H(168)	449.5(26)	19.5(fixed)	—	–5.0	19.5
*u*1601	C(63)...H(88)	449.7(36)	23.6(fixed)	—	–3.6	23.6
*u*1545	Si(145)...H(170)	449.9(25)	31.2(fixed)	—	–1.8	31.2
*u*1575	C(57)...H(88)	450.0(29)	30.8(fixed)	—	–3.0	30.8
*u*1634	Si(97)...H(137)	450.5(17)	19.1(fixed)	—	–4.7	19.1
*u*1619	C(100)...H(121)	450.7(49)	24.3(fixed)	—	–3.7	24.3
*u*1623	Si(4)...H(46)	450.7(21)	19.3(fixed)	—	–4.8	19.3
*u*1608	Si(5)...H(25)	450.8(38)	19.8(fixed)	—	–4.6	19.8
*u*1618	Si(98)...H(140)	450.9(26)	19.9(fixed)	—	–5.7	19.9
*u*1583	Si(145)...H(164)	450.9(29)	25.3(fixed)	—	–1.5	25.3

*u*1566	C(56)...H(85)	451.0(44)	33.9(fixed)	—	–4.0	33.9
*u*1642	Si(49)...H(92)	451.0(45)	27.9(fixed)	—	–1.8	27.9
*u*1632	Si(2)...H(30)	451.1(16)	22.8(fixed)	—	–8.6	22.8
*u*1603	Si(96)...H(124)	451.2(18)	19.4(fixed)	—	–5.6	19.4
*u*1586	Si(51)...H(70)	451.7(47)	27.2(fixed)	—	–1.7	27.2
*u*1580	C(9)...H(21)	452.1(63)	24.3(fixed)	—	–5.0	24.3
*u*1560	Si(96)...H(119)	452.2(27)	19.0(fixed)	—	–4.2	19.0
*u*1568	Si(5)...H(29)	452.3(34)	29.7(fixed)	—	–1.9	29.7
*u*1588	C(58)...H(72)	452.4(35)	23.5(fixed)	—	–3.6	23.5
*u*1565	Si(51)...H(76)	452.4(27)	25.4(fixed)	—	–1.4	25.4
*u*1609	Si(4)...H(41)	452.7(23)	20.5(fixed)	—	–5.3	20.5
*u*1622	Si(52)...H(81)	453.0(23)	20.5(fixed)	—	–5.6	20.5
*u*1628	C(6)...H(25)	453.0(62)	24.5(fixed)	—	–4.8	24.5
*u*1616	Si(4)...H(27)	453.3(21)	20.3(fixed)	—	–5.1	20.3
*u*1637	Si(49)...H(77)	453.4(15)	19.2(fixed)	—	–4.4	19.2
*u*1626	C(7)...H(34)	453.6(48)	26.3(fixed)	—	–7.3	26.3
*u*1648	Br(155)...H(168)	453.7(36)	27.4(fixed)	—	–5.3	27.4
*u*1582	C(16)...H(27)	453.8(49)	34.5(fixed)	—	–4.2	34.5
*u*1611	Si(98)...H(135)	453.9(23)	19.4(fixed)	—	–3.9	19.4
*u*1620	Si(5)...H(34)	454.0(24)	21.7(fixed)	—	–6.7	21.7
*u*1556	Si(49)...H(74)	454.2(27)	19.0(fixed)	—	–3.5	19.0
*u*1650	Br(14)...H(30)	454.3(45)	30.3(fixed)	—	–9.9	30.3
*u*1574	C(59)...H(74)	455.2(43)	31.2(fixed)	—	–2.7	31.2
*u*1605	C(150)...H(184)	455.2(39)	25.1(fixed)	—	–4.0	25.1
*u*1564	Si(50)...H(90)	455.6(13)	18.6(fixed)	—	–3.8	18.6
*u*1625	Si(50)...H(85)	455.9(26)	19.8(fixed)	—	–5.0	19.8
*u*1504	C(55)...H(91)	456.0(47)	32.1(fixed)	—	–2.2	32.1
*u*1647	Br(62)...H(85)	456.0(40)	27.1(fixed)	—	–5.3	27.1
*u*1621	Si(3)...H(38)	456.3(26)	18.2(fixed)	—	–3.5	18.2
*u*1617	Si(51)...H(88)	456.4(22)	19.1(fixed)	—	–3.8	19.1
*u*1606	C(148)...H(175)	457.0(45)	25.1(fixed)	—	–4.2	25.1
*u*1508	C(63)...H(73)	457.1(50)	32.1(fixed)	—	–2.4	32.1
*u*1607	Si(145)...H(166)	457.5(19)	19.2(fixed)	—	–3.9	19.2
*u*1630	Si(3)...H(40)	457.7(35)	28.3(fixed)	—	–1.7	28.3
*u*1592	C(8)...H(38)	457.7(62)	23.1(fixed)	—	–3.1	23.1
*u*1645	Br(108)...H(124)	458.3(43)	27.0(fixed)	—	–5.7	27.0
*u*1640	C(54)...H(81)	459.5(70)	26.3(fixed)	—	–5.8	26.3
*u*1615	Si(51)...H(72)	459.8(19)	19.3(fixed)	—	–3.8	19.3
*u*1602	C(56)...H(90)	461.6(39)	24.2(fixed)	—	–3.6	24.2
*u*1571	C(63)...H(72)	462.8(38)	31.1(fixed)	—	–3.0	31.1
*u*1760	H(175)...H(188)	463.3(104)	42.0(fixed)	—	–5.3	42.0
*u*1581	C(55)...H(90)	463.7(40)	30.5(fixed)	—	–2.9	30.5
*u*1598	C(103)...H(132)	465.0(53)	24.3(fixed)	—	–4.0	24.3
*u*1594	C(60)...H(74)	467.3(50)	23.1(fixed)	—	–3.2	23.1
*u*1614	C(152)...H(166)	469.2(46)	24.3(fixed)	—	–3.8	24.3
*u*1693	Si(2)...H(43)	469.6(25)	30.5(fixed)	—	–10.6	30.5

*u*1661	H(116)...H(125)	470.7(94)	38.2(fixed)	—	7.7	38.2
*u*1797	H(176)...H(188)	473.3(110)	35.6(fixed)	—	–5.9	35.6
*u*1665	Si(50)...C(64)	473.5(24)	11.6(fixed)	—	–0.6	11.6
*u*1702	H(67)...H(73)	474.0(99)	38.1(fixed)	—	4.5	38.1
*u*1653	Si(3)...C(17)	474.2(21)	12.0(tied to *u*1656)	—	–0.7	11.7
*u*1749	H(81)...H(94)	475.0(117)	44.9(fixed)	—	–6.3	44.9
*u*1685	Si(3)...H(34)	475.2(16)	24.3(fixed)	—	–6.1	24.3
*u*1658	H(120)...H(129)	475.5(84)	38.7(fixed)	—	6.2	38.7
*u*1727	H(31)...H(42)	475.7(12)	19.2(fixed)	—	–13.2	19.2
*u*1655	H(75)...H(82)	475.7(58)	37.3(fixed)	—	5.7	37.3
*u*1728	Si(52)...H(72)	476.2(36)	22.0(fixed)	—	–3.5	22.0
*u*1747	H(22)...H(25)	476.5(73)	45.9(fixed)	—	–6.0	45.9
*u*1942	H(41)...H(42)	476.7(65)	65.3(fixed)	—	–16.4	65.3
*u*1652	Si(143)...C(148)	477.3(10)	11.9(tied to *u*1656)	—	–0.7	11.6
*u*1663	Si(49)...C(54)	477.6(14)	12.0(tied to *u*1656)	—	–0.7	11.7
*u*1656	Si(2)...C(9)	477.7(20)	11.7(6)	—	–0.8	11.4
*u*1722	H(33)...H(44)	478.0(25)	18.9(fixed)	—	–12.6	18.9
*u*1675	Si(143)...C(152)	478.1(14)	11.8(tied to *u*1656)	—	–0.6	11.6
*u*1666	Si(3)...H(19)	478.1(35)	23.3(fixed)	—	–4.4	23.3
*u*1726	Si(5)...H(30)	478.3(23)	27.2(fixed)	—	–7.5	27.2
*u*1667	Si(2)...C(7)	478.5(10)	11.8(tied to *u*1656)	—	–0.7	11.5
*u*1651	H(22)...H(31)	478.6(58)	40.8(fixed)	—	10.4	40.8
*u*1697	H(26)...H(29)	478.7(21)	17.2(fixed)	—	–7.0	17.2
*u*1676	Si(143)...C(149)	479.0(21)	11.3(tied to *u*1656)	—	–0.7	11.1
*u*1705	Si(52)...C(56)	479.0(19)	11.7(tied to *u*1656)	—	–0.7	11.4
*u*1731	H(32)...H(35)	479.2(12)	17.5(fixed)	—	–9.9	17.5
*u*1696	H(83)...H(87)	479.2(22)	16.9(fixed)	—	–6.5	16.9
*u*1669	Si(96)...C(101)	479.4(10)	11.7(tied to *u*1656)	—	–0.6	11.4
*u*1707	H(36)...H(40)	479.4(21)	16.7(fixed)	—	–6.4	16.7
*u*1659	H(161)...H(167)	479.5(66)	38.7(fixed)	—	4.6	38.7
*u*1701	H(120)...H(123)	479.5(23)	16.6(fixed)	—	–6.2	16.6
*u*1660	Si(50)...H(81)	479.6(12)	23.8(fixed)	—	–4.9	23.8
*u*1710	H(167)...H(170)	479.6(21)	16.6(fixed)	—	–6.6	16.6
*u*1703	H(73)...H(76)	480.0(22)	16.4(fixed)	—	–5.7	16.4
*u*1671	Si(96)...C(105)	480.1(13)	11.7(tied to *u*1656)	—	–0.7	11.4
*u*1924	H(32)...H(46)	480.2(56)	52.6(fixed)	—	–12.1	52.6
*u*1657	Si(49)...C(55)	480.2(22)	11.6(tied to *u*1656)	—	–0.7	11.3
*u*1757	Si(96)...H(140)	480.3(19)	23.3(fixed)	—	–5.0	23.3
*u*1679	Si(49)...C(58)	480.5(12)	11.6(tied to *u*1656)	—	–0.7	11.3
*u*1687	Si(49)...H(90)	480.7(21)	21.7(fixed)	—	–3.5	21.7
*u*1654	Si(50)...C(57)	481.1(9)	11.9(tied to *u*1656)	—	–0.7	11.6
*u*1691	Si(96)...H(137)	481.1(26)	22.9(fixed)	—	–4.2	22.9
*u*1706	Si(98)...C(103)	481.1(12)	11.6(tied to *u*1656)	—	–0.7	11.4
*u*1736	Si(52)...H(85)	481.1(21)	22.7(fixed)	—	–4.6	22.7
*u*1846	H(168)...H(180)	481.2(82)	50.4(fixed)	—	–7.1	50.4
*u*1766	Si(50)...H(66)	481.2(41)	21.9(fixed)	—	–3.8	21.9

*u*1677	Si(2)...C(11)	481.2(12)	11.7(tied to *u*1656)	—	–0.7	11.4
*u*1720	H(117)...H(141)	481.3(12)	16.7(fixed)	—	–7.8	16.7
*u*1729	H(79)...H(82)	481.5(12)	16.7(fixed)	—	–7.4	16.7
*u*1716	H(23)...H(47)	481.6(12)	16.6(fixed)	—	–7.5	16.6
*u*1711	H(112)...H(116)	481.6(12)	17.0(fixed)	—	–7.4	17.0
*u*1673	Si(3)...C(10)	481.7(10)	11.7(tied to *u*1656)	—	–0.7	11.5
*u*1714	H(18)...H(22)	481.8(12)	16.7(fixed)	—	–7.3	16.7
*u*1670	Si(2)...H(25)	481.9(28)	22.0(fixed)	—	–4.2	22.0
*u*1738	Si(98)...H(115)	482.2(24)	24.4(fixed)	—	–4.9	24.4
*u*1694	Si(5)...C(13)	482.3(13)	11.9(tied to *u*1656)	—	–0.8	11.6
*u*1708	H(70)...H(94)	482.5(12)	16.3(fixed)	—	–6.4	16.3
*u*1717	H(78)...H(89)	482.6(12)	16.4(fixed)	—	–6.3	16.4
*u*1682	Si(145)...C(147)	482.7(21)	12.1(tied to *u*1656)	—	–0.6	11.8
*u*1719	H(65)...H(69)	482.8(12)	16.2(fixed)	—	–6.2	16.2
*u*1704	Si(145)...C(154)	482.9(11)	11.7(tied to *u*1656)	—	–0.7	11.4
*u*1724	H(159)...H(163)	483.0(12)	16.2(fixed)	—	–5.9	16.2
*u*1713	H(164)...H(188)	483.2(12)	16.2(fixed)	—	–5.7	16.2
*u*1725	H(114)...H(139)	483.4(25)	16.6(fixed)	—	–7.4	16.6
*u*1778	H(82)...H(93)	483.4(94)	47.0(fixed)	—	–6.8	47.0
*u*1678	Si(51)...C(53)	483.5(22)	12.0(tied to *u*1656)	—	–0.7	11.7
*u*1723	H(20)...H(45)	483.6(25)	16.9(fixed)	—	–7.2	16.9
*u*1672	H(83)...H(94)	483.7(101)	38.5(fixed)	—	6.3	38.5
*u*1718	H(80)...H(91)	483.7(25)	16.5(fixed)	—	–6.9	16.5
*u*1783	H(30)...H(39)	483.9(64)	52.2(fixed)	—	–8.9	52.2
*u*1690	Si(98)...C(106)	483.9(9)	11.6(tied to *u*1656)	—	–0.7	11.4
*u*1700	Si(52)...C(60)	483.9(11)	11.7(tied to *u*1656)	—	–0.6	11.4
*u*1715	Si(145)...H(179)	484.1(20)	21.4(fixed)	—	–3.5	21.4
*u*1712	H(67)...H(92)	484.1(25)	16.3(fixed)	—	–6.5	16.3
*u*1709	H(161)...H(186)	484.2(25)	16.2(fixed)	—	–6.4	16.2
*u*1684	Si(4)...C(6)	484.3(20)	12.0(tied to *u*1656)	—	–0.7	11.7
*u*1733	Si(98)...H(119)	484.5(22)	22.5(fixed)	—	–3.9	22.5
*u*1769	H(161)...H(179)	484.6(61)	43.1(fixed)	—	–5.0	43.1
*u*1680	Si(98)...C(100)	484.7(21)	11.8(tied to *u*1656)	—	–0.6	11.5
*u*1683	Si(4)...C(12)	484.8(9)	11.7(tied to *u*1656)	—	–0.7	11.4
*u*1698	Si(4)...C(8)	485.1(9)	11.5(tied to *u*1656)	—	–0.6	11.2
*u*1730	Si(5)...H(27)	485.1(32)	23.2(fixed)	—	–4.4	23.2
*u*1692	Si(51)...C(59)	485.2(8)	11.6(tied to *u*1656)	—	–0.7	11.3
*u*1931	H(68)...H(71)	485.3(72)	36.0(fixed)	—	–7.0	36.0
*u*1735	Si(52)...H(77)	485.5(18)	22.1(fixed)	—	–3.9	22.1
*u*1688	Si(52)...C(63)	485.7(20)	11.9(tied to *u*1656)	—	–0.6	11.7
*u*1674	Si(96)...H(121)	485.9(28)	21.0(fixed)	—	–3.5	21.0
*u*1742	H(36)...H(47)	486.2(69)	39.3(fixed)	—	4.2	39.3
*u*1689	Si(5)...C(16)	486.3(19)	12.1(tied to *u*1656)	—	–0.8	11.8
*u*1755	H(34)...H(47)	486.6(82)	49.8(fixed)	—	–7.0	49.8
*u*1734	Si(5)...H(38)	486.8(21)	21.4(fixed)	—	–3.3	21.4
*u*1927	H(66)...H(84)	486.9(57)	43.0(fixed)	—	–8.4	43.0

*u*1801	H(28)...H(43)	486.9(70)	57.0(fixed)	—	–11.4	57.0
*u*1686	Si(50)...H(88)	487.2(28)	20.6(fixed)	—	–3.4	20.6
*u*1802	H(115)...H(122)	487.3(69)	44.0(fixed)	—	–6.4	44.0
*u*1737	Si(145)...H(168)	487.4(17)	22.1(fixed)	—	–4.4	22.1
*u*1847	C(56)...H(70)	487.4(56)	32.6(fixed)	—	2.4	32.6
*u*1917	H(27)...H(33)	487.6(62)	46.5(fixed)	—	–10.6	46.5
*u*1780	C(53)...H(73)	487.9(72)	29.6(fixed)	—	2.5	29.6
*u*1668	Si(143)...H(187)	487.9(17)	22.1(fixed)	—	–3.9	22.1
*u*1771	Si(2)...H(46)	488.1(18)	22.1(fixed)	—	–4.2	22.1
*u*1764	Si(143)...H(184)	488.2(24)	21.2(fixed)	—	–3.7	21.2
*u*1758	C(101)...H(125)	488.3(71)	29.5(fixed)	—	4.2	29.5
*u*1740	Si(4)...H(21)	488.6(22)	24.3(fixed)	—	–4.7	24.3
*u*1681	H(69)...H(78)	489.0(80)	37.7(fixed)	—	4.9	37.7
*u*1803	H(21)...H(26)	489.0(82)	45.5(fixed)	—	–6.8	45.5
*u*1785	H(82)...H(94)	489.0(110)	41.1(fixed)	—	–7.4	41.1
*u*1979	H(117)...H(128)	489.7(63)	43.1(fixed)	—	–10.9	43.1
*u*1776	H(125)...H(135)	489.7(60)	47.7(fixed)	—	–6.2	47.7
*u*1976	H(175)...H(187)	490.3(80)	39.7(fixed)	—	–7.4	39.7
*u*1762	Si(49)...H(93)	490.4(29)	22.0(fixed)	—	–4.2	22.0
*u*1739	Si(51)...H(74)	490.7(18)	20.6(fixed)	—	–3.2	20.6
*u*1732	Si(145)...H(162)	490.8(23)	21.4(fixed)	—	–3.1	21.4
*u*1928	H(169)...H(180)	490.9(87)	43.7(fixed)	—	–8.8	43.7
*u*1782	C(106)...H(141)	491.1(61)	29.1(fixed)	—	3.8	29.1
*u*1751	H(73)...H(92)	491.3(95)	41.1(fixed)	—	6.7	41.1
*u*1808	C(55)...H(67)	491.4(87)	29.7(fixed)	—	2.2	29.7
*u*1772	Si(3)...H(41)	491.8(29)	22.4(fixed)	—	–4.6	22.4
*u*1741	Si(51)...H(68)	492.0(32)	22.7(fixed)	—	–3.8	22.7
*u*1744	C(56)...H(82)	492.3(40)	29.3(fixed)	—	4.4	29.3
*u*1699	H(26)...H(39)	492.4(48)	39.4(fixed)	—	5.9	39.4
*u*1767	H(128)...H(141)	492.9(109)	49.5(fixed)	—	–7.2	49.5
*u*1752	C(111)...H(130)	493.4(66)	29.3(fixed)	—	2.9	29.3
*u*1664	H(122)...H(133)	493.5(103)	37.1(fixed)	—	4.3	37.1
*u*1743	C(7)...H(31)	493.7(46)	31.2(fixed)	—	7.9	31.2
*u*1810	H(31)...H(41)	493.8(48)	60.1(fixed)	—	–9.9	60.1
*u*1695	H(20)...H(28)	493.9(77)	37.6(fixed)	—	6.1	37.6
*u*1823	Si(50)...H(92)	495.0(40)	22.4(fixed)	—	0.5	22.4
*u*1748	C(147)...H(167)	495.2(49)	28.9(fixed)	—	2.6	28.9
*u*1750	C(10)...H(22)	495.3(45)	30.0(fixed)	—	3.6	30.0
*u*1840	H(123)...H(129)	495.8(51)	45.1(fixed)	—	6.9	45.1
*u*1753	C(58)...H(75)	495.9(45)	28.1(fixed)	—	1.9	28.1
*u*1815	H(35)...H(46)	496.1(86)	50.5(fixed)	—	–7.7	50.5
*u*1763	C(64)...H(83)	496.6(72)	29.4(fixed)	—	4.0	29.4
*u*1813	H(22)...H(26)	497.1(70)	40.1(fixed)	—	–7.2	40.1
*u*1795	Si(3)...H(45)	497.1(30)	22.2(fixed)	—	0.4	22.2
*u*1920	H(162)...H(165)	497.1(49)	36.6(fixed)	—	–6.3	36.6
*u*1963	H(68)...H(72)	497.3(72)	35.9(fixed)	—	–7.1	35.9

*u*1946	H(79)...H(93)	497.7(37)	38.9(fixed)	—	–8.5	38.9
*u*1845	H(27)...H(44)	497.7(64)	68.2(fixed)	—	–12.2	68.2
*u*1938	H(72)...H(80)	497.7(51)	40.4(fixed)	—	–8.2	40.4
*u*1786	C(149)...H(161)	497.8(55)	29.4(fixed)	—	2.4	29.4
*u*1806	C(64)...H(73)	497.8(69)	32.4(fixed)	—	3.3	32.4
*u*1804	Si(49)...H(70)	497.9(30)	23.0(fixed)	—	0.0	23.0
*u*1858	H(31)...H(39)	498.1(57)	49.3(fixed)	—	–11.1	49.3
*u*1830	H(67)...H(76)	498.2(54)	41.1(fixed)	—	5.4	41.1
*u*1838	H(116)...H(122)	498.3(66)	40.7(fixed)	—	–7.3	40.7
*u*1789	Si(143)...H(164)	498.4(19)	21.6(fixed)	—	–0.3	21.6
*u*1745	H(65)...H(78)	498.7(79)	41.1(fixed)	—	6.7	41.1
*u*1790	H(40)...H(47)	498.8(55)	42.7(fixed)	—	8.4	42.7
*u*1821	H(119)...H(130)	498.9(91)	43.2(fixed)	—	–5.6	43.2
*u*1844	Si(143)...H(174)	499.0(27)	22.7(fixed)	—	0.2	22.7
*u*1894	C(60)...H(65)	499.2(30)	31.6(fixed)	—	2.6	31.6
*u*1893	C(150)...H(164)	499.4(26)	29.0(fixed)	—	1.9	29.0
*u*1966	H(88)...H(89)	499.5(50)	34.3(fixed)	—	–6.8	34.3
*u*1746	H(70)...H(83)	499.7(79)	43.9(fixed)	—	7.1	43.9
*u*1662	H(169)...H(176)	499.8(60)	38.6(fixed)	—	5.6	38.6
*u*1822	H(77)...H(86)	499.8(56)	42.2(fixed)	—	–5.3	42.2
*u*1811	H(160)...H(177)	499.8(56)	42.8(fixed)	—	–5.5	42.8
*u*1768	H(159)...H(172)	499.9(43)	39.4(fixed)	—	5.7	39.4
*u*1989	H(21)...H(25)	500.1(76)	42.2(fixed)	—	–8.8	42.2
*u*1819	H(78)...H(88)	500.1(32)	44.2(fixed)	—	–5.5	44.2
*u*1874	C(13)...H(18)	500.2(20)	34.1(fixed)	—	3.2	34.1
*u*1812	H(75)...H(85)	500.4(54)	43.5(fixed)	—	–5.6	43.5
*u*1996	H(19)...H(37)	500.5(63)	35.6(fixed)	—	–8.1	35.6
*u*1792	C(17)...H(36)	500.7(56)	29.1(fixed)	—	1.9	29.1
*u*1842	Si(2)...H(23)	500.7(18)	22.7(fixed)	—	0.6	22.7
*u*1940	H(113)...H(131)	500.8(60)	38.2(fixed)	—	–8.3	38.2
*u*1788	H(167)...H(186)	500.9(53)	39.9(fixed)	—	6.0	39.9
*u*1857	C(147)...H(174)	500.9(30)	32.2(fixed)	—	3.1	32.2
*u*1770	C(54)...H(78)	501.1(51)	28.9(fixed)	—	3.0	28.9
*u*2014	H(30)...H(46)	501.5(47)	44.8(fixed)	—	–12.7	44.8
*u*2019	H(41)...H(43)	501.5(39)	51.9(fixed)	—	–16.6	51.9
*u*1818	H(35)...H(47)	501.5(87)	45.6(fixed)	—	–8.4	45.6
*u*1889	H(28)...H(44)	501.8(68)	56.6(fixed)	—	–13.6	56.6
*u*2002	H(81)...H(93)	501.8(80)	42.6(fixed)	—	–9.4	42.6
*u*1773	H(164)...H(180)	501.9(45)	43.7(fixed)	—	6.5	43.7
*u*1798	C(59)...H(94)	502.2(81)	28.4(fixed)	—	2.8	28.4
*u*1994	H(112)...H(121)	502.2(70)	36.4(fixed)	—	–7.5	36.4
*u*1799	Si(2)...H(29)	502.4(25)	22.4(fixed)	—	0.5	22.4
*u*1836	C(12)...H(47)	502.7(49)	30.2(fixed)	—	2.7	30.2
*u*1721	H(163)...H(172)	503.1(74)	36.7(fixed)	—	3.2	36.7
*u*1777	C(9)...H(20)	503.4(65)	28.6(fixed)	—	3.4	28.6
*u*1921	C(103)...H(129)	503.5(36)	35.2(fixed)	—	4.6	35.2

*u*1816	H(161)...H(177)	503.7(60)	36.8(fixed)	—	–6.1	36.8
*u*1756	H(28)...H(45)	503.9(65)	44.5(fixed)	—	8.2	44.5
*u*1900	C(103)...H(136)	504.1(26)	32.3(fixed)	—	2.9	32.3
*u*1867	C(63)...H(92)	504.3(32)	32.9(fixed)	—	3.5	32.9
*u*1779	C(13)...H(26)	504.5(42)	29.2(fixed)	—	3.3	29.2
*u*1793	H(129)...H(141)	504.5(111)	43.5(fixed)	—	–8.4	43.5
*u*1995	H(23)...H(34)	504.8(54)	40.2(fixed)	—	–12.0	40.2
*u*1879	Si(145)...H(159)	504.8(25)	21.9(fixed)	—	0.1	21.9
*u*1834	Si(51)...H(65)	505.1(34)	22.2(fixed)	—	0.1	22.2
*u*1871	Si(52)...H(76)	505.1(25)	20.9(fixed)	—	–0.2	20.9
*u*1861	Si(96)...H(127)	505.3(27)	21.7(fixed)	—	0.7	21.7
*u*1843	Si(97)...H(126)	505.4(19)	21.8(fixed)	—	1.0	21.8
*u*1906	Si(143)...H(165)	505.4(25)	21.2(fixed)	—	–0.4	21.2
*u*1864	H(161)...H(170)	505.4(42)	42.1(fixed)	—	6.8	42.1
*u*1865	Si(98)...H(123)	505.5(25)	21.3(fixed)	—	0.0	21.3
*u*1848	H(74)...H(83)	505.5(50)	46.2(fixed)	—	–6.0	46.2
*u*1781	C(57)...H(69)	505.6(71)	29.9(fixed)	—	2.4	29.9
*u*1908	C(16)...H(45)	505.9(26)	32.8(fixed)	—	3.5	32.8
*u*1890	Si(49)...H(80)	505.9(23)	21.9(fixed)	—	0.4	21.9
*u*1925	C(56)...H(67)	506.1(55)	32.7(fixed)	—	3.1	32.7
*u*1807	C(54)...H(83)	506.4(55)	34.0(fixed)	—	4.7	34.0
*u*1774	H(18)...H(31)	506.7(43)	51.6(fixed)	—	11.4	51.6
*u*1805	C(53)...H(78)	506.7(49)	32.2(fixed)	—	3.9	32.2
*u*1851	Si(5)...H(40)	506.8(26)	22.1(fixed)	—	0.7	22.1
*u*1903	C(59)...H(79)	507.3(23)	30.8(fixed)	—	3.4	30.8
*u*1856	Si(4)...H(18)	507.4(23)	22.6(fixed)	—	0.2	22.6
*u*2025	H(168)...H(182)	507.4(66)	41.6(fixed)	—	–9.1	41.6
*u*1784	C(6)...H(28)	507.4(57)	29.5(fixed)	—	3.4	29.5
*u*1835	Si(49)...H(71)	507.4(27)	21.6(fixed)	—	–0.3	21.6
*u*2011	H(66)...H(85)	507.5(36)	37.7(fixed)	—	–8.7	37.7
*u*1824	H(114)...H(118)	507.6(58)	42.6(fixed)	—	6.5	42.6
*u*1814	Si(50)...H(79)	507.6(15)	21.0(fixed)	—	0.2	21.0
*u*1761	C(103)...H(133)	507.6(77)	28.9(fixed)	—	2.3	28.9
*u*1870	C(149)...H(181)	507.7(30)	31.1(fixed)	—	4.5	31.1
*u*1929	H(24)...H(38)	507.7(80)	39.1(fixed)	—	–7.1	39.1
*u*1826	C(152)...H(177)	507.8(37)	30.8(fixed)	—	3.3	30.8
*u*1860	C(102)...H(117)	507.9(28)	32.3(fixed)	—	4.7	32.3
*u*1993	H(18)...H(25)	508.3(70)	36.5(fixed)	—	–8.7	36.5
*u*1901	Si(3)...Br(14)	508.3(15)	11.6(tied to *u*1914)	—	–0.8	11.8
*u*1875	C(17)...H(24)	508.5(50)	32.2(fixed)	—	3.7	32.2
*u*1869	Si(145)...H(181)	508.5(21)	21.5(fixed)	—	0.5	21.5
*u*1897	C(100)...H(127)	508.6(32)	32.6(fixed)	—	4.6	32.6
*u*2024	H(115)...H(128)	508.7(47)	40.9(fixed)	—	–10.8	40.9
*u*1910	Si(98)...H(131)	508.7(18)	21.9(fixed)	—	–0.1	21.9
*u*1876	Si(2)...H(33)	508.7(24)	23.1(fixed)	—	0.7	23.1
*u*1775	H(23)...H(36)	509.0(46)	39.3(fixed)	—	6.7	39.3

*u*2032	H(70)...H(74)	509.0(66)	37.2(fixed)	—	3.3	37.2
*u*1913	C(13)...H(47)	509.3(41)	32.6(fixed)	—	4.2	32.6
*u*1872	Si(4)...H(37)	509.4(18)	21.7(fixed)	—	–0.4	21.7
*u*1922	Br(61)...H(91)	509.5(49)	29.5(fixed)	—	2.1	29.5
*u*2004	H(128)...H(140)	509.5(87)	41.8(fixed)	—	–10.2	41.8
*u*2003	H(27)...H(34)	509.7(40)	40.9(fixed)	—	–11.3	40.9
*u*1892	C(9)...H(37)	510.0(28)	30.7(fixed)	—	2.0	30.7
*u*1820	C(8)...H(39)	510.1(39)	30.2(fixed)	—	3.0	30.2
*u*2022	H(34)...H(46)	510.1(68)	43.7(fixed)	—	–10.5	43.7
*u*1862	Si(96)...Br(109)	510.3(15)	11.6(tied to *u*1914)	—	–0.8	11.8
*u*1855	H(24)...H(35)	510.4(57)	45.2(fixed)	—	8.6	45.2
*u*1888	C(8)...H(35)	510.4(38)	35.1(fixed)	—	6.3	35.1
*u*1884	H(78)...H(86)	510.4(46)	37.6(fixed)	—	–6.2	37.6
*u*1863	Si(52)...H(87)	510.4(22)	21.3(fixed)	—	0.0	21.3
*u*1947	C(101)...C(104)	510.5(54)	18.7(tied to *u*1914)	—	–0.9	19.1
*u*1853	Si(99)...H(136)	510.5(25)	22.1(fixed)	—	0.2	22.1
*u*1909	Si(4)...H(24)	510.5(19)	21.6(fixed)	—	0.0	21.6
*u*1895	C(53)...H(80)	510.5(28)	33.7(fixed)	—	4.3	33.7
*u*1827	C(6)...H(31)	510.6(31)	41.1(fixed)	—	8.8	41.1
*u*1914	Si(5)...Br(15)	510.7(19)	11.8(6)	—	–0.8	12.0
*u*1881	C(102)...H(114)	510.9(48)	33.5(fixed)	—	3.9	33.5
*u*1904	Si(52)...H(89)	510.9(22)	21.4(fixed)	—	0.0	21.4
*u*2012	H(30)...H(41)	511.0(37)	49.0(fixed)	—	–12.9	49.0
*u*1839	H(29)...H(39)	511.0(60)	45.7(fixed)	—	7.9	45.7
*u*1759	C(152)...H(169)	511.0(44)	29.8(fixed)	—	3.5	29.8
*u*1866	H(120)...H(130)	511.1(95)	36.9(fixed)	—	–6.5	36.9
*u*1833	C(147)...H(172)	511.1(25)	30.7(fixed)	—	2.6	30.7
*u*1980	C(53)...C(55)	511.2(60)	19.7(tied to *u*1656)	—	–0.9	19.3
*u*1878	Si(3)...H(32)	511.2(17)	22.6(fixed)	—	1.6	22.6
*u*1935	H(170)...H(184)	511.2(54)	43.8(fixed)	—	–8.5	43.8
*u*1859	C(105)...H(134)	511.3(34)	30.2(fixed)	—	2.8	30.2
*u*1911	Si(50)...Br(61)	511.3(15)	11.4(tied to *u*1914)	—	–0.8	11.6
*u*2000	H(115)...H(121)	511.3(43)	41.5(fixed)	—	–8.5	41.5
*u*1791	H(37)...H(44)	511.8(52)	57.5(fixed)	—	14.7	57.5
*u*1990	H(77)...H(93)	511.8(41)	36.7(fixed)	—	–8.5	36.7
*u*2030	H(27)...H(43)	511.9(45)	53.7(fixed)	—	–16.3	53.7
*u*1765	C(150)...H(176)	512.3(46)	28.8(fixed)	—	2.6	28.8
*u*1944	H(21)...H(29)	512.6(68)	39.0(fixed)	—	–9.6	39.0
*u*1852	C(148)...H(180)	512.8(33)	34.1(fixed)	—	4.5	34.1
*u*1905	Si(51)...H(84)	512.9(16)	21.3(fixed)	—	0.2	21.3
*u*1923	Br(15)...H(35)	512.9(51)	31.1(fixed)	—	5.4	31.1
*u*1930	C(150)...H(161)	512.9(37)	31.5(fixed)	—	3.2	31.5
*u*2029	H(160)...H(179)	513.1(40)	38.5(fixed)	—	–7.3	38.5
*u*1877	C(11)...H(40)	513.1(33)	33.3(fixed)	—	4.2	33.3
*u*1817	H(87)...H(94)	513.2(50)	40.3(fixed)	—	6.4	40.3
*u*1880	C(10)...H(29)	513.3(31)	34.0(fixed)	—	3.9	34.0

