Compound 25 (*N*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P) -1847.2283293730
SCF Energy (au) PBE0/def2-TZVPP -1846.898143046
Zero Point Energy (au) 0.4351654
Chemical potential (kJ mol^{-1}) 971.40

xyz Coordinates

58

Pd	0.52993	-0.10754	0.92719
P	-0.09053	0.05014	-1.29079
N	2.49327	-0.60684	0.31602
N	1.05499	0.07160	2.97304
C	-1.34358	-0.04088	1.75726
O	2.61292	-1.70511	-0.25466
C	1.29921	0.21644	-2.50663
C	-1.32697	-0.00687	3.19027
C	-1.11511	1.52726	-1.74088
C	-2.52643	-0.09944	3.93477
H	-2.50187	-0.08333	5.03712
C	1.42507	-0.61383	-3.63920
H	0.71086	-1.43531	-3.80726
C	-3.75948	-0.23247	3.28471
H	-4.68961	-0.30889	3.87136
C	-1.01221	-1.44888	-1.85154
C	-1.55135	2.42510	-0.74425
H	-1.31113	2.21919	0.31138
C	-0.41675	-2.69673	-1.54935
H	0.55330	-2.71977	-1.02075
C	2.23227	1.25716	-2.30104
H	2.15568	1.90031	-1.40941
C	0.21864	0.27663	5.21703
H	-0.63371	0.31374	5.91096
C	-2.89877	-2.61066	-2.87346
H	-3.87551	-2.57339	-3.38396
C	-2.25798	-1.41180	-2.51136
H	-2.73948	-0.44730	-2.73903
C	-0.01065	0.11225	3.83318
C	2.31444	0.22122	3.43099
H	3.10142	0.21915	2.65706
C	-1.40257	1.80972	-3.09708
H	-1.03385	1.14134	-3.89273
C	2.47242	-0.40500	-4.55420
H	2.56618	-1.06430	-5.43299
C	-2.29962	-3.84781	-2.58482
H	-2.80492	-4.78584	-2.86923
C	-1.05784	-3.88762	-1.92423
H	-0.58603	-4.85595	-1.68898
C	1.52550	0.40725	5.70048
H	1.70508	0.53575	6.78081
C	-2.60147	-0.18625	1.13698
H	-2.67676	-0.23565	0.03863
C	2.59752	0.38611	4.79300
H	3.64114	0.49853	5.12416
C	-3.79324	-0.27932	1.88023
H	-4.75656	-0.39302	1.35388
C	3.27361	1.46255	-3.21845
H	4.00169	2.27124	-3.04273

C	3.39638	0.63221	-4.34719
H	4.21993	0.79076	-5.06296
C	-2.28260	3.57375	-1.09487
H	-2.61564	4.26792	-0.30584
C	-2.58211	3.83762	-2.44125
H	-3.15405	4.73977	-2.71518
C	-2.13840	2.95428	-3.44225
H	-2.35672	3.16345	-4.50271
O	3.48380	0.09143	0.59112

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.41	1.32200	YES	YES
8	a	23.33	0.13400	YES	YES
9	a	30.97	0.20146	YES	YES
10	a	41.63	0.10629	YES	YES
11	a	46.40	0.43200	YES	YES
12	a	49.23	0.38438	YES	YES
13	a	51.58	0.10094	YES	YES
14	a	57.54	0.62062	YES	YES
15	a	65.35	0.55325	YES	YES
16	a	73.34	0.50008	YES	YES
17	a	78.24	1.17507	YES	YES
18	a	84.90	0.17798	YES	YES
19	a	93.54	0.71692	YES	YES
20	a	98.70	2.15484	YES	YES
21	a	116.60	0.42405	YES	YES
22	a	133.09	5.55041	YES	YES
23	a	157.30	0.95120	YES	YES
24	a	171.09	1.39094	YES	YES
25	a	185.89	0.88221	YES	YES
26	a	191.58	0.23451	YES	YES
27	a	208.92	0.40407	YES	YES
28	a	215.03	5.78989	YES	YES
29	a	218.82	2.66886	YES	YES
30	a	230.79	1.60555	YES	YES
31	a	244.09	0.77915	YES	YES
32	a	246.20	0.42714	YES	YES
33	a	263.29	1.82232	YES	YES
34	a	267.92	1.97083	YES	YES
35	a	285.22	2.69042	YES	YES
36	a	297.67	4.86502	YES	YES
37	a	360.38	3.46934	YES	YES
38	a	395.41	0.15500	YES	YES
39	a	398.84	0.40539	YES	YES
40	a	404.78	0.06147	YES	YES
41	a	415.55	4.53406	YES	YES
42	a	421.24	12.16084	YES	YES
43	a	425.18	1.25530	YES	YES
44	a	435.77	10.93877	YES	YES
45	a	448.02	10.76093	YES	YES
46	a	464.82	2.27823	YES	YES
47	a	469.72	0.42214	YES	YES
48	a	500.48	37.03806	YES	YES
49	a	505.45	37.37278	YES	YES
50	a	515.22	5.34314	YES	YES

Compound 25 (*O*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P) -1847.2270338910
SCF Energy (au) PBE0/def2-TZVPP -1846.897210417
Zero Point Energy (au) 0.4342369
Chemical potential (kJ mol^{-1}) 968.12

xyz Coordinates

58

Pd	0.55283	0.02536	0.93326
P	-0.09079	0.06183	-1.27013
O	2.63840	0.12158	0.44241
N	1.09928	0.15963	2.95796
C	-1.29560	-0.08104	1.77292
O	2.48971	-1.88861	-0.32560
N	3.21745	-0.94246	-0.04004
C	1.29206	0.17057	-2.49622
C	-1.26610	-0.03523	3.20804
C	-1.09956	1.54241	-1.75380
C	-2.45528	-0.15880	3.96376
H	-2.42024	-0.12651	5.06553
C	1.54120	-0.83097	-3.45592
H	0.90862	-1.73157	-3.49562
C	-3.68976	-0.33721	3.32742
H	-4.61169	-0.43527	3.92363
C	-1.06445	-1.42473	-1.78492
C	-1.62628	2.40063	-0.76575
H	-1.44486	2.17543	0.29777
C	-0.59791	-2.68377	-1.34017
H	0.31489	-2.73465	-0.72309
C	2.12618	1.31002	-2.44866
H	1.95187	2.09075	-1.69063
C	0.30484	0.25524	5.22146
H	-0.53114	0.23339	5.93584
C	-2.93428	-2.53064	-2.89935
H	-3.85481	-2.46486	-3.50314
C	-2.23905	-1.35529	-2.56382
H	-2.62517	-0.38115	-2.90383
C	0.05126	0.12889	3.83789
C	2.36491	0.32211	3.39071
H	3.12958	0.34853	2.59634
C	-1.30718	1.85470	-3.11829
H	-0.86949	1.21753	-3.90449
C	2.60438	-0.68773	-4.36492
H	2.79160	-1.47763	-5.11107
C	-2.46093	-3.78057	-2.46685
H	-3.00887	-4.70047	-2.73096
C	-1.29229	-3.85354	-1.68809
H	-0.91814	-4.83047	-1.33998
C	1.61803	0.41569	5.67942
H	1.81754	0.51481	6.75930
C	-2.55413	-0.27391	1.16682
H	-2.64011	-0.33527	0.07034
C	2.67240	0.45382	4.75090
H	3.71876	0.58312	5.06695
C	-3.73436	-0.39927	1.92400
H	-4.69806	-0.54848	1.40739
C	3.18477	1.44834	-3.35833

H	3.83171	2.33968	-3.30974
C	3.42619	0.45001	-4.31947
H	4.26193	0.55810	-5.03055
C	-2.36638	3.53816	-1.13367
H	-2.76918	4.20141	-0.35056
C	-2.58525	3.83115	-2.48968
H	-3.16348	4.72509	-2.77720
C	-2.05140	2.98855	-3.48161
H	-2.20617	3.22098	-4.54844

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.95	1.15868	YES	YES
8	a	25.92	0.05856	YES	YES
9	a	32.74	0.08857	YES	YES
10	a	37.36	0.11948	YES	YES
11	a	40.07	0.02721	YES	YES
12	a	47.58	0.49090	YES	YES
13	a	52.38	0.39076	YES	YES
14	a	55.12	0.51641	YES	YES
15	a	60.22	2.33170	YES	YES
16	a	68.52	0.48679	YES	YES
17	a	78.36	0.88282	YES	YES
18	a	86.10	0.72156	YES	YES
19	a	92.66	2.13711	YES	YES
20	a	100.63	1.74832	YES	YES
21	a	120.59	0.46039	YES	YES
22	a	126.14	1.73650	YES	YES
23	a	152.73	0.67061	YES	YES
24	a	160.66	1.31727	YES	YES
25	a	187.70	1.11546	YES	YES
26	a	191.57	0.93289	YES	YES
27	a	197.61	1.79385	YES	YES
28	a	204.57	1.65845	YES	YES
29	a	222.97	0.22910	YES	YES
30	a	243.84	1.08184	YES	YES
31	a	244.93	0.56275	YES	YES
32	a	247.62	0.89448	YES	YES
33	a	254.42	0.54335	YES	YES
34	a	268.30	1.26198	YES	YES
35	a	289.34	0.75267	YES	YES
36	a	346.15	3.97289	YES	YES
37	a	358.46	9.38326	YES	YES
38	a	365.76	2.51701	YES	YES
39	a	393.21	0.18211	YES	YES
40	a	397.03	0.31281	YES	YES
41	a	404.86	0.21408	YES	YES
42	a	416.58	5.44987	YES	YES
43	a	424.57	11.96119	YES	YES
44	a	425.47	0.70031	YES	YES
45	a	438.23	13.05482	YES	YES
46	a	447.19	11.62737	YES	YES
47	a	468.49	0.56107	YES	YES
48	a	477.71	0.75448	YES	YES
49	a	496.59	32.34177	YES	YES
50	a	507.48	43.76746	YES	YES

Compound 25 (*N*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -1847.2241281180
SCF Energy (au) PBE0/def2-TZVPP -1846.891274568
Zero Point Energy (au) 0.4348762
Chemical potential (kJ mol^{-1}) 967.87

xyz Coordinates

58

Pd	0.57792	-0.06605	0.98044
P	-0.06448	0.05098	-1.37063
N	2.46672	-0.50999	0.36538
C	1.13681	0.07288	2.93946
N	-1.34079	0.00352	1.90081
O	2.57791	-1.63200	-0.15351
C	1.28874	0.10762	-2.63361
C	-1.29981	0.02681	3.27518
C	-1.07132	1.53092	-1.85356
C	-2.50272	-0.04643	4.01408
H	-2.46393	-0.03076	5.11298
C	1.36682	-0.78797	-3.72028
H	0.62061	-1.59097	-3.83342
C	-3.73128	-0.15431	3.35608
H	-4.66771	-0.21534	3.93466
C	-1.06501	-1.43383	-1.83598
C	-1.46080	2.45313	-0.85814
H	-1.16832	2.27560	0.19075
C	-0.52777	-2.68705	-1.45217
H	0.44840	-2.72339	-0.93615
C	2.26341	1.12164	-2.49828
H	2.22709	1.81381	-1.64120
C	0.27516	0.26622	5.24534
H	-0.56832	0.31211	5.95454
C	-3.03135	-2.57466	-2.73050
H	-4.01544	-2.52607	-3.22601
C	-2.32385	-1.38610	-2.47198
H	-2.76179	-0.41860	-2.76660
C	0.04334	0.11947	3.85618
C	2.44134	0.19955	3.45171
H	3.29967	0.20345	2.76212
C	-1.40370	1.79533	-3.20268
H	-1.07023	1.10804	-3.99799
C	2.40411	-0.66647	-4.66154
H	2.45929	-1.37449	-5.50513
C	-2.48700	-3.81622	-2.36290
H	-3.04275	-4.74625	-2.56822
C	-1.23344	-3.86918	-1.72563
H	-0.80359	-4.83981	-1.42790
C	1.58256	0.37097	5.73469
H	1.75945	0.48466	6.81687
C	-2.52912	-0.11430	1.27197
H	-2.49810	-0.15110	0.17233
C	2.66410	0.34216	4.83430
H	3.69681	0.43439	5.21255
C	-3.74957	-0.19492	1.95169
H	-4.68717	-0.28888	1.38306
C	3.29392	1.24033	-3.44301
H	4.05304	2.03042	-3.32218

C	3.36693	0.34719	-4.52664
H	4.18227	0.43797	-5.26334
C	-2.19291	3.60423	-1.19994
H	-2.48517	4.31890	-0.41289
C	-2.53776	3.84756	-2.53942
H	-3.10824	4.75201	-2.80867
C	-2.13831	2.94304	-3.54060
H	-2.39125	3.13888	-4.59599
O	3.41443	0.26935	0.48106

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.92	0.32491	YES	YES
8	a	20.58	0.93245	YES	YES
9	a	27.71	0.28605	YES	YES
10	a	38.04	0.20570	YES	YES
11	a	43.33	0.23726	YES	YES
12	a	45.45	0.28140	YES	YES
13	a	48.06	0.23656	YES	YES
14	a	52.84	0.34366	YES	YES
15	a	61.45	0.52036	YES	YES
16	a	69.69	0.59354	YES	YES
17	a	74.88	0.62179	YES	YES
18	a	80.03	0.54160	YES	YES
19	a	88.58	0.75253	YES	YES
20	a	91.82	1.50812	YES	YES
21	a	107.87	0.03665	YES	YES
22	a	127.44	1.23335	YES	YES
23	a	140.87	0.90812	YES	YES
24	a	173.69	0.42647	YES	YES
25	a	180.46	0.84497	YES	YES
26	a	182.89	0.60588	YES	YES
27	a	202.43	1.37554	YES	YES
28	a	213.90	0.94243	YES	YES
29	a	225.24	3.61308	YES	YES
30	a	238.41	0.98360	YES	YES
31	a	242.18	1.08205	YES	YES
32	a	245.15	0.46449	YES	YES
33	a	264.86	1.09725	YES	YES
34	a	265.51	1.32759	YES	YES
35	a	296.73	0.10130	YES	YES
36	a	313.74	8.17973	YES	YES
37	a	361.12	0.38762	YES	YES
38	a	394.50	0.18679	YES	YES
39	a	398.13	0.34895	YES	YES
40	a	404.07	0.08877	YES	YES
41	a	412.50	4.97710	YES	YES
42	a	421.06	9.12273	YES	YES
43	a	422.30	10.54555	YES	YES
44	a	429.99	0.69875	YES	YES
45	a	438.43	8.86645	YES	YES
46	a	461.64	0.52312	YES	YES
47	a	472.85	1.42333	YES	YES
48	a	493.64	35.59263	YES	YES
49	a	502.56	27.28088	YES	YES
50	a	511.85	73.09404	YES	YES

Compound 25 (*O*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -1847.2080158060
SCF Energy (au) PBE0/def2-TZVPP -1846.877324613
Zero Point Energy (au) 0.4332919
Chemical potential (kJ mol^{-1}) 961.16

xyz Coordinates

58

Pd	0.54279	0.03425	1.00889
P	-0.12728	0.06909	-1.34235
O	2.51384	0.07200	0.47381
C	1.12055	0.18512	2.93345
N	-1.31664	-0.13923	1.93970
N	2.85860	-1.04818	-0.20738
C	1.20811	0.34933	-2.59073
C	-1.27998	-0.04272	3.31531
C	-1.33234	1.40048	-1.80909
C	-2.47012	-0.18393	4.06202
H	-2.43032	-0.09858	5.15786
C	1.38915	-0.47054	-3.72345
H	0.73844	-1.34475	-3.88438
C	-3.68262	-0.44790	3.41735
H	-4.61008	-0.56252	4.00196
C	-0.90740	-1.52887	-1.85026
C	-1.84106	2.25185	-0.80481
H	-1.52782	2.10264	0.24217
C	-0.17212	-2.70237	-1.55227
H	0.82495	-2.61436	-1.08388
C	2.06426	1.45542	-2.38967
H	1.94874	2.08582	-1.49342
C	0.32350	0.34369	5.25637
H	-0.49547	0.34249	5.99555
C	-2.72265	-2.91499	-2.71940
H	-3.72488	-2.99359	-3.17292
C	-2.18834	-1.64532	-2.43129
H	-2.77737	-0.74287	-2.66218
C	0.05414	0.17375	3.87729
C	2.43784	0.36014	3.38558
H	3.26031	0.36757	2.65076
C	-1.70060	1.63149	-3.15495
H	-1.28081	1.00215	-3.95729
C	2.40818	-0.18166	-4.64871
H	2.54403	-0.83148	-5.52907
C	-1.98302	-4.07476	-2.43599
H	-2.40269	-5.06833	-2.66535
C	-0.70618	-3.96456	-1.85442
H	-0.12189	-4.87096	-1.62480
C	1.64233	0.52044	5.69426
H	1.85159	0.65402	6.76840
C	-2.48862	-0.41266	1.32585
H	-2.45445	-0.50949	0.23032
C	2.69681	0.52684	4.75933
H	3.73545	0.66402	5.10654
C	-3.69352	-0.57646	2.01825
H	-4.61585	-0.79861	1.46060
C	3.07664	1.74116	-3.31770
H	3.74441	2.60154	-3.14762

C	3.25137	0.92367	-4.44925
H	4.05428	1.14433	-5.17195
C	-2.72024	3.29905	-1.13438
H	-3.10453	3.95973	-0.33977
C	-3.09644	3.50808	-2.47117
H	-3.78287	4.33108	-2.73094
C	-2.58212	2.67418	-3.48133
H	-2.86089	2.84463	-4.53457
O	4.05361	-1.14893	-0.36160

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.18	1.00242	YES	YES
8	a	18.48	0.35978	YES	YES
9	a	24.40	0.22491	YES	YES
10	a	36.34	0.12651	YES	YES
11	a	41.05	0.28602	YES	YES
12	a	44.49	0.11373	YES	YES
13	a	46.71	0.32472	YES	YES
14	a	49.91	0.27640	YES	YES
15	a	57.95	2.25885	YES	YES
16	a	59.05	0.17847	YES	YES
17	a	70.82	0.28915	YES	YES
18	a	77.98	0.46499	YES	YES
19	a	87.87	1.70323	YES	YES
20	a	90.51	0.89718	YES	YES
21	a	111.38	0.26947	YES	YES
22	a	132.52	0.18295	YES	YES
23	a	151.38	0.73719	YES	YES
24	a	158.31	0.36117	YES	YES
25	a	179.41	0.45298	YES	YES
26	a	183.26	0.16170	YES	YES
27	a	200.61	1.08577	YES	YES
28	a	205.54	1.59503	YES	YES
29	a	220.28	1.33965	YES	YES
30	a	230.98	1.21919	YES	YES
31	a	241.55	0.64208	YES	YES
32	a	243.25	0.84132	YES	YES
33	a	253.07	2.36449	YES	YES
34	a	259.94	1.33621	YES	YES
35	a	265.72	1.37093	YES	YES
36	a	303.07	0.93472	YES	YES
37	a	362.45	2.53568	YES	YES
38	a	379.77	11.45141	YES	YES
39	a	393.50	0.37929	YES	YES
40	a	397.35	0.34410	YES	YES
41	a	403.04	0.02681	YES	YES
42	a	414.34	6.28622	YES	YES
43	a	420.83	11.15506	YES	YES
44	a	422.96	7.30649	YES	YES
45	a	432.07	3.05518	YES	YES
46	a	439.42	6.59357	YES	YES
47	a	466.91	0.98847	YES	YES
48	a	476.64	2.21728	YES	YES
49	a	491.54	35.51237	YES	YES
50	a	504.74	26.28055	YES	YES

[Pd(2-bzpy)(NO_2)(PPh_3)] (*N*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P) -1886.5000614470
SCF Energy (au) PBE0/def2-TZVPP -1886.169112911
Zero Point Energy (au) 0.4624785
Chemical potential (kJ mol^{-1}) 1037.93

xyz Coordinates

61

C	0.25610	-1.47330	-1.51006
C	1.18802	-2.39006	-0.97712
H	1.81815	-2.10515	-0.11706
C	1.34235	-3.68444	-1.50903
H	2.08395	-4.37263	-1.06805
C	0.54990	-4.09819	-2.59089
H	0.65526	-5.11340	-3.00879
C	-0.37850	-3.20066	-3.14326
H	-1.00154	-3.51475	-4.00014
C	-0.52535	-1.90058	-2.61605
C	-1.48460	-0.91898	-3.28590
H	-2.06152	-1.41681	-4.09260
H	-2.21559	-0.52555	-2.54040
C	-0.71887	0.25208	-3.85900
C	-0.69769	0.55409	-5.23354
H	-1.29617	-0.05575	-5.92842
C	0.08275	1.62084	-5.70059
H	0.10851	1.86373	-6.77574
C	0.82707	2.37196	-4.77765
H	1.45290	3.22106	-5.09277
C	0.75503	2.02928	-3.42214
H	1.28360	2.60231	-2.64180
C	-1.07656	1.04174	2.44423
C	-2.18652	0.51682	3.13948
H	-2.44494	-0.54961	3.04890
C	-2.96852	1.34942	3.95978
H	-3.83376	0.92519	4.49587
C	-2.64844	2.70931	4.09708
H	-3.26303	3.36130	4.73988
C	-1.54353	3.23729	3.40577
H	-1.29003	4.30619	3.49704
C	-0.76417	2.41370	2.58053
H	0.08803	2.84904	2.03431
C	1.66858	0.20926	2.07862
C	1.85560	0.34781	3.47310
H	0.98580	0.34919	4.15012
C	3.14733	0.50532	4.00144
H	3.28218	0.61469	5.09046
C	4.26265	0.53510	3.14533
H	5.27514	0.66512	3.56241
C	4.08230	0.41475	1.75729
H	4.95061	0.45524	1.07939
C	2.79151	0.25765	1.22460
H	2.64362	0.18978	0.13322
C	-0.54418	-1.73129	1.78692
C	0.08494	-2.49831	2.78841
H	0.95917	-2.09921	3.32649
C	-0.38927	-3.78569	3.09687
H	0.11736	-4.37958	3.87567

C	-1.49822	-4.31372	2.41538
H	-1.86633	-5.32458	2.65740
C	-2.12831	-3.55415	1.41362
H	-2.99061	-3.96696	0.86478
C	-1.64940	-2.27409	1.09479
H	-2.12636	-1.69168	0.28934
N	-0.35242	2.52576	-0.53305
N	0.00278	0.99609	-2.98225
O	-1.50862	2.95364	-0.45208
O	0.64006	3.28350	-0.49095
P	-0.01580	-0.01317	1.34431
Pd	-0.02223	0.47713	-0.90594

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.18	0.24411	YES	YES
8	a	23.06	1.41544	YES	YES
9	a	30.27	0.42575	YES	YES
10	a	40.62	0.20354	YES	YES
11	a	42.36	0.61056	YES	YES
12	a	51.40	0.54459	YES	YES
13	a	52.96	0.50903	YES	YES
14	a	55.44	0.27767	YES	YES
15	a	58.62	0.49688	YES	YES
16	a	64.88	0.17520	YES	YES
17	a	70.53	0.48585	YES	YES
18	a	77.22	0.23705	YES	YES
19	a	83.00	1.11223	YES	YES
20	a	89.70	2.05622	YES	YES
21	a	105.07	2.51908	YES	YES
22	a	126.57	2.49444	YES	YES
23	a	133.43	1.49426	YES	YES
24	a	159.35	0.35922	YES	YES
25	a	177.80	1.58975	YES	YES
26	a	188.63	0.95353	YES	YES
27	a	197.04	1.23498	YES	YES
28	a	201.46	0.65637	YES	YES
29	a	211.54	4.26352	YES	YES
30	a	223.39	2.62341	YES	YES
31	a	236.10	0.81441	YES	YES
32	a	244.25	0.80432	YES	YES
33	a	247.67	0.59703	YES	YES
34	a	264.13	0.81028	YES	YES
35	a	267.72	0.48731	YES	YES
36	a	278.91	8.47464	YES	YES
37	a	296.13	3.45160	YES	YES
38	a	330.32	0.65498	YES	YES
39	a	390.31	2.34837	YES	YES
40	a	396.37	0.03561	YES	YES
41	a	397.72	0.38287	YES	YES
42	a	404.54	0.54128	YES	YES
43	a	419.67	11.60772	YES	YES
44	a	426.71	0.64554	YES	YES
45	a	434.71	12.97977	YES	YES
46	a	443.92	7.91249	YES	YES
47	a	447.42	10.61718	YES	YES
48	a	478.55	5.23289	YES	YES
49	a	490.81	5.94808	YES	YES
50	a	491.69	24.50787	YES	YES

[Pd(2-bzpy)(NO_2)(PPh_3)] (*O*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P) -1886.4928959420
SCF Energy (au) PBE0/def2-TZVPP -1886.162546256
Zero Point Energy (au) 0.4614247
Chemical potential (kJ mol^{-1}) 1033.54

xyz Coordinates

61

C	0.37734	1.56265	1.47758
C	1.43992	2.35571	0.99488
H	2.09770	1.97451	0.19578
C	1.68409	3.64189	1.51288
H	2.52675	4.23724	1.12144
C	0.85349	4.16655	2.51583
H	1.03006	5.17868	2.91664
C	-0.19780	3.38239	3.01952
H	-0.84288	3.77997	3.82347
C	-0.43338	2.08590	2.51676
C	-1.48784	1.19166	3.15657
H	-2.07531	1.74820	3.91592
H	-2.20088	0.82006	2.38329
C	-0.82315	-0.00508	3.80728
C	-0.96170	-0.30075	5.17583
H	-1.60932	0.33303	5.80188
C	-0.27451	-1.39287	5.72577
H	-0.37228	-1.62951	6.79827
C	0.53781	-2.17363	4.89016
H	1.09923	-3.03956	5.27359
C	0.62322	-1.83721	3.53282
H	1.21686	-2.42904	2.81323
C	-1.71739	-0.46654	-2.04917
C	-2.42868	0.35519	-2.95176
H	-2.02696	1.33627	-3.24877
C	-3.65871	-0.07419	-3.48099
H	-4.20441	0.57708	-4.18417
C	-4.18719	-1.32415	-3.11890
H	-5.15211	-1.65881	-3.53525
C	-3.47891	-2.14609	-2.22447
H	-3.88468	-3.12987	-1.93550
C	-2.25142	-1.72633	-1.68682
H	-1.69800	-2.37110	-0.98045
C	1.15951	-0.96866	-2.26462
C	0.90738	-1.44568	-3.56872
H	-0.06318	-1.24670	-4.05214
C	1.88862	-2.18456	-4.25037
H	1.68114	-2.55939	-5.26644
C	3.12437	-2.45355	-3.63661
H	3.88942	-3.04137	-4.17052
C	3.37677	-1.98660	-2.33542
H	4.33675	-2.21049	-1.84196
C	2.39744	-1.25090	-1.64868
H	2.58291	-0.91084	-0.61562
C	0.15322	1.75799	-1.98022
C	1.09907	2.06679	-2.97996
H	1.73333	1.27233	-3.40369
C	1.23725	3.38832	-3.44203
H	1.98272	3.61666	-4.22173