*u*1832	C(17)...H(28)	513.3(53)	34.9(fixed)	—	4.6	34.9
*u*1787	C(148)...H(172)	513.5(57)	29.0(fixed)	—	1.7	29.0
*u*1955	C(102)...C(105)	513.6(46)	19.2(tied to *u*1656)	—	–0.9	18.8
*u*1975	H(21)...H(27)	513.7(68)	39.6(fixed)	—	–9.5	39.6
*u*1828	C(7)...H(36)	513.7(40)	30.4(fixed)	—	2.8	30.4
*u*1912	H(75)...H(83)	513.8(47)	37.7(fixed)	—	–6.8	37.7
*u*1883	C(58)...H(87)	514.2(33)	30.0(fixed)	—	2.5	30.0
*u*1981	H(162)...H(166)	514.3(30)	34.4(fixed)	—	–6.5	34.4
*u*1850	C(12)...H(44)	514.3(44)	45.7(fixed)	—	13.4	45.7
*u*1891	C(55)...H(84)	514.4(27)	32.2(fixed)	—	4.2	32.2
*u*1926	C(7)...C(10)	514.4(36)	19.2(tied to *u*1914)	—	–1.0	19.5
*u*1886	C(59)...H(91)	514.7(43)	31.1(fixed)	—	3.0	31.1
*u*1887	C(12)...H(32)	514.7(26)	37.5(fixed)	—	8.3	37.5
*u*1898	C(148)...H(178)	514.8(28)	31.0(fixed)	—	2.8	31.0
*u*1885	C(6)...H(33)	515.1(31)	36.4(fixed)	—	5.9	36.4
*u*1754	H(112)...H(125)	515.2(46)	45.0(fixed)	—	8.2	45.0
*u*1954	H(76)...H(90)	515.3(56)	34.6(fixed)	—	–6.4	34.6
*u*1915	Si(145)...Br(156)	515.4(13)	11.7(tied to *u*1914)	—	–0.8	11.9
*u*1916	Si(51)...Br(62)	515.5(13)	11.7(tied to *u*1914)	—	–0.8	11.9
*u*1825	C(100)...H(125)	515.6(24)	35.9(fixed)	—	5.2	35.9
*u*2015	H(70)...H(81)	516.0(90)	36.6(fixed)	—	–9.3	36.6
*u*1882	Si(5)...H(42)	516.4(23)	24.5(fixed)	—	3.2	24.5
*u*1800	H(72)...H(91)	516.4(47)	41.6(fixed)	—	–4.9	41.6
*u*1919	C(56)...C(58)	516.7(30)	16.6(tied to *u*2130)	—	–0.8	18.7
*u*2009	H(19)...H(38)	516.9(37)	36.7(fixed)	—	–7.9	36.7
*u*1907	C(57)...H(71)	517.4(27)	31.8(fixed)	—	2.6	31.8
*u*1854	H(84)...H(91)	517.6(52)	40.0(fixed)	—	6.0	40.0
*u*1992	H(164)...H(175)	517.6(57)	34.3(fixed)	—	–7.1	34.3
*u*1997	H(119)...H(137)	517.8(38)	37.4(fixed)	—	–8.4	37.4
*u*1949	Si(3)...H(47)	517.8(18)	21.1(fixed)	—	–1.3	21.1
*u*1958	C(147)...C(149)	518.0(37)	19.3(tied to *u*1656)	—	–0.8	18.9
*u*1794	H(69)...H(89)	518.0(38)	40.6(fixed)	—	5.9	40.6
*u*1965	Si(50)...H(94)	518.1(18)	21.5(fixed)	—	–1.0	21.5
*u*2020	H(19)...H(25)	518.9(67)	39.5(fixed)	—	–8.9	39.5
*u*1950	Br(14)...H(44)	518.9(62)	36.2(fixed)	—	11.5	36.2
*u*1829	H(73)...H(90)	519.0(53)	41.2(fixed)	—	–5.0	41.2
*u*1796	H(117)...H(130)	519.2(49)	42.3(fixed)	—	7.5	42.3
*u*2005	H(113)...H(121)	519.3(43)	38.5(fixed)	—	–7.7	38.5
*u*1972	C(59)...C(64)	519.4(55)	19.0(tied to *u*1656)	—	–0.9	18.6
*u*1841	C(104)...H(120)	519.5(41)	32.6(fixed)	—	3.6	32.6
*u*2031	H(119)...H(132)	519.7(68)	39.6(fixed)	—	–7.5	39.6
*u*1952	Si(3)...H(31)	519.8(15)	24.8(fixed)	—	–0.5	24.8
*u*1957	Si(96)...H(116)	519.9(15)	23.4(fixed)	—	–1.0	23.4
*u*2027	H(160)...H(182)	520.1(34)	36.8(fixed)	—	–8.6	36.8
*u*2033	H(77)...H(88)	520.1(31)	39.4(fixed)	—	–7.3	39.4
*u*1936	Si(50)...H(78)	520.3(14)	20.9(fixed)	—	–1.1	20.9

*u*1968	Si(2)...H(35)	520.3(13)	22.4(fixed)	—	–0.7	22.4
*u*1932	Si(143)...H(163)	520.3(15)	20.6(fixed)	—	–1.2	20.6
*u*1899	C(8)...H(42)	520.4(23)	43.7(fixed)	—	12.7	43.7
*u*1967	Si(96)...H(129)	520.6(14)	22.7(fixed)	—	–1.1	22.7
*u*1998	H(88)...H(90)	520.6(33)	35.9(fixed)	—	–6.9	35.9
*u*1956	Si(49)...H(69)	520.6(15)	22.2(fixed)	—	–1.1	22.2
*u*1918	C(60)...H(94)	520.6(46)	31.4(fixed)	—	3.9	31.4
*u*1964	Br(108)...H(138)	520.7(65)	30.3(fixed)	—	3.0	30.3
*u*1959	Si(49)...H(82)	520.8(13)	22.6(fixed)	—	–0.7	22.6
*u*1961	Si(2)...H(22)	520.8(14)	22.5(fixed)	—	–1.0	22.5
*u*1939	C(9)...H(39)	520.9(42)	35.8(fixed)	—	4.0	35.8
*u*1962	Si(2)...H(28)	521.0(22)	22.0(fixed)	—	–1.4	22.0
*u*2017	H(21)...H(34)	521.1(50)	41.8(fixed)	—	–11.8	41.8
*u*1974	Si(143)...H(176)	521.2(15)	21.3(fixed)	—	–0.9	21.3
*u*1945	Si(143)...H(167)	521.2(21)	20.3(fixed)	—	–0.9	20.3
*u*1934	Si(49)...H(73)	521.7(22)	21.0(fixed)	—	–1.1	21.0
*u*1941	H(119)...H(134)	521.9(66)	36.1(fixed)	—	–7.2	36.1
*u*1999	C(12)...C(17)	522.0(38)	19.6(tied to *u*1656)	—	–1.0	19.2
*u*1991	H(162)...H(175)	522.4(44)	35.6(fixed)	—	–7.0	35.6
*u*1988	H(72)...H(81)	522.6(31)	39.3(fixed)	—	–8.4	39.3
*u*1868	C(63)...H(69)	523.1(40)	33.2(fixed)	—	3.2	33.2
*u*2013	Si(52)...H(75)	523.2(18)	20.3(fixed)	—	–1.2	20.3
*u*2051	H(65)...H(88)	523.3(37)	36.7(fixed)	—	3.4	36.7
*u*1953	C(54)...C(57)	523.4(46)	18.9(tied to *u*1914)	—	–0.9	19.3
*u*1951	C(6)...C(9)	523.5(46)	16.7(tied to *u*2130)	—	–0.8	18.9
*u*1948	H(74)...H(87)	523.9(61)	33.9(fixed)	—	–6.3	33.9
*u*2052	H(164)...H(168)	524.4(34)	34.0(fixed)	—	3.2	34.0
*u*2038	H(18)...H(41)	524.7(27)	39.3(fixed)	—	4.5	39.3
*u*2028	H(74)...H(85)	524.7(45)	41.3(fixed)	—	–7.7	41.3
*u*1943	Br(62)...H(86)	524.7(49)	29.0(fixed)	—	2.0	29.0
*u*2010	Si(98)...H(122)	524.9(13)	21.2(fixed)	—	–1.2	21.2
*u*1982	Si(98)...H(114)	525.2(19)	22.2(fixed)	—	–1.0	22.2
*u*1987	Si(5)...H(44)	525.2(19)	26.8(fixed)	—	–0.6	26.8
*u*1970	H(166)...H(174)	525.3(61)	36.5(fixed)	—	–7.4	36.5
*u*2001	Si(145)...H(180)	525.3(13)	21.6(fixed)	—	–1.4	21.6
*u*1984	Si(145)...H(161)	525.6(19)	21.3(fixed)	—	–1.2	21.3
*u*1873	C(16)...H(22)	525.9(33)	34.6(fixed)	—	4.4	34.6
*u*1983	Si(52)...H(91)	525.9(18)	21.0(fixed)	—	–1.0	21.0
*u*2016	Si(5)...H(39)	525.9(13)	22.8(fixed)	—	–1.6	22.8
*u*1977	Si(51)...H(67)	526.0(18)	21.8(fixed)	—	–1.2	21.8
*u*2008	Si(52)...H(86)	526.0(12)	21.1(fixed)	—	–1.2	21.1
*u*1985	Si(4)...H(20)	526.3(18)	21.7(fixed)	—	–0.8	21.7
*u*2026	H(68)...H(81)	526.4(64)	38.7(fixed)	—	–9.3	38.7
*u*1978	C(8)...C(13)	526.4(32)	16.9(tied to *u*2130)	—	–0.9	19.1
*u*1837	H(71)...H(86)	526.6(54)	40.2(fixed)	—	5.1	40.2
*u*1896	C(55)...H(86)	527.0(45)	31.7(fixed)	—	2.9	31.7

*u*1971	Si(51)...H(83)	527.1(14)	21.3(fixed)	—	–0.9	21.3
*u*1933	C(103)...C(107)	527.2(59)	16.7(tied to *u*2130)	—	–0.8	18.8
*u*1973	Si(98)...H(130)	527.2(13)	21.1(fixed)	—	–1.0	21.1
*u*2068	C(54)...C(56)	527.6(46)	15.1(tied to *u*2130)	—	–0.9	17.0
*u*1902	C(57)...H(75)	528.0(26)	30.6(fixed)	—	2.6	30.6
*u*1831	H(75)...H(79)	528.0(28)	39.3(fixed)	—	5.5	39.3
*u*1969	Si(4)...H(36)	528.5(13)	20.2(fixed)	—	–1.0	20.2
*u*1986	Si(4)...H(26)	528.5(13)	20.4(fixed)	—	–0.9	20.4
*u*2007	H(25)...H(38)	528.6(57)	36.1(fixed)	—	–7.4	36.1
*u*2060	C(55)...H(92)	528.6(79)	28.2(fixed)	—	2.6	28.2
*u*1849	H(73)...H(91)	529.3(49)	35.5(fixed)	—	–5.6	35.5
*u*2084	H(70)...H(84)	529.3(79)	46.8(fixed)	—	3.4	46.8
*u*2167	H(71)...H(92)	529.3(87)	41.2(fixed)	—	4.2	41.2
*u*1937	C(150)...C(152)	529.5(32)	16.9(tied to *u*2130)	—	–0.9	19.1
*u*2034	H(160)...H(174)	529.6(30)	36.7(fixed)	—	4.2	36.7
*u*2057	H(112)...H(135)	529.6(33)	37.2(fixed)	—	3.8	37.2
*u*1960	C(148)...C(151)	531.3(44)	17.1(tied to *u*2130)	—	–0.9	19.3
*u*1809	H(22)...H(42)	531.7(45)	47.8(fixed)	—	14.1	47.8
*u*2023	H(74)...H(90)	532.1(32)	34.4(fixed)	—	–6.6	34.4
*u*2043	C(59)...H(70)	532.6(67)	29.2(fixed)	—	1.7	29.2
*u*2040	H(166)...H(181)	533.0(28)	35.8(fixed)	—	5.7	35.8
*u*2036	H(72)...H(90)	533.1(35)	38.8(fixed)	—	–6.8	38.8
*u*2018	H(119)...H(135)	533.2(50)	35.3(fixed)	—	–7.4	35.3
*u*2046	H(90)...H(92)	533.4(34)	37.7(fixed)	—	4.5	37.7
*u*2082	Br(61)...C(63)	533.4(34)	17.9(tied to *u*2130)	—	–1.0	20.2
*u*2099	H(66)...H(73)	533.5(76)	37.8(fixed)	—	1.9	37.8
*u*2119	C(55)...C(64)	533.6(55)	18.4(fixed)	—	–0.6	18.4
*u*2074	Br(15)...H(23)	533.6(50)	34.1(fixed)	—	3.9	34.1
*u*2140	H(65)...H(79)	533.8(73)	43.6(fixed)	—	3.4	43.6
*u*2059	H(79)...H(85)	534.0(31)	35.6(fixed)	—	4.9	35.6
*u*2035	H(126)...H(132)	534.3(37)	37.2(fixed)	—	6.0	37.2
*u*2180	H(165)...H(186)	534.4(52)	41.3(fixed)	—	3.6	41.3
*u*2137	H(18)...H(32)	534.4(44)	55.0(fixed)	—	4.8	55.0
*u*2085	C(11)...Br(15)	534.9(39)	18.3(tied to *u*2130)	—	–1.0	20.7
*u*2159	C(105)...H(123)	535.3(45)	27.9(fixed)	—	1.6	27.9
*u*2094	C(149)...H(186)	535.5(45)	27.8(fixed)	—	2.1	27.8
*u*2130	Br(14)...C(16)	535.5(43)	19.1(10)	21.6(20)	–1.2	21.6
*u*2047	C(57)...H(65)	535.7(67)	28.3(fixed)	—	1.8	28.3
*u*2055	Br(15)...H(20)	535.9(54)	33.7(fixed)	—	4.1	33.7
*u*2049	H(27)...H(37)	535.9(30)	35.9(fixed)	—	3.1	35.9
*u*2006	H(74)...H(88)	536.0(49)	34.9(fixed)	—	–6.4	34.9
*u*2254	H(123)...H(127)	536.1(55)	43.9(fixed)	—	3.3	43.9
*u*2163	H(37)...H(42)	536.1(57)	64.5(fixed)	—	3.9	64.5
*u*2095	C(53)...C(60)	536.2(26)	14.9(tied to *u*2130)	—	–0.8	16.9
*u*2021	H(166)...H(175)	536.9(40)	36.6(fixed)	—	–7.5	36.6
*u*2096	C(148)...C(150)	537.1(18)	14.4(tied to *u*2130)	—	–0.9	16.2

*u*2088	H(116)...H(124)	537.2(73)	39.7(fixed)	—	3.6	39.7
*u*2083	C(147)...C(152)	537.7(27)	15.1(tied to *u*2130)	—	–0.8	17.0
*u*2120	H(132)...H(141)	537.9(62)	37.8(fixed)	—	3.5	37.8
*u*2109	C(6)...C(13)	538.0(15)	15.2(tied to *u*2130)	—	–1.0	17.2
*u*2048	H(74)...H(82)	538.1(40)	36.6(fixed)	—	4.4	36.6
*u*2081	H(43)...H(45)	538.3(25)	38.3(fixed)	—	7.3	38.3
*u*2042	H(24)...H(46)	538.4(60)	37.0(fixed)	—	5.1	37.0
*u*2101	C(54)...C(59)	538.6(44)	16.6(tied to *u*2130)	—	–0.8	18.8
*u*2078	H(113)...H(127)	538.7(33)	37.8(fixed)	—	5.7	37.8
*u*2058	C(150)...H(173)	538.9(36)	28.6(fixed)	—	1.2	28.6
*u*2076	C(63)...C(64)	539.1(32)	14.8(tied to *u*2130)	—	–0.7	16.8
*u*2168	H(67)...H(72)	539.2(98)	37.5(fixed)	—	1.6	37.5
*u*2067	C(10)...H(18)	539.3(38)	28.7(fixed)	—	2.2	28.7
*u*2128	C(149)...C(154)	539.5(29)	15.0(tied to *u*2130)	—	–0.9	17.0
*u*2187	C(103)...C(105)	539.5(30)	18.0(fixed)	—	–0.8	18.0
*u*2131	C(17)...H(40)	539.6(48)	29.1(fixed)	—	3.1	29.1
*u*2104	C(148)...H(183)	539.8(35)	28.3(fixed)	—	2.0	28.3
*u*2105	C(16)...C(17)	540.0(26)	14.9(tied to *u*2130)	—	–0.9	16.8
*u*2171	C(53)...H(76)	540.4(46)	27.4(fixed)	—	1.3	27.4
*u*2134	Br(155)...H(159)	540.9(22)	31.0(fixed)	—	3.0	31.0
*u*2142	C(149)...C(158)	541.2(30)	15.8(tied to *u*2130)	—	–0.6	17.8
*u*2061	H(66)...H(80)	541.2(27)	38.5(fixed)	—	5.4	38.5
*u*2107	C(100)...C(107)	541.2(20)	14.8(tied to *u*2130)	—	–0.9	16.7
*u*2039	H(123)...H(140)	541.7(42)	35.4(fixed)	—	4.0	35.4
*u*2208	H(24)...H(33)	541.7(56)	50.4(fixed)	—	4.2	50.4
*u*2092	C(16)...H(37)	541.7(44)	28.9(fixed)	—	1.1	28.9
*u*2045	H(72)...H(84)	541.8(29)	36.9(fixed)	—	5.4	36.9
*u*2041	H(21)...H(31)	541.8(50)	41.8(fixed)	—	8.1	41.8
*u*2190	H(73)...H(93)	541.8(73)	38.6(fixed)	—	2.1	38.6
*u*2123	C(6)...C(10)	541.8(28)	16.8(tied to *u*2130)	—	–0.8	19.0
*u*2113	C(53)...C(57)	541.9(41)	16.3(tied to *u*2130)	—	–0.8	18.5
*u*2054	H(32)...H(38)	542.0(35)	42.1(fixed)	—	10.2	42.1
*u*2080	C(101)...C(102)	542.1(19)	14.7(tied to *u*2130)	—	–0.9	16.6
*u*2065	C(9)...H(45)	542.1(54)	29.0(fixed)	—	2.7	29.0
*u*2089	C(60)...Br(62)	542.2(33)	17.8(tied to *u*2130)	—	–1.0	20.1
*u*2122	C(57)...C(59)	542.4(14)	14.8(tied to *u*2130)	—	–0.9	16.7
*u*2144	C(12)...C(16)	542.4(34)	16.9(tied to *u*2130)	—	–0.8	19.1
*u*2244	H(70)...H(76)	542.4(60)	35.0(fixed)	—	1.5	35.0
*u*2112	C(100)...C(105)	542.5(29)	15.2(tied to *u*2130)	—	–0.8	17.2
*u*2178	C(56)...H(69)	542.5(60)	34.3(fixed)	—	–0.5	34.3
*u*2127	C(100)...Br(109)	542.6(44)	17.8(tied to *u*2130)	—	–1.0	20.1
*u*2100	C(12)...H(23)	542.6(39)	28.5(fixed)	—	2.8	28.5
*u*2110	C(11)...C(13)	542.8(26)	15.6(tied to *u*2130)	—	–0.9	17.7
*u*2044	Br(62)...H(82)	542.8(26)	35.4(fixed)	—	5.1	35.4
*u*2126	H(164)...H(181)	542.8(42)	45.7(fixed)	—	2.8	45.7
*u*2072	H(120)...H(128)	542.9(71)	38.9(fixed)	—	2.1	38.9

*u*2103	C(9)...C(10)	543.0(24)	15.1(tied to *u*2130)	—	–0.8	17.1
*u*2037	Br(14)...H(26)	543.0(44)	32.5(fixed)	—	4.0	32.5
*u*2229	H(159)...H(173)	543.4(33)	39.2(fixed)	—	3.1	39.2
*u*2202	H(23)...H(37)	543.4(53)	40.7(fixed)	—	4.3	40.7
*u*2075	H(83)...H(93)	543.4(74)	38.6(fixed)	—	3.7	38.6
*u*2114	C(103)...C(111)	543.5(26)	15.0(tied to *u*2130)	—	–0.8	17.0
*u*2050	H(160)...H(167)	543.5(51)	36.8(fixed)	—	2.2	36.8
*u*2206	C(53)...C(56)	543.6(43)	15.9(tied to *u*2130)	—	–0.8	18.0
*u*2115	C(8)...C(17)	543.6(38)	15.1(tied to *u*2130)	—	–0.8	17.0
*u*2195	Si(50)...H(93)	543.7(23)	16.1(fixed)	—	–3.7	16.1
*u*2249	H(40)...H(45)	543.7(57)	44.6(fixed)	—	4.5	44.6
*u*2056	H(34)...H(40)	543.7(41)	38.4(fixed)	—	6.0	38.4
*u*2160	C(8)...C(11)	543.8(30)	15.9(tied to *u*2130)	—	–0.7	17.9
*u*2267	H(112)...H(118)	543.9(62)	42.5(fixed)	—	3.0	42.5
*u*2166	C(100)...H(118)	544.0(48)	28.3(fixed)	—	1.6	28.3
*u*2064	H(29)...H(30)	544.5(39)	38.8(fixed)	—	6.1	38.8
*u*2152	Si(3)...H(46)	544.5(21)	16.6(fixed)	—	–3.5	16.6
*u*2156	C(11)...H(24)	544.6(47)	27.6(fixed)	—	2.0	27.6
*u*2184	C(13)...C(17)	545.0(33)	16.3(tied to *u*2130)	—	–0.8	18.4
*u*2063	H(81)...H(87)	545.0(41)	35.1(fixed)	—	3.6	35.1
*u*2111	C(53)...C(58)	545.0(26)	15.2(tied to *u*2130)	—	–0.9	17.1
*u*2179	C(147)...H(170)	545.1(36)	28.4(fixed)	—	2.6	28.4
*u*2161	Si(2)...H(27)	545.4(21)	16.6(fixed)	—	–3.8	16.6
*u*2173	C(100)...C(102)	545.6(37)	16.0(tied to *u*2130)	—	–0.8	18.1
*u*2221	Si(52)...H(74)	545.8(19)	16.0(fixed)	—	–2.9	16.0
*u*2093	H(22)...H(30)	545.8(48)	42.6(fixed)	—	2.1	42.6
*u*2091	C(9)...C(12)	546.0(28)	14.7(tied to *u*2130)	—	–0.8	16.6
*u*2073	H(162)...H(178)	546.0(33)	35.5(fixed)	—	3.6	35.5
*u*2148	C(7)...C(12)	546.0(31)	16.2(tied to *u*2130)	—	–0.8	18.3
*u*2129	C(10)...C(12)	546.1(18)	15.2(tied to *u*2130)	—	–0.9	17.2
*u*2117	C(58)...C(60)	546.3(25)	15.0(tied to *u*2130)	—	–0.8	17.0
*u*2133	C(148)...C(154)	546.4(26)	16.6(tied to *u*2130)	—	–0.7	18.8
*u*2125	C(55)...C(59)	546.6(27)	15.0(tied to *u*2130)	—	–0.8	16.9
*u*2185	Si(143)...H(166)	546.8(22)	15.4(fixed)	—	–3.0	15.4
*u*2149	C(147)...C(151)	547.0(23)	16.2(tied to *u*2130)	—	–0.8	18.3
*u*2070	H(19)...H(33)	547.0(31)	40.9(fixed)	—	7.4	40.9
*u*2102	H(20)...H(27)	547.1(74)	37.8(fixed)	—	2.8	37.8
*u*2285	H(65)...H(76)	547.1(62)	40.1(fixed)	—	2.4	40.1
*u*2135	C(9)...C(17)	547.4(41)	16.5(tied to *u*2130)	—	–0.7	18.7
*u*2069	Br(108)...H(122)	547.4(30)	33.0(fixed)	—	3.0	33.0
*u*2071	H(75)...H(81)	547.5(50)	38.8(fixed)	—	0.9	38.8
*u*2136	H(161)...H(166)	547.6(62)	36.8(fixed)	—	1.8	36.8
*u*2118	C(6)...C(11)	547.7(28)	15.4(tied to *u*2130)	—	–0.8	17.4
*u*2328	H(70)...H(75)	547.9(51)	35.7(fixed)	—	0.0	35.7
*u*2139	C(8)...C(16)	547.9(17)	15.9(tied to *u*2130)	—	–0.9	17.9
*u*2216	C(147)...C(150)	548.1(28)	15.7(tied to *u*2130)	—	–0.8	17.8

*u*2155	Si(49)...H(72)	548.2(23)	15.8(fixed)	—	–3.2	15.8
*u*2143	C(100)...C(104)	548.4(23)	16.6(tied to *u*2130)	—	–0.8	18.8
*u*2294	Br(62)...C(64)	548.5(30)	16.1(tied to *u*2130)	—	–0.9	18.2
*u*2116	Br(108)...H(118)	548.5(35)	31.4(fixed)	—	3.1	31.4
*u*2097	H(26)...H(41)	548.5(47)	37.8(fixed)	—	2.8	37.8
*u*2299	H(135)...H(141)	548.7(39)	39.2(fixed)	—	4.1	39.2
*u*2170	H(117)...H(136)	549.0(36)	46.2(fixed)	—	3.7	46.2
*u*2158	Si(143)...H(162)	549.0(8)	16.1(fixed)	—	–2.9	16.1
*u*2066	C(101)...H(136)	549.2(37)	28.5(fixed)	—	2.0	28.5
*u*2231	Si(98)...H(121)	549.2(8)	16.0(fixed)	—	–3.1	16.0
*u*2090	H(68)...H(78)	549.2(48)	37.5(fixed)	—	2.4	37.5
*u*2196	C(60)...H(67)	549.2(45)	34.8(fixed)	—	–0.6	34.8
*u*2141	H(36)...H(46)	549.3(62)	37.4(fixed)	—	1.2	37.4
*u*2098	C(148)...C(153)	549.3(20)	15.2(tied to *u*2130)	—	–0.8	17.2
*u*2207	Si(49)...H(68)	549.3(11)	16.0(fixed)	—	–3.5	16.0
*u*2062	Br(155)...H(188)	549.4(28)	32.5(fixed)	—	3.3	32.5
*u*2298	H(159)...H(170)	549.4(47)	41.3(fixed)	—	4.4	41.3
*u*2175	C(59)...C(63)	549.4(32)	15.7(tied to *u*2130)	—	–0.8	17.8
*u*2077	H(71)...H(77)	549.5(32)	36.5(fixed)	—	3.6	36.5
*u*2200	Si(5)...H(41)	549.5(10)	16.8(fixed)	—	–3.9	16.8
*u*2217	Si(2)...H(21)	549.6(7)	16.2(fixed)	—	–3.9	16.2
*u*2053	H(25)...H(42)	549.7(32)	48.2(fixed)	—	15.9	48.2
*u*2218	Si(143)...H(175)	549.7(10)	15.9(fixed)	—	–3.4	15.9
*u*2219	Si(96)...H(115)	549.7(7)	16.1(fixed)	—	–4.0	16.1
*u*2154	C(13)...H(29)	549.9(51)	29.1(fixed)	—	2.8	29.1
*u*2106	C(55)...C(57)	550.1(19)	15.3(tied to *u*2130)	—	–0.7	17.3
*u*2138	Br(62)...H(89)	550.3(18)	30.1(fixed)	—	2.3	30.1
*u*2177	H(29)...H(45)	550.4(58)	45.1(fixed)	—	4.2	45.1
*u*2183	C(63)...H(94)	550.5(53)	35.5(fixed)	—	–0.3	35.5
*u*2213	C(16)...H(47)	550.8(43)	36.5(fixed)	—	–0.4	36.5
*u*2222	Si(145)...H(182)	550.8(7)	16.2(fixed)	—	–3.4	16.2
*u*2151	C(101)...C(106)	550.9(31)	16.0(tied to *u*2130)	—	–0.7	18.1
*u*2186	Si(96)...H(128)	551.0(9)	16.2(fixed)	—	–3.9	16.2
*u*2239	H(25)...H(35)	551.0(40)	39.2(fixed)	—	6.3	39.2
*u*2201	Si(3)...H(30)	551.1(7)	16.3(fixed)	—	–5.1	16.3
*u*2210	Si(49)...H(81)	551.3(8)	16.0(fixed)	—	–3.9	16.0
*u*2198	Si(2)...H(34)	551.5(8)	16.1(fixed)	—	–4.4	16.1
*u*2153	C(64)...H(87)	551.5(45)	27.0(fixed)	—	1.6	27.0
*u*2255	C(7)...Br(14)	551.6(28)	15.9(tied to *u*2130)	—	–0.9	18.0
*u*2269	H(159)...H(174)	551.6(40)	34.5(fixed)	—	2.1	34.5
*u*2315	H(67)...H(74)	551.7(71)	37.3(fixed)	—	2.3	37.3
*u*2223	Si(52)...H(88)	551.8(8)	16.1(fixed)	—	–3.1	16.1
*u*2209	Si(98)...H(132)	551.8(8)	15.9(fixed)	—	–3.3	15.9
*u*2087	Br(61)...H(76)	551.9(35)	29.4(fixed)	—	2.3	29.4
*u*2188	C(150)...H(163)	552.0(30)	31.9(fixed)	—	–0.7	31.9
*u*2203	H(68)...H(83)	552.1(56)	39.0(fixed)	—	4.0	39.0

*u*2215	Si(4)...H(25)	552.2(8)	15.9(fixed)	—	–3.3	15.9
*u*2182	H(38)...H(47)	552.2(51)	37.6(fixed)	—	2.5	37.6
*u*2204	Si(4)...H(38)	552.3(9)	15.8(fixed)	—	–3.0	15.8
*u*2162	Si(50)...H(77)	552.4(7)	16.1(fixed)	—	–3.3	16.1
*u*2124	C(102)...H(126)	552.4(40)	27.9(fixed)	—	3.3	27.9
*u*2292	H(164)...H(170)	552.4(29)	33.0(fixed)	—	0.5	33.0
*u*2214	Si(51)...H(85)	552.4(8)	16.0(fixed)	—	–3.5	16.0
*u*2345	C(64)...H(71)	552.5(63)	33.0(fixed)	—	–1.0	33.0
*u*2258	H(18)...H(40)	552.7(31)	36.3(fixed)	—	2.5	36.3
*u*2233	C(147)...H(176)	552.8(41)	34.5(fixed)	—	–0.6	34.5
*u*2176	C(63)...H(84)	553.0(42)	27.1(fixed)	—	2.3	27.1
*u*2174	H(85)...H(94)	553.1(89)	37.3(fixed)	—	2.0	37.3
*u*2266	C(149)...H(180)	553.3(41)	40.1(fixed)	—	–1.0	40.1
*u*2306	C(54)...H(84)	553.6(57)	38.3(fixed)	—	–1.1	38.3
*u*2227	C(10)...H(28)	553.6(37)	38.4(fixed)	—	–0.6	38.4
*u*2205	Si(145)...H(160)	553.6(24)	16.3(fixed)	—	–3.2	16.3
*u*2242	C(11)...H(39)	553.7(43)	40.0(fixed)	—	–0.8	40.0
*u*2262	H(114)...H(119)	553.8(58)	38.4(fixed)	—	3.1	38.4
*u*2147	C(54)...H(89)	553.9(37)	27.6(fixed)	—	1.6	27.6
*u*2278	H(84)...H(89)	553.9(54)	39.6(fixed)	—	4.0	39.6
*u*2232	Si(5)...H(43)	553.9(22)	17.7(fixed)	—	–6.6	17.7
*u*2295	C(101)...Br(108)	553.9(22)	15.9(tied to *u*2130)	—	–0.9	17.9
*u*2193	C(60)...C(64)	554.0(37)	15.4(tied to *u*2130)	—	–0.7	17.4
*u*2191	H(66)...H(78)	554.1(45)	37.9(fixed)	—	2.9	37.9
*u*2197	C(9)...C(13)	554.2(37)	16.3(tied to *u*2130)	—	–0.8	18.4
*u*2211	H(167)...H(187)	554.3(40)	36.5(fixed)	—	2.4	36.5
*u*2265	H(65)...H(87)	554.6(44)	34.0(fixed)	—	1.8	34.0
*u*2199	Si(51)...H(66)	554.7(24)	16.4(fixed)	—	–3.4	16.4
*u*2334	C(12)...H(42)	554.8(47)	56.3(fixed)	—	–1.2	56.3
*u*2322	C(6)...H(32)	555.0(35)	46.8(fixed)	—	–1.0	46.8
*u*2226	Si(98)...H(113)	555.0(23)	16.3(fixed)	—	–3.6	16.3
*u*2228	Si(4)...H(19)	555.1(23)	16.3(fixed)	—	–3.7	16.3
*u*2240	C(13)...H(20)	555.1(29)	35.9(fixed)	—	–0.6	35.9
*u*2086	H(121)...H(133)	555.3(81)	36.7(fixed)	—	1.9	36.7
*u*2250	H(85)...H(91)	555.5(51)	37.1(fixed)	—	2.1	37.1
*u*2349	H(44)...H(45)	555.6(33)	38.5(fixed)	—	–1.4	38.5
*u*2169	C(54)...C(63)	556.0(34)	16.5(tied to *u*2130)	—	–0.8	18.7
*u*2192	H(117)...H(131)	556.2(50)	41.4(fixed)	—	5.3	41.4
*u*2279	Br(61)...H(80)	556.6(38)	29.0(fixed)	—	3.0	29.0
*u*2251	C(100)...H(129)	556.6(44)	40.9(fixed)	—	–0.8	40.9
*u*2297	C(152)...Br(155)	556.7(20)	16.0(tied to *u*2130)	—	–0.9	18.1
*u*2284	H(41)...H(47)	556.7(45)	39.8(fixed)	—	2.9	39.8
*u*2236	H(38)...H(44)	556.8(54)	46.8(fixed)	—	14.7	46.8
*u*2302	Br(155)...H(165)	556.8(27)	29.3(fixed)	—	1.4	29.3
*u*2230	Si(52)...H(90)	556.9(22)	16.1(fixed)	—	–3.0	16.1
*u*2172	C(7)...C(16)	557.1(29)	17.0(tied to *u*2130)	—	–1.0	19.2