C	0.42871	4.40907	-2.91654
H	0.53749	5.44435	-3.28037
C	-0.51567	4.10771	-1.91831
H	-1.14573	4.90554	-1.49226
C	-0.64650	2.79366	-1.44504
H	-1.37151	2.57148	-0.64559
N	0.83660	-3.17935	0.70576
N	-0.03913	-0.78076	3.01467
O	-0.24019	-2.41887	0.47278
O	0.70194	-4.33815	0.36717
P	-0.07819	0.03934	-1.33865
Pd	0.06699	-0.35561	0.92845

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.61	0.64007	YES	YES
8	a	21.96	0.99524	YES	YES
9	a	26.49	0.37683	YES	YES
10	a	35.60	0.49180	YES	YES
11	a	42.57	0.74355	YES	YES
12	a	45.64	0.93454	YES	YES
13	a	49.43	0.47134	YES	YES
14	a	52.68	0.24421	YES	YES
15	a	55.12	0.34047	YES	YES
16	a	63.95	0.70949	YES	YES
17	a	74.26	2.80795	YES	YES
18	a	75.62	0.72638	YES	YES
19	a	89.04	1.79969	YES	YES
20	a	93.41	0.46400	YES	YES
21	a	113.40	0.43106	YES	YES
22	a	130.95	1.41874	YES	YES
23	a	144.41	0.61092	YES	YES
24	a	151.52	1.10166	YES	YES
25	a	172.89	2.90258	YES	YES
26	a	181.23	1.74276	YES	YES
27	a	188.48	0.56783	YES	YES
28	a	199.21	0.27383	YES	YES
29	a	211.06	1.73817	YES	YES
30	a	214.16	1.78525	YES	YES
31	a	226.72	1.46881	YES	YES
32	a	243.00	0.20966	YES	YES
33	a	247.82	0.64149	YES	YES
34	a	252.86	2.48169	YES	YES
35	a	254.70	2.30462	YES	YES
36	a	265.22	0.45890	YES	YES
37	a	302.49	2.21572	YES	YES
38	a	322.02	15.47602	YES	YES
39	a	338.32	4.88927	YES	YES
40	a	389.59	2.06118	YES	YES
41	a	395.57	0.10534	YES	YES
42	a	396.75	0.25280	YES	YES
43	a	402.00	0.55532	YES	YES
44	a	425.89	14.06372	YES	YES
45	a	428.69	5.25869	YES	YES
46	a	434.13	3.43140	YES	YES
47	a	446.56	17.61624	YES	YES
48	a	450.06	1.03636	YES	YES
49	a	478.98	3.27773	YES	YES
50	a	496.22	28.56208	YES	YES

[Pd(2-bzpy)(NO_2)(PPh_3)] (*N*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -1886.4963825260
SCF Energy (au) PBE0/def2-TZVPP -1886.162232339
Zero Point Energy (au) 0.4625474
Chemical potential (kJ mol^{-1}) 1036.60

xyz Coordinates

61

N	0.22619	-1.43930	-1.67117
C	1.15107	-2.27747	-1.15203
H	1.74818	-1.88201	-0.31518
C	1.35833	-3.57403	-1.63452
H	2.12980	-4.21088	-1.17530
C	0.56185	-4.02555	-2.69775
H	0.68628	-5.04246	-3.10504
C	-0.39210	-3.15416	-3.23909
H	-1.03014	-3.46816	-4.08011
C	-0.54108	-1.85469	-2.71626
C	-1.49282	-0.84895	-3.32495
H	-2.07210	-1.33390	-4.13802
H	-2.21558	-0.51578	-2.54394
C	-0.71363	0.35455	-3.84703
C	-0.69558	0.66231	-5.22284
H	-1.29199	0.05637	-5.92856
C	0.07058	1.73970	-5.69951
H	0.07561	1.97864	-6.77626
C	0.82732	2.50524	-4.79729
H	1.43401	3.35179	-5.16281
C	0.80837	2.20230	-3.42144
H	1.39194	2.82253	-2.72059
C	-1.10932	0.96905	2.58232
C	-2.10695	0.36719	3.37920
H	-2.27232	-0.72066	3.33455
C	-2.89602	1.15022	4.24039
H	-3.67190	0.66577	4.85639
C	-2.69513	2.53772	4.31775
H	-3.31601	3.15099	4.99177
C	-1.70141	3.14162	3.52738
H	-1.54076	4.23126	3.57348
C	-0.91401	2.36784	2.66123
H	-0.14662	2.86295	2.04410
C	1.63850	0.17165	2.18944
C	1.83345	0.11150	3.58840
H	0.97035	-0.02887	4.26032
C	3.12198	0.24891	4.12893
H	3.26492	0.20197	5.22148
C	4.22562	0.45888	3.28149
H	5.23515	0.57505	3.70982
C	4.03682	0.53932	1.89199
H	4.89438	0.72663	1.22507
C	2.74818	0.40065	1.34722
H	2.58927	0.50013	0.25852
C	-0.54108	-1.75430	1.72150
C	0.20911	-2.67482	2.48282
H	1.14883	-2.35780	2.96270
C	-0.23371	-4.00169	2.63245
H	0.36380	-4.71030	3.23010

C	-1.43032	-4.42243	2.02925
H	-1.77621	-5.46236	2.15057
C	-2.18253	-3.51237	1.26436
H	-3.12033	-3.83574	0.78279
C	-1.73653	-2.19137	1.10293
H	-2.32071	-1.48642	0.48618
N	-0.30350	2.51525	-0.50900
C	0.04127	1.12654	-2.93485
O	-1.46050	2.93506	-0.46176
O	0.68492	3.21420	-0.23501
P	-0.03513	0.00205	1.41848
Pd	-0.01507	0.55931	-0.95595

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.21	0.92868	YES	YES
8	a	21.07	0.10977	YES	YES
9	a	29.78	0.37967	YES	YES
10	a	39.97	0.25714	YES	YES
11	a	41.66	0.32167	YES	YES
12	a	45.59	0.30608	YES	YES
13	a	47.60	0.19456	YES	YES
14	a	53.07	0.05902	YES	YES
15	a	58.34	0.26059	YES	YES
16	a	61.66	1.18858	YES	YES
17	a	70.86	0.31245	YES	YES
18	a	77.60	0.14179	YES	YES
19	a	80.71	0.80757	YES	YES
20	a	85.08	0.32840	YES	YES
21	a	98.35	2.73192	YES	YES
22	a	125.52	0.30744	YES	YES
23	a	129.02	0.41380	YES	YES
24	a	139.51	0.10248	YES	YES
25	a	180.71	0.42587	YES	YES
26	a	185.63	0.93775	YES	YES
27	a	197.02	1.55171	YES	YES
28	a	198.91	0.79906	YES	YES
29	a	211.52	1.34457	YES	YES
30	a	216.91	2.32664	YES	YES
31	a	235.91	3.88326	YES	YES
32	a	242.31	1.11466	YES	YES
33	a	245.89	0.06268	YES	YES
34	a	265.83	0.73845	YES	YES
35	a	282.79	0.67561	YES	YES
36	a	291.21	1.55559	YES	YES
37	a	311.68	4.81951	YES	YES
38	a	331.71	1.15842	YES	YES
39	a	390.56	1.69737	YES	YES
40	a	396.56	0.14833	YES	YES
41	a	399.27	0.28408	YES	YES
42	a	403.55	0.31563	YES	YES
43	a	417.28	8.84811	YES	YES
44	a	420.89	8.85229	YES	YES
45	a	427.55	1.87908	YES	YES
46	a	442.20	14.11052	YES	YES
47	a	444.51	1.29897	YES	YES
48	a	478.78	1.70582	YES	YES
49	a	489.08	28.67224	YES	YES
50	a	498.98	7.18768	YES	YES

[Pd(2-bzpy)(NO_2)(PPh_3)] (*O*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -1886.4812187060
SCF Energy (au) PBE0/def2-TZVPP -1886.148034150
Zero Point Energy (au) 0.4609825
Chemical potential (kJ mol^{-1}) 1031.08

xyz Coordinates

1297.42 0.90163

T (K)	P (MPa)	Cv (kJ/mol-K)	Cp (kJ/mol-K)
298.15	0.1000000	0.5333319	0.5416462

******* HOMO & LUMO energies *******

HOMO-LUMO Separation
HOMO: 134. 134 a -0.15581953 H = -4.24007 eV
LUMO: 135. 135 a -0.09819912 H = -2.67214 eV
Gap : +0.05762041 H = +1.56793 eV

******* xyz coordinates *******

61

N	0.30293	1.51665	1.67993
C	1.31078	2.27595	1.18855
H	1.91542	1.81885	0.39087
C	1.58172	3.56618	1.65474
H	2.41894	4.13519	1.22306
C	0.76358	4.10047	2.66172
H	0.93727	5.11699	3.05112
C	-0.27535	3.31073	3.17202
H	-0.93223	3.68948	3.97061
C	-0.48506	2.00981	2.67649
C	-1.51689	1.07602	3.26362
H	-2.09219	1.60545	4.05101
H	-2.23413	0.77753	2.46351
C	-0.82256	-0.16050	3.82849
C	-0.93225	-0.48952	5.19533
H	-1.56698	0.12621	5.85752
C	-0.24494	-1.59925	5.71554
H	-0.33733	-1.85222	6.78498
C	0.55892	-2.37874	4.86737
H	1.10674	-3.24840	5.26917
C	0.66435	-2.06052	3.49888
H	1.27978	-2.69064	2.83511
C	-1.66590	-0.47638	-2.23529
C	-2.30142	0.30668	-3.22500
H	-1.87376	1.27555	-3.52873
C	-3.48752	-0.14388	-3.83073
H	-3.97477	0.47618	-4.60184
C	-4.04709	-1.37770	-3.45769
H	-4.97800	-1.72935	-3.93318
C	-3.41543	-2.16075	-2.47554
H	-3.84697	-3.13045	-2.17698
C	-2.23264	-1.71748	-1.86100
H	-1.73872	-2.33170	-1.08712
C	1.23290	-0.83230	-2.35480

C	1.09204	-1.16766	-3.71918
H	0.15690	-0.92919	-4.25252
C	2.13635	-1.81684	-4.39767
H	2.01593	-2.08017	-5.46170
C	3.32533	-2.14168	-3.72025
H	4.13965	-2.66052	-4.25282
C	3.46718	-1.81982	-2.36002
H	4.38790	-2.09160	-1.81821
C	2.42364	-1.17270	-1.67737
H	2.51937	-0.95469	-0.59976
C	0.09206	1.81605	-1.91229
C	1.13865	2.27825	-2.73900
H	1.86354	1.56242	-3.15851
C	1.25829	3.64768	-3.03876
H	2.07967	3.99209	-3.68906
C	0.33284	4.57010	-2.52335
H	0.42521	5.64215	-2.76414
C	-0.71329	4.11856	-1.69757
H	-1.44370	4.83552	-1.28728
C	-0.82764	2.75484	-1.38692
H	-1.64648	2.41278	-0.73113
N	0.80691	-3.18472	0.51943
C	-0.02210	-0.95157	2.97405
O	-0.28089	-2.37799	0.46308
O	0.59009	-4.28170	0.05695
P	-0.08972	0.04247	-1.40822
Pd	0.02888	-0.43040	1.00632

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.66	1.03371	YES	YES
8	a	19.12	0.29866	YES	YES
9	a	26.99	0.20968	YES	YES
10	a	37.81	0.16628	YES	YES
11	a	43.15	0.19357	YES	YES
12	a	45.39	0.77077	YES	YES
13	a	48.84	0.21816	YES	YES
14	a	51.09	0.16683	YES	YES
15	a	56.22	0.12066	YES	YES
16	a	60.64	0.50666	YES	YES
17	a	68.14	1.34149	YES	YES
18	a	71.14	1.88357	YES	YES
19	a	80.56	0.63003	YES	YES
20	a	86.58	0.48617	YES	YES
21	a	121.32	0.92981	YES	YES
22	a	121.62	0.16096	YES	YES
23	a	131.62	0.68340	YES	YES
24	a	153.76	0.93133	YES	YES
25	a	174.74	1.24312	YES	YES
26	a	181.43	0.83955	YES	YES
27	a	192.04	0.59771	YES	YES
28	a	198.78	1.17698	YES	YES
29	a	205.76	1.24523	YES	YES
30	a	209.57	4.53714	YES	YES
31	a	223.95	0.60707	YES	YES
32	a	240.50	1.12909	YES	YES
33	a	248.14	0.32675	YES	YES
34	a	254.28	0.49810	YES	YES
35	a	264.54	0.38778	YES	YES
36	a	275.59	3.86956	YES	YES
37	a	292.58	1.84526	YES	YES
38	a	330.66	1.72535	YES	YES
39	a	361.29	8.91197	YES	YES
40	a	389.20	1.54142	YES	YES
41	a	395.33	0.31096	YES	YES
42	a	397.61	0.55455	YES	YES
43	a	401.74	0.17503	YES	YES
44	a	414.47	7.07440	YES	YES
45	a	425.45	9.69835	YES	YES
46	a	431.51	0.63987	YES	YES
47	a	439.68	11.36042	YES	YES
48	a	448.78	4.00741	YES	YES
49	a	479.91	3.31850	YES	YES
50	a	490.02	25.13703	YES	YES