*u*2220	H(19)...H(31)	557.1(35)	44.8(fixed)	—	8.7	44.8
*u*2355	H(65)...H(86)	557.2(27)	34.9(fixed)	—	0.0	34.9
*u*2121	H(19)...H(28)	557.2(61)	39.6(fixed)	—	2.9	39.6
*u*2245	C(59)...H(78)	557.2(21)	35.9(fixed)	—	–0.6	35.9
*u*2305	H(79)...H(83)	557.4(25)	36.0(fixed)	—	0.8	36.0
*u*2259	H(70)...H(89)	557.4(50)	40.9(fixed)	—	2.5	40.9
*u*2145	H(69)...H(77)	557.5(81)	38.0(fixed)	—	1.6	38.0
*u*2268	H(87)...H(92)	557.5(60)	42.3(fixed)	—	2.8	42.3
*u*2189	C(102)...H(116)	557.6(30)	41.6(fixed)	—	–0.6	41.6
*u*2392	C(107)...H(139)	557.9(41)	35.8(fixed)	—	–0.9	35.8
*u*2348	C(152)...H(178)	558.0(38)	33.1(fixed)	—	–0.9	33.1
*u*2331	C(53)...H(79)	558.0(48)	35.2(fixed)	—	–1.0	35.2
*u*2342	H(164)...H(169)	558.0(26)	32.9(fixed)	—	–1.1	32.9
*u*2164	C(55)...C(60)	558.6(39)	17.8(fixed)	—	–0.7	17.8
*u*2264	C(105)...H(133)	558.9(42)	34.3(fixed)	—	-0.9	34.3
*u*2354	C(8)...H(33)	558.9(41)	42.6(fixed)	—	–1.2	42.6
*u*2165	C(56)...C(57)	559.2(19)	15.8(tied to *u*2130)	—	–0.7	17.9
*u*2289	C(54)...Br(61)	559.5(25)	16.1(tied to *u*2130)	—	–1.0	18.2
*u*2347	H(18)...H(39)	559.7(25)	37.8(fixed)	—	–0.2	37.8
*u*2281	H(89)...H(92)	559.8(42)	34.3(fixed)	—	2.7	34.3
*u*2243	H(21)...H(36)	559.8(47)	38.0(fixed)	—	1.2	38.0
*u*2252	Br(109)...H(139)	559.9(52)	29.5(fixed)	—	3.3	29.5
*u*2346	H(112)...H(133)	560.0(28)	36.1(fixed)	—	0.2	36.1
*u*2353	H(114)...H(127)	560.0(35)	36.9(fixed)	—	1.6	36.9
*u*2108	H(168)...H(176)	560.1(51)	36.9(fixed)	—	1.9	36.9
*u*2247	H(29)...H(40)	560.1(59)	43.4(fixed)	—	4.6	43.4
*u*2300	H(161)...H(168)	560.2(47)	36.9(fixed)	—	2.4	36.9
*u*2286	H(123)...H(136)	560.3(36)	34.4(fixed)	—	1.9	34.4
*u*2338	H(91)...H(92)	560.5(29)	36.8(fixed)	—	0.8	36.8
*u*2079	H(169)...H(175)	560.6(47)	39.0(fixed)	—	3.2	39.0
*u*2157	C(60)...H(71)	560.7(50)	27.5(fixed)	—	1.4	27.5
*u*2212	C(103)...H(138)	560.8(32)	36.5(fixed)	—	–0.6	36.5
*u*2146	C(56)...H(79)	561.0(22)	27.1(fixed)	—	2.1	27.1
*u*2237	H(160)...H(172)	561.2(25)	36.6(fixed)	—	1.4	36.6
*u*2241	H(116)...H(137)	561.2(25)	41.1(fixed)	—	4.3	41.1
*u*2319	C(58)...Br(61)	561.3(26)	17.4(tied to *u*2130)	—	–0.9	19.6
*u*2181	H(25)...H(39)	561.4(45)	38.9(fixed)	—	2.5	38.9
*u*2329	C(149)...Br(155)	561.8(14)	17.8(tied to *u*2130)	—	–0.9	20.1
*u*2296	H(117)...H(120)	561.8(25)	37.4(fixed)	—	1.8	37.4
*u*2325	H(161)...H(174)	561.9(30)	36.3(fixed)	—	0.4	36.3
*u*2273	C(12)...H(31)	562.1(29)	50.2(fixed)	—	–0.8	50.2
*u*2283	H(24)...H(45)	562.1(54)	34.1(fixed)	—	2.5	34.1
*u*2274	H(29)...H(37)	562.2(31)	33.9(fixed)	—	0.9	33.9
*u*2288	H(167)...H(181)	562.6(34)	36.2(fixed)	—	1.9	36.2
*u*2253	C(58)...H(86)	562.6(39)	34.4(fixed)	—	–0.8	34.4
*u*2224	H(28)...H(46)	562.6(58)	40.3(fixed)	—	3.7	40.3

*u*2256	C(53)...H(82)	562.7(45)	39.9(fixed)	—	–0.6	39.9
*u*2248	H(162)...H(180)	562.8(35)	38.0(fixed)	—	4.1	38.0
*u*2308	Br(155)...Br(156)	563.1(34)	19.5(tied to *u*2130)	—	–1.2	22.1
*u*2270	C(8)...H(44)	563.2(30)	60.3(fixed)	—	–0.4	60.3
*u*2380	C(102)...H(112)	563.5(51)	33.9(fixed)	—	–1.3	33.9
*u*2132	H(162)...H(172)	563.6(59)	36.2(fixed)	—	1.2	36.2
*u*2312	H(42)...H(45)	563.7(27)	36.7(fixed)	—	1.6	36.7
*u*2263	C(55)...H(83)	563.8(35)	38.9(fixed)	—	–0.8	38.9
*u*2280	H(65)...H(80)	564.0(36)	34.5(fixed)	—	3.5	34.5
*u*2320	H(165)...H(181)	564.2(33)	32.7(fixed)	—	2.9	32.7
*u*2363	C(7)...H(37)	564.4(45)	31.9(fixed)	—	–1.3	31.9
*u*2304	H(73)...H(84)	564.7(34)	37.2(fixed)	—	1.6	37.2
*u*2313	H(32)...H(36)	564.8(27)	43.4(fixed)	—	4.7	43.4
*u*2301	H(117)...H(118)	564.9(35)	33.7(fixed)	—	3.4	33.7
*u*2277	H(127)...H(134)	564.9(39)	32.8(fixed)	—	1.6	32.8
*u*2275	C(6)...H(35)	565.1(47)	42.8(fixed)	—	–0.7	42.8
*u*2408	C(13)...H(45)	565.2(42)	35.8(fixed)	—	–1.3	35.8
*u*2316	H(29)...H(31)	565.3(29)	38.6(fixed)	—	0.5	38.6
*u*2150	C(7)...H(42)	565.3(40)	31.9(fixed)	—	8.5	31.9
*u*2339	H(24)...H(47)	565.4(45)	37.0(fixed)	—	0.6	37.0
*u*2238	H(115)...H(130)	565.4(48)	39.4(fixed)	—	2.4	39.4
*u*2387	C(54)...H(74)	565.5(56)	23.1(fixed)	—	–1.7	23.1
*u*2287	Br(14)...H(33)	565.6(46)	30.6(fixed)	—	4.1	30.6
*u*2314	C(105)...Br(108)	566.1(34)	17.3(tied to *u*2130)	—	–0.8	19.6
*u*2351	C(100)...H(126)	566.3(25)	37.7(fixed)	—	–1.1	37.7
*u*2336	H(71)...H(78)	566.6(26)	35.8(fixed)	—	0.2	35.8
*u*2272	C(17)...H(26)	566.7(43)	35.7(fixed)	—	–0.8	35.7
*u*2311	H(26)...H(42)	566.9(26)	50.3(fixed)	—	7.9	50.3
*u*2225	H(76)...H(79)	567.0(28)	38.6(fixed)	—	3.6	38.6
*u*2344	H(67)...H(80)	567.1(37)	38.1(fixed)	—	1.4	38.1
*u*2437	C(56)...H(65)	567.1(56)	32.1(fixed)	—	–1.2	32.1
*u*2367	C(147)...H(173)	567.3(26)	30.6(fixed)	—	–1.2	30.6
*u*2323	C(148)...H(181)	567.4(33)	37.5(fixed)	—	–0.9	37.5
*u*2290	H(164)...H(178)	567.4(33)	33.2(fixed)	—	1.7	33.2
*u*2330	H(20)...H(33)	567.5(37)	41.1(fixed)	—	2.8	41.1
*u*2194	C(9)...H(36)	567.6(40)	31.5(fixed)	—	–0.6	31.5
*u*2385	H(116)...H(126)	567.7(65)	32.4(fixed)	—	–1.0	32.4
*u*2333	H(35)...H(40)	567.7(32)	37.6(fixed)	—	1.0	37.6
*u*2318	H(129)...H(134)	567.7(33)	34.3(fixed)	—	0.0	34.3
*u*2337	H(79)...H(84)	567.8(25)	32.4(fixed)	—	1.6	32.4
*u*2276	H(112)...H(127)	567.8(41)	33.9(fixed)	—	3.7	33.9
*u*2335	C(11)...Br(14)	567.9(31)	18.1(tied to *u*2130)	—	–1.0	20.4
*u*2234	H(71)...H(87)	568.1(61)	39.8(fixed)	—	2.8	39.8
*u*2235	C(57)...H(73)	568.2(28)	34.2(fixed)	—	–0.5	34.2
*u*2384	C(59)...H(89)	568.2(43)	31.5(fixed)	—	–1.1	31.5
*u*2324	H(82)...H(87)	568.2(32)	34.0(fixed)	—	0.0	34.0

*u*2350	H(28)...H(37)	568.3(30)	34.4(fixed)	—	–0.9	34.4
*u*2293	H(33)...H(40)	568.4(35)	35.4(fixed)	—	2.8	35.4
*u*2459	C(150)...H(159)	568.7(40)	32.8(fixed)	—	–1.2	32.8
*u*2307	H(88)...H(94)	568.9(59)	36.5(fixed)	—	3.0	36.5
*u*2341	C(7)...Br(15)	569.4(37)	14.7(tied to *u*2130)	—	–1.0	16.6
*u*2303	H(80)...H(87)	569.8(34)	32.6(fixed)	—	1.2	32.6
*u*2340	C(10)...Br(15)	569.9(31)	18.6(tied to *u*2130)	—	–0.9	21.1
*u*2257	H(23)...H(42)	569.9(47)	48.2(fixed)	—	12.1	48.2
*u*2416	H(65)...H(73)	569.9(65)	31.1(fixed)	—	–1.4	31.1
*u*2368	H(22)...H(32)	570.1(42)	36.5(fixed)	—	–3.8	36.5
*u*2326	H(27)...H(39)	570.1(43)	41.6(fixed)	—	2.9	41.6
*u*2317	H(29)...H(32)	570.4(35)	36.3(fixed)	—	2.3	36.3
*u*2370	C(6)...Br(15)	571.1(41)	16.9(tied to *u*2130)	—	–1.0	19.1
*u*2309	Br(15)...H(32)	571.3(38)	31.6(fixed)	—	5.5	31.6
*u*2260	H(72)...H(86)	571.4(51)	36.6(fixed)	—	2.0	36.6
*u*2425	H(131)...H(141)	571.5(55)	31.5(fixed)	—	–0.9	31.5
*u*2261	H(22)...H(43)	571.6(35)	45.7(fixed)	—	2.1	45.7
*u*2357	C(104)...H(118)	571.7(41)	33.4(fixed)	—	–1.0	33.4
*u*2291	H(18)...H(33)	571.7(32)	36.8(fixed)	—	4.7	36.8
*u*2343	H(163)...H(178)	571.8(28)	34.9(fixed)	—	0.5	34.9
*u*2352	C(17)...H(29)	572.0(45)	36.4(fixed)	—	–1.1	36.4
*u*2495	H(67)...H(71)	572.1(75)	31.8(fixed)	—	–1.7	31.8
*u*2246	C(148)...H(177)	572.4(28)	34.0(fixed)	—	–0.8	34.0
*u*2379	H(120)...H(127)	572.4(59)	32.1(fixed)	—	–2.1	32.1
*u*2282	H(69)...H(90)	572.7(52)	38.3(fixed)	—	2.3	38.3
*u*2372	H(23)...H(31)	572.8(42)	32.8(fixed)	—	2.1	32.8
*u*2457	C(55)...H(66)	573.1(60)	28.6(fixed)	—	–3.4	28.6
*u*2356	C(8)...Br(14)	573.3(37)	16.5(tied to *u*2130)	—	–0.9	18.7
*u*2386	H(75)...H(80)	573.4(41)	31.2(fixed)	—	–3.1	31.2
*u*2327	H(71)...H(84)	574.1(35)	33.2(fixed)	—	2.7	33.2
*u*2310	H(32)...H(37)	574.2(28)	36.7(fixed)	—	7.0	36.7
*u*2415	C(101)...H(124)	574.6(55)	30.3(fixed)	—	–4.1	30.3
*u*2365	H(76)...H(82)	574.6(36)	30.5(fixed)	—	0.5	30.5
*u*2366	C(58)...Br(62)	575.0(21)	16.6(tied to *u*2130)	—	–0.9	18.8
*u*2480	C(53)...H(72)	575.1(67)	28.0(fixed)	—	–3.3	28.0
*u*2358	C(147)...Br(155)	575.1(17)	14.9(tied to *u*2130)	—	–0.9	16.9
*u*2383	H(159)...H(167)	575.4(44)	30.7(fixed)	—	–1.6	30.7
*u*2271	H(75)...H(77)	575.9(32)	36.4(fixed)	—	1.6	36.4
*u*2424	C(105)...H(119)	576.1(45)	28.4(fixed)	—	–3.5	28.4
*u*2436	C(53)...H(88)	576.3(34)	23.2(fixed)	—	–1.7	23.2
*u*2430	C(60)...H(92)	576.3(50)	34.2(fixed)	—	–1.2	34.2
*u*2493	C(7)...H(32)	576.3(35)	33.9(fixed)	—	–6.1	33.9
*u*2321	H(71)...H(79)	576.4(29)	33.9(fixed)	—	1.3	33.9
*u*2399	H(69)...H(75)	576.6(57)	38.4(fixed)	—	0.5	38.4
*u*2468	C(54)...H(75)	576.6(42)	22.4(fixed)	—	–1.7	22.4
*u*2374	C(63)...H(70)	576.7(46)	32.9(fixed)	—	–1.3	32.9

*u*2395	H(83)...H(92)	576.8(64)	31.2(fixed)	—	–0.6	31.2
*u*2427	H(161)...H(165)	576.8(48)	31.9(fixed)	—	–1.7	31.9
*u*2382	C(16)...H(23)	576.9(36)	37.3(fixed)	—	–1.5	37.3
*u*2375	C(10)...H(21)	577.1(37)	30.9(fixed)	—	–4.0	30.9
*u*2541	C(101)...H(126)	577.2(51)	27.1(fixed)	—	–4.2	27.1
*u*2444	C(148)...H(168)	577.7(27)	22.6(fixed)	—	–1.5	22.6
*u*2431	C(6)...H(41)	578.0(22)	23.7(fixed)	—	–1.9	23.7
*u*2435	H(44)...H(47)	578.2(55)	42.3(fixed)	—	3.1	42.3
*u*2376	C(58)...H(74)	578.2(29)	26.7(fixed)	—	–2.9	26.7
*u*2423	C(106)...H(140)	578.3(48)	29.8(fixed)	—	–4.0	29.8
*u*2404	H(73)...H(94)	578.6(61)	35.1(fixed)	—	–0.7	35.1
*u*2522	H(69)...H(74)	578.6(75)	39.3(fixed)	—	–1.5	39.3
*u*2410	C(7)...H(30)	579.1(36)	33.7(fixed)	—	–5.6	33.7
*u*2586	C(53)...H(71)	579.2(52)	25.5(fixed)	—	–3.5	25.5
*u*2442	H(84)...H(94)	579.3(71)	32.5(fixed)	—	–2.1	32.5
*u*2510	C(54)...H(76)	579.5(45)	22.3(fixed)	—	–1.8	22.3
*u*2394	C(9)...H(40)	579.6(45)	34.6(fixed)	—	–1.0	34.6
*u*2561	C(106)...H(139)	579.7(42)	26.7(fixed)	—	–4.2	26.7
*u*2450	H(36)...H(45)	580.0(49)	31.6(fixed)	—	–2.6	31.6
*u*2413	H(91)...H(94)	580.3(52)	39.4(fixed)	—	1.0	39.4
*u*2525	C(56)...H(80)	580.5(28)	27.1(fixed)	—	–4.3	27.1
*u*2369	C(103)...Br(108)	580.6(23)	21.7(tied to *u*2567)	—	–0.8	19.1
*u*2393	H(70)...H(78)	580.6(47)	30.3(fixed)	—	–1.0	30.3
*u*2463	H(67)...H(86)	580.7(41)	38.8(fixed)	—	0.4	38.8
*u*2470	C(150)...H(179)	580.7(26)	23.2(fixed)	—	–1.7	23.2
*u*2501	C(17)...H(44)	580.8(36)	23.7(fixed)	—	–1.7	23.7
*u*2590	C(55)...H(65)	580.8(57)	24.5(fixed)	—	–3.5	24.5
*u*2398	H(28)...H(31)	581.1(37)	43.3(fixed)	—	2.5	43.3
*u*2332	H(24)...H(42)	581.2(27)	41.6(fixed)	—	11.1	41.6
*u*2359	C(102)...Br(108)	581.4(27)	16.9(fixed)	—	–0.9	16.9
*u*2432	C(59)...H(93)	581.7(54)	28.9(fixed)	—	–3.6	28.9
*u*2417	C(152)...H(160)	581.7(28)	23.0(fixed)	—	–1.7	23.0
*u*2538	C(10)...H(23)	581.8(34)	26.4(fixed)	—	–4.3	26.4
*u*2563	C(105)...H(118)	581.8(44)	25.6(fixed)	—	–3.8	25.6
*u*2531	H(37)...H(47)	582.0(45)	31.4(fixed)	—	–1.0	31.4
*u*2401	C(149)...H(160)	582.0(36)	27.8(fixed)	—	–3.2	27.8
*u*2397	H(78)...H(83)	582.2(31)	40.6(fixed)	—	1.5	40.6
*u*2364	C(57)...H(76)	582.4(26)	30.7(fixed)	—	–1.0	30.7
*u*2371	C(152)...Br(156)	582.5(22)	16.8(tied to *u*2130)	—	–0.9	19.0
*u*2526	C(53)...H(86)	582.6(23)	22.4(fixed)	—	–1.7	22.4
*u*2407	C(6)...H(27)	582.6(53)	29.1(fixed)	—	–3.8	29.1
*u*2360	C(56)...Br(61)	582.7(29)	14.8(tied to *u*2130)	—	–1.0	16.7
*u*2440	H(167)...H(180)	582.8(50)	43.6(fixed)	—	0.9	43.6
*u*2400	H(69)...H(79)	583.0(61)	32.3(fixed)	—	–1.8	32.3
*u*2456	C(100)...H(135)	583.0(27)	23.0(fixed)	—	–1.8	23.0
*u*2523	H(114)...H(129)	583.0(54)	44.3(fixed)	—	1.0	44.3

*u*2482	H(35)...H(39)	583.0(45)	44.7(fixed)	—	1.4	44.7
*u*2439	C(57)...H(83)	583.2(21)	23.2(fixed)	—	–1.3	23.2
*u*2377	C(56)...H(81)	583.3(33)	30.4(fixed)	—	–4.0	30.4
*u*2361	Br(62)...C(63)	583.3(14)	18.9(tied to *u*2567)	—	–1.0	16.6
*u*2362	C(55)...H(87)	583.3(48)	31.4(fixed)	—	–1.0	31.4
*u*2575	H(122)...H(129)	583.3(33)	37.5(fixed)	—	0.4	37.5
*u*2433	C(147)...H(166)	583.4(40)	27.3(fixed)	—	–3.2	27.3
*u*2555	C(64)...H(84)	583.5(49)	28.5(fixed)	—	–4.2	28.5
*u*2465	C(64)...H(91)	583.5(32)	22.6(fixed)	—	–1.4	22.6
*u*2418	C(64)...H(90)	583.7(36)	22.7(fixed)	—	–1.6	22.7
*u*2391	H(20)...H(29)	583.7(56)	31.2(fixed)	—	–1.4	31.2
*u*2528	C(105)...H(114)	584.0(36)	23.1(fixed)	—	–1.5	23.1
*u*2443	C(150)...H(177)	584.0(35)	23.0(fixed)	—	–1.3	23.0
*u*2557	C(147)...H(165)	584.1(33)	25.9(fixed)	—	–3.5	25.9
*u*2412	C(101)...H(119)	584.3(28)	22.9(fixed)	—	–1.8	22.9
*u*2403	Br(15)...H(22)	584.3(40)	37.8(fixed)	—	–0.5	37.8
*u*2490	C(148)...H(169)	584.4(21)	22.3(fixed)	—	–1.9	22.3
*u*2446	C(9)...H(31)	584.4(24)	23.3(fixed)	—	–1.1	23.3
*u*2402	H(163)...H(169)	584.7(34)	37.0(fixed)	—	0.3	37.0
*u*2485	C(57)...H(85)	584.8(22)	23.0(fixed)	—	–1.7	23.0
*u*2546	C(152)...H(159)	585.0(32)	22.4(fixed)	—	–1.8	22.4
*u*2420	H(18)...H(28)	585.2(51)	31.5(fixed)	—	–1.2	31.5
*u*2396	H(26)...H(40)	585.3(38)	31.2(fixed)	—	–1.4	31.2
*u*2577	C(149)...H(159)	585.4(36)	24.9(fixed)	—	–3.7	24.9
*u*2580	Br(14)...H(24)	585.4(50)	37.3(fixed)	—	–1.0	37.3
*u*2500	C(64)...H(85)	585.5(59)	28.4(fixed)	—	–3.9	28.4
*u*2409	H(67)...H(78)	585.6(44)	34.8(fixed)	—	0.0	34.8
*u*2478	C(17)...H(43)	585.7(26)	23.5(fixed)	—	–1.4	23.5
*u*2461	C(8)...H(41)	585.8(34)	28.7(fixed)	—	–3.8	28.7
*u*2406	H(69)...H(83)	586.0(48)	36.2(fixed)	—	0.6	36.2
*u*2574	H(67)...H(75)	586.0(47)	35.0(fixed)	—	–0.4	35.0
*u*2496	C(12)...H(46)	586.1(41)	28.5(fixed)	—	–3.6	28.5
*u*2508	C(13)...H(35)	586.1(28)	23.7(fixed)	—	–1.4	23.7
*u*2613	Br(62)...H(80)	586.1(28)	38.5(fixed)	—	–1.2	38.5
*u*2618	Br(15)...H(18)	586.4(49)	36.7(fixed)	—	–1.4	36.7
*u*2556	H(39)...H(47)	586.6(36)	36.3(fixed)	—	–0.9	36.3
*u*2405	C(101)...H(120)	586.6(21)	23.1(fixed)	—	–1.5	23.1
*u*2509	H(24)...H(39)	586.7(35)	33.3(fixed)	—	–1.9	33.3
*u*2506	C(58)...H(76)	586.7(29)	23.4(fixed)	—	–3.1	23.4
*u*2537	C(6)...H(39)	586.8(21)	23.0(fixed)	—	–2.2	23.0
*u*2589	Br(61)...Br(62)	586.9(26)	23.8(tied to *u*2567)	—	–1.0	20.9
*u*2532	C(6)...H(40)	586.9(24)	22.9(fixed)	—	–1.7	22.9
*u*2411	C(57)...H(68)	587.0(41)	28.6(fixed)	—	–3.4	28.6
*u*2504	C(17)...H(38)	587.1(36)	27.3(fixed)	—	–3.1	27.3
*u*2473	C(152)...H(161)	587.1(32)	23.2(fixed)	—	–1.7	23.2
*u*2619	Br(62)...H(93)	587.1(40)	24.4(fixed)	—	–1.7	24.4

*u*2551	C(148)...H(170)	587.2(20)	22.0(fixed)	—	–2.0	22.0
*u*2451	H(167)...H(188)	587.3(34)	33.3(fixed)	—	–0.5	33.3
*u*2378	H(116)...H(120)	587.3(35)	45.4(fixed)	—	1.4	45.4
*u*2514	C(100)...H(133)	587.3(23)	22.6(fixed)	—	–1.7	22.6
*u*2588	C(59)...H(92)	587.3(51)	25.1(fixed)	—	–3.8	25.1
*u*2458	C(59)...H(73)	587.4(34)	23.2(fixed)	—	–1.4	23.2
*u*2381	H(122)...H(134)	587.4(68)	30.5(fixed)	—	–1.5	30.5
*u*2559	H(67)...H(88)	587.4(58)	40.0(fixed)	—	–1.6	40.0
*u*2426	C(12)...H(27)	587.5(30)	23.1(fixed)	—	–1.8	23.1
*u*2539	C(54)...H(79)	587.8(38)	26.1(fixed)	—	–3.7	26.1
*u*2466	Br(155)...H(161)	587.8(25)	35.4(fixed)	—	–0.7	35.4
*u*2494	C(105)...H(113)	588.1(31)	23.4(fixed)	—	–1.9	23.4
*u*2475	C(13)...H(34)	588.1(34)	24.0(fixed)	—	–1.7	24.0
*u*2414	C(9)...H(19)	588.1(47)	30.0(fixed)	—	–3.7	30.0
*u*2474	H(161)...H(176)	588.4(49)	39.3(fixed)	—	0.5	39.3
*u*2535	C(53)...H(87)	588.4(33)	22.2(fixed)	—	–1.7	22.2
*u*2601	C(12)...H(45)	588.4(33)	26.4(fixed)	—	–4.1	26.4
*u*2597	C(17)...H(37)	588.5(37)	24.5(fixed)	—	–3.4	24.5
*u*2487	C(9)...H(30)	588.5(31)	23.3(fixed)	—	–1.7	23.3
*u*2449	H(20)...H(31)	588.6(27)	43.0(fixed)	—	3.5	43.0
*u*2488	C(10)...H(38)	588.6(26)	23.3(fixed)	—	–1.9	23.3
*u*2389	H(169)...H(174)	588.6(38)	31.4(fixed)	—	–1.0	31.4
*u*2507	C(103)...H(141)	588.7(28)	22.9(fixed)	—	–1.6	22.9
*u*2469	C(10)...H(36)	588.7(23)	23.0(fixed)	—	–1.5	23.0
*u*2567	Br(14)...Br(15)	588.8(19)	20.7(15)	18.1(18)	–1.2	18.1
*u*2438	H(161)...H(172)	588.8(25)	33.6(fixed)	—	–1.2	33.6
*u*2455	C(8)...H(46)	589.0(47)	23.3(fixed)	—	–1.7	23.3
*u*2448	H(73)...H(83)	589.0(45)	42.8(fixed)	—	1.1	42.8
*u*2553	C(9)...H(18)	589.0(44)	25.5(fixed)	—	–3.9	25.5
*u*2471	C(55)...H(78)	589.1(20)	23.2(fixed)	—	–1.3	23.2
*u*2472	C(16)...H(26)	589.1(23)	23.6(fixed)	—	–1.3	23.6
*u*2467	C(103)...H(140)	589.2(34)	23.4(fixed)	—	–1.8	23.4
*u*2484	C(60)...H(82)	589.5(25)	23.1(fixed)	—	–1.3	23.1
*u*2521	H(122)...H(141)	589.6(46)	38.9(fixed)	—	0.6	38.9
*u*2464	C(59)...H(72)	589.8(28)	23.4(fixed)	—	–1.9	23.4
*u*2584	H(161)...H(169)	589.8(32)	35.3(fixed)	—	–1.8	35.3
*u*2527	H(20)...H(39)	590.1(38)	40.3(fixed)	—	0.6	40.3
*u*2578	C(13)...H(24)	590.1(33)	27.5(fixed)	—	–4.1	27.5
*u*2529	H(26)...H(35)	590.2(33)	36.8(fixed)	—	1.6	36.8
*u*2373	H(170)...H(176)	590.2(40)	32.2(fixed)	—	–2.2	32.2
*u*2441	C(54)...H(77)	590.4(53)	28.4(fixed)	—	–3.5	28.4
*u*2486	H(31)...H(36)	590.4(37)	52.2(fixed)	—	2.0	52.2
*u*2554	C(57)...H(70)	590.5(45)	24.5(fixed)	—	–3.5	24.5
*u*2390	C(103)...H(135)	590.5(60)	27.2(fixed)	—	–3.1	27.2
*u*2530	C(8)...H(47)	590.5(33)	23.2(fixed)	—	–1.8	23.2
*u*2564	H(163)...H(168)	590.6(39)	37.4(fixed)	—	–1.5	37.4

*u*2542	C(64)...H(89)	590.6(34)	22.0(fixed)	—	–1.7	22.0
*u*2503	H(114)...H(120)	590.7(41)	35.7(fixed)	—	–0.2	35.7
*u*2454	H(28)...H(47)	590.7(47)	37.6(fixed)	—	0.0	37.6
*u*2460	H(82)...H(86)	590.9(40)	39.2(fixed)	—	1.1	39.2
*u*2477	H(163)...H(180)	590.9(31)	36.2(fixed)	—	0.7	36.2
*u*2479	C(58)...H(66)	591.0(25)	23.3(fixed)	—	–2.0	23.3
*u*2512	C(11)...H(20)	591.2(37)	23.0(fixed)	—	–1.2	23.0
*u*2492	C(16)...H(25)	591.3(25)	24.3(fixed)	—	–1.7	24.3
*u*2429	H(73)...H(78)	591.3(27)	39.0(fixed)	—	0.9	39.0
*u*2462	H(26)...H(44)	591.4(38)	61.6(fixed)	—	4.1	61.6
*u*2518	C(58)...H(67)	591.4(39)	23.2(fixed)	—	–1.6	23.2
*u*2595	Br(14)...H(21)	591.5(38)	24.5(fixed)	—	–1.7	24.5
*u*2421	H(163)...H(173)	591.6(50)	30.1(fixed)	—	–1.6	30.1
*u*2598	C(150)...H(178)	591.7(29)	21.9(fixed)	—	–2.2	21.9
*u*2428	H(22)...H(36)	591.8(36)	33.6(fixed)	—	–1.5	33.6
*u*2447	H(114)...H(133)	591.8(37)	40.6(fixed)	—	0.7	40.6
*u*2552	C(8)...H(45)	591.9(41)	22.6(fixed)	—	–1.8	22.6
*u*2549	C(110)...H(123)	591.9(27)	22.1(fixed)	—	–1.9	22.1
*u*2630	C(55)...H(93)	592.0(57)	26.2(fixed)	—	–3.5	26.2
*u*2544	C(6)...H(29)	592.4(39)	26.2(fixed)	—	–4.0	26.2
*u*2419	C(152)...H(168)	592.4(34)	28.0(fixed)	—	–3.7	28.0
*u*2497	C(60)...H(81)	592.5(33)	23.3(fixed)	—	–1.9	23.3
*u*2499	C(13)...H(25)	592.5(33)	28.7(fixed)	—	–3.7	28.7
*u*2434	H(116)...H(138)	592.8(23)	38.6(fixed)	—	0.7	38.6
*u*2516	H(83)...H(91)	593.1(36)	33.9(fixed)	—	–1.5	33.9
*u*2545	C(58)...H(65)	593.1(29)	22.3(fixed)	—	–1.7	22.3
*u*2548	H(90)...H(94)	593.2(63)	41.0(fixed)	—	–1.3	41.0
*u*2585	H(20)...H(41)	593.3(36)	41.3(fixed)	—	–1.8	41.3
*u*2569	C(103)...H(139)	593.4(27)	22.2(fixed)	—	–1.7	22.2
*u*2513	C(12)...H(28)	593.5(33)	22.6(fixed)	—	–1.8	22.6
*u*2566	C(17)...H(42)	593.6(23)	22.9(fixed)	—	–2.4	22.9
*u*2568	C(101)...H(118)	593.7(23)	22.0(fixed)	—	–2.1	22.0
*u*2612	H(166)...H(180)	593.7(41)	46.6(fixed)	—	–2.3	46.6
*u*2624	Br(108)...H(115)	593.8(30)	24.3(fixed)	—	–1.6	24.3
*u*2453	H(36)...H(44)	593.9(37)	46.5(fixed)	—	7.8	46.5
*u*2388	C(150)...H(175)	594.0(33)	28.9(fixed)	—	–3.4	28.9
*u*2533	H(20)...H(35)	594.4(58)	45.7(fixed)	—	1.8	45.7
*u*2511	C(11)...H(19)	594.5(29)	23.6(fixed)	—	–2.0	23.6
*u*2534	C(12)...H(29)	594.5(27)	22.7(fixed)	—	–1.8	22.7
*u*2571	C(13)...H(33)	594.5(24)	23.0(fixed)	—	–2.2	23.0
*u*2582	H(160)...H(176)	594.6(44)	39.9(fixed)	—	–1.6	39.9
*u*2519	C(103)...H(134)	594.7(52)	24.2(fixed)	—	–3.3	24.2
*u*2627	Br(14)...H(43)	594.8(41)	39.5(fixed)	—	–7.0	39.5
*u*2547	C(150)...H(174)	594.9(29)	25.4(fixed)	—	–3.7	25.4
*u*2520	H(67)...H(82)	594.9(64)	43.6(fixed)	—	1.0	43.6
*u*2594	Br(61)...H(90)	595.0(33)	29.7(fixed)	—	–3.1	29.7

*u*2587	H(43)...H(47)	595.2(44)	43.4(fixed)	—	–1.0	43.4
*u*2573	C(8)...H(40)	595.3(30)	25.7(fixed)	—	–4.0	25.7
*u*2505	C(152)...H(170)	595.4(28)	27.7(fixed)	—	–4.1	27.7
*u*2515	H(22)...H(44)	595.6(30)	42.5(fixed)	—	–4.9	42.5
*u*2543	C(105)...H(112)	595.7(33)	22.3(fixed)	—	–1.7	22.3
*u*2452	H(120)...H(125)	595.7(36)	36.2(fixed)	—	–1.5	36.2
*u*2498	C(149)...H(172)	595.7(22)	22.9(fixed)	—	–1.5	22.9
*u*2483	C(149)...H(171)	596.2(25)	23.0(fixed)	—	–1.8	23.0
*u*2540	C(149)...H(173)	596.4(24)	22.5(fixed)	—	–1.8	22.5
*u*2581	C(9)...H(32)	596.4(23)	22.3(fixed)	—	–2.2	22.3
*u*2614	Br(15)...H(34)	596.4(43)	34.6(fixed)	—	–4.7	34.6
*u*2422	C(148)...H(171)	596.7(45)	27.3(fixed)	—	–3.0	27.3
*u*2591	H(28)...H(39)	596.9(41)	38.9(fixed)	—	–0.9	38.9
*u*2637	C(16)...H(38)	596.9(41)	25.1(fixed)	—	–2.9	25.1
*u*2562	C(148)...H(173)	596.9(40)	23.7(fixed)	—	–3.1	23.7
*u*2683	Br(14)...H(42)	597.0(42)	39.4(fixed)	—	–9.1	39.4
*u*2583	C(60)...H(80)	597.0(23)	22.1(fixed)	—	–2.0	22.1
*u*2593	C(57)...H(84)	597.1(15)	21.5(fixed)	—	–2.3	21.5
*u*2622	Br(155)...H(175)	597.2(28)	24.3(fixed)	—	–1.8	24.3
*u*2651	Br(62)...H(94)	597.2(36)	23.4(fixed)	—	–1.7	23.4
*u*2600	H(34)...H(39)	597.3(54)	45.5(fixed)	—	–1.8	45.5
*u*2634	Br(108)...H(116)	597.4(24)	23.5(fixed)	—	–1.7	23.5
*u*2599	H(28)...H(30)	597.5(47)	44.3(fixed)	—	–1.8	44.3
*u*2558	C(11)...H(18)	597.7(25)	22.7(fixed)	—	–1.9	22.7
*u*2675	C(105)...H(121)	597.8(31)	24.7(fixed)	—	–3.1	24.7
*u*2481	C(55)...H(77)	597.8(25)	23.4(fixed)	—	–1.7	23.4
*u*2570	H(86)...H(94)	597.8(38)	34.3(fixed)	—	0.1	34.3
*u*2635	C(11)...H(25)	598.0(31)	25.0(fixed)	—	–3.0	25.0
*u*2631	C(59)...H(68)	598.2(44)	25.9(fixed)	—	–3.4	25.9
*u*2579	C(10)...H(37)	598.4(18)	22.4(fixed)	—	–2.1	22.4
*u*2625	Br(14)...H(22)	598.7(26)	23.7(fixed)	—	–1.7	23.7
*u*2621	Br(155)...H(186)	598.9(30)	35.3(fixed)	—	–1.2	35.3
*u*2550	H(26)...H(47)	599.3(42)	40.3(fixed)	—	0.5	40.3
*u*2517	Br(61)...H(75)	599.3(39)	32.6(fixed)	—	–0.9	32.6
*u*2560	H(116)...H(119)	599.4(39)	47.5(fixed)	—	–1.8	47.5
*u*2606	Br(62)...H(88)	599.5(34)	29.0(fixed)	—	–3.1	29.0
*u*2604	Br(108)...H(123)	599.5(25)	33.4(fixed)	—	–1.0	33.4
*u*2489	H(69)...H(91)	599.5(34)	35.4(fixed)	—	–0.3	35.4
*u*2603	H(78)...H(85)	599.9(25)	42.2(fixed)	—	–1.8	42.2
*u*2502	Br(108)...H(120)	600.4(31)	36.0(fixed)	—	–0.8	36.0
*u*2592	C(59)...H(71)	600.5(30)	21.9(fixed)	—	–2.1	21.9
*u*2476	Br(62)...H(91)	600.6(21)	33.6(fixed)	—	–0.7	33.6
*u*2623	Br(61)...H(68)	600.7(33)	24.6(fixed)	—	–2.0	24.6
*u*2632	C(10)...H(19)	600.8(31)	26.8(fixed)	—	–3.6	26.8
*u*2596	C(16)...H(24)	600.8(18)	22.7(fixed)	—	–2.3	22.7
*u*2680	Br(62)...H(92)	600.8(35)	23.4(fixed)	—	–2.0	23.4

*u*2445	H(28)...H(36)	600.9(46)	36.3(fixed)	—	0.5	36.3
*u*2676	Br(15)...H(33)	601.0(35)	30.3(fixed)	—	–5.6	30.3
*u*2638	C(149)...H(187)	601.5(30)	25.1(fixed)	—	–3.2	25.1
*u*2682	C(53)...H(74)	601.8(54)	24.5(fixed)	—	–3.0	24.5
*u*2639	C(55)...H(94)	601.9(47)	24.7(fixed)	—	–3.0	24.7
*u*2605	H(113)...H(129)	601.9(47)	46.6(fixed)	—	–2.0	46.6
*u*2576	H(121)...H(138)	602.2(40)	41.6(fixed)	—	–1.7	41.6
*u*2661	C(100)...H(119)	602.3(44)	25.0(fixed)	—	–3.3	25.0
*u*2628	C(57)...H(66)	602.7(38)	25.8(fixed)	—	–3.4	25.8
*u*2572	C(55)...H(79)	603.1(20)	22.1(fixed)	—	–1.8	22.1
*u*2611	H(122)...H(140)	603.2(53)	39.9(fixed)	—	–2.0	39.9
*u*2536	H(75)...H(78)	603.4(24)	33.4(fixed)	—	–1.4	33.4
*u*2686	Br(61)...H(89)	603.6(33)	24.6(fixed)	—	–3.6	24.6
*u*2491	H(163)...H(177)	604.1(31)	38.2(fixed)	—	0.4	38.2
*u*2668	Br(14)...H(23)	604.3(25)	23.4(fixed)	—	–2.2	23.4
*u*2657	C(63)...H(85)	604.3(38)	25.2(fixed)	—	–3.3	25.2
*u*2645	Br(155)...H(176)	604.4(25)	23.5(fixed)	—	–1.5	23.5
*u*2524	H(73)...H(86)	604.6(40)	33.9(fixed)	—	–0.8	33.9
*u*2671	C(17)...H(41)	604.6(35)	27.2(fixed)	—	–3.9	27.2
*u*2616	Br(108)...H(137)	604.8(42)	30.9(fixed)	—	–3.5	30.9
*u*2620	H(31)...H(38)	604.8(35)	57.0(fixed)	—	–2.5	57.0
*u*2629	C(59)...H(69)	605.7(38)	24.8(fixed)	—	–2.9	24.8
*u*2660	C(12)...H(21)	606.0(36)	26.7(fixed)	—	–3.9	26.7
*u*2644	Br(61)...H(69)	606.1(33)	23.8(fixed)	—	–1.7	23.8
*u*2617	H(25)...H(44)	606.4(38)	68.4(fixed)	—	–2.5	68.4
*u*2609	H(72)...H(83)	606.9(38)	45.4(fixed)	—	–2.2	45.4
*u*2690	C(111)...H(133)	606.9(26)	24.2(fixed)	—	–3.0	24.2
*u*2655	C(101)...H(137)	607.3(23)	26.5(fixed)	—	–3.6	26.5
*u*2608	H(66)...H(82)	607.6(45)	45.7(fixed)	—	–2.1	45.7
*u*2658	C(149)...H(188)	607.7(27)	23.8(fixed)	—	–2.8	23.8
*u*2678	C(147)...H(168)	607.8(35)	25.0(fixed)	—	–3.3	25.0
*u*2636	C(57)...H(67)	607.8(37)	24.7(fixed)	—	–3.0	24.7
*u*2565	H(27)...H(36)	607.9(46)	37.1(fixed)	—	–1.7	37.1
*u*2643	C(10)...H(20)	608.1(24)	25.0(fixed)	—	–3.1	25.0
*u*2607	H(81)...H(86)	608.2(49)	40.1(fixed)	—	–1.9	40.1
*u*2673	H(69)...H(76)	608.3(54)	34.6(fixed)	—	–2.9	34.6
*u*2691	Br(155)...H(174)	608.3(21)	23.4(fixed)	—	–2.1	23.4
*u*2633	C(9)...H(46)	608.9(45)	26.2(fixed)	—	–3.4	26.2
*u*2641	C(150)...H(171)	609.1(27)	25.0(fixed)	—	–2.8	25.0
*u*2687	C(17)...H(39)	609.7(28)	26.5(fixed)	—	–3.8	26.5
*u*2649	C(148)...H(184)	609.7(24)	25.3(fixed)	—	–3.2	25.3
*u*2652	C(102)...H(124)	610.1(36)	26.5(fixed)	—	–3.8	26.5
*u*2695	Br(108)...H(117)	610.1(22)	23.1(fixed)	—	–2.1	23.1
*u*2696	C(53)...H(75)	610.6(33)	23.5(fixed)	—	–2.8	23.5
*u*2697	Br(108)...H(136)	610.9(43)	25.3(fixed)	—	–4.0	25.3
*u*2674	Br(61)...H(70)	611.0(28)	23.5(fixed)	—	–2.1	23.5

*u*2648	C(12)...H(22)	611.2(26)	25.6(fixed)	—	–3.3	25.6
*u*2656	C(148)...H(185)	611.4(23)	24.4(fixed)	—	–3.0	24.4
*u*2615	H(26)...H(46)	611.5(54)	41.7(fixed)	—	–2.0	41.7
*u*2626	H(19)...H(35)	611.5(49)	49.4(fixed)	—	–2.4	49.4
*u*2640	C(16)...H(36)	611.5(26)	23.6(fixed)	—	–2.7	23.6
*u*2642	C(150)...H(172)	611.6(23)	23.9(fixed)	—	–2.6	23.9
*u*2650	C(9)...H(47)	612.0(35)	25.1(fixed)	—	–3.2	25.1
*u*2666	C(11)...H(26)	612.1(24)	23.6(fixed)	—	–3.1	23.6
*u*2699	C(147)...H(169)	612.3(23)	25.7(fixed)	—	–3.8	25.7
*u*2665	C(100)...H(120)	613.0(28)	24.0(fixed)	—	–3.1	24.0
*u*2646	C(101)...H(138)	613.3(22)	25.6(fixed)	—	–3.1	25.6
*u*2704	H(159)...H(176)	614.2(39)	34.7(fixed)	—	–3.2	34.7
*u*2677	Br(62)...H(87)	614.3(30)	24.2(fixed)	—	–3.5	24.2
*u*2679	C(64)...H(88)	614.4(45)	24.4(fixed)	—	–3.1	24.4
*u*2654	C(106)...H(116)	614.4(25)	26.6(fixed)	—	–3.7	26.6
*u*2653	C(102)...H(125)	614.4(25)	26.6(fixed)	—	–3.7	26.6
*u*2700	H(42)...H(47)	614.4(37)	37.4(fixed)	—	–5.8	37.4
*u*2664	C(7)...H(43)	614.6(30)	31.6(fixed)	—	–6.3	31.6
*u*2681	C(13)...H(27)	614.9(36)	26.7(fixed)	—	–3.8	26.7
*u*2685	H(67)...H(87)	614.9(43)	35.1(fixed)	—	–2.9	35.1
*u*2787	H(38)...H(42)	615.1(55)	60.6(fixed)	—	–6.4	60.6
*u*2692	H(89)...H(94)	615.3(49)	35.7(fixed)	—	–2.8	35.7
*u*2670	C(7)...H(44)	615.4(26)	34.2(fixed)	—	–6.6	34.2
*u*2688	H(163)...H(170)	615.6(24)	32.8(fixed)	—	–3.5	32.8
*u*2669	C(63)...H(83)	615.7(24)	24.5(fixed)	—	–3.4	24.5
*u*2719	Br(155)...H(166)	615.7(17)	26.6(fixed)	—	–2.9	26.6
*u*2602	H(73)...H(77)	616.0(34)	39.6(fixed)	—	–1.7	39.6
*u*2647	C(60)...H(72)	616.5(43)	24.3(fixed)	—	–3.0	24.3
*u*2728	H(71)...H(94)	617.3(60)	38.4(fixed)	—	–2.8	38.4
*u*2693	C(13)...H(28)	617.4(35)	26.2(fixed)	—	–3.5	26.2
*u*2698	H(20)...H(40)	617.5(25)	36.1(fixed)	—	–3.2	36.1
*u*2708	H(33)...H(39)	617.8(34)	40.0(fixed)	—	–4.5	40.0
*u*2723	Br(61)...H(81)	618.1(27)	28.5(fixed)	—	–3.8	28.5
*u*2689	C(64)...H(86)	618.1(28)	24.0(fixed)	—	–2.8	24.0
*u*2722	H(165)...H(180)	618.2(37)	39.3(fixed)	—	–4.0	39.3
*u*2672	C(54)...H(90)	618.3(42)	25.3(fixed)	—	–3.2	25.3
*u*2707	H(28)...H(32)	618.4(32)	38.6(fixed)	—	–4.6	38.6
*u*2714	H(69)...H(84)	618.4(55)	41.5(fixed)	—	–2.5	41.5
*u*2827	H(71)...H(93)	618.5(64)	38.2(fixed)	—	–5.2	38.2
*u*2662	C(54)...H(91)	619.0(29)	24.2(fixed)	—	–2.7	24.2
*u*2610	H(162)...H(177)	619.0(34)	39.6(fixed)	—	–1.9	39.6
*u*2774	H(19)...H(32)	619.9(38)	52.4(fixed)	—	–6.4	52.4
*u*2797	H(25)...H(33)	619.9(42)	47.1(fixed)	—	–5.5	47.1
*u*2764	H(68)...H(84)	620.3(57)	43.3(fixed)	—	–5.3	43.3
*u*2659	C(56)...H(77)	620.4(24)	25.0(fixed)	—	–3.1	25.0
*u*2724	H(20)...H(32)	620.5(33)	48.3(fixed)	—	–2.0	48.3

*u*2725	H(67)...H(79)	620.6(50)	39.5(fixed)	—	–2.6	39.5
*u*2742	H(165)...H(188)	621.2(38)	37.5(fixed)	—	–2.6	37.5
*u*2701	H(116)...H(118)	621.4(26)	40.8(fixed)	—	–3.6	40.8
*u*2712	H(122)...H(139)	621.4(34)	34.6(fixed)	—	–3.6	34.6
*u*2667	C(56)...H(78)	621.4(17)	24.3(fixed)	—	–3.0	24.3
*u*2703	H(112)...H(129)	621.5(41)	40.3(fixed)	—	–3.6	40.3
*u*2784	H(122)...H(127)	622.3(37)	39.7(fixed)	—	–2.3	39.7
*u*2709	H(78)...H(84)	623.0(17)	35.8(fixed)	—	–3.8	35.8
*u*2663	C(60)...H(73)	623.4(34)	23.6(fixed)	—	–2.8	23.6
*u*2705	H(65)...H(82)	623.5(36)	39.3(fixed)	—	–3.3	39.3
*u*2694	H(123)...H(138)	624.0(28)	36.5(fixed)	—	–3.1	36.5
*u*2889	H(121)...H(127)	624.3(44)	40.3(fixed)	—	–4.9	40.3
*u*2715	Br(108)...H(128)	624.6(34)	28.7(fixed)	—	–3.7	28.7
*u*2775	C(56)...H(68)	624.7(43)	19.9(fixed)	—	–5.6	19.9
*u*2791	H(39)...H(45)	625.1(38)	42.0(fixed)	—	–3.5	42.0
*u*2711	H(80)...H(86)	625.3(32)	34.7(fixed)	—	–3.7	34.7
*u*2721	H(36)...H(42)	625.6(39)	54.6(fixed)	—	–1.1	54.6
*u*2716	H(31)...H(37)	625.8(23)	48.1(fixed)	—	–4.1	48.1
*u*2822	H(165)...H(187)	625.9(40)	38.3(fixed)	—	–4.8	38.3
*u*2726	Br(14)...H(34)	625.9(32)	30.0(fixed)	—	–4.2	30.0
*u*2741	H(22)...H(37)	626.2(39)	38.5(fixed)	—	–3.3	38.5
*u*2792	H(66)...H(79)	626.4(43)	40.0(fixed)	—	–5.1	40.0
*u*2720	H(24)...H(44)	626.6(23)	56.9(fixed)	—	–4.6	56.9
*u*2727	Br(15)...H(30)	626.6(37)	30.5(fixed)	—	–4.7	30.5
*u*2748	H(161)...H(173)	626.7(29)	36.1(fixed)	—	–2.9	36.1
*u*2713	H(18)...H(35)	626.7(39)	41.7(fixed)	—	–3.8	41.7
*u*2750	H(26)...H(33)	627.0(38)	44.8(fixed)	—	–2.7	44.8
*u*2710	H(26)...H(45)	627.1(39)	35.6(fixed)	—	–3.6	35.6
*u*2874	H(112)...H(119)	628.0(58)	38.1(fixed)	—	–5.2	38.1
*u*2718	H(163)...H(181)	628.6(32)	39.8(fixed)	—	–2.0	39.8
*u*2843	H(159)...H(169)	628.7(33)	39.4(fixed)	—	–3.6	39.4
*u*2756	H(112)...H(120)	628.9(42)	38.4(fixed)	—	–2.9	38.4
*u*2684	H(29)...H(36)	629.0(34)	32.7(fixed)	—	–3.3	32.7
*u*2717	H(71)...H(83)	629.0(33)	38.0(fixed)	—	–3.6	38.0
*u*2751	Br(61)...H(82)	629.1(24)	26.9(fixed)	—	–3.8	26.9
*u*2763	H(72)...H(92)	629.3(79)	30.8(fixed)	—	–2.5	30.8
*u*2729	H(117)...H(138)	629.8(28)	42.1(fixed)	—	–2.5	42.1
*u*2762	C(64)...H(72)	629.8(53)	22.7(fixed)	—	–5.0	22.7
*u*2800	C(12)...H(43)	629.8(30)	30.7(fixed)	—	–14.0	30.7
*u*2816	H(65)...H(75)	630.0(43)	36.4(fixed)	—	–2.6	36.4
*u*2869	H(85)...H(89)	630.5(49)	36.7(fixed)	—	–5.2	36.7
*u*2861	H(21)...H(37)	632.0(50)	37.6(fixed)	—	–5.8	37.6
*u*2702	H(164)...H(177)	632.0(26)	34.1(fixed)	—	–3.1	34.1
*u*2732	H(29)...H(47)	632.0(40)	41.6(fixed)	—	–2.8	41.6
*u*2845	H(117)...H(137)	632.2(27)	42.7(fixed)	—	–5.7	42.7
*u*2706	H(73)...H(79)	632.2(26)	34.4(fixed)	—	–3.2	34.4

*u*2761	H(23)...H(44)	632.2(35)	52.6(fixed)	—	–6.6	52.6
*u*2753	Br(155)...H(167)	632.3(13)	24.6(fixed)	—	–3.1	24.6
*u*2829	H(37)...H(43)	632.4(43)	36.8(fixed)	—	–14.0	36.8
*u*2759	H(70)...H(85)	632.6(66)	32.0(fixed)	—	–4.9	32.0
*u*2749	Br(108)...H(129)	632.6(30)	27.1(fixed)	—	–4.0	27.1
*u*2745	H(118)...H(125)	632.6(35)	40.8(fixed)	—	–3.4	40.8
*u*2744	C(56)...C(64)	633.0(13)	12.2(tied to *u*2982)	—	–1.3	13.5
*u*2758	Br(14)...H(35)	633.0(28)	28.1(fixed)	—	–4.4	28.1
*u*2767	H(83)...H(89)	633.4(37)	37.5(fixed)	—	–3.4	37.5
*u*2817	C(13)...H(19)	633.4(13)	21.2(fixed)	—	–6.6	21.2
*u*2757	Br(15)...H(31)	633.4(25)	32.0(fixed)	—	–5.4	32.0
*u*2906	H(41)...H(45)	633.5(44)	41.3(fixed)	—	–6.2	41.3
*u*2860	H(123)...H(128)	633.5(44)	31.8(fixed)	—	–5.6	31.8
*u*2786	C(6)...H(30)	633.8(26)	27.4(fixed)	—	–10.1	27.4
*u*2813	C(60)...H(66)	633.8(21)	19.6(fixed)	—	–5.7	19.6
*u*2734	C(101)...C(107)	633.8(9)	12.4(tied to *u*2982)	—	–1.3	13.7
*u*2859	C(103)...H(128)	633.9(27)	24.3(fixed)	—	–6.9	24.3
*u*2736	C(6)...C(16)	634.0(22)	12.7(tied to *u*2982)	—	–1.5	14.0
*u*2730	C(54)...C(60)	634.2(9)	12.5(tied to *u*2982)	—	–1.3	13.8
*u*2740	C(53)...C(63)	634.3(22)	12.4(tied to *u*2982)	—	–1.3	13.7
*u*2837	C(8)...H(43)	634.3(15)	26.3(fixed)	—	–14.5	26.3
*u*2752	C(147)...C(157)	634.4(22)	12.4(tied to *u*2982)	—	–1.3	13.7
*u*2766	C(54)...H(85)	634.4(40)	23.4(fixed)	—	–6.5	23.4
*u*2739	C(150)...C(158)	634.4(9)	12.4(tied to *u*2982)	—	–1.3	13.7
*u*2746	C(102)...C(111)	634.4(9)	12.4(tied to *u*2982)	—	–1.3	13.7
*u*2731	C(100)...C(110)	634.4(22)	12.3(tied to *u*2982)	—	–1.3	13.6
*u*2776	C(147)...H(175)	634.6(25)	20.3(fixed)	—	–5.7	20.3
*u*2940	H(65)...H(74)	634.7(69)	36.1(fixed)	—	–4.7	36.1
*u*2781	H(18)...H(30)	634.7(38)	34.2(fixed)	—	–8.5	34.2
*u*2735	C(149)...C(153)	634.8(28)	12.1(tied to *u*2982)	—	–1.3	13.3
*u*2743	C(7)...C(13)	634.9(8)	12.4(tied to *u*2982)	—	–1.5	13.7
*u*2737	C(58)...C(59)	635.1(9)	12.3(tied to *u*2982)	—	–1.3	13.6
*u*2820	C(150)...H(162)	635.1(16)	18.6(fixed)	—	–4.9	18.6
*u*2811	C(149)...H(182)	635.6(26)	20.0(fixed)	—	–6.6	20.0
*u*2733	C(11)...C(12)	635.7(8)	12.3(tied to *u*2982)	—	–1.4	13.6
*u*2738	C(8)...C(10)	635.7(9)	12.4(tied to *u*2982)	—	–1.4	13.6
*u*2847	H(66)...H(72)	636.1(66)	38.3(fixed)	—	–6.1	38.3
*u*2760	H(65)...H(77)	636.1(67)	31.1(fixed)	—	–3.8	31.1
*u*2755	H(70)...H(91)	636.1(37)	37.6(fixed)	—	–2.6	37.6
*u*2826	C(103)...H(137)	636.1(18)	19.9(fixed)	—	–6.3	19.9
*u*2803	H(86)...H(92)	636.3(38)	38.8(fixed)	—	–2.5	38.8
*u*2818	H(166)...H(186)	636.5(45)	30.3(fixed)	—	–3.1	30.3
*u*2777	C(63)...H(93)	636.5(27)	20.2(fixed)	—	–6.2	20.2
*u*2936	H(159)...H(168)	636.8(47)	37.9(fixed)	—	–5.4	37.9
*u*2821	C(12)...H(30)	636.9(16)	23.3(fixed)	—	–10.5	23.3
*u*2779	C(102)...H(115)	637.1(18)	20.1(fixed)	—	–7.2	20.1

*u*2790	C(17)...H(25)	637.2(37)	20.5(fixed)	—	–6.1	20.5
*u*2835	C(8)...H(34)	637.3(27)	24.2(fixed)	—	–8.2	24.2
*u*2863	C(56)...H(66)	637.5(39)	22.9(fixed)	—	–5.5	22.9
*u*2819	C(16)...H(46)	637.5(22)	19.9(fixed)	—	–6.5	19.9
*u*2825	H(115)...H(124)	637.5(55)	42.1(fixed)	—	–7.7	42.1
*u*2773	H(164)...H(182)	637.5(36)	31.3(fixed)	—	–5.2	31.3
*u*2778	C(152)...H(179)	637.8(27)	22.1(fixed)	—	–5.0	22.1
*u*2807	C(100)...H(128)	637.8(26)	20.5(fixed)	—	–7.2	20.5
*u*2770	H(28)...H(40)	637.9(46)	40.8(fixed)	—	–2.8	40.8
*u*2783	H(162)...H(181)	637.9(35)	41.8(fixed)	—	–4.6	41.8
*u*2838	H(40)...H(46)	637.9(47)	32.4(fixed)	—	–3.3	32.4
*u*2768	C(53)...H(77)	638.2(39)	22.9(fixed)	—	–5.7	22.9
*u*2844	H(115)...H(131)	638.3(47)	39.3(fixed)	—	–5.8	39.3
*u*2872	H(21)...H(32)	638.4(38)	43.3(fixed)	—	–10.1	43.3
*u*2867	H(160)...H(173)	638.5(27)	35.2(fixed)	—	–5.0	35.2
*u*2865	H(66)...H(76)	639.1(45)	30.5(fixed)	—	–4.1	30.5
*u*2832	C(59)...H(77)	639.3(14)	19.6(fixed)	—	–5.9	19.6
*u*2798	C(11)...H(41)	639.3(21)	21.1(fixed)	—	–7.0	21.1
*u*2848	C(13)...H(46)	639.3(30)	23.7(fixed)	—	–6.1	23.7
*u*2805	C(53)...H(81)	639.4(22)	21.1(fixed)	—	–7.2	21.1
*u*2941	H(117)...H(126)	639.4(43)	31.6(fixed)	—	–6.1	31.6
*u*2772	C(17)...H(27)	639.5(40)	24.1(fixed)	—	–6.3	24.1
*u*2769	H(27)...H(45)	639.5(54)	32.5(fixed)	—	–3.9	32.5
*u*2919	H(23)...H(32)	639.6(31)	36.2(fixed)	—	–7.6	36.2
*u*2801	C(10)...H(27)	639.9(20)	20.7(fixed)	—	–6.7	20.7
*u*2836	H(119)...H(128)	640.0(45)	40.4(fixed)	—	–7.1	40.4
*u*2878	H(23)...H(43)	640.2(37)	46.0(fixed)	—	–10.0	46.0
*u*2788	C(148)...H(182)	640.2(24)	23.0(fixed)	—	–6.2	23.0
*u*2802	H(159)...H(171)	640.4(37)	30.8(fixed)	—	–2.6	30.8
*u*2795	H(21)...H(30)	640.4(38)	45.7(fixed)	—	–9.4	45.7
*u*2808	C(6)...H(34)	640.6(23)	22.2(fixed)	—	–8.4	22.2
*u*2794	C(105)...H(135)	640.7(22)	20.0(fixed)	—	–5.3	20.0
*u*2833	C(102)...H(113)	641.1(33)	23.5(fixed)	—	–5.9	23.5
*u*2943	H(115)...H(126)	641.4(54)	36.1(fixed)	—	–8.0	36.1
*u*2796	C(9)...H(38)	641.5(25)	19.1(fixed)	—	–4.9	19.1
*u*2900	H(74)...H(80)	641.6(30)	33.9(fixed)	—	–7.1	33.9
*u*2840	H(29)...H(46)	641.6(48)	40.6(fixed)	—	–5.6	40.6
*u*2814	C(55)...H(85)	641.7(25)	20.3(fixed)	—	–6.6	20.3
*u*2970	H(66)...H(71)	642.0(55)	32.6(fixed)	—	–6.4	32.6
*u*2949	H(132)...H(139)	642.0(45)	34.4(fixed)	—	–7.4	34.4
*u*2866	H(24)...H(34)	642.1(46)	31.3(fixed)	—	–6.7	31.3
*u*2754	H(76)...H(78)	642.2(23)	36.2(fixed)	—	–2.8	36.2
*u*2780	C(7)...H(38)	642.5(27)	22.0(fixed)	—	–4.7	22.0
*u*2782	C(110)...H(115)	642.7(23)	24.8(fixed)	—	–6.9	24.8
*u*2959	H(131)...H(139)	642.8(34)	31.0(fixed)	—	–5.8	31.0
*u*2985	H(65)...H(71)	642.9(43)	29.6(fixed)	—	–5.1	29.6

*u*2785	C(147)...H(171)	643.0(24)	22.3(fixed)	—	–4.5	22.3
*u*2868	C(150)...H(160)	643.1(25)	22.5(fixed)	—	–5.4	22.5
*u*2815	C(58)...H(88)	643.2(21)	19.6(fixed)	—	–5.2	19.6
*u*2789	C(148)...H(179)	643.6(18)	19.7(fixed)	—	–5.3	19.7
*u*2864	H(113)...H(118)	643.8(47)	31.5(fixed)	—	–4.4	31.5
*u*2804	H(23)...H(38)	643.9(37)	30.6(fixed)	—	–1.9	30.6
*u*2765	H(74)...H(81)	644.3(30)	39.4(fixed)	—	–6.5	39.4
*u*2881	H(160)...H(170)	644.3(35)	31.3(fixed)	—	–3.1	31.3
*u*2793	C(101)...H(132)	645.5(27)	22.9(fixed)	—	–5.5	22.9
*u*2839	C(59)...H(90)	645.6(28)	22.3(fixed)	—	–5.0	22.3
*u*2914	H(76)...H(80)	645.6(24)	30.0(fixed)	—	–5.5	30.0
*u*2938	H(88)...H(92)	645.7(60)	38.3(fixed)	—	–5.0	38.3
*u*2988	H(65)...H(72)	645.7(69)	31.4(fixed)	—	–6.4	31.4
*u*2747	H(73)...H(87)	645.8(44)	36.0(fixed)	—	–2.5	36.0
*u*2977	H(159)...H(165)	645.8(28)	30.0(fixed)	—	–5.4	30.0
*u*2967	H(84)...H(92)	646.0(38)	32.1(fixed)	—	–5.9	32.1
*u*2862	C(9)...H(41)	646.0(33)	23.8(fixed)	—	–6.5	23.8
*u*2806	H(19)...H(27)	646.0(53)	41.3(fixed)	—	–7.1	41.3
*u*2926	H(84)...H(93)	646.0(54)	36.6(fixed)	—	–7.4	36.6
*u*2799	C(57)...H(72)	646.3(17)	19.7(fixed)	—	–5.3	19.7
*u*2855	H(29)...H(41)	646.8(49)	32.5(fixed)	—	–4.0	32.5
*u*2812	H(160)...H(166)	647.0(36)	37.2(fixed)	—	–5.9	37.2
*u*2851	H(85)...H(93)	647.2(56)	39.5(fixed)	—	–7.1	39.5
*u*2897	H(70)...H(90)	647.2(56)	36.8(fixed)	—	–4.9	36.8
*u*2952	H(23)...H(30)	647.4(36)	37.0(fixed)	—	–9.5	37.0
*u*2946	H(118)...H(128)	647.6(51)	33.9(fixed)	—	–7.3	33.9
*u*2856	C(60)...H(93)	647.7(32)	22.7(fixed)	—	–5.8	22.7
*u*2771	H(112)...H(124)	647.9(38)	32.3(fixed)	—	–5.0	32.3
*u*2937	H(70)...H(79)	648.7(34)	30.0(fixed)	—	–5.2	30.0
*u*2928	H(160)...H(165)	648.7(38)	33.0(fixed)	—	–6.2	33.0
*u*2993	H(37)...H(45)	648.9(28)	30.3(fixed)	—	–5.4	30.3
*u*2905	H(27)...H(40)	649.0(45)	39.9(fixed)	—	–5.8	39.9
*u*2842	H(72)...H(87)	649.2(52)	35.6(fixed)	—	–4.6	35.6
*u*2899	C(16)...H(18)	649.5(26)	26.5(fixed)	—	–0.7	26.5
*u*2944	H(18)...H(27)	649.6(53)	33.1(fixed)	—	–7.3	33.1
*u*2853	H(87)...H(93)	650.0(42)	30.3(fixed)	—	–4.3	30.3
*u*2951	H(24)...H(41)	650.1(38)	35.0(fixed)	—	–7.4	35.0
*u*2912	C(63)...H(65)	650.1(29)	25.1(fixed)	—	–0.6	25.1
*u*2884	C(60)...H(70)	650.2(25)	25.8(fixed)	—	–0.8	25.8
*u*2854	H(38)...H(46)	650.7(37)	37.7(fixed)	—	–6.1	37.7
*u*2828	C(16)...H(21)	650.9(27)	24.6(fixed)	—	–6.7	24.6
*u*2823	C(63)...H(68)	650.9(30)	23.2(fixed)	—	–5.3	23.2
*u*2929	C(56)...H(92)	650.9(29)	25.5(fixed)	—	–0.3	25.5
*u*2852	H(76)...H(77)	651.1(31)	35.6(fixed)	—	–4.7	35.6
*u*2975	H(159)...H(166)	651.2(44)	31.8(fixed)	—	–6.5	31.8
*u*2934	H(18)...H(29)	651.6(33)	31.2(fixed)	—	–5.7	31.2