2-bzpy/iso/O-bound

SCF Energy (au) (RI)BP86/SV(P) -1886.4812187060
SCF Energy (au) PBE0/def2-TZVPP -1886.148034150
Zero Point Energy (au) 0.4609825
Chemical potential (kJ mol^{-1}) 1031.08

xyz Coordinates

1297.42 0.90163

T (K)	P (MPa)	Cv (kJ/mol-K)	Cp (kJ/mol-K)
298.15	0.1000000	0.5333319	0.5416462

******* HOMO & LUMO energies *******

HOMO-LUMO Separation
HOMO: 134. 134 a -0.15581953 H = -4.24007 eV
LUMO: 135. 135 a -0.09819912 H = -2.67214 eV
Gap : +0.05762041 H = +1.56793 eV

******* xyz coordinates *******

61

N	0.30293	1.51665	1.67993
C	1.31078	2.27595	1.18855
H	1.91542	1.81885	0.39087
C	1.58172	3.56618	1.65474
H	2.41894	4.13519	1.22306
C	0.76358	4.10047	2.66172
H	0.93727	5.11699	3.05112
C	-0.27535	3.31073	3.17202
H	-0.93223	3.68948	3.97061
C	-0.48506	2.00981	2.67649
C	-1.51689	1.07602	3.26362
H	-2.09219	1.60545	4.05101
H	-2.23413	0.77753	2.46351
C	-0.82256	-0.16050	3.82849
C	-0.93225	-0.48952	5.19533
H	-1.56698	0.12621	5.85752
C	-0.24494	-1.59925	5.71554
H	-0.33733	-1.85222	6.78498
C	0.55892	-2.37874	4.86737
H	1.10674	-3.24840	5.26917
C	0.66435	-2.06052	3.49888
H	1.27978	-2.69064	2.83511
C	-1.66590	-0.47638	-2.23529
C	-2.30142	0.30668	-3.22500
H	-1.87376	1.27555	-3.52873
C	-3.48752	-0.14388	-3.83073
H	-3.97477	0.47618	-4.60184
C	-4.04709	-1.37770	-3.45769
H	-4.97800	-1.72935	-3.93318
C	-3.41543	-2.16075	-2.47554
H	-3.84697	-3.13045	-2.17698
C	-2.23264	-1.71748	-1.86100
H	-1.73872	-2.33170	-1.08712
C	1.23290	-0.83230	-2.35480

C	1.09204	-1.16766	-3.71918
H	0.15690	-0.92919	-4.25252
C	2.13635	-1.81684	-4.39767
H	2.01593	-2.08017	-5.46170
C	3.32533	-2.14168	-3.72025
H	4.13965	-2.66052	-4.25282
C	3.46718	-1.81982	-2.36002
H	4.38790	-2.09160	-1.81821
C	2.42364	-1.17270	-1.67737
H	2.51937	-0.95469	-0.59976
C	0.09206	1.81605	-1.91229
C	1.13865	2.27825	-2.73900
H	1.86354	1.56242	-3.15851
C	1.25829	3.64768	-3.03876
H	2.07967	3.99209	-3.68906
C	0.33284	4.57010	-2.52335
H	0.42521	5.64215	-2.76414
C	-0.71329	4.11856	-1.69757
H	-1.44370	4.83552	-1.28728
C	-0.82764	2.75484	-1.38692
H	-1.64648	2.41278	-0.73113
N	0.80691	-3.18472	0.51943
C	-0.02210	-0.95157	2.97405
O	-0.28089	-2.37799	0.46308
O	0.59009	-4.28170	0.05695
P	-0.08972	0.04247	-1.40822
Pd	0.02888	-0.43040	1.00632

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.66	1.03371	YES	YES
8	a	19.12	0.29866	YES	YES
9	a	26.99	0.20968	YES	YES
10	a	37.81	0.16628	YES	YES
11	a	43.15	0.19357	YES	YES
12	a	45.39	0.77077	YES	YES
13	a	48.84	0.21816	YES	YES
14	a	51.09	0.16683	YES	YES
15	a	56.22	0.12066	YES	YES
16	a	60.64	0.50666	YES	YES
17	a	68.14	1.34149	YES	YES
18	a	71.14	1.88357	YES	YES
19	a	80.56	0.63003	YES	YES
20	a	86.58	0.48617	YES	YES
21	a	121.32	0.92981	YES	YES
22	a	121.62	0.16096	YES	YES
23	a	131.62	0.68340	YES	YES
24	a	153.76	0.93133	YES	YES
25	a	174.74	1.24312	YES	YES
26	a	181.43	0.83955	YES	YES
27	a	192.04	0.59771	YES	YES
28	a	198.78	1.17698	YES	YES
29	a	205.76	1.24523	YES	YES
30	a	209.57	4.53714	YES	YES
31	a	223.95	0.60707	YES	YES
32	a	240.50	1.12909	YES	YES
33	a	248.14	0.32675	YES	YES
34	a	254.28	0.49810	YES	YES
35	a	264.54	0.38778	YES	YES
36	a	275.59	3.86956	YES	YES
37	a	292.58	1.84526	YES	YES
38	a	330.66	1.72535	YES	YES
39	a	361.29	8.91197	YES	YES
40	a	389.20	1.54142	YES	YES
41	a	395.33	0.31096	YES	YES
42	a	397.61	0.55455	YES	YES
43	a	401.74	0.17503	YES	YES
44	a	414.47	7.07440	YES	YES
45	a	425.45	9.69835	YES	YES
46	a	431.51	0.63987	YES	YES
47	a	439.68	11.36042	YES	YES
48	a	448.78	4.00741	YES	YES
49	a	479.91	3.31850	YES	YES
50	a	490.02	25.13703	YES	YES

[Pd(2-PhCH$_2$Py)(NO$_2$)(PPh$_3$)] (*N*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P) -1925.7786872050
SCF Energy (au) PBE0/def2-TZVPP -1925.443712970
Zero Point Energy (au) 0.4900827
Chemical potential (kJ mol^{-1}) 1105.71

xyz Coordinates

64

C	0.34015	-1.46959	-1.42821
C	1.55691	-2.13691	-1.15468
H	2.30352	-1.66127	-0.49519
C	1.85147	-3.40107	-1.69430
H	2.81314	-3.88981	-1.46128
C	0.91372	-4.03379	-2.52546
H	1.12467	-5.02615	-2.95852
C	-0.29491	-3.38269	-2.81233
H	-1.02777	-3.87474	-3.47779
C	-0.60201	-2.10596	-2.28110
C	-2.04215	0.02570	-2.87442
H	-2.99357	0.25288	-3.40330
H	-2.07881	0.54133	-1.88745
C	-0.88324	0.61207	-3.64049
C	-0.89720	0.80969	-5.03383
H	-1.79600	0.53553	-5.60870
C	0.22434	1.36021	-5.67147
H	0.22257	1.51975	-6.76237
C	1.34071	1.71507	-4.89859
H	2.23774	2.16465	-5.35153
C	1.29431	1.49551	-3.51598
H	2.11816	1.78371	-2.84367
C	-1.79246	0.22425	1.95737
C	-2.43019	-0.65086	2.86363
H	-1.89187	-1.52247	3.26841
C	-3.76134	-0.41707	3.25176
H	-4.25237	-1.10912	3.95624
C	-4.46144	0.69143	2.74679
H	-5.50545	0.87231	3.05314
C	-3.82515	1.56949	1.85138
H	-4.36532	2.44534	1.45497
C	-2.49835	1.34039	1.45130
H	-1.99756	2.04173	0.75672
C	0.93669	1.11540	2.52067
C	0.48535	1.45173	3.81578
H	-0.48824	1.08077	4.17552
C	1.27078	2.26758	4.64623
H	0.90763	2.53250	5.65311
C	2.51122	2.75090	4.19296
H	3.12332	3.39676	4.84440
C	2.96262	2.42161	2.90361
H	3.92481	2.81319	2.53521
C	2.17810	1.61047	2.06665
H	2.51383	1.39014	1.04040
C	0.40854	-1.69359	2.01068
C	1.43375	-1.90454	2.95671
H	1.98559	-1.04757	3.37366
C	1.75705	-3.20786	3.37544
H	2.56157	-3.35746	4.11452

C	1.05680	-4.31042	2.86024
H	1.31033	-5.33152	3.19055
C	0.03475	-4.10749	1.91537
H	-0.51315	-4.96765	1.49709
C	-0.28159	-2.81022	1.48543
H	-1.06958	-2.66526	0.72984
N	0.36370	2.58186	-0.51813
N	0.21460	0.95333	-2.91533
O	-0.60044	3.31762	-0.25054
O	1.48699	3.05203	-0.77557
P	-0.03534	-0.00004	1.41193
Pd	0.21415	0.48771	-0.82277
C	-1.95731	-1.50980	-2.65455
H	-2.31344	-2.01846	-3.57757
H	-2.70633	-1.75891	-1.86556

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.34	0.12842	YES	YES
8	a	21.65	0.68394	YES	YES
9	a	23.54	0.80625	YES	YES
10	a	38.56	0.73667	YES	YES
11	a	42.47	0.28152	YES	YES
12	a	44.95	0.82790	YES	YES
13	a	50.58	0.05910	YES	YES
14	a	52.70	0.09970	YES	YES
15	a	58.29	0.02026	YES	YES
16	a	60.61	0.61588	YES	YES
17	a	75.26	0.62696	YES	YES
18	a	80.13	0.62922	YES	YES
19	a	84.15	0.31346	YES	YES
20	a	98.86	2.31859	YES	YES
21	a	100.40	2.22233	YES	YES
22	a	111.00	3.95772	YES	YES
23	a	122.23	2.30795	YES	YES
24	a	143.70	0.23120	YES	YES
25	a	152.45	0.17065	YES	YES
26	a	174.85	2.02929	YES	YES
27	a	188.25	0.51197	YES	YES
28	a	188.66	1.49282	YES	YES
29	a	201.31	0.92098	YES	YES
30	a	212.88	3.99856	YES	YES
31	a	219.00	1.86362	YES	YES
32	a	223.79	1.21511	YES	YES
33	a	244.04	0.88076	YES	YES
34	a	252.53	1.12312	YES	YES
35	a	259.70	0.40617	YES	YES
36	a	267.11	1.45151	YES	YES
37	a	273.69	0.61987	YES	YES
38	a	277.20	10.91905	YES	YES
39	a	309.02	1.30045	YES	YES
40	a	376.61	1.34699	YES	YES
41	a	395.20	0.21181	YES	YES
42	a	399.22	0.39743	YES	YES
43	a	403.77	0.34947	YES	YES
44	a	406.38	0.20899	YES	YES
45	a	424.93	14.44667	YES	YES
46	a	433.10	8.19531	YES	YES
47	a	436.79	1.33055	YES	YES
48	a	444.08	12.05820	YES	YES
49	a	450.97	8.39515	YES	YES
50	a	485.04	0.77761	YES	YES

[Pd(2-PhCH$_2$Py)(NO$_2$)(PPh$_3$)] (*O*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P) -1925.7669841250
SCF Energy (au) PBE0/def2-TZVPP -1925.433976990
Zero Point Energy (au) 0.4887736
Chemical potential (kJ mol^{-1}) 1099.36

xyz Coordinates

64

C	0.41091	-1.50463	-1.41072
C	1.66747	-2.06077	-1.07224
H	2.34895	-1.50363	-0.40701
C	2.08268	-3.31332	-1.55536
H	3.07151	-3.71204	-1.27126
C	1.23023	-4.04822	-2.39421
H	1.53590	-5.03340	-2.78457
C	-0.01591	-3.50810	-2.74287
H	-0.68273	-4.08048	-3.41322
C	-0.44775	-2.24424	-2.26913
C	-2.09402	-0.27628	-2.91343
H	-3.05712	-0.15454	-3.45531
H	-2.20234	0.22494	-1.92412
C	-0.99804	0.44068	-3.66111
C	-1.03498	0.67544	-5.04833
H	-1.90408	0.33135	-5.63124
C	0.02573	1.35170	-5.66864
H	0.00597	1.54246	-6.75445
C	1.10311	1.79150	-4.88464
H	1.95109	2.33965	-5.32326
C	1.08051	1.52961	-3.50821
H	1.87349	1.88190	-2.82937
C	-1.73931	0.38859	2.08540
C	-2.44245	-0.46447	2.96362
H	-2.00870	-1.43002	3.26833
C	-3.70452	-0.08629	3.45575
H	-4.24560	-0.76047	4.14067
C	-4.27082	1.14294	3.07986
H	-5.26048	1.43764	3.46739
C	-3.56967	1.99664	2.20920
H	-4.00603	2.96471	1.91167
C	-2.31078	1.62760	1.70849
H	-1.75909	2.29928	1.02567
C	1.09921	1.01412	2.37817
C	0.80453	1.42825	3.69487
H	-0.15697	1.15286	4.15859
C	1.73031	2.20176	4.41463
H	1.48894	2.52713	5.44019
C	2.95361	2.56767	3.82641
H	3.67539	3.18174	4.39028
C	3.24826	2.16320	2.51311
H	4.19756	2.46377	2.04022
C	2.32349	1.39390	1.78854
H	2.53903	1.10597	0.74583
C	0.24584	-1.75355	2.01508
C	1.21250	-2.03705	3.00260
H	1.80538	-1.22114	3.44494
C	1.42559	-3.36094	3.42751
H	2.18658	-3.56894	4.19791