*u*2857	H(25)...H(41)	651.8(33)	39.4(fixed)	—	–7.1	39.4
*u*2921	C(150)...H(186)	651.9(21)	26.0(fixed)	—	–0.6	26.0
*u*2841	H(119)...H(126)	652.0(39)	30.9(fixed)	—	–2.4	30.9
*u*2930	H(68)...H(79)	652.1(35)	33.6(fixed)	—	–6.8	33.6
*u*2831	C(55)...H(88)	652.6(36)	21.6(fixed)	—	–4.9	21.6
*u*2834	H(68)...H(77)	653.0(48)	38.6(fixed)	—	–6.4	38.6
*u*2933	C(59)...H(80)	653.1(18)	26.2(fixed)	—	–0.2	26.2
*u*2896	C(101)...H(134)	653.3(19)	24.3(fixed)	—	–0.7	24.3
*u*2885	C(53)...H(91)	653.3(29)	25.2(fixed)	—	–0.6	25.2
*u*2924	C(10)...H(24)	653.4(19)	25.6(fixed)	—	–0.6	25.6
*u*2958	H(24)...H(40)	653.4(31)	31.5(fixed)	—	–5.8	31.5
*u*2810	H(121)...H(135)	653.5(60)	36.6(fixed)	—	–5.8	36.6
*u*2909	C(100)...H(136)	653.5(26)	25.4(fixed)	—	–0.7	25.4
*u*2989	H(37)...H(46)	653.6(45)	31.7(fixed)	—	–6.4	31.7
*u*2969	C(147)...H(183)	653.6(24)	24.5(fixed)	—	–0.7	24.5
*u*2916	C(11)...H(37)	653.6(16)	24.6(fixed)	—	–1.2	24.6
*u*2875	H(84)...H(90)	653.7(41)	29.8(fixed)	—	–2.9	29.8
*u*2846	H(68)...H(89)	653.8(35)	30.4(fixed)	—	–3.7	30.4
*u*2995	H(38)...H(45)	653.8(35)	33.1(fixed)	—	–6.9	33.1
*u*2830	C(57)...H(74)	653.9(17)	21.3(fixed)	—	–4.6	21.3
*u*2932	C(102)...H(139)	654.1(19)	25.5(fixed)	—	0.1	25.5
*u*2888	C(6)...H(44)	654.1(29)	33.5(fixed)	—	2.0	33.5
*u*2994	H(85)...H(92)	654.2(61)	32.8(fixed)	—	–7.3	32.8
*u*2954	C(111)...H(118)	654.4(16)	25.0(fixed)	—	–0.8	25.0
*u*2895	H(76)...H(81)	654.4(35)	32.3(fixed)	—	–6.6	32.3
*u*2913	H(170)...H(174)	654.4(23)	31.4(fixed)	—	–5.7	31.4
*u*2950	C(13)...H(23)	654.9(19)	26.2(fixed)	—	–0.5	26.2
*u*2968	H(65)...H(91)	654.9(39)	34.5(fixed)	—	1.5	34.5
*u*2939	C(149)...H(178)	654.9(32)	24.6(fixed)	—	–0.9	24.6
*u*2876	C(103)...H(125)	655.1(16)	28.3(fixed)	—	–0.1	28.3
*u*2948	H(164)...H(173)	655.2(34)	27.7(fixed)	—	–4.6	27.7
*u*2886	C(54)...H(86)	655.4(19)	25.7(fixed)	—	–0.8	25.7
*u*2880	C(100)...H(138)	655.4(28)	26.9(fixed)	—	–0.4	26.9
*u*2891	H(123)...H(134)	655.8(42)	28.4(fixed)	—	–4.8	28.4
*u*2964	C(53)...H(89)	655.8(28)	24.0(fixed)	—	–0.9	24.0
*u*2883	C(8)...H(31)	656.1(19)	30.6(fixed)	—	0.8	30.6
*u*2917	C(102)...H(141)	656.1(15)	27.8(fixed)	—	–0.5	27.8
*u*2824	H(168)...H(175)	656.1(34)	38.6(fixed)	—	–6.7	38.6
*u*2901	C(152)...H(180)	656.3(15)	26.3(fixed)	—	–0.6	26.3
*u*2918	C(103)...H(126)	656.4(16)	25.5(fixed)	—	0.2	25.5
*u*2893	C(12)...H(35)	656.6(14)	27.4(fixed)	—	0.3	27.4
*u*2923	C(147)...H(185)	656.8(28)	25.3(fixed)	—	–0.7	25.3
*u*2922	C(58)...H(84)	656.8(14)	25.6(fixed)	—	–0.4	25.6
*u*2915	C(64)...H(75)	656.9(18)	24.4(fixed)	—	–0.8	24.4
*u*2927	C(12)...H(33)	656.9(19)	28.2(fixed)	—	0.0	28.2
*u*2911	C(63)...H(67)	657.0(30)	26.2(fixed)	—	–0.8	26.2

*u*2894	C(16)...H(20)	657.1(29)	26.5(fixed)	—	–0.3	26.5
*u*2907	C(7)...H(40)	657.1(17)	25.3(fixed)	—	–0.1	25.3
*u*2956	H(18)...H(44)	657.2(38)	40.4(fixed)	—	6.6	40.4
*u*2955	H(70)...H(86)	657.4(35)	35.2(fixed)	—	1.2	35.2
*u*2882	C(59)...H(82)	657.7(14)	27.6(fixed)	—	0.0	27.6
*u*2935	C(64)...H(76)	657.7(18)	23.3(fixed)	—	–0.9	23.3
*u*2873	C(58)...H(83)	657.7(16)	26.2(fixed)	—	–0.2	26.2
*u*2879	C(105)...H(130)	658.1(16)	25.8(fixed)	—	–0.6	25.8
*u*2904	C(152)...H(181)	658.1(17)	25.0(fixed)	—	–0.2	25.0
*u*2892	C(13)...H(22)	658.2(14)	27.2(fixed)	—	–0.3	27.2
*u*2920	C(6)...H(42)	658.3(28)	31.7(fixed)	—	2.1	31.7
*u*2898	C(101)...H(133)	658.4(13)	25.7(fixed)	—	–0.8	25.7
*u*2903	C(150)...H(188)	658.4(14)	25.5(fixed)	—	–0.5	25.5
*u*2925	C(8)...H(32)	658.5(14)	28.3(fixed)	—	1.0	28.3
*u*2931	C(7)...H(39)	658.6(16)	27.8(fixed)	—	–0.9	27.8
*u*2877	C(60)...H(69)	658.6(15)	26.7(fixed)	—	–0.7	26.7
*u*2902	C(54)...H(87)	658.8(16)	24.2(fixed)	—	–0.8	24.2
*u*2971	H(70)...H(77)	658.9(56)	31.6(fixed)	—	–6.6	31.6
*u*2942	H(19)...H(29)	659.0(42)	34.6(fixed)	—	–7.6	34.6
*u*2908	H(121)...H(134)	659.1(58)	31.0(fixed)	—	–6.0	31.0
*u*2990	Br(15)...C(17)	659.4(13)	12.9(tied to *u*2982)	—	–1.5	14.2
*u*2870	C(149)...H(177)	659.5(34)	24.4(fixed)	—	–0.5	24.4
*u*2947	H(168)...H(174)	659.5(35)	32.4(fixed)	—	–6.8	32.4
*u*2910	C(56)...H(94)	659.5(14)	25.6(fixed)	—	–0.4	25.6
*u*2976	H(114)...H(136)	659.9(36)	36.0(fixed)	—	2.0	36.0
*u*2858	H(71)...H(88)	660.3(48)	29.7(fixed)	—	–3.6	29.7
*u*2966	H(24)...H(31)	660.4(30)	38.2(fixed)	—	4.6	38.2
*u*3028	H(68)...H(74)	660.4(55)	26.8(fixed)	—	–6.7	26.8
*u*2978	H(35)...H(37)	660.6(25)	35.0(fixed)	—	2.7	35.0
*u*2871	C(11)...H(36)	660.6(16)	24.5(fixed)	—	–0.8	24.5
*u*2986	C(57)...Br(62)	660.7(13)	12.9(tied to *u*2982)	—	–1.4	14.2
*u*2983	H(169)...H(186)	660.8(29)	35.7(fixed)	—	2.1	35.7
*u*2945	H(116)...H(134)	661.2(27)	35.6(fixed)	—	2.5	35.6
*u*2982	C(9)...Br(14)	661.2(15)	12.9(9)	14.2(10)	–1.5	14.2
*u*2850	H(74)...H(79)	661.2(21)	29.2(fixed)	—	–2.6	29.2
*u*2809	H(162)...H(171)	661.2(46)	36.3(fixed)	—	–5.3	36.3
*u*2890	C(10)...H(26)	661.2(14)	25.1(fixed)	—	–0.4	25.1
*u*2991	H(75)...H(92)	661.3(35)	34.6(fixed)	—	1.7	34.6
*u*2887	H(170)...H(175)	661.4(33)	35.9(fixed)	—	–7.3	35.9
*u*2965	H(80)...H(83)	661.4(26)	36.2(fixed)	—	3.1	36.2
*u*2980	C(148)...Br(155)	661.5(13)	12.7(tied to *u*2982)	—	–1.5	14.1
*u*2987	C(55)...Br(61)	662.0(16)	12.8(tied to *u*2982)	—	–1.4	14.2
*u*2979	H(25)...H(40)	662.4(34)	33.5(fixed)	—	–7.3	33.5
*u*2998	H(118)...H(141)	662.4(26)	35.9(fixed)	—	2.0	35.9
*u*3002	H(159)...H(185)	662.7(36)	34.0(fixed)	—	1.4	34.0
*u*2849	H(21)...H(42)	663.2(39)	34.8(fixed)	—	1.0	34.8

*u*2961	H(120)...H(139)	663.8(28)	35.5(fixed)	—	2.8	35.5
*u*2953	H(162)...H(173)	664.4(43)	30.0(fixed)	—	–5.7	30.0
*u*3004	H(67)...H(89)	664.6(44)	34.3(fixed)	—	1.1	34.3
*u*3015	Br(15)...H(21)	664.9(37)	20.5(fixed)	—	–7.1	20.5
*u*2963	H(165)...H(177)	664.9(41)	33.6(fixed)	—	1.6	33.6
*u*2962	H(82)...H(84)	665.5(21)	36.5(fixed)	—	3.2	36.5
*u*3003	H(23)...H(39)	665.7(32)	37.4(fixed)	—	2.1	37.4
*u*3017	Br(15)...H(19)	666.7(40)	24.0(fixed)	—	–6.5	24.0
*u*2984	H(117)...H(133)	667.2(25)	35.5(fixed)	—	2.6	35.5
*u*2957	H(33)...H(36)	667.6(29)	37.5(fixed)	—	2.7	37.5
*u*2960	H(22)...H(40)	668.0(24)	36.1(fixed)	—	3.0	36.1
*u*2981	H(20)...H(42)	668.4(40)	42.6(fixed)	—	6.6	42.6
*u*2974	H(170)...H(188)	669.5(25)	34.6(fixed)	—	2.5	34.6
*u*2972	H(69)...H(87)	670.0(30)	34.7(fixed)	—	1.4	34.7
*u*3014	Br(14)...H(25)	670.0(33)	22.9(fixed)	—	–6.2	22.9
*u*2973	H(26)...H(32)	670.2(24)	37.8(fixed)	—	4.7	37.8
*u*3039	H(68)...H(76)	671.1(43)	26.0(fixed)	—	–6.2	26.0
*u*3016	Br(62)...H(81)	671.2(20)	24.5(fixed)	—	–7.1	24.5
*u*2992	H(76)...H(94)	671.4(32)	33.0(fixed)	—	1.6	33.0
*u*3036	H(19)...H(41)	671.5(21)	28.7(fixed)	—	–8.0	28.7
*u*3006	H(67)...H(91)	671.9(35)	36.8(fixed)	—	0.2	36.8
*u*3048	H(66)...H(88)	672.1(30)	26.6(fixed)	—	–6.9	26.6
*u*3022	Br(155)...H(160)	672.5(16)	19.5(fixed)	—	–5.9	19.5
*u*3007	H(20)...H(44)	673.5(34)	47.7(fixed)	—	3.4	47.7
*u*2997	H(114)...H(138)	673.8(33)	39.2(fixed)	—	0.8	39.2
*u*3013	H(161)...H(185)	673.8(34)	36.1(fixed)	—	0.2	36.1
*u*3052	H(162)...H(168)	674.2(26)	25.4(fixed)	—	–5.7	25.4
*u*3060	H(25)...H(43)	674.4(24)	33.6(fixed)	—	–16.3	33.6
*u*3000	H(69)...H(86)	675.0(20)	37.5(fixed)	—	0.2	37.5
*u*3012	H(169)...H(188)	675.1(20)	38.1(fixed)	—	0.4	38.1
*u*3045	H(166)...H(182)	675.4(24)	26.7(fixed)	—	–7.8	26.7
*u*3005	H(116)...H(133)	675.5(18)	39.9(fixed)	—	0.7	39.9
*u*3059	H(113)...H(135)	675.8(25)	26.9(fixed)	—	–7.5	26.9
*u*3026	Br(62)...H(78)	676.1(18)	26.1(fixed)	—	–0.5	26.1
*u*3009	H(120)...H(141)	676.1(20)	39.7(fixed)	—	0.4	39.7
*u*3053	H(159)...H(175)	676.1(32)	26.7(fixed)	—	–6.1	26.7
*u*3010	H(22)...H(39)	676.4(19)	40.7(fixed)	—	0.6	40.7
*u*3044	H(19)...H(40)	676.5(27)	27.8(fixed)	—	–6.6	27.8
*u*3021	Br(108)...H(119)	676.7(26)	19.6(fixed)	—	–5.9	19.6
*u*3057	H(30)...H(38)	676.7(26)	30.3(fixed)	—	–12.1	30.3
*u*3019	Br(108)...H(121)	676.7(23)	22.4(fixed)	—	–5.2	22.4
*u*3030	H(160)...H(175)	677.1(26)	26.9(fixed)	—	–6.8	26.9
*u*3029	Br(155)...H(164)	677.1(17)	24.6(fixed)	—	–1.1	24.6
*u*3031	H(115)...H(119)	677.2(28)	27.0(fixed)	—	–8.6	27.0
*u*3047	Br(15)...H(45)	677.5(20)	26.2(fixed)	—	–0.6	26.2
*u*3096	H(68)...H(75)	677.6(40)	23.5(fixed)	—	–6.8	23.5

*u*2999	H(82)...H(83)	677.7(20)	40.1(fixed)	—	1.2	40.1
*u*3018	Br(155)...H(187)	678.5(21)	23.0(fixed)	—	–5.7	23.0
*u*3011	H(75)...H(94)	678.6(17)	35.8(fixed)	—	0.4	35.8
*u*3001	H(35)...H(36)	679.0(19)	38.3(fixed)	—	1.0	38.3
*u*3043	H(25)...H(45)	679.0(43)	27.0(fixed)	—	–6.2	27.0
*u*3008	H(26)...H(31)	679.2(20)	43.0(fixed)	—	1.8	43.0
*u*3033	Br(15)...H(47)	679.3(17)	26.4(fixed)	—	–0.7	26.4
*u*3064	H(77)...H(85)	679.5(24)	26.5(fixed)	—	–7.0	26.5
*u*3094	H(26)...H(43)	679.5(21)	28.4(fixed)	—	–15.9	28.4
*u*3020	Br(61)...H(74)	679.5(26)	19.4(fixed)	—	–5.1	19.4
*u*3034	H(90)...H(93)	679.6(31)	26.8(fixed)	—	–7.5	26.8
*u*3079	H(162)...H(170)	679.6(21)	25.1(fixed)	—	–5.5	25.1
*u*3024	Br(61)...H(73)	679.9(24)	26.4(fixed)	—	–0.6	26.4
*u*3133	H(38)...H(43)	679.9(39)	39.2(fixed)	—	–15.8	39.2
*u*3023	Br(62)...H(90)	680.1(13)	19.2(fixed)	—	–5.4	19.2
*u*3035	Br(62)...H(79)	680.1(17)	25.2(fixed)	—	–0.6	25.2
*u*3027	Br(14)...H(28)	680.3(20)	28.0(fixed)	—	–0.5	28.0
*u*3054	H(66)...H(87)	680.7(31)	25.9(fixed)	—	–6.0	25.9
*u*3025	Br(155)...H(163)	680.8(17)	25.3(fixed)	—	–1.0	25.3
*u*3082	H(18)...H(42)	680.8(33)	41.1(fixed)	—	–1.0	41.1
*u*3105	H(44)...H(46)	680.8(33)	24.9(fixed)	—	–8.3	24.9
*u*3074	H(113)...H(134)	681.0(29)	26.1(fixed)	—	–6.7	26.1
*u*3037	H(25)...H(46)	681.0(48)	27.6(fixed)	—	–7.3	27.6
*u*3071	H(113)...H(128)	681.4(28)	27.5(fixed)	—	–8.7	27.5
*u*3072	H(43)...H(46)	681.4(23)	27.1(fixed)	—	–7.4	27.1
*u*3050	H(65)...H(81)	681.7(33)	27.3(fixed)	—	–7.3	27.3
*u*3093	H(112)...H(136)	681.7(33)	32.8(fixed)	—	–1.9	32.8
*u*3038	H(27)...H(38)	682.0(27)	26.2(fixed)	—	–6.2	26.2
*u*2996	H(167)...H(177)	682.1(41)	34.9(fixed)	—	0.3	34.9
*u*3121	H(65)...H(89)	682.2(32)	31.3(fixed)	—	–1.8	31.3
*u*3107	H(165)...H(182)	682.5(28)	25.8(fixed)	—	–7.1	25.8
*u*3117	H(114)...H(128)	683.0(34)	24.6(fixed)	—	–8.4	24.6
*u*3051	Br(61)...H(71)	683.0(19)	25.7(fixed)	—	–1.0	25.7
*u*3114	H(24)...H(43)	683.1(20)	31.4(fixed)	—	–14.2	31.4
*u*3065	H(89)...H(93)	683.1(29)	26.2(fixed)	—	–6.5	26.2
*u*3042	H(72)...H(85)	683.1(27)	27.3(fixed)	—	–8.0	27.3
*u*3032	Br(14)...H(29)	683.2(22)	26.7(fixed)	—	–0.5	26.7
*u*3100	H(80)...H(84)	683.4(17)	35.0(fixed)	—	–1.6	35.0
*u*3088	H(115)...H(118)	683.5(25)	26.4(fixed)	—	–7.8	26.4
*u*3069	H(167)...H(182)	683.5(33)	24.2(fixed)	—	–7.5	24.2
*u*3046	H(29)...H(38)	683.5(27)	25.8(fixed)	—	–5.3	25.8
*u*3061	H(66)...H(81)	683.5(23)	28.0(fixed)	—	–8.7	28.0
*u*3119	H(66)...H(86)	683.5(21)	23.6(fixed)	—	–7.0	23.6
*u*3075	H(27)...H(31)	683.7(22)	24.7(fixed)	—	–7.9	24.7
*u*3099	H(33)...H(37)	683.7(17)	35.4(fixed)	—	–2.0	35.4
*u*3123	H(72)...H(93)	683.8(57)	31.4(fixed)	—	–7.4	31.4

*u*3090	H(24)...H(32)	683.8(17)	37.7(fixed)	—	–1.2	37.7
*u*3085	H(30)...H(36)	683.8(21)	26.0(fixed)	—	–11.7	26.0
*u*3076	H(77)...H(83)	683.9(20)	24.2(fixed)	—	–6.9	24.2
*u*3120	H(118)...H(139)	683.9(16)	33.1(fixed)	—	–1.5	33.1
*u*3056	H(34)...H(41)	684.0(31)	28.1(fixed)	—	–8.1	28.1
*u*3040	H(164)...H(179)	684.0(24)	25.9(fixed)	—	–5.7	25.9
*u*3126	H(159)...H(183)	684.0(30)	31.4(fixed)	—	–1.9	31.4
*u*3089	H(91)...H(93)	684.1(30)	24.1(fixed)	—	–7.3	24.1
*u*3118	H(165)...H(178)	684.5(37)	32.4(fixed)	—	–2.0	32.4
*u*3084	H(30)...H(37)	684.5(20)	29.2(fixed)	—	–10.5	29.2
*u*3067	H(27)...H(30)	684.6(29)	27.6(fixed)	—	–8.0	27.6
*u*3066	H(121)...H(139)	684.8(27)	26.1(fixed)	—	–5.5	26.1
*u*3103	H(35)...H(41)	685.1(24)	24.9(fixed)	—	–8.3	24.9
*u*3070	H(19)...H(34)	685.3(25)	29.2(fixed)	—	–10.1	29.2
*u*3063	H(18)...H(34)	685.4(23)	28.3(fixed)	—	–8.4	28.3
*u*3041	H(121)...H(140)	685.5(30)	27.0(fixed)	—	–6.6	27.0
*u*3055	H(115)...H(120)	685.5(20)	24.6(fixed)	—	–8.4	24.6
*u*3104	H(162)...H(169)	685.8(19)	23.3(fixed)	—	–6.4	23.3
*u*3078	H(33)...H(41)	685.9(23)	27.5(fixed)	—	–7.5	27.5
*u*3122	H(19)...H(39)	685.9(19)	24.7(fixed)	—	–8.4	24.7
*u*3073	H(70)...H(87)	686.0(17)	31.8(fixed)	—	–1.8	31.8
*u*3077	H(117)...H(134)	686.0(16)	32.7(fixed)	—	–1.3	32.7
*u*3049	H(112)...H(128)	686.2(32)	26.7(fixed)	—	–7.3	26.7
*u*3081	H(73)...H(85)	686.4(32)	24.5(fixed)	—	–7.7	24.5
*u*3115	H(113)...H(133)	686.5(21)	24.1(fixed)	—	–7.5	24.1
*u*3080	H(170)...H(186)	686.6(16)	33.8(fixed)	—	–1.5	33.8
*u*3108	H(76)...H(92)	686.9(15)	31.4(fixed)	—	–1.6	31.4
*u*3149	H(121)...H(128)	687.1(28)	32.5(fixed)	—	–8.9	32.5
*u*3086	H(42)...H(46)	687.2(22)	26.8(fixed)	—	–6.7	26.8
*u*3091	H(161)...H(175)	687.3(29)	24.4(fixed)	—	–7.0	24.4
*u*3130	H(25)...H(34)	687.3(29)	32.7(fixed)	—	–10.1	32.7
*u*3110	H(23)...H(40)	687.9(16)	33.5(fixed)	—	–1.5	33.5
*u*3106	H(20)...H(34)	688.0(33)	25.1(fixed)	—	–9.5	25.1
*u*3095	H(80)...H(88)	688.2(22)	25.5(fixed)	—	–5.7	25.5
*u*3113	H(25)...H(47)	688.3(31)	24.4(fixed)	—	–7.6	24.4
*u*3068	H(81)...H(88)	688.4(30)	26.4(fixed)	—	–6.5	26.4
*u*3098	H(27)...H(32)	688.5(21)	26.9(fixed)	—	–7.2	26.9
*u*3131	H(19)...H(30)	688.8(30)	36.6(fixed)	—	–12.6	36.6
*u*3102	H(121)...H(141)	688.8(24)	24.0(fixed)	—	–6.7	24.0
*u*3087	H(72)...H(78)	689.2(19)	24.0(fixed)	—	–6.3	24.0
*u*3116	H(77)...H(84)	689.2(18)	25.1(fixed)	—	–6.6	25.1
*u*3058	H(162)...H(179)	689.3(24)	26.2(fixed)	—	–6.5	26.2
*u*3112	H(67)...H(81)	689.5(34)	24.8(fixed)	—	–8.4	24.8
*u*3092	H(82)...H(88)	689.7(22)	24.1(fixed)	—	–6.2	24.1
*u*3101	H(71)...H(85)	690.2(31)	26.1(fixed)	—	–7.1	26.1
*u*3155	H(66)...H(74)	690.2(50)	30.7(fixed)	—	–7.3	30.7

*u*3129	H(68)...H(85)	690.2(40)	31.7(fixed)	—	–8.9	31.7
*u*3111	Br(108)...Br(109)	690.8(15)	13.2(tied to *u*2982)	—	–1.6	14.6
*u*3062	H(72)...H(77)	692.8(24)	26.5(fixed)	—	–6.4	26.5
*u*3109	H(28)...H(38)	693.0(30)	23.5(fixed)	—	–6.4	23.5
*u*3139	H(113)...H(119)	693.4(41)	31.7(fixed)	—	–8.0	31.7
*u*3083	H(72)...H(79)	693.6(19)	25.4(fixed)	—	–5.8	25.4
*u*3142	H(41)...H(46)	694.0(32)	33.3(fixed)	—	–8.6	33.3
*u*3097	H(163)...H(179)	694.3(20)	23.9(fixed)	—	–6.4	23.9
*u*3127	H(166)...H(187)	694.3(28)	30.1(fixed)	—	–7.2	30.1
*u*3125	H(66)...H(77)	694.9(37)	31.4(fixed)	—	–7.9	31.4
*u*3124	H(27)...H(46)	696.3(45)	33.1(fixed)	—	–8.6	33.1
*u*3132	H(85)...H(90)	696.4(36)	30.6(fixed)	—	–7.1	30.6
*u*3138	H(113)...H(124)	697.5(24)	33.8(fixed)	—	–9.3	33.8
*u*3145	H(72)...H(94)	698.1(42)	26.1(fixed)	—	–7.4	26.1
*u*3148	H(160)...H(168)	698.1(31)	30.5(fixed)	—	–7.4	30.5
*u*3137	H(162)...H(182)	698.5(25)	30.5(fixed)	—	–8.1	30.5
*u*3135	H(21)...H(38)	698.9(31)	31.1(fixed)	—	–7.4	31.1
*u*3151	H(36)...H(43)	699.2(22)	30.4(fixed)	—	–15.5	30.4
*u*3159	H(20)...H(30)	700.3(23)	29.2(fixed)	—	–12.2	29.2
*u*3136	H(115)...H(132)	701.0(32)	32.1(fixed)	—	–8.1	32.1
*u*3144	H(69)...H(85)	701.2(31)	26.6(fixed)	—	–8.6	26.6
*u*3128	H(160)...H(171)	701.3(25)	30.2(fixed)	—	–6.6	30.2
*u*3160	H(27)...H(41)	701.7(33)	33.1(fixed)	—	–9.0	33.1
*u*3185	H(122)...H(128)	701.8(23)	26.9(fixed)	—	–9.1	26.9
*u*3150	H(88)...H(93)	703.1(39)	30.9(fixed)	—	–7.9	30.9
*u*3158	H(166)...H(188)	704.2(24)	25.5(fixed)	—	–7.1	25.5
*u*3146	H(67)...H(77)	704.4(32)	26.2(fixed)	—	–7.9	26.2
*u*3154	H(27)...H(47)	704.6(33)	26.8(fixed)	—	–9.0	26.8
*u*3175	H(39)...H(46)	705.0(24)	28.0(fixed)	—	–9.1	28.0
*u*3192	H(66)...H(75)	705.2(30)	25.5(fixed)	—	–7.5	25.5
*u*3140	H(21)...H(43)	705.3(28)	37.2(fixed)	—	–10.8	37.2
*u*3166	H(26)...H(34)	705.4(20)	26.5(fixed)	—	–10.3	26.5
*u*3153	H(163)...H(182)	705.8(21)	25.7(fixed)	—	–8.1	25.7
*u*3134	H(72)...H(88)	706.0(39)	29.3(fixed)	—	–6.9	29.3
*u*3156	H(115)...H(138)	707.2(22)	27.9(fixed)	—	–9.2	27.9
*u*3147	H(22)...H(38)	707.3(22)	26.4(fixed)	—	–7.3	26.4
*u*3195	H(160)...H(169)	707.8(20)	26.9(fixed)	—	–8.4	26.9
*u*3157	H(161)...H(171)	708.2(23)	25.8(fixed)	—	–6.9	25.8
*u*3162	H(113)...H(120)	708.2(23)	26.1(fixed)	—	–8.2	26.1
*u*3152	H(116)...H(132)	708.4(21)	27.8(fixed)	—	–8.4	27.8
*u*3167	H(21)...H(44)	708.8(24)	33.7(fixed)	—	–12.4	33.7
*u*3143	H(68)...H(90)	709.0(37)	31.1(fixed)	—	–7.3	31.1
*u*3173	C(64)...H(74)	709.4(20)	16.3(fixed)	—	–4.3	16.3
*u*3183	H(28)...H(41)	709.9(31)	27.7(fixed)	—	–9.2	27.7
*u*3184	C(6)...H(43)	710.6(20)	18.5(fixed)	—	–9.9	18.5
*u*3164	H(83)...H(90)	711.1(19)	25.9(fixed)	—	–7.6	25.9

*u*3141	H(74)...H(77)	711.2(22)	29.3(fixed)	—	–6.7	29.3
*u*3169	C(7)...H(41)	711.8(8)	16.7(fixed)	—	–5.7	16.7
*u*3194	C(56)...H(93)	711.8(16)	16.4(fixed)	—	–5.3	16.4
*u*3176	C(152)...H(182)	711.8(11)	16.5(fixed)	—	–5.1	16.5
*u*3168	C(54)...H(88)	712.1(12)	16.4(fixed)	—	–4.6	16.4
*u*3179	H(86)...H(93)	712.2(24)	26.0(fixed)	—	–8.0	26.0
*u*3172	C(101)...H(135)	712.7(9)	16.2(fixed)	—	–4.6	16.2
*u*3193	C(103)...H(124)	713.1(10)	16.6(fixed)	—	–5.8	16.6
*u*3170	C(149)...H(179)	713.1(23)	16.1(fixed)	—	–4.5	16.1
*u*3177	C(105)...H(132)	713.3(10)	16.5(fixed)	—	–4.9	16.5
*u*3178	C(58)...H(85)	713.3(10)	16.4(fixed)	—	–5.3	16.4
*u*3163	H(68)...H(91)	713.8(26)	25.9(fixed)	—	–7.3	25.9
*u*3198	C(8)...H(30)	714.2(8)	17.1(fixed)	—	–7.5	17.1
*u*3197	C(13)...H(21)	714.4(9)	16.7(fixed)	—	–5.7	16.7
*u*3174	C(10)...H(25)	714.5(9)	16.4(fixed)	—	–5.1	16.4
*u*3188	C(102)...H(140)	714.7(8)	16.6(fixed)	—	–5.8	16.6
*u*3171	C(11)...H(38)	714.8(9)	16.2(fixed)	—	–4.5	16.2
*u*3196	C(150)...H(187)	714.9(8)	16.3(fixed)	—	–5.0	16.3
*u*3165	H(74)...H(78)	715.0(17)	25.3(fixed)	—	–6.9	25.3
*u*3191	C(147)...H(184)	715.1(21)	16.6(fixed)	—	–4.8	16.6
*u*3182	C(12)...H(34)	715.1(8)	16.7(fixed)	—	–6.6	16.7
*u*3186	C(60)...H(68)	715.2(8)	16.3(fixed)	—	–5.0	16.3
*u*3180	C(100)...H(137)	715.7(21)	16.5(fixed)	—	–5.3	16.5
*u*3190	C(59)...H(81)	715.7(7)	16.5(fixed)	—	–5.8	16.5
*u*3181	C(53)...H(90)	715.7(21)	16.6(fixed)	—	–4.5	16.6
*u*3189	C(16)...H(19)	715.8(20)	16.7(fixed)	—	–5.7	16.7
*u*3187	C(63)...H(66)	716.2(20)	16.4(fixed)	—	–5.0	16.4
*u*3161	H(73)...H(88)	716.2(30)	25.0(fixed)	—	–7.0	25.0
*u*3204	H(18)...H(43)	727.0(24)	29.7(fixed)	—	–8.9	29.7
*u*3202	H(74)...H(92)	727.2(41)	26.8(fixed)	—	–3.1	26.8
*u*3199	H(70)...H(88)	727.8(33)	27.3(fixed)	—	–3.9	27.3
*u*3210	H(168)...H(186)	729.0(28)	27.2(fixed)	—	–4.3	27.2
*u*3215	H(23)...H(41)	731.5(21)	27.4(fixed)	—	–4.5	27.4
*u*3200	H(65)...H(90)	731.9(32)	27.0(fixed)	—	–3.6	27.0
*u*3205	H(115)...H(134)	732.7(25)	26.3(fixed)	—	–5.1	26.3
*u*3216	H(80)...H(85)	733.0(22)	27.2(fixed)	—	–4.2	27.2
*u*3220	H(24)...H(30)	733.2(22)	27.7(fixed)	—	–6.9	27.7
*u*3206	H(127)...H(132)	734.1(25)	27.0(fixed)	—	–3.3	27.0
*u*3212	H(34)...H(37)	734.1(20)	27.0(fixed)	—	–6.3	27.0
*u*3221	H(159)...H(184)	734.3(23)	26.5(fixed)	—	–3.9	26.5
*u*3218	H(165)...H(179)	734.8(28)	26.2(fixed)	—	–4.1	26.2
*u*3222	H(118)...H(140)	735.4(19)	26.8(fixed)	—	–5.2	26.8
*u*3209	H(117)...H(135)	736.2(20)	26.3(fixed)	—	–3.0	26.3
*u*3201	H(21)...H(40)	736.2(24)	27.2(fixed)	—	–4.2	27.2
*u*3203	H(112)...H(137)	736.3(23)	27.1(fixed)	—	–4.4	27.1
*u*3214	H(76)...H(93)	736.7(24)	25.4(fixed)	—	–4.7	25.4

*u*3211	H(33)...H(38)	738.2(23)	28.4(fixed)	—	–2.9	28.4
*u*3208	H(170)...H(187)	738.6(22)	26.3(fixed)	—	–3.9	26.3
*u*3224	H(66)...H(89)	738.7(24)	25.8(fixed)	—	–4.4	25.8
*u*3219	H(81)...H(84)	739.0(17)	26.9(fixed)	—	–4.8	26.9
*u*3242	H(20)...H(43)	739.3(26)	28.5(fixed)	—	–11.4	28.5
*u*3213	H(25)...H(32)	739.7(16)	28.2(fixed)	—	–2.7	28.2
*u*3234	Br(14)...H(27)	740.2(14)	16.8(fixed)	—	–5.8	16.8
*u*3207	H(68)...H(87)	740.2(21)	25.8(fixed)	—	–4.3	25.8
*u*3250	Br(15)...H(46)	741.2(15)	16.9(fixed)	—	–5.5	16.9
*u*3228	H(25)...H(31)	741.3(18)	30.0(fixed)	—	–4.7	30.0
*u*3240	H(19)...H(44)	741.5(26)	32.5(fixed)	—	–4.6	32.5
*u*3225	H(116)...H(135)	741.7(16)	28.0(fixed)	—	–4.7	28.0
*u*3217	H(19)...H(42)	742.2(25)	30.7(fixed)	—	–1.8	30.7
*u*3233	H(66)...H(91)	742.4(26)	25.6(fixed)	—	–5.4	25.6
*u*3244	H(119)...H(141)	742.5(14)	27.7(fixed)	—	–5.4	27.7
*u*3235	H(35)...H(38)	742.9(14)	27.2(fixed)	—	–4.2	27.2
*u*3241	Br(61)...H(72)	742.9(14)	16.5(fixed)	—	–4.9	16.5
*u*3232	H(82)...H(85)	743.0(13)	27.6(fixed)	—	–5.4	27.6
*u*3229	H(22)...H(41)	743.1(14)	27.3(fixed)	—	–6.0	27.3
*u*3252	H(75)...H(93)	743.4(18)	25.0(fixed)	—	–5.9	25.0
*u*3236	H(113)...H(138)	743.5(25)	27.1(fixed)	—	–5.6	27.1
*u*3243	H(68)...H(86)	743.8(17)	25.9(fixed)	—	–5.5	25.9
*u*3237	H(168)...H(188)	744.1(13)	25.9(fixed)	—	–5.6	25.9
*u*3247	H(169)...H(187)	744.3(14)	26.5(fixed)	—	–5.6	26.5
*u*3251	Br(62)...H(77)	744.4(13)	16.7(fixed)	—	–5.2	16.7
*u*3238	H(74)...H(94)	744.5(14)	25.8(fixed)	—	–4.5	25.8
*u*3230	H(81)...H(83)	744.6(15)	26.5(fixed)	—	–6.2	26.5
*u*3227	H(69)...H(88)	744.9(15)	26.7(fixed)	—	–5.0	26.7
*u*3248	H(115)...H(133)	744.9(13)	26.3(fixed)	—	–6.6	26.3
*u*3223	H(166)...H(177)	745.0(29)	24.8(fixed)	—	–4.8	24.8
*u*3249	H(160)...H(185)	745.2(25)	25.8(fixed)	—	–5.3	25.8
*u*3231	H(120)...H(140)	745.2(15)	26.2(fixed)	—	–6.4	26.2
*u*3246	Br(155)...H(162)	745.4(13)	16.5(fixed)	—	–4.6	16.5
*u*3253	H(21)...H(39)	745.5(15)	28.0(fixed)	—	–6.7	28.0
*u*3239	H(26)...H(30)	745.7(14)	26.2(fixed)	—	–8.4	26.2
*u*3245	H(67)...H(90)	746.0(26)	26.5(fixed)	—	–5.1	26.5
*u*3226	H(34)...H(36)	746.6(15)	25.3(fixed)	—	–7.4	25.3
*u*3257	H(74)...H(93)	781.7(23)	20.0(fixed)	—	–7.7	20.0
*u*3254	H(166)...H(179)	784.4(23)	19.4(fixed)	—	–7.2	19.4
*u*3256	H(21)...H(41)	785.4(10)	20.5(fixed)	—	–9.2	20.5
*u*3265	H(115)...H(135)	785.8(11)	19.9(fixed)	—	–8.4	19.9
*u*3262	H(168)...H(187)	786.5(11)	19.9(fixed)	—	–8.1	19.9
*u*3260	H(68)...H(88)	786.9(12)	19.8(fixed)	—	–7.8	19.8
*u*3261	H(25)...H(30)	787.1(11)	20.3(fixed)	—	–10.2	20.3
*u*3267	H(19)...H(43)	787.5(23)	21.5(fixed)	—	–12.6	21.5
*u*3255	H(119)...H(140)	787.6(11)	20.2(fixed)	—	–8.6	20.2

*u*3264	H(81)...H(85)	787.9(11)	20.0(fixed)	—	–9.0	20.0
*u*3258	H(34)...H(38)	788.2(11)	19.9(fixed)	—	–8.8	19.9
*u*3259	H(160)...H(184)	790.2(24)	20.2(fixed)	—	–7.6	20.2
*u*3266	H(113)...H(137)	791.0(24)	20.1(fixed)	—	–8.6	20.1
*u*3263	H(66)...H(90)	791.9(24)	20.1(fixed)	—	–7.7	20.1

Table S14. Final refined Cartesian coordinates (in Å) for all six conformers of **1**

	1a				**1b**		
	x	*y*	*z*		*x*	*y*	*z*
C(1)	0.0000	0.0000	0.0000	C(48)	0.0000	0.0000	0.0000
Si(2)	–0.6058	1.3054	1.2419	Si(49)	–0.6058	1.3371	1.2077
Si(3)	–0.6058	–1.7082	0.5729	Si(50)	–0.6058	–1.6929	0.6169
Si(4)	1.9097	0.0000	0.0000	Si(51)	1.9097	0.0000	0.0000
Si(5)	–0.6086	0.4893	–1.7428	Si(52)	–0.6086	0.4441	–1.7548
C(6)	–2.3827	1.1404	–1.7527	C(53)	–2.3622	1.1482	–1.7804
C(7)	–0.5295	–0.9349	–2.9825	C(54)	–0.5844	–1.0226	–2.9463
C(8)	–2.4037	–2.1050	0.1577	C(55)	0.3395	–3.1793	–0.0609
C(9)	0.2953	–3.1796	–0.1924	C(56)	–0.4843	–1.9581	2.4816
C(10)	2.6509	1.7384	0.0000	C(57)	2.6558	1.7363	0.0000
C(11)	2.6509	–0.9232	–1.4730	C(58)	2.6558	–0.9223	–1.4712
C(12)	–2.3525	1.0361	1.9042	C(59)	–2.3936	1.1488	1.7827
C(13)	0.3933	1.4210	2.8390	C(60)	0.3313	1.4250	2.8437
H(14)	–0.5660	2.6773	0.5600	H(61)	–0.4767	2.7011	0.5210
H(15)	–0.4427	–1.7944	2.0943	H(62)	–2.0766	–1.8533	0.2174
C(16)	2.6509	–0.9232	1.4730	C(63)	2.6558	–0.9223	1.4712
C(17)	0.3581	1.9323	–2.4875	C(64)	0.3912	1.8293	–2.5630
H(18)	–2.5253	2.0321	–1.1388	H(65)	–2.4723	2.0669	–1.2005
H(19)	–2.6522	1.3960	–2.7795	H(66)	–2.6290	1.3732	–2.8151
H(20)	–3.1158	0.4193	–1.3854	H(67)	–3.1139	0.4625	–1.3840
H(21)	–0.8922	–0.5749	–3.9474	H(68)	–0.9450	–0.6831	–3.9195
H(22)	0.4774	–1.3304	–3.1314	H(69)	0.4092	–1.4519	–3.0903
H(23)	–1.1369	–1.7968	–2.6986	H(70)	–1.2167	–1.8541	–2.6282
H(24)	–2.5891	–2.1032	–0.9183	H(71)	1.3982	–3.1623	0.2059
H(25)	–2.6338	–3.1040	0.5338	H(72)	–0.0961	–4.0873	0.3613
H(26)	–3.1192	–1.4092	0.6007	H(73)	0.2977	–3.2643	–1.1487
H(27)	–0.1370	–4.0980	0.2099	H(74)	–0.8582	–2.9575	2.7134
H(28)	0.1891	–3.2093	–1.2787	H(75)	0.5413	–1.8921	2.8504
H(29)	1.3665	–3.1951	0.0188	H(76)	–1.0671	–1.2410	3.0635
H(30)	3.7394	1.6510	0.0000	H(77)	3.7439	1.6447	0.0000
H(31)	2.3647	2.3365	–0.8676	H(78)	2.3717	2.3337	–0.8688
H(32)	2.3647	2.3365	0.8676	H(79)	2.3717	2.3337	0.8688
H(33)	2.3647	–0.5056	–2.4405	H(80)	2.3717	–0.5034	–2.4387
H(34)	3.7394	–0.8767	–1.3990	H(81)	3.7439	–0.8736	–1.3935
H(35)	2.3647	–1.9759	–1.5191	H(82)	2.3717	–1.9756	–1.5158
H(36)	–3.1200	1.0347	1.1275	H(83)	–3.1199	1.1802	0.9680
H(37)	–2.4489	0.0908	2.4423	H(84)	–2.5683	0.2112	2.3145
H(38)	–2.5865	1.8423	2.6024	H(85)	–2.6245	1.9679	2.4668
H(39)	0.3775	0.4871	3.4045	H(86)	0.2646	0.4984	3.4175
H(40)	1.4436	1.6745	2.6810	H(87)	1.3958	1.6381	2.7262
H(41)	–0.0463	2.1985	3.4672	H(88)	–0.1036	2.2235	3.4484
H(42)	2.3647	–1.9759	1.5191	H(89)	2.3717	–1.9756	1.5158
H(43)	3.7394	–0.8767	1.3990	H(90)	3.7439	–0.8736	1.3935

H(44)	2.3647	–0.5056	2.4405	H(91)	2.3717	–0.5034	2.4387
H(45)	1.4252	1.7314	–2.6028	H(92)	1.4503	1.5916	–2.6812
H(46)	–0.0492	2.1482	–3.4773	H(93)	–0.0209	2.0184	–3.5563
H(47)	0.3012	2.8488	–1.8966	H(94)	0.3646	2.7686	–2.0068
	1c				**1d**		
	x	*y*	*z*		*x*	*y*	*z*
C(95)	0.0000	0.0000	0.0000	C(142)	0.0000	0.0000	0.0000
Si(96)	–0.6067	1.2934	1.2539	Si(143)	–1.5436	1.1093	0.0000
Si(97)	–0.6067	–1.7139	0.5546	Si(144)	0.0000	–1.1093	1.5436
Si(98)	1.9097	0.0000	0.0000	Si(145)	1.5508	1.1145	0.0000
Si(99)	–0.6095	0.5035	–1.7384	Si(146)	0.0000	–1.1145	–1.5508
C(100)	–2.3971	1.1167	–1.7476	C(147)	–1.7121	–1.7885	–1.9818
C(101)	–0.4932	–0.8995	–2.9991	C(148)	1.1599	–2.5988	–1.3995
C(102)	–2.4268	–2.0769	0.2112	C(149)	–0.5622	–0.2669	3.1363
C(103)	0.2659	–3.1801	–0.2523	C(150)	–1.1587	–2.5969	1.4618
C(104)	2.6503	1.7387	0.0000	C(151)	1.3995	2.5988	–1.1599
C(105)	2.6503	–0.9232	–1.4733	C(152)	3.1289	0.1923	–0.4802
C(106)	–0.6984	3.0644	0.6076	C(153)	–3.1363	0.2669	0.5622
C(107)	–2.3462	1.0101	1.9294	C(154)	–1.4618	2.5969	1.1587
H(108)	0.3574	1.2866	2.4451	H(155)	–1.7652	1.6330	–1.4231
H(109)	–0.3918	–1.8253	2.0679	H(156)	1.4231	–1.6330	1.7652
C(110)	2.6503	–0.9232	1.4733	C(157)	1.9818	1.7885	1.7121
C(111)	0.3307	1.9781	–2.4546	C(158)	0.4802	–0.1923	–3.1289
H(112)	–2.5580	1.9963	–1.1210	H(159)	–2.4491	–1.0101	–2.1899
H(113)	–2.6676	1.3829	–2.7715	H(160)	–1.6245	–2.4113	–2.8744
H(114)	–3.1140	0.3715	–1.3966	H(161)	–2.1536	–2.3992	–1.1916
H(115)	–0.8582	–0.5332	–3.9609	H(162)	1.1005	–3.1802	–2.3219
H(116)	0.5241	–1.2677	–3.1470	H(163)	2.2053	–2.3233	–1.2461
H(117)	–1.0860	–1.7761	–2.7297	H(164)	0.9128	–3.2644	–0.5698
H(118)	–2.6734	–2.0401	–0.8519	H(165)	–1.5882	0.1012	3.0717
H(119)	–2.6544	–3.0822	0.5715	H(166)	–0.5206	–0.9968	3.9474
H(120)	–3.1092	–1.3830	0.7063	H(167)	0.0577	0.5852	3.4229
H(121)	–0.1659	–4.1017	0.1431	H(168)	–1.0730	–3.1545	2.3968
H(122)	0.1508	–3.1972	–1.3380	H(169)	–2.2038	–2.3034	1.3436
H(123)	1.3404	–3.2060	–0.0596	H(170)	–0.9328	–3.2830	0.6430
H(124)	3.7389	1.6524	0.0000	H(171)	2.3219	3.1802	–1.1005
H(125)	2.3632	2.3333	–0.8696	H(172)	1.2461	2.3233	–2.2053
H(126)	2.3632	2.3333	0.8696	H(173)	0.5698	3.2644	–0.9128
H(127)	2.3632	–0.5020	–2.4390	H(174)	3.0926	–0.2461	–1.4796
H(128)	3.7389	–0.8774	–1.4002	H(175)	3.9628	0.8968	–0.4556
H(129)	2.3632	–1.9759	–1.5155	H(176)	3.3726	–0.6356	0.1888
H(130)	0.2644	3.4547	0.2716	H(177)	–3.4229	–0.5852	–0.0577
H(131)	–1.3824	3.1730	–0.2366	H(178)	–3.0717	–0.1012	1.5882
H(132)	–1.0571	3.7095	1.4123	H(179)	–3.9474	0.9968	0.5206
H(133)	–3.1106	1.0184	1.1498	H(180)	–1.3436	2.3034	2.2038
H(134)	–2.4584	0.0600	2.4559	H(181)	–0.6430	3.2830	0.9328

H(135)	–2.5798	1.8110	2.6338	H(182)	–2.3968	3.1545	1.0730
H(136)	2.3632	–1.9759	1.5155	H(183)	2.1899	1.0101	2.4491
H(137)	3.7389	–0.8774	1.4002	H(184)	2.8744	2.4113	1.6245
H(138)	2.3632	–0.5020	2.4390	H(185)	1.1916	2.3992	2.1536
H(139)	1.4017	1.7975	–2.5670	H(186)	1.4796	0.2461	–3.0926
H(140)	–0.0752	2.2016	–3.4434	H(187)	0.4556	–0.8968	–3.9628
H(141)	0.2478	2.8824	–1.8482	H(188)	–0.1888	0.6356	–3.3726
	1e				**1f**		
	x	*y*	*z*		*x*	*y*	*z*
C(189)	0.0000	0.0000	0.0000	C(236)	0.0000	0.0000	0.0000
Si(190)	–1.5434	1.1096	0.0000	S(237)	–1.5434	1.1096	0.0000
Si(191)	0.0000	–1.1096	1.5434	S(238)	0.0000	–1.1096	1.5434
Si(192)	1.5506	1.1147	0.0000	S(239)	1.5506	1.1147	0.0000
Si(193)	0.0000	–1.1147	–1.5506	S(240)	0.0000	–1.1147	–1.5506
C(194)	–1.7062	–1.8165	–1.9605	C(241)	–1.7042	–1.8230	–1.9577
C(195)	1.1860	–2.5796	–1.4119	C(242)	1.1910	–2.5759	–1.4164
C(196)	1.6821	–1.8179	2.0242	C(243)	–1.1625	–2.5944	1.4641
C(197)	–0.5516	–0.2666	3.1394	C(244)	1.6655	–1.8868	1.9728
C(198)	1.4119	2.5796	–1.1860	C(245)	1.4164	2.5759	–1.1910
C(199)	3.1338	0.1845	–0.4467	C(246)	3.1358	0.1843	–0.4390
C(200)	–2.0242	1.8179	–1.6821	C(247)	–1.4641	2.5944	1.1625
C(201)	–3.1394	0.2666	0.5516	C(248)	–1.9728	1.8868	–1.6655
H(202)	–1.2831	2.2861	0.9470	H(249)	–2.7450	0.2604	0.4287
H(203)	–0.9470	–2.2861	1.2831	H(250)	–0.4287	–0.2604	2.7450
C(204)	1.9605	1.8165	1.7062	C(251)	1.9577	1.8230	1.7042
C(205)	0.4467	–0.1845	–3.1338	C(252)	0.4390	–0.1843	–3.1358
H(206)	–2.4574	–1.0492	–2.1586	H(253)	–2.4570	–1.0574	–2.1563
H(207)	–1.6213	–2.4385	–2.8539	H(254)	–1.6171	–2.4443	–2.8514
H(208)	–2.1273	–2.4330	–1.1637	H(255)	–2.1192	–2.4428	–1.1603
H(209)	1.1270	–3.1637	–2.3326	H(256)	1.1301	–3.1588	–2.3378
H(210)	2.2279	–2.2854	–1.2699	H(257)	2.2322	–2.2769	–1.2796
H(211)	0.9590	–3.2473	–0.5783	H(258)	0.9659	–3.2452	–0.5835
H(212)	2.4088	–1.0365	2.2558	H(259)	–0.9260	–3.2773	0.6455
H(213)	1.5582	–2.4334	2.9176	H(260)	–1.0766	–3.1525	2.3987
H(214)	2.1304	–2.4422	1.2486	H(261)	–2.2113	–2.3190	1.3357
H(215)	–0.5110	–0.9964	3.9506	H(262)	1.5425	–2.4971	2.8699
H(216)	0.0960	0.5697	3.4106	H(263)	2.0511	–2.5323	1.1811
H(217)	–1.5692	0.1271	3.0958	H(264)	2.4487	–1.1530	2.1740
H(218)	2.3326	3.1637	–1.1270	H(265)	2.3378	3.1588	–1.1301
H(219)	1.2699	2.2854	–2.2279	H(266)	1.2796	2.2769	–2.2322
H(220)	0.5783	3.2473	–0.9590	H(267)	0.5835	3.2452	–0.9659
H(221)	3.1073	–0.2704	–1.4391	H(268)	3.1118	–0.2716	–1.4310
H(222)	3.9688	0.8877	–0.4245	H(269)	3.9694	0.8893	–0.4166
H(223)	3.3678	–0.6327	0.2386	H(270)	3.3684	–0.6285	0.2521
H(224)	–1.2486	2.4422	–2.1304	H(271)	–1.3357	2.3190	2.2113
H(225)	–2.2558	1.0365	–2.4088	H(272)	–0.6455	3.2773	0.9260

H(226)	–2.9176	2.4334	–1.5582	H(273)	–2.3987	3.1525	1.0766
H(227)	–3.4106	–0.5697	–0.0960	H(274)	–1.1811	2.5323	–2.0511
H(228)	–3.0958	–0.1271	1.5692	H(275)	–2.1740	1.1530	–2.4487
H(229)	–3.9506	0.9964	0.5110	H(276)	–2.8699	2.4971	–1.5425
H(230)	2.1586	1.0492	2.4574	H(277)	2.1563	1.0574	2.4570
H(231)	2.8539	2.4385	1.6213	H(278)	2.8514	2.4443	1.6171
H(232)	1.1637	2.4330	2.1273	H(279)	1.1603	2.4428	2.1192
H(233)	1.4391	0.2704	–3.1073	H(280)	1.4310	0.2716	–3.1118
H(234)	0.4245	–0.8877	–3.9688	H(281)	0.4166	–0.8893	–3.9694
H(235)	–0.2386	0.6327	–3.3678	H(282)	–0.2521	0.6285	–3.3684

Table S15. Final refined Cartesian coordinates (in Å) for all four conformers of **2**.

	2a				**2b**		
	x	*y*	*z*		*x*	*y*	*z*
C(1)	0.0000	0.0000	0.0000	C(48)	0.0000	0.0000	0.0000
Si(2)	–0.6614	1.2219	1.2970	Si(49)	–0.6614	1.2652	1.2548
Si(3)	–0.6614	–1.7490	0.3412	Si(50)	–0.6614	–1.7364	0.4003
Si(4)	1.9378	0.0000	0.0000	Si(51)	1.9378	0.0000	0.0000
Si(5)	–0.6743	0.4535	–1.7592	Si(52)	–0.6743	0.3935	–1.7736
C(6)	–2.4766	1.0090	–1.6984	C(53)	–2.4602	1.0014	–1.7297
C(7)	–0.6295	–1.0251	–2.9308	C(54)	–0.6795	–1.1346	–2.8807
C(8)	–2.4764	–2.0339	–0.0423	C(55)	0.1479	–3.1462	–0.5379
C(9)	0.3174	–3.1625	–0.4116	C(56)	–0.6798	–2.1951	2.2202
C(10)	2.6398	1.7516	0.0000	C(57)	2.6426	1.7505	0.0000
C(11)	2.6398	–0.8371	–1.5386	C(58)	2.6426	–0.8368	–1.5375
C(12)	–2.4615	1.0124	1.7854	C(59)	–2.4874	1.1201	1.6636
C(13)	0.3495	1.3824	2.8702	C(60)	0.2821	1.3673	2.8741
Cl(14)	–0.6175	3.1559	0.5237	Cl(61)	–0.5022	3.1986	0.4957
Cl(15)	–0.5545	–2.1523	2.3823	Cl(62)	–2.6559	–1.8976	–0.1426
C(16)	2.6398	–0.8371	1.5386	C(63)	2.6426	–0.8368	1.5375
C(17)	0.3632	1.7967	–2.5839	C(64)	0.3917	1.6697	–2.6657
H(18)	–2.6385	1.9001	–1.0783	H(65)	–2.5931	1.9239	–1.1500
H(19)	–2.7849	1.2470	–2.7247	H(66)	–2.7672	1.2014	–2.7644
H(20)	–3.1573	0.2421	–1.3068	H(67)	–3.1592	0.2715	–1.3014
H(21)	–1.0238	–0.6924	–3.8996	H(68)	–1.0719	–0.8322	–3.8602
H(22)	0.3802	–1.4242	–3.0922	H(69)	0.3178	–1.5677	–3.0314
H(23)	–1.2368	–1.8727	–2.5880	H(70)	–1.3083	–1.9487	–2.4978
H(24)	–2.7025	–1.8756	–1.1047	H(71)	1.2237	–3.2224	–0.3338
H(25)	–2.7072	–3.0785	0.2037	H(72)	–0.3285	–4.0789	–0.2093
H(26)	–3.1515	–1.3900	0.5361	H(73)	0.0309	–3.0687	–1.6265
H(27)	–0.1822	–4.0984	–0.1301	H(74)	–1.0817	–3.2133	2.3008
H(28)	0.3447	–3.1065	–1.5075	H(75)	0.3241	–2.1885	2.6642
H(29)	1.3560	–3.2108	–0.0598	H(76)	–1.3065	–1.5318	2.8302
H(30)	3.7344	1.6700	0.0000	H(77)	3.7370	1.6666	0.0000
H(31)	2.3416	2.3418	–0.8761	H(78)	2.3457	2.3395	–0.8774
H(32)	2.3416	2.3418	0.8761	H(79)	2.3457	2.3395	0.8774
H(33)	2.3416	–0.3496	–2.4758	H(80)	2.3457	–0.3477	–2.4743
H(34)	3.7344	–0.7981	–1.4669	H(81)	3.7370	–0.7967	–1.4638
H(35)	2.3416	–1.8888	–1.6383	H(82)	2.3457	–1.8890	–1.6355
H(36)	–3.1586	1.1314	0.9459	H(83)	–3.1409	1.2535	0.7918
H(37)	–2.6543	0.0298	2.2350	H(84)	–2.7410	0.1504	2.1112
H(38)	–2.6937	1.7815	2.5333	H(85)	–2.7268	1.9051	2.3925
H(39)	0.4116	0.4334	3.4183	H(86)	0.2695	0.4191	3.4270
H(40)	1.3766	1.7283	2.6962	H(87)	1.3343	1.6530	2.7478
H(41)	–0.1531	2.1159	3.5138	H(88)	–0.2064	2.1301	3.4941
H(42)	2.3416	–1.8888	1.6383	H(89)	2.3457	–1.8890	1.6355
H(43)	3.7344	–0.7981	1.4669	H(90)	3.7370	–0.7967	1.4638

H(44)	2.3416	–0.3496	2.4758	H(91)	2.3457	–0.3477	2.4743
H(45)	1.4123	1.5096	–2.7316	H(92)	1.4312	1.3472	–2.8080
H(46)	–0.0774	1.9980	–3.5689	H(93)	–0.0520	1.8377	–3.6555
H(47)	0.3854	2.7389	–2.0211	H(94)	0.4427	2.6354	–2.1463
	2c				**2d**		
	x	*y*	*z*		*x*	*y*	*z*
C(95)	0.0000	0.0000	0.0000	C(142)	0.0000	0.0000	0.0000
Si(96)	–1.5604	1.0853	0.0000	Si(143)	–1.5605	1.0851	0.0000
Si(97)	0.0000	–1.0853	1.5604	Si(144)	0.0000	–1.0851	1.5605
Si(98)	1.5909	1.1064	0.0000	Si(145)	1.5910	1.1063	0.0000
Si(99)	0.0000	–1.1064	–1.5909	Si(146)	0.0000	–1.1063	–1.5910
C(100)	–1.6921	–1.8791	–1.9082	C(147)	–1.7228	–1.7593	–1.9986
C(101)	1.2069	–2.5493	–1.4421	C(148)	1.0899	–2.6336	–1.3906
C(102)	–0.4604	–0.2052	3.1529	C(149)	1.6252	–1.9410	1.9464
C(103)	–1.0495	–2.6381	1.4608	C(150)	–0.6030	–0.2442	3.1263
C(104)	1.4421	2.5493	–1.2069	C(151)	1.3906	2.6336	–1.0899
C(105)	3.1188	0.1385	–0.5380	C(152)	3.0918	0.1873	–0.6810
C(106)	–3.1529	0.2052	0.4604	C(153)	–1.9464	1.9410	–1.6252
C(107)	–1.4608	2.6381	1.0495	C(154)	–3.1263	0.2442	0.6030
Cl(108)	–1.9600	1.8223	–1.8963	Cl(155)	–1.3402	2.6754	1.3277
Cl(109)	1.8963	–1.8223	1.9600	Cl(156)	–1.3277	–2.6754	1.3402
C(110)	1.9082	1.8791	1.6921	C(157)	1.9986	1.7593	1.7228
C(111)	0.5380	–0.1385	–3.1188	C(158)	0.6810	–0.1873	–3.0918
H(112)	–2.4882	–1.1389	–2.0604	H(159)	–2.4566	–0.9656	–2.1897
H(113)	–1.6133	–2.4867	–2.8189	H(160)	–1.6389	–2.3719	–2.9056
H(114)	–2.0346	–2.5296	–1.0932	H(161)	–2.1526	–2.3829	–1.2042
H(115)	1.1507	–3.1258	–2.3745	H(162)	1.0368	–3.2037	–2.3272
H(116)	2.2485	–2.2340	–1.2988	H(163)	2.1435	–2.3956	–1.1954
H(117)	0.9775	–3.2261	–0.6088	H(164)	0.7724	–3.2922	–0.5719
H(118)	–1.4756	0.2110	3.1219	H(165)	2.4378	–1.2245	2.1230
H(119)	–0.4198	–0.9442	3.9635	H(166)	1.4815	–2.5268	2.8635
H(120)	0.2184	0.6186	3.4087	H(167)	1.9580	–2.6238	1.1540
H(121)	–0.9570	–3.1626	2.4206	H(168)	–0.5497	–0.9800	3.9391
H(122)	–2.1115	–2.4148	1.2956	H(169)	0.0230	0.6144	3.4017
H(123)	–0.7368	–3.3263	0.6650	H(170)	–1.6381	0.1147	3.0583
H(124)	2.3745	3.1258	–1.1507	H(171)	2.3272	3.2037	–1.0368
H(125)	1.2988	2.2340	–2.2485	H(172)	1.1954	2.3956	–2.1435
H(126)	0.6088	3.2261	–0.9775	H(173)	0.5719	3.2922	–0.7724
H(127)	3.0409	–0.2708	–1.5535	H(174)	2.9644	–0.1485	–1.7183
H(128)	3.9731	0.8273	–0.5130	H(175)	3.9454	0.8765	–0.6478
H(129)	3.3484	–0.7130	0.1154	H(176)	3.3540	–0.7087	–0.1037
H(130)	–3.4087	–0.6186	–0.2184	H(177)	–1.1540	2.6238	–1.9580
H(131)	–3.1219	–0.2110	1.4756	H(178)	–2.1230	1.2245	–2.4378
H(132)	–3.9635	0.9442	0.4198	H(179)	–2.8635	2.5268	–1.4815
H(133)	–1.2956	2.4148	2.1115	H(180)	–3.4017	–0.6144	–0.0230
H(134)	–0.6650	3.3263	0.7368	H(181)	–3.0583	–0.1147	1.6381

H(135)	–2.4206	3.1626	0.9570	H(182)	–3.9391	0.9800	0.5497
H(136)	2.0604	1.1389	2.4882	H(183)	2.1897	0.9656	2.4566
H(137)	2.8189	2.4867	1.6133	H(184)	2.9056	2.3719	1.6389
H(138)	1.0932	2.5296	2.0346	H(185)	1.2042	2.3829	2.1526
H(139)	1.5535	0.2708	–3.0409	H(186)	1.7183	0.1485	–2.9644
H(140)	0.5130	–0.8273	–3.9731	H(187)	0.6478	–0.8765	–3.9454
H(141)	–0.1154	0.7130	–3.3484	H(188)	0.1037	0.7087	–3.3540

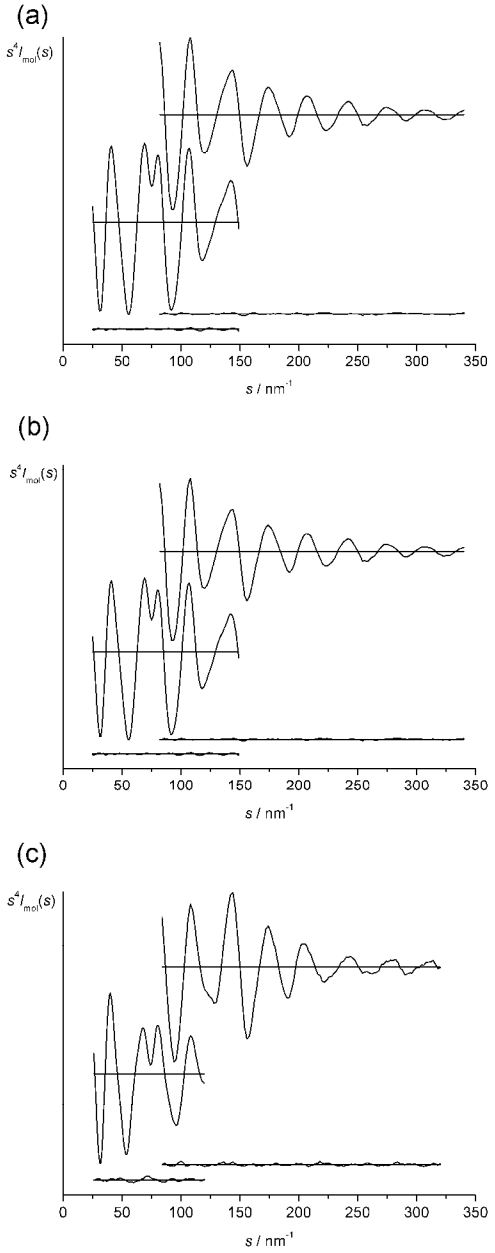
Table S16. Final refined Cartesian coordinates (in Å) for all four conformers of **3**.