C	0.67334	-4.41043	2.87601
H	0.84224	-5.44785	3.20952
C	-0.29134	-4.13471	1.88995
H	-0.87799	-4.95426	1.44366
C	-0.49823	-2.81721	1.45529
H	-1.23881	-2.61352	0.66574
O	-0.19443	2.47227	-0.37907
N	0.06104	0.86622	-2.92455
N	0.87193	3.19361	-0.74866
P	-0.06738	-0.03652	1.40697
Pd	0.07285	0.40992	-0.84223
C	-1.84106	-1.79223	-2.70393
H	-2.09281	-2.32376	-3.64881
H	-2.59505	-2.13971	-1.95722
O	0.76882	4.37986	-0.50972

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.18	0.48487	YES	YES
8	a	22.15	0.92819	YES	YES
9	a	23.60	0.57559	YES	YES
10	a	36.83	1.22884	YES	YES
11	a	39.68	0.63004	YES	YES
12	a	41.48	0.47811	YES	YES
13	a	43.49	0.82854	YES	YES
14	a	50.57	0.49965	YES	YES
15	a	52.69	0.14086	YES	YES
16	a	54.28	0.24635	YES	YES
17	a	64.74	2.19653	YES	YES
18	a	70.77	1.18170	YES	YES
19	a	84.28	0.71792	YES	YES
20	a	85.50	0.42120	YES	YES
21	a	98.22	2.09896	YES	YES
22	a	107.15	0.88890	YES	YES
23	a	126.66	1.30495	YES	YES
24	a	143.96	0.25896	YES	YES
25	a	149.71	1.27314	YES	YES
26	a	158.74	3.28247	YES	YES
27	a	177.78	0.74724	YES	YES
28	a	187.29	0.69786	YES	YES
29	a	192.72	0.15869	YES	YES
30	a	209.99	0.82205	YES	YES
31	a	213.15	2.98867	YES	YES
32	a	226.92	1.08319	YES	YES
33	a	230.44	0.88558	YES	YES
34	a	238.92	1.33456	YES	YES
35	a	243.88	2.48569	YES	YES
36	a	252.23	0.54567	YES	YES
37	a	265.17	0.69194	YES	YES
38	a	273.83	2.07255	YES	YES
39	a	309.79	3.98198	YES	YES
40	a	332.39	18.47681	YES	YES
41	a	379.65	1.73819	YES	YES
42	a	395.51	0.12329	YES	YES
43	a	397.09	0.23649	YES	YES
44	a	401.52	0.41725	YES	YES
45	a	413.81	0.26418	YES	YES
46	a	427.07	14.54902	YES	YES
47	a	432.67	7.37372	YES	YES
48	a	439.33	2.12666	YES	YES
49	a	445.36	12.85747	YES	YES
50	a	451.73	4.30256	YES	YES

[Pd(2-PhCH$_2$Py)(NO$_2$)(PPh$_3$)] (*N*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -1925.7711326310
SCF Energy (au) PBE0/def2-TZVPP -1925.433182431
Zero Point Energy (au) 0.4898810
Chemical potential (kJ mol^{-1}) 1101.12

xyz Coordinates

64

N	0.24646	-1.46785	-1.59306
C	1.42814	-2.07950	-1.33364
H	2.08612	-1.56337	-0.61723
C	1.81717	-3.28192	-1.92917
H	2.79273	-3.72585	-1.67913
C	0.93939	-3.88291	-2.84336
H	1.20499	-4.82603	-3.34879
C	-0.28288	-3.25470	-3.10531
H	-0.99543	-3.69800	-3.81887
C	-0.62507	-2.04184	-2.46673
C	-2.10558	0.10303	-2.93003
H	-3.04295	0.29041	-3.49963
H	-2.22966	0.59374	-1.93954
C	-0.91562	0.73654	-3.62771
C	-0.91479	0.99333	-5.01518
H	-1.80984	0.74777	-5.61534
C	0.20484	1.57386	-5.63638
H	0.19044	1.77693	-6.72049
C	1.33165	1.90906	-4.86732
H	2.20820	2.38023	-5.34494
C	1.33910	1.66028	-3.47969
H	2.21235	1.95628	-2.87444
C	-1.76872	0.21196	2.13029
C	-2.33512	-0.61884	3.12272
H	-1.75294	-1.45178	3.54922
C	-3.64958	-0.39361	3.56689
H	-4.08371	-1.04901	4.34058
C	-4.40519	0.66453	3.03259
H	-5.43592	0.83954	3.38390
C	-3.84422	1.49519	2.04691
H	-4.43009	2.32766	1.62314
C	-2.53444	1.27165	1.59030
H	-2.09240	1.93357	0.82260
C	0.99905	1.01727	2.64600
C	0.61263	1.28991	3.97672
H	-0.35505	0.92408	4.35691
C	1.45363	2.03688	4.81721
H	1.14072	2.25082	5.85271
C	2.68632	2.51637	4.33880
H	3.34231	3.10817	4.99883
C	3.07260	2.25464	3.01323
H	4.02691	2.64653	2.62501
C	2.23132	1.51309	2.16612
H	2.51587	1.35091	1.11391
C	0.38394	-1.73730	1.96103
C	1.51225	-2.05751	2.74663
H	2.14099	-1.25194	3.15809
C	1.83575	-3.39960	3.01655
H	2.71842	-3.63168	3.63548

C	1.03591	-4.43785	2.51138
H	1.28752	-5.48895	2.72967
C	-0.09014	-4.12838	1.72692
H	-0.72531	-4.93603	1.32660
C	-0.40835	-2.79055	1.44593
H	-1.29277	-2.56096	0.82818
N	0.34140	2.54593	-0.50757
C	0.22538	1.06930	-2.85857
O	-0.67648	3.21226	-0.27672
O	1.47182	3.04047	-0.54088
P	-0.04052	0.00775	1.49811
Pd	0.17810	0.54781	-0.86257
C	-1.99149	-1.43450	-2.72974
H	-2.39430	-1.95017	-3.62729
H	-2.66069	-1.73069	-1.88573

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.59	0.45325	YES	YES
8	a	15.72	0.30089	YES	YES
9	a	21.61	0.29087	YES	YES
10	a	30.04	0.43557	YES	YES
11	a	39.05	0.18591	YES	YES
12	a	42.53	0.39833	YES	YES
13	a	44.76	0.26310	YES	YES
14	a	51.05	0.03764	YES	YES
15	a	58.35	0.50629	YES	YES
16	a	60.33	0.51107	YES	YES
17	a	67.78	0.32688	YES	YES
18	a	76.55	0.61289	YES	YES
19	a	78.02	0.19460	YES	YES
20	a	88.35	0.42275	YES	YES
21	a	102.08	2.58563	YES	YES
22	a	106.58	3.34142	YES	YES
23	a	122.38	0.63552	YES	YES
24	a	126.85	0.09855	YES	YES
25	a	138.34	0.01225	YES	YES
26	a	171.50	0.38578	YES	YES
27	a	183.72	0.62789	YES	YES
28	a	187.24	0.26518	YES	YES
29	a	194.51	1.43213	YES	YES
30	a	203.96	2.69721	YES	YES
31	a	218.38	1.59615	YES	YES
32	a	230.46	3.26455	YES	YES
33	a	241.08	1.01159	YES	YES
34	a	249.45	1.09903	YES	YES
35	a	255.10	0.21492	YES	YES
36	a	266.53	0.42248	YES	YES
37	a	285.42	1.96562	YES	YES
38	a	301.10	3.03329	YES	YES
39	a	313.49	0.93885	YES	YES
40	a	367.60	1.85024	YES	YES
41	a	395.97	0.36789	YES	YES
42	a	398.79	0.41560	YES	YES
43	a	402.11	0.24397	YES	YES
44	a	403.47	0.27145	YES	YES
45	a	415.74	9.79069	YES	YES
46	a	425.58	10.61682	YES	YES
47	a	436.09	5.64704	YES	YES
48	a	441.98	6.65183	YES	YES
49	a	452.43	2.60691	YES	YES
50	a	476.68	2.24388	YES	YES

[Pd(2-PhCH$_2$Py)(NO$_2$)(PPh$_3$)] (*O*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -1925.7519014620
SCF Energy (au) PBE0/def2-TZVPP -1925.415631266
Zero Point Energy (au) 0.4882682
Chemical potential (kJ mol^{-1}) 1095.25

xyz Coordinates

64

N	0.33111	-1.47723	-1.63009
C	1.54241	-2.00502	-1.31463
H	2.14899	-1.41786	-0.60908
C	2.01686	-3.20796	-1.83994
H	3.01089	-3.57710	-1.54526
C	1.19932	-3.90748	-2.74010
H	1.53175	-4.85738	-3.18995
C	-0.05019	-3.36734	-3.05898
H	-0.71824	-3.88858	-3.76278
C	-0.48362	-2.14635	-2.49294
C	-2.15548	-0.13974	-2.97972
H	-3.10246	-0.03515	-3.55427
H	-2.34031	0.30667	-1.97725
C	-1.03229	0.62998	-3.64901
C	-1.06350	0.96300	-5.01964
H	-1.93940	0.67695	-5.62997
C	-0.00020	1.66848	-5.60961
H	-0.03791	1.92907	-6.68059
C	1.10016	2.05278	-4.82534
H	1.93228	2.61954	-5.27779
C	1.13886	1.73213	-3.45282
H	1.98898	2.06759	-2.83630
C	-1.69505	0.38771	2.27054
C	-2.35700	-0.43817	3.20543
H	-1.92005	-1.40592	3.50037
C	-3.58085	-0.03146	3.76577
H	-4.09000	-0.68380	4.49501
C	-4.15040	1.20038	3.40179
H	-5.11027	1.51755	3.84252
C	-3.49209	2.02636	2.47334
H	-3.93242	2.99454	2.18266
C	-2.27214	1.62682	1.90355
H	-1.75467	2.27357	1.17172
C	1.17703	0.84927	2.48589
C	0.98125	1.15226	3.85083
H	0.04091	0.86539	4.35014
C	1.97662	1.82968	4.57353
H	1.81265	2.06759	5.63774
C	3.17240	2.21319	3.94050
H	3.94883	2.75266	4.50802
C	3.36867	1.92391	2.57963
H	4.29417	2.24257	2.07247
C	2.37311	1.25020	1.85252
H	2.50963	1.06006	0.77409
C	0.17121	-1.83458	1.95538
C	1.22018	-2.26608	2.79565
H	1.89914	-1.52659	3.24940
C	1.40175	-3.63506	3.06383
H	2.22511	-3.95507	3.72413

C	0.53652	-4.58860	2.50297
H	0.67707	-5.66071	2.71906
C	-0.51186	-4.16823	1.66402
H	-1.19525	-4.90997	1.21814
C	-0.68723	-2.80429	1.38477
H	-1.50838	-2.48558	0.72027
O	-0.20096	2.41730	-0.35416
C	0.07974	1.01868	-2.86692
N	0.89477	3.20653	-0.50298
P	-0.07963	-0.06134	1.48500
Pd	0.04707	0.46508	-0.90819
C	-1.88449	-1.65849	-2.82604
H	-2.17300	-2.17320	-3.76765
H	-2.57187	-2.06280	-2.04305
O	0.71612	4.32186	-0.07178

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.85	0.97749	YES	YES
8	a	17.93	0.18100	YES	YES
9	a	21.72	0.54182	YES	YES
10	a	32.76	0.20653	YES	YES
11	a	39.70	0.12804	YES	YES
12	a	42.31	0.98683	YES	YES
13	a	44.02	0.12158	YES	YES
14	a	47.97	0.38350	YES	YES
15	a	51.64	0.33224	YES	YES
16	a	53.91	0.26350	YES	YES
17	a	59.16	1.53159	YES	YES
18	a	65.78	1.08756	YES	YES
19	a	73.75	0.10712	YES	YES
20	a	81.31	0.25550	YES	YES
21	a	87.56	0.55890	YES	YES
22	a	111.71	1.76397	YES	YES
23	a	117.59	2.08519	YES	YES
24	a	132.43	0.13843	YES	YES
25	a	148.56	0.36992	YES	YES
26	a	163.60	1.22356	YES	YES
27	a	181.18	0.51013	YES	YES
28	a	183.26	0.92544	YES	YES
29	a	196.39	0.62553	YES	YES
30	a	201.01	1.27347	YES	YES
31	a	206.58	4.36326	YES	YES
32	a	221.29	0.33882	YES	YES
33	a	236.64	1.38360	YES	YES
34	a	240.38	0.97733	YES	YES
35	a	249.43	0.42695	YES	YES
36	a	257.80	1.01229	YES	YES
37	a	263.15	1.53741	YES	YES
38	a	265.35	0.83727	YES	YES
39	a	306.73	1.88228	YES	YES
40	a	356.79	8.13252	YES	YES
41	a	374.87	2.91530	YES	YES
42	a	395.68	0.32613	YES	YES
43	a	397.72	0.47487	YES	YES
44	a	401.56	0.11045	YES	YES
45	a	410.06	0.09371	YES	YES
46	a	414.30	6.79218	YES	YES
47	a	428.00	9.93491	YES	YES
48	a	439.68	10.65106	YES	YES
49	a	442.50	2.85243	YES	YES
50	a	456.37	2.00364	YES	YES

[Pd(8MQ)(OAc)(PPh_3)] (*cis*)

SCF Energy (au) (RI)BP86/SV(P) -929.3794214489
SCF Energy (au) PBE0/def2-TZVPP -929.1949321643
Zero Point Energy (au) 0.2442443
Chemical potential (kJ mol^{-1}) 509.41

xyz Coordinates

33

Pd	0.01925	-0.15372	-0.59005
N	1.83126	-0.03173	-1.87821
O	-0.88224	-0.55780	-2.38266
N	0.87689	0.10838	1.22484
C	-1.69113	-0.33680	0.47968
C	-1.36604	-0.23645	1.95185
C	-2.28149	-0.35867	2.99939
C	-1.86737	-0.23242	4.35461
C	1.95613	-0.20286	-3.03087
C	0.43482	0.14837	3.64697
C	-0.53872	0.01923	4.68022
C	1.92014	-0.42739	-4.46394
C	-0.00677	0.01114	2.28832
C	2.17090	0.34255	1.46558
H	2.82274	0.40494	0.57997
C	1.82054	0.40106	3.86758
H	2.19649	0.51518	4.89819
C	2.67987	0.49796	2.78035
H	3.75540	0.69073	2.91682
C	-1.35200	0.31668	-3.24232
H	2.45905	0.37432	-5.01251
H	0.82616	-0.40396	-4.73702
H	2.35942	-1.41448	-4.72256
H	-3.34327	-0.55399	2.77297
H	-2.61660	-0.33445	5.15714
H	-0.22394	0.11888	5.73199
H	-2.14969	-1.31603	0.21292
H	-2.38819	0.47000	0.15879
C	-2.21257	1.46334	-2.69839
O	-1.13996	0.21881	-4.46032
H	-3.09709	1.05714	-2.15946
H	-2.55610	2.11016	-3.53067
H	-1.63393	2.07231	-1.96896

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.68	0.08796	YES	YES
8	a	31.96	1.81149	YES	YES
9	a	44.49	6.42169	YES	YES
10	a	54.68	0.86307	YES	YES
11	a	70.14	3.85015	YES	YES
12	a	100.77	1.44974	YES	YES
13	a	116.00	1.33281	YES	YES
14	a	119.55	0.38418	YES	YES
15	a	134.98	15.42435	YES	YES
16	a	143.79	8.36876	YES	YES
17	a	162.05	1.53444	YES	YES
18	a	169.91	5.24991	YES	YES
19	a	209.47	8.66023	YES	YES
20	a	213.68	6.52056	YES	YES
21	a	225.36	1.36913	YES	YES
22	a	229.55	1.60953	YES	YES
23	a	236.47	0.67339	YES	YES
24	a	280.91	2.69301	YES	YES
25	a	359.23	29.61027	YES	YES
26	a	374.66	3.21448	YES	YES
27	a	397.00	8.89029	YES	YES
28	a	418.35	2.00680	YES	YES
29	a	426.99	1.11291	YES	YES
30	a	446.88	0.24760	YES	YES
31	a	469.58	0.03347	YES	YES
32	a	497.69	0.10537	YES	YES
33	a	529.22	0.32190	YES	YES
34	a	530.72	0.65797	YES	YES
35	a	576.90	0.47649	YES	YES
36	a	583.99	7.00857	YES	YES
37	a	621.49	0.25298	YES	YES
38	a	628.30	1.02018	YES	YES
39	a	648.64	11.53215	YES	YES
40	a	667.42	9.39698	YES	YES
41	a	723.85	1.15309	YES	YES
42	a	754.42	3.19288	YES	YES
43	a	783.03	50.68416	YES	YES
44	a	798.41	1.22387	YES	YES
45	a	831.14	13.87545	YES	YES
46	a	894.82	3.23532	YES	YES
47	a	895.12	0.60612	YES	YES
48	a	900.33	8.64511	YES	YES
49	a	925.98	0.05499	YES	YES
50	a	947.20	0.25812	YES	YES

Compound 33 (*N*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P)	-906.0579555018
SCF Energy (au) PBE0/def2-TZVPP	-905.8660134102
Zero Point Energy (au)	0.2059819
Chemical potential (kJ mol^{-1})	410.30

xyz Coordinates

29

Pd	-0.24524	0.01010	-0.82133
N	1.30062	-0.14216	-2.26904
N	-1.58199	0.00609	-2.36815
N	0.91902	0.04514	0.92605
C	-1.79172	0.16135	0.50381
O	-2.57678	-0.72296	-2.33594
C	-1.25997	0.07046	1.91126
C	-2.04659	0.02124	3.06567
C	-1.46212	-0.03691	4.36069
C	1.84750	-0.12692	-3.30150
C	0.76783	-0.00830	3.38087
C	-0.08140	-0.04488	4.52481
C	2.46688	-0.08342	-4.61853
C	0.15648	0.04002	2.08009
C	2.24936	0.02354	1.01852
H	2.80357	0.02670	0.06590
C	2.19156	-0.02752	3.44027
H	2.69397	-0.06131	4.42199
C	2.92893	-0.00806	2.26362
H	4.02993	-0.02332	2.27697
O	-1.31367	0.74203	-3.32937
H	3.32971	0.61710	-4.62568
H	1.71515	0.26781	-5.35906
H	2.82139	-1.09253	-4.92070
H	-3.14518	0.03449	2.96740
H	-2.11843	-0.07185	5.24611
H	0.37022	-0.08462	5.52973
H	-2.53409	-0.63234	0.26834
H	-2.28764	1.14525	0.32842

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.72	0.99576	YES	YES
8	a	28.31	5.45380	YES	YES
9	a	39.00	3.22213	YES	YES
10	a	47.60	0.37486	YES	YES
11	a	55.12	0.43152	YES	YES
12	a	69.10	1.44028	YES	YES
13	a	95.05	1.40944	YES	YES
14	a	143.83	0.13343	YES	YES
15	a	164.18	0.73767	YES	YES
16	a	174.47	0.03026	YES	YES
17	a	189.06	3.09718	YES	YES
18	a	207.32	1.33816	YES	YES
19	a	226.33	2.05137	YES	YES
20	a	229.27	1.91835	YES	YES
21	a	245.71	1.82955	YES	YES
22	a	299.04	9.62067	YES	YES
23	a	312.04	1.23563	YES	YES
24	a	379.48	0.60146	YES	YES
25	a	383.69	1.92682	YES	YES
26	a	416.23	0.80093	YES	YES
27	a	426.97	0.75859	YES	YES
28	a	467.45	0.24161	YES	YES
29	a	495.75	0.23957	YES	YES
30	a	523.46	0.50216	YES	YES
31	a	527.54	1.12600	YES	YES
32	a	548.75	4.95712	YES	YES
33	a	577.07	2.90191	YES	YES
34	a	619.15	0.83963	YES	YES
35	a	631.58	1.48941	YES	YES
36	a	661.29	14.27502	YES	YES
37	a	716.36	1.92238	YES	YES
38	a	751.74	2.86018	YES	YES
39	a	785.19	51.72092	YES	YES
40	a	799.48	1.03181	YES	YES
41	a	813.86	75.32450	YES	YES
42	a	832.30	11.83940	YES	YES
43	a	889.97	0.10117	YES	YES
44	a	893.81	0.15528	YES	YES
45	a	923.17	0.11293	YES	YES
46	a	949.54	2.44720	YES	YES
47	a	962.11	0.14283	YES	YES
48	a	972.75	0.59250	YES	YES
49	a	1012.61	4.99718	YES	YES
50	a	1022.95	5.26783	YES	YES

Compound 33 (*N*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P)	-906.0547775410
SCF Energy (au) PBE0/def2-TZVPP	-905.8636767570
Zero Point Energy (au)	0.2062457
Chemical potential (kJ mol^{-1})	412.83

xyz Coordinates

29

Pd	-0.09844	0.10081	-0.85397
N	-1.05210	0.06864	-2.59126
N	1.72713	-0.16481	-1.97426
N	0.73573	0.13032	1.02408
C	-1.86071	0.33261	0.24217
O	1.65170	-0.76735	-3.05337
C	-1.55812	0.07208	1.69184
C	-2.49955	-0.11157	2.70840
C	-2.10004	-0.28166	4.06302
C	-1.47462	-0.00677	-3.67612
C	0.24446	-0.09286	3.42177
C	-0.75705	-0.25770	4.42332
C	-1.95356	-0.12358	-5.04538
C	-0.18164	0.04243	2.05735
C	2.04327	0.15416	1.29352
H	2.69819	0.24958	0.40455
C	1.64637	-0.07515	3.67869
H	2.00905	-0.17113	4.71629
C	2.53565	0.05965	2.62135
H	3.62399	0.08284	2.78714
O	2.81540	0.29034	-1.56747
H	-1.84698	0.84726	-5.57629
H	-3.02270	-0.42622	-5.06634
H	-1.35143	-0.88745	-5.58439
H	-3.57367	-0.10926	2.45664
H	-2.87172	-0.42221	4.83828
H	-0.45093	-0.37806	5.47548
H	-2.69902	-0.29558	-0.13265
H	-2.14248	1.40249	0.08925

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.00	1.10840	YES	YES
8	a	28.75	1.53348	YES	YES
9	a	37.37	6.48857	YES	YES
10	a	40.14	3.64327	YES	YES
11	a	51.14	0.39813	YES	YES
12	a	94.39	1.25924	YES	YES
13	a	134.01	2.00177	YES	YES
14	a	155.35	5.06411	YES	YES
15	a	166.94	0.23282	YES	YES
16	a	201.01	2.60511	YES	YES
17	a	202.86	0.39983	YES	YES
18	a	216.88	7.83237	YES	YES
19	a	233.23	8.91397	YES	YES
20	a	235.97	0.73010	YES	YES
21	a	257.90	0.34364	YES	YES
22	a	286.10	8.92160	YES	YES
23	a	331.28	5.22535	YES	YES
24	a	388.62	0.88670	YES	YES
25	a	403.14	5.94635	YES	YES
26	a	414.19	0.82983	YES	YES
27	a	428.61	0.69429	YES	YES
28	a	462.99	7.46830	YES	YES
29	a	473.75	0.76332	YES	YES
30	a	501.69	1.28457	YES	YES
31	a	519.72	9.64512	YES	YES
32	a	530.55	0.88620	YES	YES
33	a	581.78	1.86049	YES	YES
34	a	600.82	6.87189	YES	YES
35	a	626.07	2.96400	YES	YES
36	a	649.80	18.90940	YES	YES
37	a	724.54	0.78596	YES	YES
38	a	754.83	10.13652	YES	YES
39	a	790.58	40.44082	YES	YES
40	a	798.75	5.60161	YES	YES
41	a	812.50	47.53477	YES	YES
42	a	834.87	15.88367	YES	YES
43	a	890.83	0.63851	YES	YES
44	a	895.06	0.28582	YES	YES
45	a	960.43	0.00516	YES	YES
46	a	966.81	15.94767	YES	YES
47	a	968.59	0.30765	YES	YES
48	a	1008.08	1.09293	YES	YES
49	a	1012.37	5.76124	YES	YES
50	a	1019.89	5.46912	YES	YES

Compound 33 (*O*-bound isomer, *cis*)

SCF Energy (au) (RI)BP86/SV(P) -906.0425059711
SCF Energy (au) PBE0/def2-TZVPP -905.8523027963
Zero Point Energy (au) 0.2046258
Chemical potential (kJ mol^{-1}) 403.43

xyz Coordinates

29

Pd	-0.25373	-0.00266	-0.73262
N	1.36440	0.00633	-2.09812
O	-1.65628	-0.00415	-2.20808
N	0.83739	-0.00725	1.00154
C	-1.83955	-0.01354	0.53305
C	-1.34931	-0.00737	1.95917
C	-2.15881	-0.00408	3.09810
C	-1.59423	0.00611	4.40305
C	2.02531	0.00362	-3.06053
C	0.65370	0.00576	3.45913
C	-0.21590	0.01164	4.58860
C	2.75809	-0.00669	-4.31832
C	0.06067	-0.00330	2.15091
C	2.16909	-0.00601	1.11616
H	2.73757	-0.01002	0.17295
C	2.07655	0.00859	3.54031
H	2.56659	0.01644	4.52850
C	2.82737	0.00186	2.37181
H	3.92818	0.00352	2.39885
N	-1.19654	0.01993	-3.47568
H	3.10013	1.01820	-4.57862
H	2.07966	-0.36712	-5.12301
H	3.64207	-0.67739	-4.26176
H	-3.25556	-0.00672	2.98102
H	-2.26356	0.01070	5.27907
H	0.21893	0.01976	5.60159
H	-2.44236	-0.91970	0.29843
H	-2.46221	0.87850	0.29726
O	-2.09458	0.00987	-4.29094