	3a				**3b**		
	x	*y*	*z*		*x*	*y*	*z*
C(1)	0.0000	0.0000	0.0000	C(48)	0.0000	0.0000	0.0000
Si(2)	–0.6473	1.1858	1.3296	Si(49)	–0.6470	1.2527	1.2669
Si(3)	–0.6473	–1.7518	0.3243	Si(50)	–0.6470	–1.7327	0.4149
Si(4)	1.9504	0.0000	0.0000	Si(51)	1.9504	0.0000	0.0000
Si(5)	–0.6660	0.5370	–1.7527	Si(52)	–0.6657	0.4469	–1.7780
C(6)	–2.4622	1.1108	–1.6854	C(53)	–2.4410	1.0844	–1.7348
C(7)	–0.6170	–0.8807	–2.9967	C(54)	–0.6775	–1.0467	–2.9308
C(8)	–2.4530	–2.0545	–0.0770	C(55)	0.1771	–3.1478	–0.4970
C(9)	0.3350	–3.1522	–0.4418	C(56)	–0.6433	–2.1878	2.2331
C(10)	2.6612	1.7477	0.0000	C(57)	2.6631	1.7470	0.0000
C(11)	2.6612	–0.8528	–1.5256	C(58)	2.6631	–0.8523	–1.5250
C(12)	–2.4476	0.9858	1.8115	C(59)	–2.4725	1.1285	1.6734
C(13)	0.3468	1.2725	2.9163	C(60)	0.2676	1.3009	2.9022
Br(14)	–0.5718	3.3348	0.5810	Br(61)	–0.4366	3.3855	0.4985
Br(15)	–0.5471	–2.2358	2.5469	Br(62)	–2.8279	–1.9543	–0.1625
C(16)	2.6612	–0.8528	1.5256	C(63)	2.6631	–0.8523	1.5250
C(17)	0.3599	1.9293	–2.5070	C(64)	0.3972	1.7526	–2.6295
H(18)	–2.6182	1.9663	–1.0410	H(65)	–2.5608	1.9848	–1.1461
H(19)	–2.7523	1.3887	–2.6904	H(66)	–2.7306	1.3073	–2.7536
H(20)	–3.1462	0.3480	–1.3362	H(67)	–3.1460	0.3679	–1.3335
H(21)	–1.0001	–0.5023	–3.9357	H(68)	–1.0576	–0.7145	–3.8882
H(22)	0.3786	–1.2680	–3.1708	H(69)	0.3033	–1.4763	–3.0886
H(23)	–1.2194	–1.7315	–2.7056	H(70)	–1.3064	–1.8553	–2.5812
H(24)	–2.6631	–1.8978	–1.1271	H(71)	1.2360	–3.2112	–0.2820
H(25)	–2.6693	–3.0884	0.1592	H(72)	–0.2899	–4.0652	–0.1623
H(26)	–3.1317	–1.4304	0.4899	H(73)	0.0690	–3.0880	–1.5723
H(27)	–0.1541	–4.0788	–0.1699	H(74)	–1.0347	–3.1934	2.3167
H(28)	0.3542	–3.0859	–1.5219	H(75)	0.3535	–2.1785	2.6549
H(29)	1.3602	–3.1990	–0.0978	H(76)	–1.2571	–1.5360	2.8412
H(30)	3.7400	1.6597	0.0000	H(77)	3.7417	1.6574	0.0000
H(31)	2.3710	2.3318	–0.8638	H(78)	2.3737	2.3299	–0.8649
H(32)	2.3710	2.3318	0.8638	H(79)	2.3737	2.3299	0.8649
H(33)	2.3710	–0.3838	–2.4568	H(80)	2.3737	–0.3817	–2.4558
H(34)	3.7400	–0.8098	–1.4487	H(81)	3.7417	–0.8086	–1.4468
H(35)	2.3710	–1.8918	–1.6138	H(82)	2.3737	–1.8916	–1.6119
H(36)	–3.1341	1.1374	0.9886	H(83)	–3.1157	1.2802	0.8161
H(37)	–2.6459	0.0066	2.2280	H(84)	–2.7309	0.1703	2.1053
H(38)	–2.6644	1.7253	2.5716	H(85)	–2.6957	1.8973	2.4019
H(39)	0.3784	0.3169	3.4236	H(86)	0.2167	0.3558	3.4272
H(40)	1.3680	1.5992	2.7685	H(87)	1.3140	1.5590	2.8027
H(41)	–0.1434	1.9839	3.5683	H(88)	–0.2077	2.0538	3.5177
H(42)	2.3710	–1.8918	1.6138	H(89)	2.3737	–1.8916	1.6119
H(43)	3.7400	–0.8098	1.4487	H(90)	3.7417	–0.8086	1.4468

H(44)	2.3710	–0.3838	2.4568	H(91)	2.3737	–0.3817	2.4558
H(45)	1.3987	1.6662	–2.6594	H(92)	1.4245	1.4439	–2.7744
H(46)	–0.0725	2.1660	–3.4706	H(93)	–0.0380	1.9412	–3.6024
H(47)	0.3672	2.8322	–1.9102	H(94)	0.4391	2.6911	–2.0919
	3c				**3d**		
	x	*y*	*z*		*x*	*y*	*z*
C(95)	0.0000	0.0000	0.0000	C(142)	0.0000	0.0000	0.0000
Si(96)	–1.5524	1.0877	0.0000	Si(143)	–1.5526	1.0874	0.0000
Si(97)	0.0000	–1.0877	1.5524	Si(144)	0.0000	–1.0874	1.5526
Si(98)	1.5974	1.1192	0.0000	Si(145)	1.5976	1.1189	0.0000
Si(99)	0.0000	–1.1192	–1.5974	Si(146)	0.0000	–1.1189	–1.5976
C(100)	–1.6886	–1.8957	–1.9223	C(147)	–1.7245	–1.7517	–2.0281
C(101)	1.2167	–2.5547	–1.4606	C(148)	1.0784	–2.6539	–1.3962
C(102)	–0.4825	–0.2200	3.1422	C(149)	1.6216	–1.9434	1.9409
C(103)	–1.0632	–2.6282	1.4550	C(150)	–0.5710	–0.2481	3.1283
C(104)	1.4606	2.5547	–1.2167	C(151)	1.3962	2.6539	–1.0784
C(105)	3.1409	0.1565	–0.5006	C(152)	3.1081	0.2097	–0.6720
C(106)	–3.1422	0.2200	0.4825	C(153)	–1.9409	1.9434	–1.6216
C(107)	–1.4550	2.6282	1.0632	C(154)	–3.1283	0.2481	0.5710
Br(108)	–2.0241	1.9143	–2.0574	Br(155)	–1.3387	2.8232	1.4579
Br(109)	2.0574	–1.9143	2.0241	Br(156)	–1.4579	–2.8232	1.3387
C(110)	1.9223	1.8957	1.6886	C(157)	2.0281	1.7517	1.7245
C(111)	0.5006	–0.1565	–3.1409	C(158)	0.6720	–0.2097	–3.1081
H(112)	–2.4752	–1.1689	–2.0787	H(159)	–2.4363	–0.9615	–2.2295
H(113)	–1.6027	–2.4960	–2.8189	H(160)	–1.6342	–2.3587	–2.9197
H(114)	–2.0305	–2.5370	–1.1202	H(161)	–2.1677	–2.3598	–1.2501
H(115)	1.1548	–3.1215	–2.3807	H(162)	1.0219	–3.2137	–2.3209
H(116)	2.2437	–2.2393	–1.3288	H(163)	2.1190	–2.4278	–1.2025
H(117)	1.0029	–3.2251	–0.6381	H(164)	0.7600	–3.3022	–0.5901
H(118)	–1.4897	0.1743	3.1023	H(165)	2.4188	–1.2341	2.1220
H(119)	–0.4398	–0.9526	3.9378	H(166)	1.4747	–2.5226	2.8434
H(120)	0.1752	0.5988	3.4040	H(167)	1.9527	–2.6154	1.1597
H(121)	–0.9692	–3.1478	2.3998	H(168)	–0.5193	–0.9808	3.9232
H(122)	–2.1089	–2.3933	1.3034	H(169)	0.0668	0.5845	3.3956
H(123)	–0.7670	–3.3082	0.6667	H(170)	–1.5870	0.1215	3.0765
H(124)	2.3807	3.1215	–1.1548	H(171)	2.3209	3.2137	–1.0219
H(125)	1.3288	2.2393	–2.2437	H(172)	1.2025	2.4278	–2.1190
H(126)	0.6381	3.2251	–1.0029	H(173)	0.5901	3.3022	–0.7600
H(127)	3.0832	–0.2647	–1.4960	H(174)	2.9906	–0.1252	–1.6945
H(128)	3.9755	0.8451	–0.4752	H(175)	3.9430	0.8975	–0.6368
H(129)	3.3674	–0.6703	0.1602	H(176)	3.3722	–0.6701	–0.0995
H(130)	–3.4040	–0.5988	–0.1752	H(177)	–1.1597	2.6154	–1.9527
H(131)	–3.1023	–0.1743	1.4897	H(178)	–2.1220	1.2341	–2.4188
H(132)	–3.9378	0.9526	0.4398	H(179)	–2.8434	2.5226	–1.4747
H(133)	–1.3034	2.3933	2.1089	H(180)	–3.3956	–0.5845	–0.0668
H(134)	–0.6667	3.3082	0.7670	H(181)	–3.0765	–0.1215	1.5870

H(135)	–2.3998	3.1478	0.9692	H(182)	–3.9232	0.9808	0.5193
H(136)	2.0787	1.1689	2.4752	H(183)	2.2295	0.9615	2.4363
H(137)	2.8189	2.4960	1.6027	H(184)	2.9197	2.3587	1.6342
H(138)	1.1202	2.5370	2.0305	H(185)	1.2501	2.3598	2.1677
H(139)	1.4960	0.2647	–3.0832	H(186)	1.6945	0.1252	–2.9906
H(140)	0.4752	–0.8451	–3.9755	H(187)	0.6368	–0.8975	–3.9430
H(141)	–0.1602	0.6703	–3.3674	H(188)	0.0995	0.6701	–3.3722

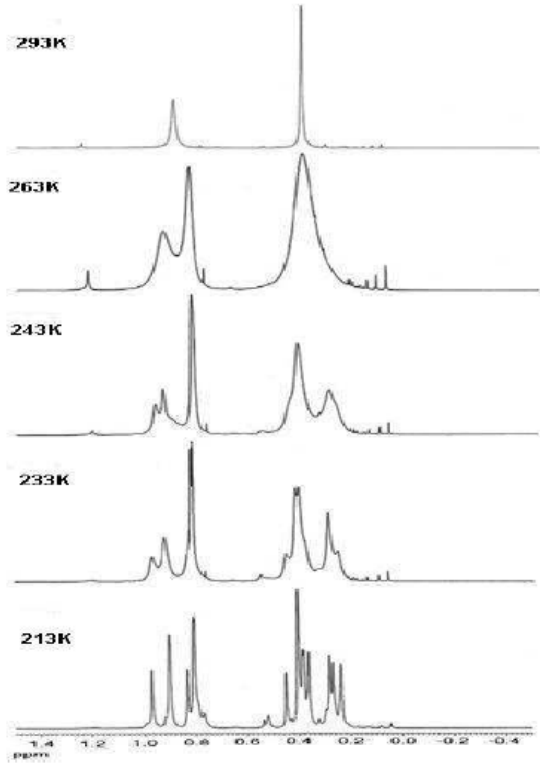
Figure S1 Molecular scattering curves and difference curves between theoretical and experimental data for (a) **1**, (b) **2**, and (c) **3**.



NMR Studies

$(BrMe_2Si)_2C(SiMe_3)_2$. Variable temperature ^1H NMR spectra for $(BrMe_2Si)_2C(SiMe_3)_2$ were recorded in the range of 293 to 213 K and are shown in Figure S2. The spectrum at 293 K shows broad resonances for $SiMe_2Br$ and $SiMe_3$ at 0.90 and 0.41 ppm, respectively. On lowering the temperature, both signals broaden further and begin to split between 273 and 263 K. At 213 K, both the $SiMe_2Br$ and $SiMe_3$ regions of the spectrum have split out into a multitude of larger and smaller signals.

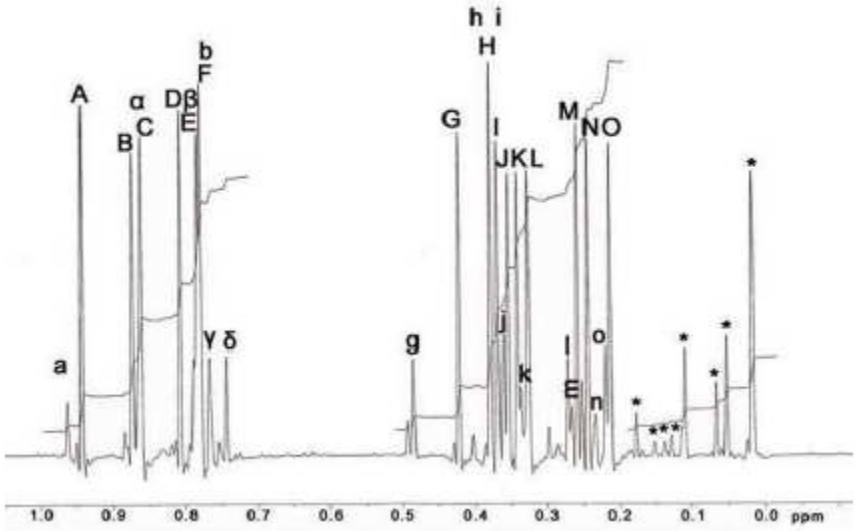
Figure S2 400 MHz ^1H NMR spectra of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ in the range 293 to 213 K.



A better resolved 500 MHz ^1H NMR spectrum (with a line-narrowing function applied) of $(BrMe_2Si)_2C(SiMe_3)_2$ at 201 K is shown in Figure S3. The labels on Figure S3 were assigned using 2D $^1H/^{29}Si$ NMR shift correlation spectroscopy and ^1H NMR saturation transfer experiments described below. Six large signals labelled A to F are seen in the $SiMe_2Br$ region of the spectrum extending from 0.97 to 0.75 ppm. There are also six small signals in this region, which fall into two separate sets labelled α to δ, and a and b.

Integration of these signals suggests that the large signals are due to a major C_1-symmetric conformer and a major C_2-symmetric conformer present in proportions of approximately 54% and 27%, respectively. The small signals are due to minor conformers of C_1 (*ca.* 15 %) and C_2 symmetry (*ca.* 4%). These have been assigned on the basis that a C_1-symmetric conformer should give rise to four different ^{1}H NMR signals in the $SiMe_2Br$ region due to the presence of four different methyl groups, while a C_2 conformer should give rise to two ^{1}H NMR signals in this region of the spectrum. Other less abundant conformers, which have not been investigated, may also present in solution at this temperature as there are other small, unlabelled peaks present as well as several signals known to be due to impurities.

Figure S3 Expansion of the 500 MHz ^{1}H NMR spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 201 K. A star denotes impurities not observed in Figure S2 as a different sample was used for Figure S3.



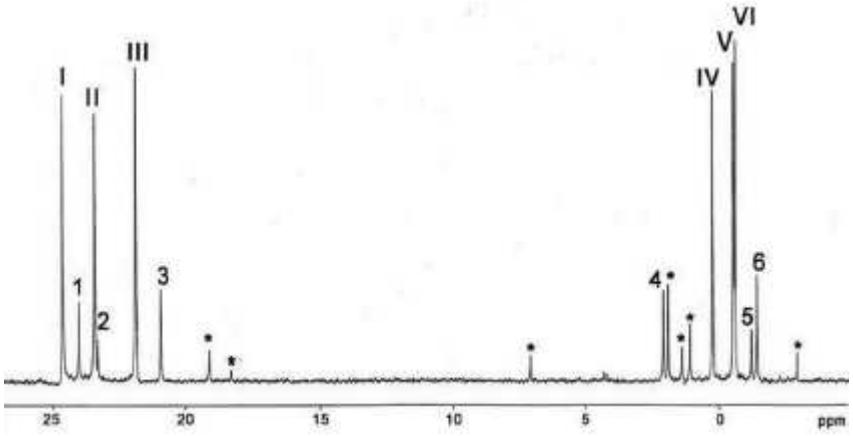
The $SiMe_3$ region of the spectrum in Figure S3 extends from 0.49 to 0.21 ppm and shows nine large signals labelled G to O, as well as nine small signals labelled g to o, some of which coincide with the larger resonances. A C_1 and a C_2 conformer of $(BrMe_2Si)_2C(SiMe_3)_2$ are expected to give rise to six and three different proton signals in this region, respectively. The presence of nine large and nine small proton signals in the ^{1}H NMR spectrum again supports the assumption that are two C_1 and two C_2 conformers present. There are several ^{1}H NMR signals in the region of 0.18 to 0.02 ppm marked with

asterisks that could not be assigned; these are assumed to be due to impurities not present in Figure S2 for which a different samples was used.

A 119 MHz $^{29}Si\{^1H\}$ inverse-gated NMR spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ recorded at 300 K showed a broad signal at –0.35 ppm, corresponding to the $SiMe_3$ groups and a broad signal due to the $SiMe_2Br$ region, which had begun to split out into several signals, extending from 24.38 to 22.11 ppm.

An INEPT NMR spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ was recorded at 201 K and shows that both the $SiMe_2Br$ and $SiMe_3$ signals have split out into several distinct resonances. The labels given to resonances in Figure S4 were obtained with the help of 2D $^1H/^{29}Si$ NMR shift correlation spectroscopy and are described below.

Figure S4 99 MHz $^{29}Si\{^1H\}$ INEPT NMR spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 201 K. A star denotes a signal that could not be assigned.

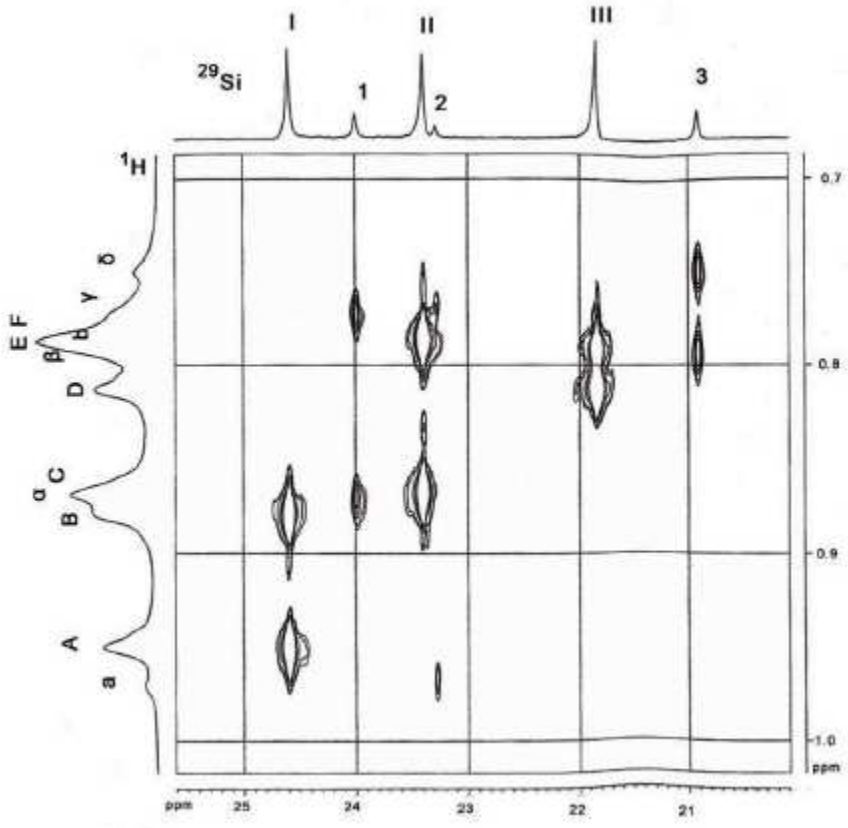


In the $SiMe_2Br$ region, three large signals are seen at 24.60 (I), 23.40 (II), and 21.85 ppm (III), as well as three small signals at 24.00 (1), 23.29 (2), and 20.92 ppm (3). A C_1 conformer of $(BrMe_2Si)_2C(SiMe_3)_2$ is expected to give rise to two ^{29}Si NMR signals in the $SiMe_2Br$ region, whereas a C_2 conformer should give rise to only one ^{29}Si NMR resonance. These results are therefore consistent with those from ^1H NMR spectrum at 201 K. The $SiMe_3$ region of the $^{29}Si\{^1H\}$ NMR spectrum at 201 K shows three large signals at 0.23 (IV), –0.53 (V) and –0.61 ppm (VI), as well as three smaller signals at 2.08 (4), –1.20 (5) and –1.42 ppm (6). In this region of the spectrum, two signals would be expected to be seen for a C_1 conformer and one for a C_2-symmetric conformer, meaning that the $SiMe_3$ region

is also in agreement with the findings from the ^{1}H NMR experiments. Several small, unidentified ^{29}Si NMR signals are observed and labelled with asterisks. These are likely to be due to impurities present as they do not correlate with ^{1}H NMR signals in the same way as the other ^{29}Si NMR signals.

A 2D $^{1}H/^{29}Si$ NMR shift correlation spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ was recorded at 201 K in order to assign ^{1}H NMR signals to ^{29}Si NMR signals. Each ^{29}Si NMR signal in the $SiMe_2Br$ region of the spectrum shown in Figure S5 is expected to be associated with two different proton signals. This spectrum shows that proton signals at 0.94 and 0.87 ppm labelled A and B, correlate with the ^{29}Si NMR resonance at 24.60 ppm labelled I. The ^{29}Si NMR signal at 23.40 ppm (II) is associated with proton signals C and F at 0.86 and 0.779 ppm. The third, large silicon signal III at 21.85 ppm is linked to proton signals at 0.81 ppm (D) and 0.784 ppm (E). Proton signals α and γ concealed under a large peak at 0.86 ppm and at 0.767 ppm, correlate with the small silicon signal 1 at 24.00 ppm. Silicon signal 2 at 23.29 ppm is linked with the ^{1}H NMR signals a and b at 0.96 ppm and hidden under a large peak at 0.779 ppm. Proton signals β and δ at 0.788 and 0.74 ppm, are associated with the ^{29}Si NMR signal at 20.92 ppm labelled 3.

Figure S5 2D $^{1}H/^{29}Si$ NMR shift correlation spectrum of the $SiMe_2Br$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 201 K. This is Figure 4 in the manuscript.



As proton signals a and b are assumed to be due to a minor C_2 conformer of $(BrMe_2Si)_2C(SiMe_3)_2$, silicon signal 2 must also be associated with this conformer. Likewise, proton signals α, β, γ and δ assigned to minor conformer C_1 are linked to silicon signals 1 and 3, which must therefore be due to the same conformer.

For the $SiMe_3$ region of the ^{29}Si NMR spectrum (see Figure S6) each signal is expected to be associated with three ^{1}H NMR signals. Interpretation of the shift correlation spectrum in a manner similar to that used for the $SiMe_2Br$ region yields the assignments summarised in Table S17. Several small signals labelled by asterisks do not seem to correlate in a similar way to the ^{1}H NMR signals and are assumed to be due to impurities.

Figure S6 2D $^{1}H/^{29}Si$ NMR shift correlation spectrum of the $SiMe_3$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 201 K. A star denotes a peak assigned to an impurity. This is Figure 5 in the manuscript.

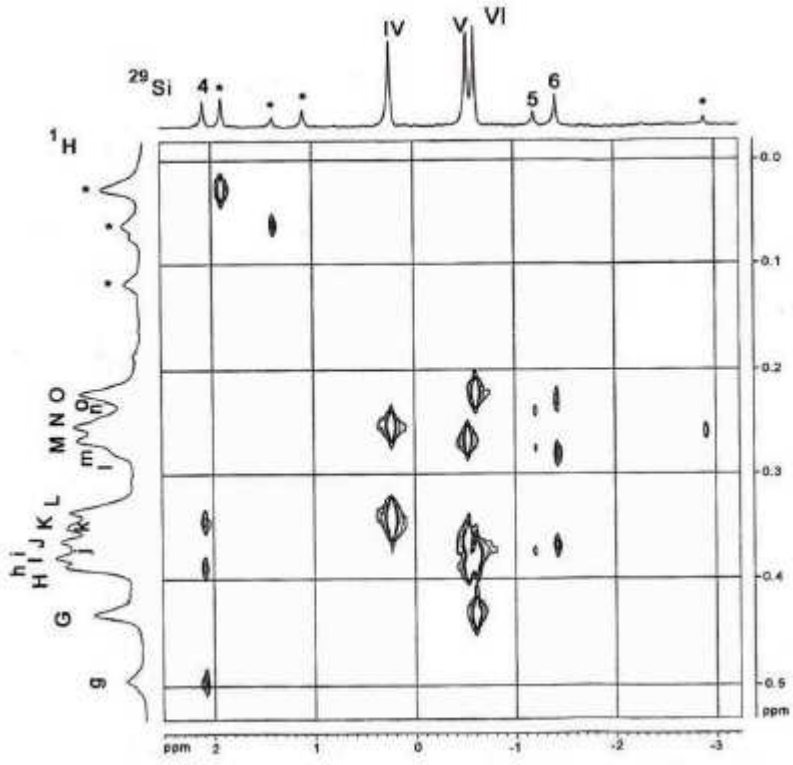


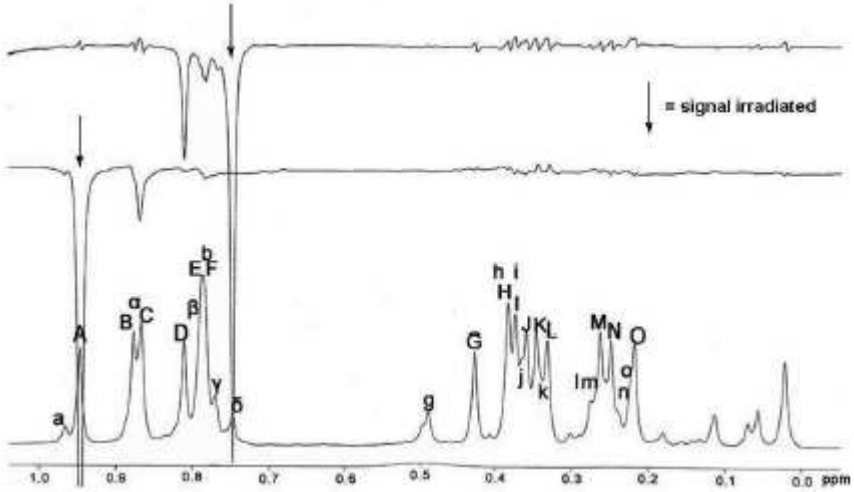
Table S17 Summary of the 2D $^{1}H/^{29}Si$ NMR shift correlation assignments in $(BrMe_2Si)_2C(SiMe_3)_2$.

Major Conformers (C_1 and C_2)		Minor Conformers (C_1 and C_2)	
^{29}Si	^{1}H	^{29}Si	^{1}H
I	A and B	1	α and γ
II	C and F	2	a and b
III	D and E	3	β and δ
IV	K, L and N	4	g, h and k
V	H, J and M	5	i, m and n
VI	G, I and O	6	j, l and o

Several ^{1}H NMR saturation transfer experiments on $(BrMe_2Si)_2C(SiMe_3)_2$ were recorded at 201 K to probe the exchange processes between different conformers at low temperature. Both large and small proton signals in the $SiMe_2Br$ region of the proton spectrum were irradiated but the assignment of the enhanced signals is ambiguous in some cases. Figure S7 shows two saturation transfer experiments in which signals δ (upper spectrum) and A

(middle spectrum) were irradiated. Irradiation of signal δ, which has been assigned to a minor conformer of C_1 symmetry, led to an increase in signal D assigned to a major conformer. There may also be an increase in a signal due to a minor conformer concealed by a large peak of either proton E or F. This enhanced signal could either be signal be due to a minor C_2 conformer or signal β due to a minor C_1 conformer. Irradiation of signal A of a major conformer gave rise to an increased signal of α belonging to a minor C_1 conformer.

Figure S7 ^{1}H NMR saturation transfer experiments of the $SiMe_2Br$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 201 K. Irradiation of δ (top) and A (centre).



Further saturation transfer experiments led to the following observations. Irradiation of signal a, which has been assigned to a minor conformer of C_2 symmetry, resulted in the increase of signal C assigned to a major conformer. There also appears to be a slight enhancement of signal A, although this assignment is tentative. Irradiation of signal D due to a major conformer led to an increase of signal δ belonging to a minor C_1 conformer. A small signal hidden under large signals E or F also appears to be increased. This enhanced signal may be β belonging to a minor C_1 conformer but could also be due to b arising from a small C_2 conformer. When signal γ, due to a minor C_1 conformer, was irradiated, signal F belonging to a major conformer appeared to be enhanced. However, it cannot be discounted that the enhanced signal seen is due to proton b of a minor C_2 conformer. There also appears to be a small enhancement of a signal that is either due to proton α of a minor C_2 conformer or proton B due to a major conformer. Irradiation of signal B due to a major

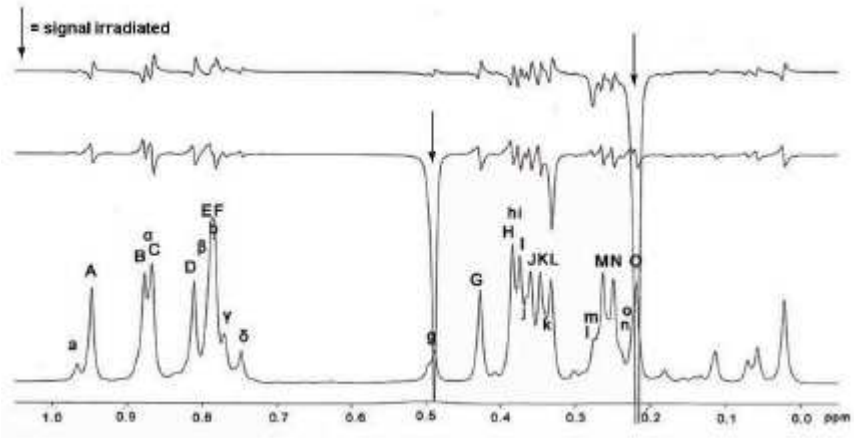
conformer possibly led to a very slight increase of signals b or γ, but this was inconclusive. Table S18 summarises the results of these saturation transfer spectra. It can be seen that major and minor conformers of $(BrMe_2Si)_2C(SiMe_3)_2$ undergo energy exchange processes with each other at 201 K. There is also a possibility of energy exchange processes between the minor conformers but the experiments do not provide clear evidence for this.

Table S18 Summary of the results of the ^{1}H NMR saturation transfer experiments on $(BrMe_2Si)_2C(SiMe_3)_2$ for the $SiMe_2Br$ region of at 201 K.

^{1}H NMR signal irradiated	^{1}H NMR signal increased
A	α
B	possibly b or γ
D	δ and possibly b or β
A	C and possibly A
γ	F (or b) and possibly B or α
δ	D and possibly b or β

Three ^{1}H NMR saturation transfer experiments at 201 K were recorded, in which signals in the $SiMe_3$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ were irradiated. Figure S8 shows the irradiations of signals O (spectrum at the top) and g (spectrum at the centre).

Figure S8 ^{1}H NMR saturation transfer experiments of the $SiMe_3$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 201 K. Irradiation of O (top) and g (centre).



Irradiation of signal g due to a minor conformer led to an increase in signal L due to a major conformer and when signal O, due to a major conformer, was irradiated, small signal m due to a minor conformer appeared to increase. Irradiation of signal G belonging to a

major conformer resulted in the increase of signal j due to a minor conformer. In all three experiments it was found that major conformers undergo energy exchange processes with minor conformers in solution at 201 K. The results of the ^{1}H NMR saturation transfer experiments of the $SiMe_3$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ are summarised in Table S19.

Table S19 Results of the ^{1}H NMR saturation transfer experiments of the $SiMe_3$ region of $(BrMe_2Si)_2C(SiMe_3)_2$ at 201 K.

^{1}H NMR signal irradiated	^{1}H NMR signal increased
G	j
O	m
g	L

The ^{1}H NMR saturation transfer spectra of $(BrMe_2Si)_2C(SiMe_3)_2$ at 201 K led to the conclusion that energy transfer processes occur between major and minor conformers, but not between the major conformers. As individual ^{1}H NMR signals could not be assigned to either C_1 or C_2 conformers, it is not known which conformers participate in these transfer processes. Furthermore, there is a possibility that minor conformers undergo exchange processes with one another.

A series of 126 MHz $^{13}C\{^1H\}$ NMR spectra of $(BrMe_2Si)_2C(SiMe_3)_2$ was recorded from 293 to 213 K, as shown in Figure S9. At 293 K two signals are seen at 9.89 and 4.97 ppm corresponding to the $SiMe_2Br$ and $SiMe_3$ groups, respectively. A very small signal at 6.86 ppm due to a quaternary carbon is also present but cannot be seen in the spectrum shown in Figure S9. On lowering the temperature, these three signals broaden and begin to split out between 263 and 243 K. An expansion of the spectrum recorded at 213 K is shown in Figure S10.

Figure S9 126 MHz $^{13}C\{^{1}H\}$ NMR spectra of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ in the range 293 to 213 K.

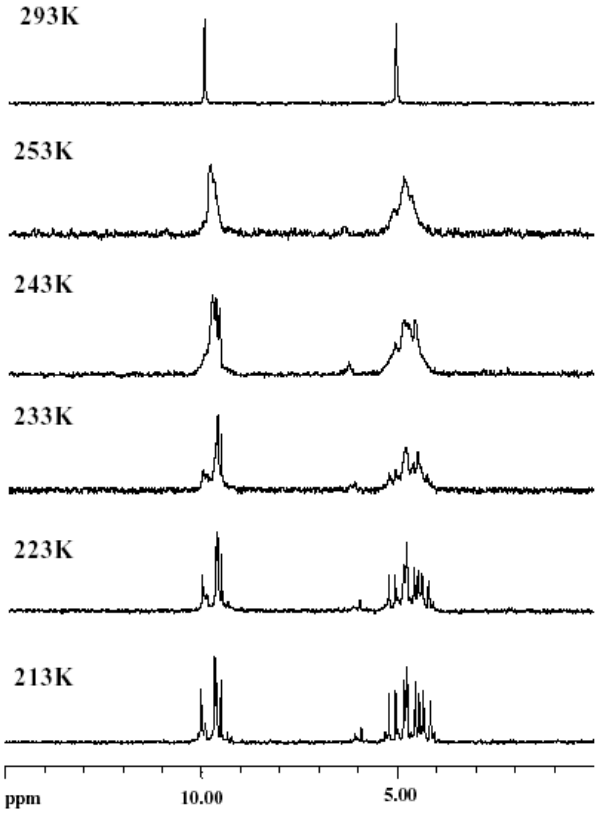
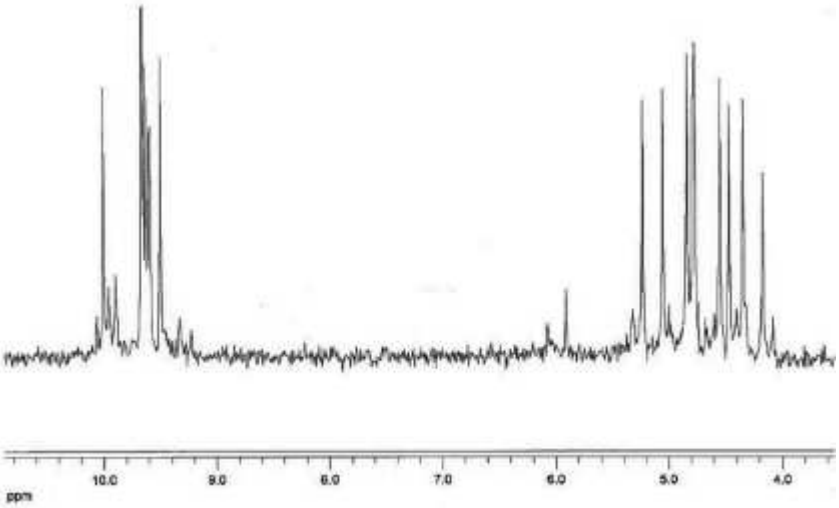


Figure S10 Expansion of the $^{13}C\{^{1}H\}$ NMR spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ at 213 K.