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.44	3.52930	YES	YES
8	a	17.33	1.05089	YES	YES
9	a	23.67	0.98088	YES	YES
10	a	43.87	0.68465	YES	YES
11	a	50.30	3.99389	YES	YES
12	a	81.92	1.03177	YES	YES
13	a	92.15	0.44861	YES	YES
14	a	143.58	0.00695	YES	YES
15	a	159.09	0.90012	YES	YES
16	a	174.75	0.26949	YES	YES
17	a	185.02	0.61263	YES	YES
18	a	201.20	7.89736	YES	YES
19	a	220.11	0.57243	YES	YES
20	a	223.22	5.50228	YES	YES
21	a	233.18	0.01808	YES	YES
22	a	238.56	0.36876	YES	YES
23	a	296.97	0.62093	YES	YES
24	a	360.83	4.50752	YES	YES
25	a	367.06	20.11877	YES	YES
26	a	382.51	0.29323	YES	YES
27	a	420.71	2.43707	YES	YES
28	a	429.57	0.70216	YES	YES
29	a	468.54	0.01875	YES	YES
30	a	498.74	0.26591	YES	YES
31	a	529.86	0.31954	YES	YES
32	a	530.46	0.56032	YES	YES
33	a	577.84	1.68780	YES	YES
34	a	621.70	0.02754	YES	YES
35	a	636.46	1.17910	YES	YES
36	a	670.41	10.29368	YES	YES
37	a	721.16	2.07513	YES	YES
38	a	753.72	2.59880	YES	YES
39	a	782.90	51.33440	YES	YES
40	a	798.61	3.87276	YES	YES
41	a	802.12	52.33195	YES	YES
42	a	830.54	13.38230	YES	YES
43	a	894.34	0.16157	YES	YES
44	a	894.74	0.44821	YES	YES
45	a	919.95	0.14613	YES	YES
46	a	951.30	17.94377	YES	YES
47	a	960.28	0.11150	YES	YES
48	a	970.12	556.47072	YES	YES
49	a	972.62	0.61318	YES	YES
50	a	1008.88	12.53810	YES	YES

Compound 33 (*O*-bound isomer, *trans*)

SCF Energy (au) (RI)BP86/SV(P)	-906.0430044044
SCF Energy (au) PBE0/def2-TZVPP	-905.8538940935
Zero Point Energy (au)	0.2052074
Chemical potential (kJ mol^{-1})	408.10

xyz Coordinates

29

Pd	-0.22908	0.02462	-0.85128
N	-1.28714	-0.00771	-2.53278
O	1.40116	-0.29000	-2.17881
N	0.71337	0.06296	0.96357
C	-1.91056	0.24366	0.31180
C	-1.53506	0.07598	1.76191
C	-2.42535	-0.01434	2.83440
C	-1.95577	-0.11783	4.17315
C	-1.77351	-0.04564	-3.59312
C	0.35436	-0.04426	3.39519
C	-0.59423	-0.12262	4.45664
C	-2.34408	-0.09911	-4.93175
C	-0.14383	0.03493	2.05172
C	2.03454	0.05925	1.15939
H	2.64839	0.11661	0.23661
C	1.76872	-0.05269	3.57290
H	2.18844	-0.11015	4.59178
C	2.59791	0.00989	2.46174
H	3.69429	0.01272	2.56399
N	2.60630	0.14126	-1.84899
H	-2.27811	0.89824	-5.41851
H	-3.41120	-0.40728	-4.89297
H	-1.78221	-0.83106	-5.55205
H	-3.51128	0.00422	2.64051
H	-2.68623	-0.18724	4.99622
H	-0.23317	-0.19554	5.49557
H	-2.70630	-0.47263	0.00539
H	-2.29301	1.27557	0.12214
O	3.44566	0.00237	-2.72246

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.00	0.24577	YES	YES
8	a	28.07	0.53502	YES	YES
9	a	35.68	4.51578	YES	YES
10	a	37.94	5.82285	YES	YES
11	a	47.66	2.41834	YES	YES
12	a	96.69	2.36212	YES	YES
13	a	112.85	3.48394	YES	YES
14	a	140.38	1.13300	YES	YES
15	a	165.50	0.40512	YES	YES
16	a	181.21	1.50986	YES	YES
17	a	195.58	4.23678	YES	YES
18	a	208.14	0.15485	YES	YES
19	a	220.63	4.41906	YES	YES
20	a	234.41	1.96493	YES	YES
21	a	237.80	2.00274	YES	YES
22	a	257.02	2.06944	YES	YES
23	a	302.91	15.90714	YES	YES
24	a	335.23	15.07155	YES	YES
25	a	391.97	0.47226	YES	YES
26	a	416.77	2.52354	YES	YES
27	a	420.15	0.70554	YES	YES
28	a	429.16	0.27603	YES	YES
29	a	472.56	0.35691	YES	YES
30	a	501.90	0.71525	YES	YES
31	a	524.55	3.36722	YES	YES
32	a	530.49	1.78624	YES	YES
33	a	580.84	0.48209	YES	YES
34	a	615.15	3.49123	YES	YES
35	a	627.07	2.56390	YES	YES
36	a	671.16	10.21719	YES	YES
37	a	726.35	2.06745	YES	YES
38	a	757.79	11.90231	YES	YES
39	a	791.33	37.98115	YES	YES
40	a	799.17	1.46537	YES	YES
41	a	810.18	15.26242	YES	YES
42	a	836.36	16.23033	YES	YES
43	a	893.86	0.28513	YES	YES
44	a	895.44	0.20315	YES	YES
45	a	960.47	0.56606	YES	YES
46	a	963.69	18.41866	YES	YES
47	a	969.94	0.54845	YES	YES
48	a	1013.70	5.92550	YES	YES
49	a	1015.13	19.30616	YES	YES
50	a	1019.15	5.53115	YES	YES

Compound 34 (*cis*)

SCF Energy (au) (RI)BP86/SV(P) -981.1956293530
SCF Energy (au) PBE0/def2-TZVPP -981.0104853842
Zero Point Energy (au) 0.2105540
Chemical potential (kJ mol^{-1}) 420.60

xyz Coordinates

30

Pd	-0.12954	-0.24696	-0.57554
N	1.56565	-0.28491	-1.89803
O	-1.38534	-0.56639	-2.17580
N	0.85575	-0.07562	1.19783
C	-1.78657	-0.13397	0.58604
C	-1.37725	0.00850	2.03152
C	-2.24729	0.11813	3.11872
C	-1.75258	0.24744	4.44620
C	2.08642	-0.05743	-2.91894
C	0.54289	0.16294	3.62934
C	-0.38624	0.27015	4.70495
C	2.63449	0.28206	-4.22357
C	0.01951	0.03223	2.29867
C	2.17974	-0.05890	1.37799
H	2.79434	-0.14878	0.46876
C	1.95977	0.17723	3.78298
H	2.39797	0.27696	4.79034
C	2.77088	0.06701	2.66085
H	3.86872	0.07413	2.74532
N	-1.32970	0.29639	-3.19983
H	3.55729	0.89224	-4.12088
H	1.86700	0.87422	-4.76993
H	2.86906	-0.63456	-4.80619
H	-3.33634	0.10346	2.94449
H	-2.46823	0.33151	5.28074
H	-0.00732	0.37213	5.73499
H	-2.37940	-1.05890	0.40381
H	-2.38831	0.73404	0.23270
O	-0.59754	1.29666	-3.10686
O	-2.02436	0.01642	-4.17317

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.24	1.92562	YES	YES
8	a	27.81	4.34642	YES	YES
9	a	38.50	4.79499	YES	YES
10	a	53.08	0.42458	YES	YES
11	a	64.14	2.88959	YES	YES
12	a	67.46	1.23672	YES	YES
13	a	93.99	0.05936	YES	YES
14	a	130.44	2.63657	YES	YES
15	a	146.58	0.79190	YES	YES
16	a	158.28	4.21628	YES	YES
17	a	173.10	0.22492	YES	YES
18	a	179.68	2.16241	YES	YES
19	a	209.40	5.11150	YES	YES
20	a	224.01	0.98849	YES	YES
21	a	228.88	2.25773	YES	YES
22	a	232.33	0.49414	YES	YES
23	a	284.35	0.59722	YES	YES
24	a	329.62	14.47303	YES	YES
25	a	362.34	5.66188	YES	YES
26	a	384.57	0.71307	YES	YES
27	a	418.63	1.35127	YES	YES
28	a	428.25	0.84014	YES	YES
29	a	468.70	0.03487	YES	YES
30	a	498.34	0.16317	YES	YES
31	a	528.69	0.33405	YES	YES
32	a	530.66	0.48470	YES	YES
33	a	577.73	1.32349	YES	YES
34	a	621.43	0.03707	YES	YES
35	a	632.17	0.91507	YES	YES
36	a	670.60	9.76459	YES	YES
37	a	697.67	1.31363	YES	YES
38	a	722.96	1.35068	YES	YES
39	a	744.01	1.36750	YES	YES
40	a	754.76	3.12483	YES	YES
41	a	777.52	11.49217	YES	YES
42	a	783.27	49.90242	YES	YES
43	a	798.61	1.11105	YES	YES
44	a	831.59	12.62391	YES	YES
45	a	895.42	0.07643	YES	YES
46	a	896.15	0.41479	YES	YES
47	a	922.16	0.17324	YES	YES
48	a	948.09	8.49963	YES	YES
49	a	957.41	194.21051	YES	YES
50	a	962.03	0.09113	YES	YES

Compound 34 (*trans*)

SCF Energy (au) (RI)BP86/SV(P)	-981.1999967255
SCF Energy (au) PBE0/def2-TZVPP	-981.0156500325
Zero Point Energy (au)	0.2110517
Chemical potential (kJ mol^{-1})	421.76

xyz Coordinates

30

Pd	-0.33418	-0.19655	-0.63541
N	-1.43880	-0.21147	-2.28427
O	1.49028	-0.51864	-1.70010
N	0.71441	-0.17017	1.09671
C	-1.94859	0.01826	0.61112
C	-1.45363	0.12033	2.03723
C	-2.24942	0.31113	3.16885
C	-1.67488	0.38561	4.46862
C	-1.92193	-0.14215	-3.34391
C	0.55502	0.07412	3.53391
C	-0.30168	0.26864	4.65669
C	-2.45839	-0.01595	-4.69071
C	-0.05014	0.00696	2.23504
C	2.04086	-0.29103	1.18693
H	2.56485	-0.43535	0.22551
C	1.97337	-0.05613	3.60410
H	2.47528	-0.00932	4.58547
C	2.70734	-0.23950	2.43873
H	3.80299	-0.34432	2.46325
N	1.82991	0.36303	-2.64645
H	-1.77971	0.62704	-5.29331
H	-3.46875	0.44637	-4.67143
H	-2.53006	-1.01252	-5.17777
H	-3.34246	0.40611	3.05385
H	-2.33385	0.53839	5.33926
H	0.13769	0.32619	5.66602
H	-2.62117	-0.86165	0.48174
H	-2.52216	0.92713	0.31603
O	1.03086	1.27129	-2.92789
O	2.92933	0.20192	-3.17452

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.91	0.63739	YES	YES
8	a	28.20	4.57965	YES	YES
9	a	36.53	5.63133	YES	YES
10	a	41.94	1.22818	YES	YES
11	a	52.41	2.63739	YES	YES
12	a	58.03	0.44240	YES	YES
13	a	83.11	2.05086	YES	YES
14	a	144.44	0.12459	YES	YES
15	a	152.47	2.90833	YES	YES
16	a	169.49	4.60186	YES	YES
17	a	179.37	3.42448	YES	YES
18	a	199.64	0.09078	YES	YES
19	a	218.54	5.65587	YES	YES
20	a	228.64	0.58509	YES	YES
21	a	235.12	0.57357	YES	YES
22	a	245.29	4.52523	YES	YES
23	a	307.63	18.21776	YES	YES
24	a	325.05	5.05141	YES	YES
25	a	389.45	2.78446	YES	YES
26	a	411.33	3.66285	YES	YES
27	a	418.86	0.05471	YES	YES
28	a	430.09	0.54314	YES	YES
29	a	472.43	0.07345	YES	YES
30	a	500.79	0.46419	YES	YES
31	a	526.90	0.79631	YES	YES
32	a	528.98	3.26273	YES	YES
33	a	579.50	0.29611	YES	YES
34	a	621.05	6.37740	YES	YES
35	a	623.18	1.02335	YES	YES
36	a	667.00	6.59779	YES	YES
37	a	704.63	1.35009	YES	YES
38	a	725.12	0.69897	YES	YES
39	a	732.33	6.16401	YES	YES
40	a	757.95	9.76928	YES	YES
41	a	784.45	6.40259	YES	YES
42	a	789.52	45.51605	YES	YES
43	a	799.31	0.78253	YES	YES
44	a	835.16	16.44575	YES	YES
45	a	896.98	0.26722	YES	YES
46	a	897.98	1.60830	YES	YES
47	a	955.46	0.13724	YES	YES
48	a	963.05	114.50404	YES	YES
49	a	968.80	125.20565	YES	YES
50	a	970.67	0.50643	YES	YES

[Pd(2-phpy)(OAc)$_2$]$_2$ (Ritter bimetallic dimer, head-to-head)