The $SiMe_2Br$ region in Figure S10 shows five large signals at 10.00, 9.67, 9.63, 9.61 and 9.45 ppm and five small signals at 10.05, 9.95, 9.87, 9.35 and 9.23 ppm. Eight large signals at 5.25, 5.09, 4.84, 4.75, 4.55, 4.48, 4.34 and 4.19 ppm and six small signals at 5.30, 4.99, 4.70, 4.60, 4.39 and 4.09 ppm are observed in the $SiMe_3$ region of the spectrum. Another two small signals are seen at 6.07 and 5.93 ppm, in the region known to be due to quaternary carbon atoms in such compounds. From the ^1H and $^{29}Si\{^1H\}$ NMR spectra of $(BrMe_2Si)_2C(SiMe_3)_2$ recorded at 201 K and the $^1H/^{29}Si$ shift correlation spectrum discussed above, it was concluded that a major C_1 and a major C_2 conformer as well as a minor C_1 and a minor C_2 symmetry conformer exist in solution at 201 K. The $^{13}C\{^1H\}$ NMR spectrum at a similar temperature would thus be expected to show six large and six small signals in the $SiMe_2Br$ region corresponding to a major C_1 and C_2 conformer and a minor C_1 and C_2 conformer, respectively. Nine large and nine small signals due to the same conformers should be seen in the $SiMe_3$ region of the spectrum. Thus, in both cases, a slightly smaller number of signals is actually observed. However, it is likely that in such a complicated spectrum signal overlap occurs in both the $SiMe_2Br$ and $SiMe_3$ regions and that the spectrum is broadly consistent with the ^1H spectra.

The 50 MHz $^{13}C\{^1H\}$ and 40 MHz $^{29}Si\{^1H\}$ MAS solid-state NMR spectra of $(BrMe_2Si)_2C(SiMe_3)_2$ were recorded at 293 K. The ^{13}C spectrum displayed two large, broad NMR signals at 11.79 and 7.10 ppm due to carbon atoms of the $SiMe_2Br$ and $SiMe_3$ groups of the molecule, respectively. Both signals have slight shoulders indicating more than one environment being present for each carbon. This may be due to different conformers being present in the solid at this temperature give rise to the splitting or due to crystal packing effects (an asymmetric unit cell) or different polymorphs of $(BrMe_2Si)_2C(SiMe_3)_2$ leading to inequivalent ^{13}C NMR signals. There are also three small, broad peaks observed at 33.40, 31.10 and 25.70 ppm, which may be due to quaternary carbon atom environments. The solid-state $^{29}Si\{^1H\}$ NMR spectrum of $(BrMe_2Si)_2C(SiMe_3)_2$ showed three broad resonances at 22.60, 20.90 and 0.15 ppm. The peaks at 22.60 and 20.90 ppm are due to the $SiMe_2Br$ environments and the signal at 0.15 ppm is due to the $SiMe_3$ region. The splitting of the $SiMe_2Br$ region may again attributed to crystal packing effects in the solid or different polymorphs, although the presence of different conformers cannot be discounted.

$(ClMe_2Si)_2C(SiMe_3)_2$. The steric crowding in $(ClMe_2Si)_2C(SiMe_3)_2$ is between that of $(HMe_2Si)_2C(SiMe_3)_2$ and $(BrMe_2Si)_2C(SiMe_3)_2$, but, at readily accessible temperatures, its NMR spectra are much more similar to those of the bromide. Variable-temperature ^1H NMR spectra are shown in Figure S11. The spectrum at 203 K has a complicated splitting pattern reminiscent of the better-resolved spectrum for $(BrMe_2Si)_2C(SiMe_3)_2$ described above and again suggests that more than one conformation is present at this temperature.

Figure S11 500 MHz ^1H NMR spectra of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ in the range 298 to 203 K.

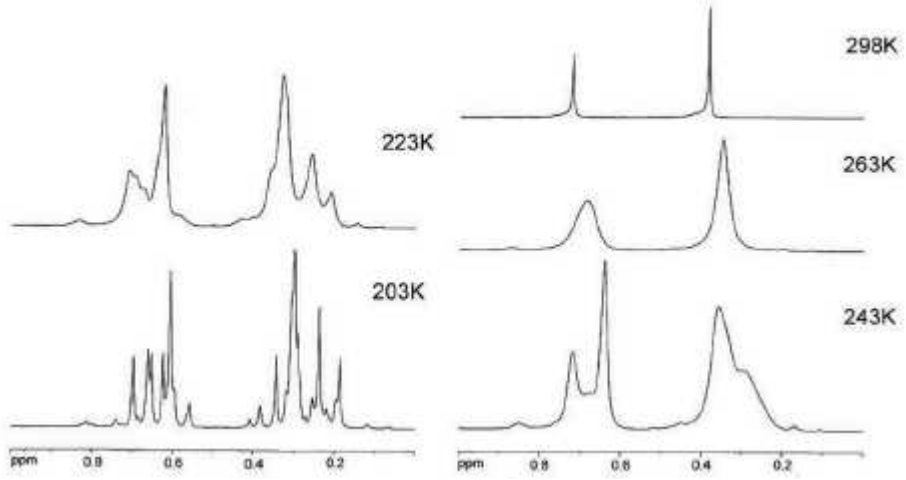
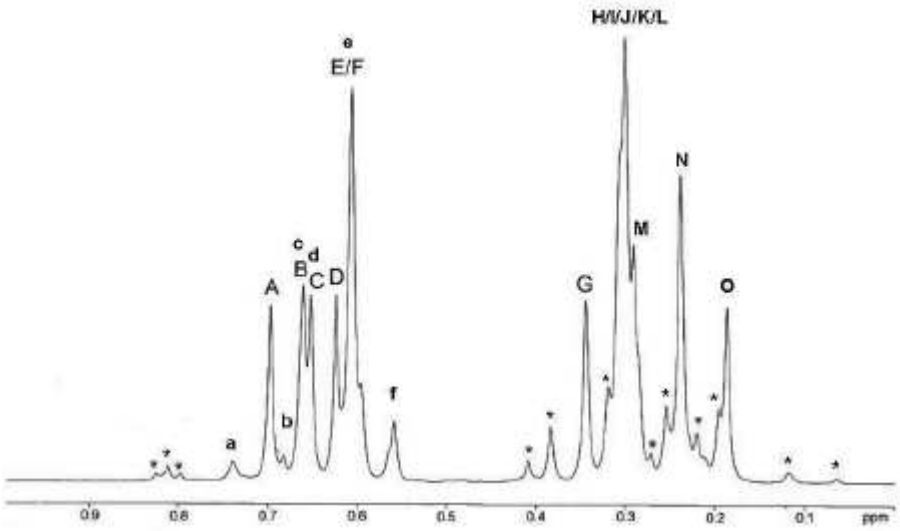


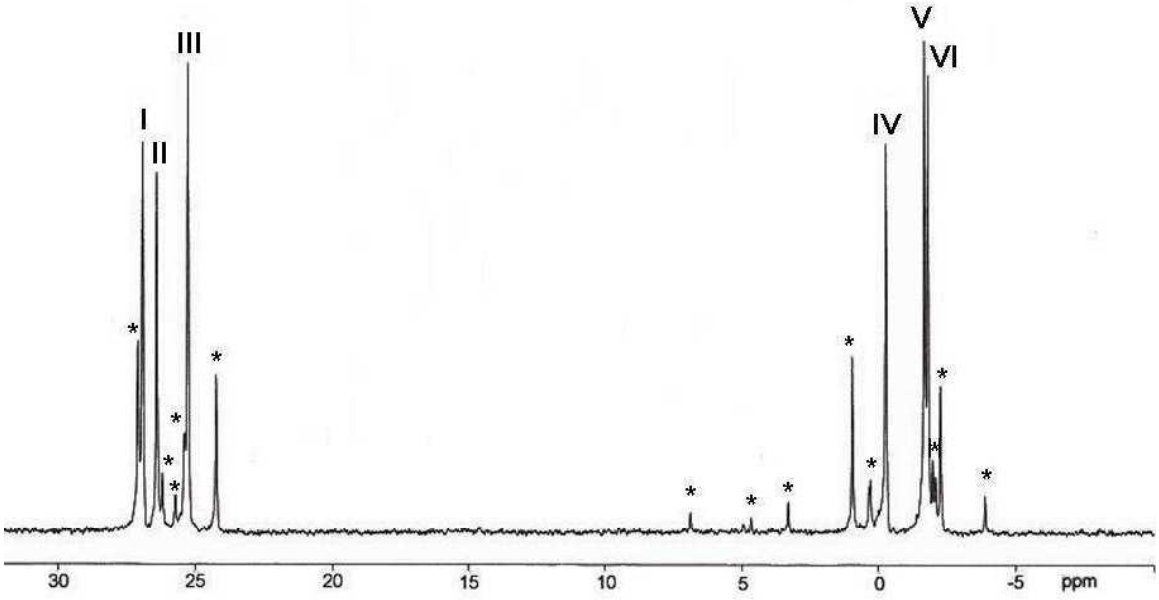
Figure S12 shows an expansion of the spectrum at 203 K, which as well as showing signals for various conformers described in more detail above for the analogous bromide, also shows several small unassigned signals which may be due to as yet unidentified conformers, or to impurities.

Figure S12 500 MHz ^{1}H NMR spectrum of $(Me_3Si)_2C(SiMe_2Cl)_2$ in $CDCl_3/CD_2Cl_2$ at 203 K. A star denotes unidentified signals.



The $^{29}Si\{^1H\}$ inverse-gated NMR spectrum of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ at 300 K shows two broad resonances at 25.66 and –1.09 ppm, corresponding to the $SiMe_2Cl$ and $SiMe_3$ groups, respectively. On lowering the temperature, these signals split into several new peaks as shown in Figure S13, with an overall chemical shift pattern similar to that seen for $(BrMe_2Si)_2C(SiMe_3)_2$ at 201 K (see Figure S4). The signal labeling shown on the spectrum was made with the help of the 2D $^1H/^{29}Si$ NMR shift correlation spectra described above for the analogous bromide. As in the proton spectrum, the ^{29}Si NMR spectrum showed several signals that could not be identified. In the $SiMe_2Cl$ region, three large signals at 26.91 (I), 26.41 (II) and 25.27 ppm (III) were identified as belonging to the most abundant conformers. As both the ^1H and $^{29}Si\{^1H\}$ NMR spectra of $(ClMe_2Si)_2C(SiMe_3)_2$ resemble those of $(ClMe_2Si)_2C(SiMe_3)_2$, discussed above, it is likely that similar major C_1 and C_2 and a minor C_1 and C_2 conformers are present for $(ClMe_2Si)_2C(SiMe_3)_2$ solution at 203 K. A C_1 conformer in the $SiMe_2Cl$ region would give rise to two ^{29}Si NMR signals, one resonance being observed for a C_2 conformer. The three signals labeled I to III in Figure S13 are thus consistent with the presence of major C_1 and C_2 conformers of $(ClMe_2Si)_2C(SiMe_3)_2$ in solution. However, it was not possible to assign these three signals to individual conformers.

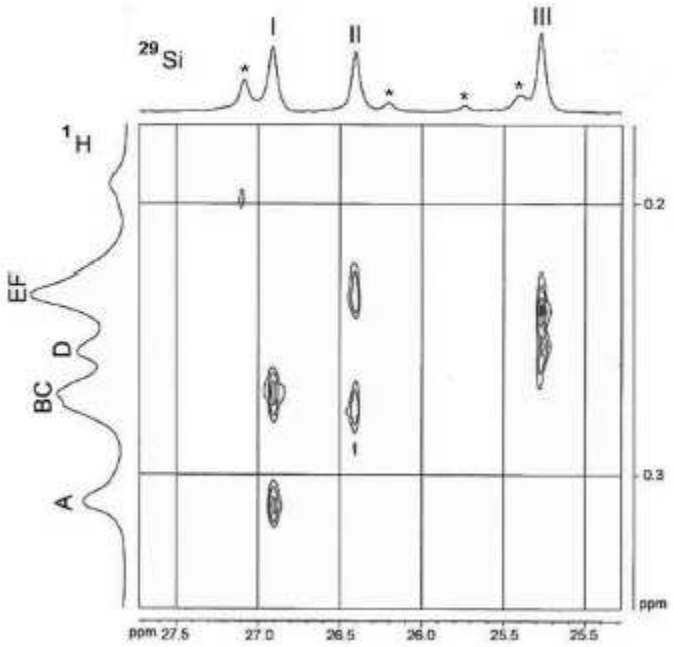
Figure S13 99 MHz 29Si{1H} INEPT NMR spectrum of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$/acetone-d_6 at 203 K. Stars denote unidentified signals.



In the $SiMe_3$ region, from approximately 0.95 to –3.88 ppm, the large signals at –0.29 (IV), –1.69 (V) and –1.82 ppm (VI) are assigned to the major conformers of $(ClMe_2Si)_2C(SiMe_3)_2$. In this region, a C_1 conformer is expected to give rise to two ^{29}Si signals and only one resonance for a C_2 conformer. None of the three signals labeled could be assigned individually to the major C_2 or C_1 conformer. There are several small ^{29}Si NMR signals in both the $SiMe_2Cl$ and $SiMe_3$ regions and some of these are assumed to be due to less abundant C_1 and C_2 conformers. Unfortunately, no assignments of signals due to minor conformers could be made using the 2D $^1H/^{29}Si$ shift correlation NMR spectra discussed below.

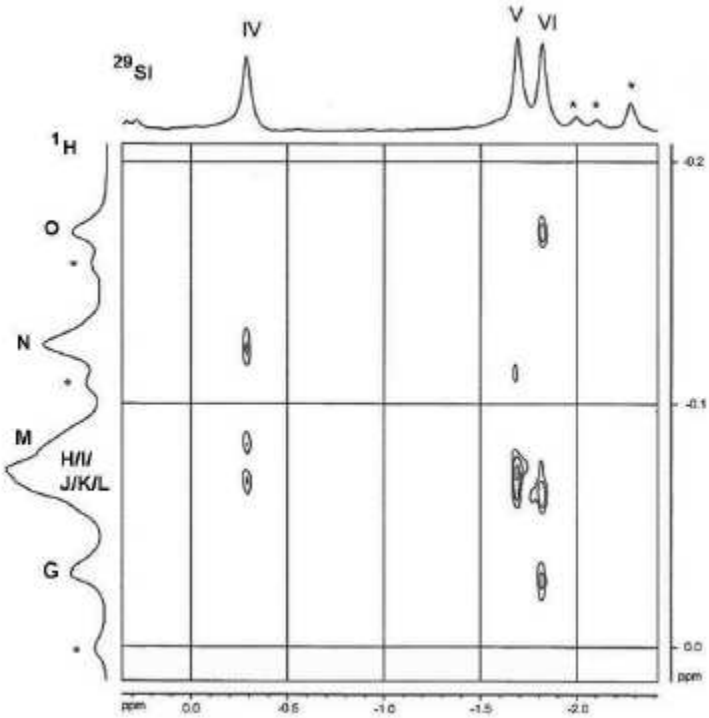
2D $^1H/^{29}Si$ NMR shift correlation spectra of $(ClMe_2Si)_2C(SiMe_3)_2$ in a $CDCl_3$/acetone-d_6 solvent mixture were recorded at 203 K. Figure S14 shows the $SiMe_2Cl$ region of the spectrum.

Figure S14 2D $^{1}H/^{29}Si$ NMR shift correlation spectrum of the $SiMe_2Cl$ region of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$/acetone-d_6 at 203 K. Stars denote unidentified signals.



Any silicon signal in this region should be associated with two different proton signals due to the two methyl groups in the $SiMe_2Cl$ groups. Only the three largest signals, at 26.91 (I), 26.41 (II) and 25.27 ppm (III), can be linked to ^{1}H NMR signals with the help of this shift correlation spectrum. Thus, signal I correlates to proton signals at 0.70 and 0.65 ppm, labeled A and C. Signals B at 0.66 ppm, and F hidden under the peak at 0.61 ppm, are due to protons associated with silicon II. Silicon III is linked to protons D and E at 0.62 and 0.61 ppm, respectively. These three silicon and six proton signals are consistent with the assumption that a major C_1 and a major C_2 conformer of $(ClMe_2Si)_2C(SiMe_3)_2$ are observed at this temperature in solution by analogy with the bromide described above. Several smaller signals are observed in the $SiMe_2Cl$ regions of both the ^{29}Si NMR and the ^{1}H NMR spectra at 203 K. However, the ^{1}H NMR spectrum is not well resolved and further small signals may be hidden by the larger resonances. Furthermore, the 2D $^{1}H/^{29}Si$ NMR shift correlation spectrum does not show any correlation between small ^{1}H and ^{29}Si NMR signals. Thus no assumptions can be made regarding less abundant conformers. Figure S15 shows the $SiMe_3$ region of the correlation spectrum for $(ClMe_2Si)_2C(SiMe_3)_2$.

Figure S15 2D $^{1}H/^{29}Si$ NMR shift correlation spectrum of the $SiMe_3$ region of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$/acetone-d_6 at 203 K. Stars denote unidentified signals.



Any ^{29}Si NMR signal in this region should be associated with three proton signals due to three different methyl substituents on $SiMe_3$ groups. The shift correlation spectrum in Figure S15 only permits the assignment of the largest silicon and proton signals. The ^{29}Si NMR signal seen at –0.29 ppm, labeled IV, is associated with proton signals N at 0.24 ppm, M at 0.29 ppm and one of the signals hidden under the broad peak at 0.30 ppm, tentatively labeled I. Silicon V at –1.69 ppm is linked to three proton signals covered by the broad peak at 0.30 ppm. These signals have been tentatively labeled J, K and L. The ^{29}Si NMR resonance at –1.82 ppm (VI) correlates with proton signal G at 0.34 ppm, a signal hidden under the broad peak at 0.30 ppm, tentatively labeled H and resonance O at 0.19 ppm. These three silicon and nine proton signals are consistent with the assumption that a major C_1 and a major C_2 conformer of $(ClMe_2Si)_2C(SiMe_3)_2$ are present at this temperature in solution, as seen for the analogous bromide. Several smaller signals are observed in the $SiMe_3$ regions of both the ^{29}Si NMR and ^{1}H NMR spectra but it has not been possible to assign them as the shift correlation spectrum yields no information regarding these resonances. Furthermore, other small signals may be hidden under broad signals in the

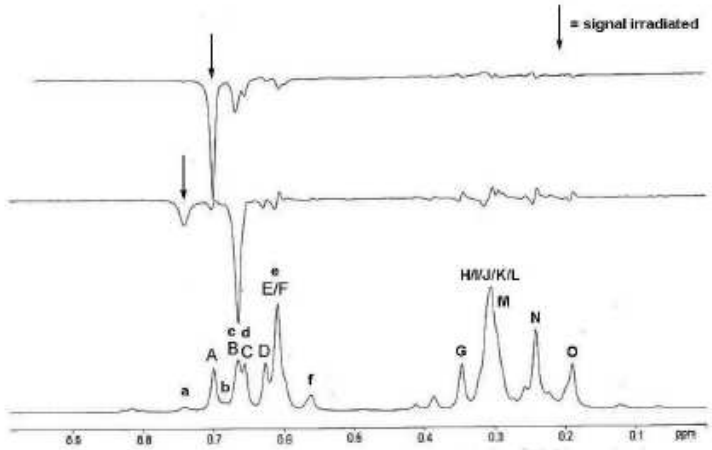
$SiMe_3$ region of the ^1H NMR spectrum. Thus no assumptions can be made regarding less abundant conformers of $(ClMe_2Si)_2C(SiMe_3)_2$. Table S20 summarizes the assignments from the shift correlation spectrum of $(ClMe_2Si)_2C(SiMe_3)_2$.

Table S20 Summary of 2D $^1H/^{29}Si$ NMR shift correlation assignments for $(ClMe_2Si)_2C(SiMe_3)_2$ at 203 K.

^{29}Si NMR Signal	^1H NMR Signals
I	A and C
II	B and F
III	D and E
IV	I, M and N
V	J, K and L
VI	G, H and O

Several ^1H NMR saturation transfer experiments at 203 K were carried out in a similar manner to those described above for $(BrMe_2Si)_2C(SiMe_3)_2$. When the proton signal labeled A at 0.70 ppm was irradiated, two small signals labeled c and d coinciding with large signals B and C at 0.66 and 0.65 ppm, respectively, appeared to increase (Figure S16). Figure S16 also shows a saturation transfer experiment in which a small signal at 0.74 ppm, labeled a, was irradiated resulting in an increase of large signal B at 0.66 ppm.

Figure S16 ^1H NMR saturation transfer experiments on the $SiMe_2Cl$ region of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 203 K. Irradiation of signal A (upper spectrum) and signal a (middle spectrum).



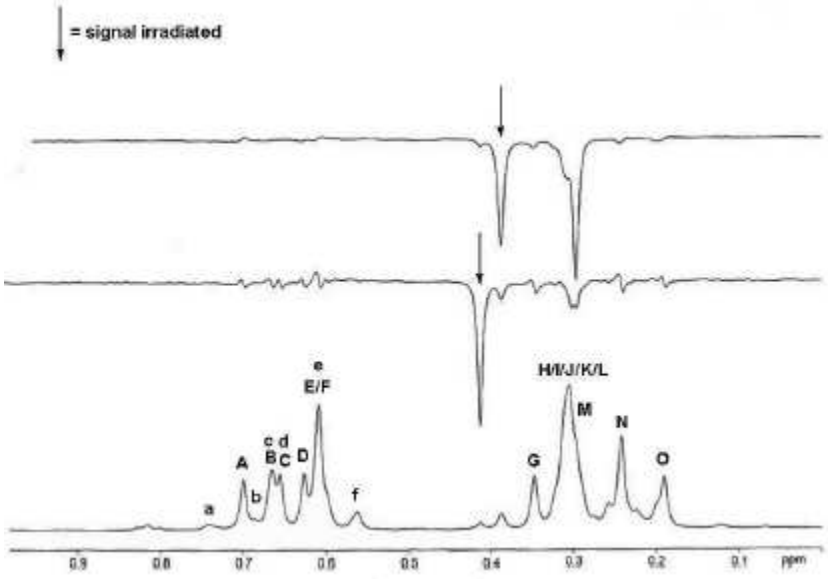
Irradiation of large signal D at 0.62 ppm gave rise to an increase in a small signal at 0.56 ppm, labeled f, and another small signal labeled e hidden under a broad peak at 0.61 ppm, while irradiation at small signal b led to increases in large signals A, B and possibly signal e. When small signal f at 0.56 ppm was irradiated the reverse process was seen with an increase in signals D at 0.62 ppm and e at 0.61 ppm. These saturation transfer experiments allow six ^{1}H NMR signals due to less abundant conformers of $(ClMe_2Si)_2C(SiMe_3)_2$ to be identified and labeled. These findings further support the assumption that $(ClMe_2Si)_2C(SiMe_3)_2$ in solution at 203 K behaves like its analogue $(BrMe_2Si)_2C(SiMe_3)_2$. The six small ^{1}H NMR signals are assumed to arise from a C_1 and a C_2 conformer but it has not been possible to assign the individual signals. These spectra also show that exchange processes occur between more and less abundant conformers as well as amongst the less abundant conformers. Table S21 summarizes the results of the saturation transfer experiments for the $SiMe_2Cl$ region.

Table S21 Results of the ^{1}H NMR saturation transfer experiments for $(ClMe_2Si)_2C(SiMe_3)_2$ at 203 K.

Irradiated Signal	Increased Signals
A	c and d
D	e and f
a	B
b	A, B and possibly e
f	D and e

Figure S17 shows ^{1}H NMR saturation transfer spectra at 203 K carried out by irradiation of signals in the $SiMe_3$ region of the spectrum. Irradiation of the small signal at 0.34 ppm (upper spectrum in Figure S17) resulted in the increase of a large signal hidden under the broad, large signal at 0.30 ppm and possibly in the increase of a smaller signal covered by the same signal at 0.30 ppm. When small signal 0.41 ppm was irradiated (Figure S17, centre spectrum), there appears to be an increase in two small signals covered by the large, broad peak at 0.30 ppm.

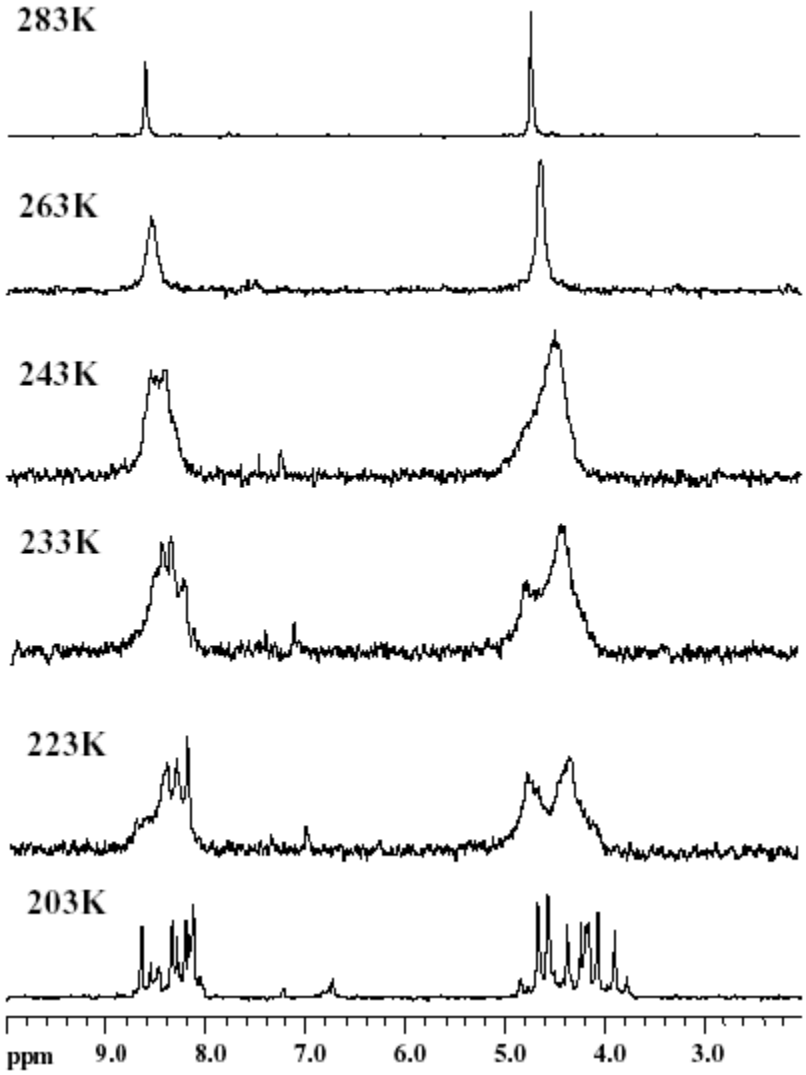
Figure S17 ^{1}H NMR saturation transfer experiments of the $SiMe_3$ region of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3/CD_2Cl_2$ at 203 K. Irradiation of the signal at 0.34 ppm (upper spectrum) and at 0.41 ppm (middle spectrum).



The results of these two saturation transfer experiments again appear to confirm that energy exchange processes at 203 K occur between small and large population conformers as well as between different low abundance conformers. It is not known what the symmetries of these conformers are. Comparison of all ^{1}H NMR saturation transfer experiments of $(ClMe_2Si)_2C(SiMe_3)_2$ with those of the analogous compound $(BrMe_2Si)_2C(SiMe_3)_2$ show that the energy exchange processes occur, as might be expected, in similar ways in both compounds in solution at low temperature, although exchange processes between minor conformers of $(ClMe_2Si)_2C(SiMe_3)_2$ cannot be confirmed.

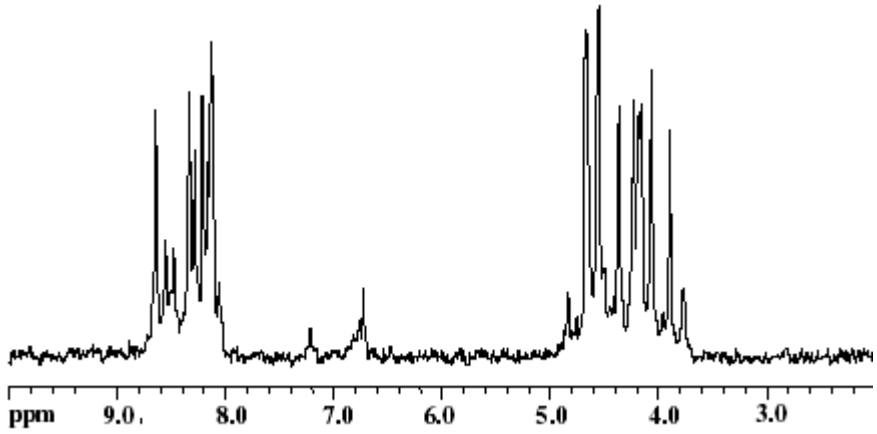
A series of 126 MHz ^{13}C $\{^{1}H\}$NMR spectra of $(ClMe_2Si)_2C(SiMe_3)_2$ was recorded from 293 to 203 K, see Figure S18.

Figure S18 126 MHz $^{13}C\{^{1}H\}$ NMR spectra of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ in the range 283 to 203 K.



At 293 K only two resonances were observed, at 8.65 and 4.77 ppm, due to $SiMe_2Cl$ and Me_3Si, respectively. At 273 K, both resonances broadened and another small resonance occurred at 7.65 ppm, which split into two small signals between 273 and 263 K. It is not known if quaternary carbons give rise to these small signals. Splitting of the two large resonances occurs between 253 and 243 K and continues on lowering the temperature further. An expansion of the spectrum at 203 K is shown in Figure S19.

Figure S19 Expansion of the 126 MHz $^{13}C\{^1H\}$ NMR spectrum of $(ClMe_2Si)_2C(SiMe_3)_2$ in $CDCl_3$ at 203 K.



In the $SiMe_2Cl$ region, six large signals are seen at 8.65, 8.34, 8.29, 8.21, 8.16 and 8.13 ppm as well as three small resonances at 8.56, 8.48 and 8.06 ppm. In the Me_3Si region, there are seven large signals at 4.67, 4.57, 4.24, 4.19, 4.17, 4.07 and 3.90 ppm and four smaller signals at 4.84, 4.37, 3.97 and 3.78 ppm. The $^1H/^{29}Si$ shift correlation spectrum and comparison with results of equivalent spectra for $(BrMe_2Si)_2C(SiMe_3)_2$ indicate that a major C_1 and C_2 and a minor C_1 and C_2 conformers of $(ClMe_2Si)_2C(SiMe_3)_2$ appear to be present in solution at 203 K. A $^{13}C\{^1H\}$ NMR spectrum of $(ClMe_2Si)_2C(SiMe_3)_2$ at 203 K should, therefore, display six large and six small carbon signals in the $SiMe_2Cl$ region and nine large and nine small carbon signals in the $SiMe_3$ region. As for the analogous bromide, several resonances appear to be missing from this ideal total, see Figure S19, but it is likely that overlap of signals occurs in this complicated spectrum and the spectrum is, therefore, broadly consistent with the expected conformers. The two small signals at 7.23 and *ca.* 6.73 ppm in Figure S19, the latter of which appears to be split into three peaks, are probably due to quaternary carbon atoms.

$(HMe_2Si)_2C(SiMe_3)_2$. The 500 MHz ^1H NMR and 99 MHz ^{29}Si NMR spectra of $(HMe_2Si)_2C(SiMe_3)_2$ in a $CDCl_3$ and CD_2Cl_2 solvent mixture recorded at 213 K showed no significant changes when compared to the corresponding spectra recorded at ambient temperature. The ^1H NMR spectrum at 213 K showed a singlet at 0.15 ppm ($SiMe_3$), a doublet ($Si\underline{Me}_2H$) at 0.24 ppm and a septet ($SiMe_2\underline{H}$) at 4.04 ppm. Two signals were seen

in the $^{29}Si\{^{1}H\}$ INEPT NMR spectrum of $(HMe_2Si)_2C(SiMe_3)_2$, one at –16.49 ppm due to the $SiMe_2H$ groups and one at –0.46 ppm due to the $SiMe_3$ groups. The proton coupled ^{29}Si NMR spectrum shows complicated multiplets. The signal at –16.49 ppm splits into two multiplets which selective decoupling ^{29}Si DEPT NMR experiments show are due to the expected large doublet $^{1}J_{Si–H}$ (182.3 Hz), a septet $^{2}J_{Si–H}$ (6.4 Hz, coupling to two Me groups) and smaller doublet $^{3}J_{Si–H}$ (3.2 Hz, coupling to Si–H on remote Si). The lack of dynamic processes being observed at this temperature is presumably due to the relatively small size of the H compared to the halides.

Reference 41 in full:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al:Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision C.01; Gaussian, Inc.; Wallingford, CT, 2004.