SCF Energy (au) (RI)BP86/SV(P) -2126.2446029620
SCF Energy (au) PBE0/def2-TZVPP -2125.849778620
Zero Point Energy (au) 0.5123556
Chemical potential (kJ mol^{-1}) 1135.92

xyz Coordinates

70

Pd	-0.18289	1.45433	-0.84265
Pd	-0.47697	-1.21176	-0.91425
O	-0.32316	3.63744	-0.99486
O	0.02266	5.74165	-1.50846
C	0.44493	4.57955	-1.48967
C	1.83490	4.22788	-2.00217
H	1.79764	3.35101	-2.68153
H	2.49188	3.95598	-1.14587
H	2.27138	5.10415	-2.52379
O	-0.79008	-3.24619	-1.56578
O	-1.34931	-4.12953	0.46063
C	-1.15848	-4.20443	-0.75681
C	-1.33086	-5.53800	-1.51171
H	-1.78641	-6.28927	-0.83551
H	-0.33730	-5.90220	-1.85377
H	-1.96221	-5.39970	-2.41491
O	-1.92012	1.41499	-2.17194
O	-2.46372	-0.72554	-1.66851
C	-2.66804	0.38644	-2.25645
C	-3.89868	0.48330	-3.14603
H	-3.67433	-0.02134	-4.11214
H	-4.16388	1.53969	-3.35002
H	-4.75215	-0.05647	-2.68563
O	0.99101	1.14851	-2.51677
O	0.29413	-0.98820	-2.84022
C	0.86320	0.08480	-3.21566
C	1.43315	0.12322	-4.61914
H	0.76280	0.73930	-5.25821
H	1.50246	-0.89757	-5.04320
H	2.42909	0.61315	-4.61348
C	1.32637	1.48149	0.46029
N	-1.07631	-1.38643	1.02092
N	-1.24484	1.87977	0.84470
C	-2.54723	2.21763	0.81185
H	-3.02717	2.16852	-0.17691
C	-3.22270	2.63144	1.96513
H	-4.28761	2.90166	1.90553
C	-2.50560	2.70722	3.17219
H	-3.00527	3.03086	4.09980
C	-1.14135	2.39689	3.18295
H	-0.55349	2.48925	4.10787
C	-0.50246	1.99702	1.99038
C	0.92391	1.74056	1.80081
C	1.89811	1.79614	2.82474
H	1.59957	1.99906	3.86668
C	3.25030	1.60576	2.51629
H	4.00844	1.65011	3.31475
C	3.63969	1.36756	1.18350
H	4.70562	1.22289	0.94007

C	2.68181	1.30852	0.15381
H	2.99483	1.12016	-0.88406
C	1.25909	-1.78340	-0.12005
C	2.42198	-2.08708	-0.83635
H	2.43799	-2.00554	-1.93353
C	3.56854	-2.51810	-0.14104
H	4.48693	-2.75532	-0.70457
C	3.54824	-2.65773	1.25963
H	4.45009	-2.99505	1.79568
C	2.37162	-2.39065	1.97188
H	2.35283	-2.53169	3.06507
C	1.21061	-1.96426	1.28889
C	-0.09584	-1.74777	1.90638
C	-0.43030	-1.92972	3.26291
H	0.35252	-2.22016	3.97874
C	-1.75539	-1.76974	3.68130
H	-2.02297	-1.92244	4.73959
C	-2.74191	-1.43351	2.73740
H	-3.79925	-1.32086	3.02014
C	-2.35902	-1.25476	1.40469
H	-3.07101	-1.01347	0.60043

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.01	0.94283	YES	YES
8	a	23.99	0.13496	YES	YES
9	a	31.41	1.31445	YES	YES
10	a	34.74	1.71956	YES	YES
11	a	39.68	1.41749	YES	YES
12	a	40.47	0.55234	YES	YES
13	a	42.96	1.35847	YES	YES
14	a	48.24	1.13359	YES	YES
15	a	50.07	1.86463	YES	YES
16	a	54.22	0.14527	YES	YES
17	a	57.81	0.29136	YES	YES
18	a	60.34	1.87017	YES	YES
19	a	66.72	0.30121	YES	YES
20	a	70.73	0.39870	YES	YES
21	a	76.53	0.36199	YES	YES
22	a	77.61	0.69144	YES	YES
23	a	88.15	1.66184	YES	YES
24	a	94.53	0.12378	YES	YES
25	a	113.61	0.51658	YES	YES
26	a	116.21	0.05527	YES	YES
27	a	118.37	0.24753	YES	YES
28	a	125.72	0.33808	YES	YES
29	a	132.45	1.97616	YES	YES
30	a	136.93	0.21835	YES	YES
31	a	139.29	0.29909	YES	YES
32	a	141.81	0.39619	YES	YES
33	a	145.50	3.50345	YES	YES
34	a	150.82	2.34625	YES	YES
35	a	163.16	0.34316	YES	YES
36	a	168.59	1.13743	YES	YES
37	a	178.89	1.17824	YES	YES
38	a	186.04	3.02315	YES	YES
39	a	194.89	5.57608	YES	YES
40	a	202.21	6.20776	YES	YES
41	a	205.87	15.48534	YES	YES
42	a	218.13	1.37728	YES	YES
43	a	220.03	31.78962	YES	YES
44	a	233.58	6.43862	YES	YES
45	a	242.77	6.14649	YES	YES
46	a	264.00	5.94802	YES	YES
47	a	267.41	2.64910	YES	YES
48	a	269.87	5.34359	YES	YES
49	a	273.86	4.45825	YES	YES
50	a	279.53	19.41204	YES	YES

[Pd(2-phpy)(OAc)$_2$]$_2$ (Ritter bimetallic dimer, head-to-tail)

SCF Energy (au) (RI)BP86/SV(P) -2126.2425494860
SCF Energy (au) PBE0/def2-TZVPP -2125.847914679
Zero Point Energy (au) 0.5123646
Chemical potential (kJ mol^{-1}) 1137.07

xyz Coordinates

70

Pd	-0.14617	1.40208	-1.08148
Pd	-0.49564	-1.26000	-0.97009
O	-0.07758	3.44943	-1.82524
O	0.29633	5.57212	-2.24209
C	0.43632	4.60430	-1.48591
C	1.20278	4.74470	-0.17122
H	2.11914	4.11453	-0.18320
H	0.57795	4.42320	0.68978
H	1.50049	5.80376	-0.03104
O	-0.91106	-3.31556	-1.47526
O	-1.13099	-4.13434	0.64270
C	-1.14251	-4.24624	-0.58650
C	-1.43977	-5.59965	-1.26325
H	-1.77256	-6.32995	-0.49830
H	-0.51933	-5.97671	-1.76055
H	-2.21637	-5.48355	-2.04871
O	-1.81198	1.34387	-2.31607
O	-2.48601	-0.72993	-1.68857
C	-2.62201	0.34812	-2.33799
C	-3.83048	0.49325	-3.24546
H	-3.66499	-0.12890	-4.15269
H	-3.98120	1.54705	-3.55140
H	-4.73358	0.09805	-2.73502
O	1.11290	0.85767	-2.77438
O	0.17945	-1.20268	-2.93734
C	0.84955	-0.21067	-3.40073
C	1.34331	-0.34245	-4.82998
H	0.72545	0.31866	-5.47690
H	1.26369	-1.38635	-5.19152
H	2.39089	0.01836	-4.89988
N	1.39391	1.43576	0.25324
N	-1.02948	-1.31884	0.99672
C	-1.17035	1.95271	0.53138
C	-2.52017	2.32698	0.55963
H	-3.11123	2.33614	-0.36814
C	-3.10693	2.71931	1.77829
H	-4.16905	3.01696	1.79686
C	-2.34913	2.74855	2.96510
H	-2.81704	3.05740	3.91381
C	-0.99051	2.40796	2.93459
H	-0.39527	2.45999	3.86126
C	-0.38430	2.02002	1.71729
C	1.04033	1.73259	1.54516
C	2.04025	1.78172	2.53823
H	1.76272	2.01910	3.57578
C	3.37543	1.54349	2.19464
H	4.16038	1.58399	2.96719
C	3.70561	1.26136	0.85689
H	4.74349	1.07493	0.54394

C	2.67817	1.21390	-0.09101
H	2.85283	0.99804	-1.15614
C	1.25533	-1.82474	-0.20959
C	2.39198	-2.17572	-0.94809
H	2.37045	-2.14862	-2.04770
C	3.55577	-2.59376	-0.27252
H	4.45049	-2.87165	-0.85523
C	3.57865	-2.67458	1.13244
H	4.49086	-3.00786	1.65351
C	2.42890	-2.35838	1.86967
H	2.44233	-2.45749	2.96763
C	1.25223	-1.94251	1.20765
C	-0.02886	-1.67276	1.86112
C	-0.31548	-1.79103	3.23422
H	0.48378	-2.07923	3.93267
C	-1.61946	-1.57410	3.69365
H	-1.85189	-1.67643	4.76617
C	-2.62815	-1.24074	2.77442
H	-3.66845	-1.07442	3.09111
C	-2.29003	-1.12402	1.42190
H	-3.02413	-0.87619	0.64055

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.58	2.19553	YES	YES
8	a	27.08	0.57432	YES	YES
9	a	28.70	1.51967	YES	YES
10	a	32.96	1.32928	YES	YES
11	a	35.24	0.34761	YES	YES
12	a	44.37	0.27645	YES	YES
13	a	47.05	1.20486	YES	YES
14	a	49.65	1.83639	YES	YES
15	a	51.91	0.33846	YES	YES
16	a	56.32	0.58162	YES	YES
17	a	59.80	0.21434	YES	YES
18	a	60.75	1.73613	YES	YES
19	a	63.51	0.76381	YES	YES
20	a	71.78	0.12154	YES	YES
21	a	77.60	0.17344	YES	YES
22	a	78.04	0.24269	YES	YES
23	a	89.42	2.77707	YES	YES
24	a	96.00	0.18206	YES	YES
25	a	110.92	0.69901	YES	YES
26	a	121.85	0.39391	YES	YES
27	a	127.17	3.24064	YES	YES
28	a	130.06	0.23335	YES	YES
29	a	131.03	0.57671	YES	YES
30	a	134.13	0.03038	YES	YES
31	a	142.34	0.45948	YES	YES
32	a	145.10	2.74702	YES	YES
33	a	152.50	0.74057	YES	YES
34	a	155.55	0.85899	YES	YES
35	a	159.76	0.32847	YES	YES
36	a	173.82	0.25297	YES	YES
37	a	184.81	1.51850	YES	YES
38	a	188.69	8.65420	YES	YES
39	a	193.91	4.21212	YES	YES
40	a	204.43	1.29479	YES	YES
41	a	207.59	8.02804	YES	YES
42	a	217.38	5.36806	YES	YES
43	a	221.03	44.57990	YES	YES
44	a	235.52	0.76499	YES	YES
45	a	248.43	1.53061	YES	YES
46	a	265.68	0.75927	YES	YES
47	a	268.15	6.55451	YES	YES
48	a	271.26	4.53129	YES	YES
49	a	273.45	1.55433	YES	YES
50	a	275.54	23.86338	YES	YES

Compound 59a

SCF Energy (au) (RI)BP86/SV(P) -2050.0934946350
SCF Energy (au) PBE0/def2-TZVPP -2049.718362610
Zero Point Energy (au) 0.5004945
Chemical potential (kJ mol^{-1}) 1109.09

xyz Coordinates

68

Pd	-0.24613	1.44670	-1.06256
Pd	-0.60537	-1.19054	-1.16359
O	-0.24962	3.65724	-1.15454
O	0.13283	5.74799	-1.72663
C	0.48672	4.56374	-1.75226
C	1.79111	4.14782	-2.42677
H	1.68469	3.18732	-2.97185
H	2.57705	4.01235	-1.64823
H	2.12777	4.95283	-3.11231
O	-1.12957	-3.20197	-1.79274
O	-0.62839	-4.27932	0.14983
C	-1.04833	-4.24556	-1.01424
C	-1.55312	-5.52243	-1.71446
H	-1.44551	-6.39032	-1.03288
H	-0.97843	-5.70102	-2.64893
H	-2.61923	-5.40089	-2.00520
O	-1.85997	1.49493	-2.34310
O	-2.61593	-0.58113	-1.82970
C	-2.71329	0.53594	-2.41451
C	-3.91306	0.78371	-3.31170
H	-3.73931	0.26738	-4.28187
H	-4.05960	1.86548	-3.50012
H	-4.82159	0.33780	-2.85670
O	1.10224	1.01736	-2.75493
O	0.13558	-1.00607	-3.08611
C	0.85118	-0.00975	-3.45537
C	1.41365	-0.07512	-4.86456
H	0.83096	0.61760	-5.51133
H	1.34630	-1.10033	-5.27828
H	2.46629	0.27734	-4.86702
N	1.24523	1.54569	0.31756
N	-1.17320	-1.47793	0.76592
C	-1.45903	1.85644	0.53498
C	-1.08070	2.14404	3.06671
C	-0.18550	2.27132	4.16524
C	-0.60594	1.91922	1.77330
C	0.80022	1.80087	1.59848
C	1.72448	1.94465	2.68678
C	1.19053	2.18165	3.98685
C	3.11363	1.84356	2.38618
H	3.85360	1.95442	3.19636
C	3.52253	1.61439	1.07810
H	4.58889	1.54430	0.81438
C	2.55003	1.46698	0.05642
H	2.82091	1.28771	-0.99645
C	1.23144	-1.76703	-0.46625
C	2.24434	-2.07796	1.88421
C	2.04973	-2.26346	3.28261
C	1.16281	-1.84733	1.03500

C	-0.13053	-1.76985	1.61728
C	-0.35801	-1.99066	3.01382
C	0.77742	-2.23424	3.84146
C	-1.70725	-1.96015	3.47093
H	-1.92341	-2.13859	4.53761
C	-2.73612	-1.71869	2.56943
H	-3.78917	-1.70829	2.88975
C	-2.42961	-1.47361	1.20605
H	-3.20558	-1.26726	0.45125
H	-2.28471	1.11864	0.60196
H	-1.84975	2.85913	0.25939
H	-0.59515	2.45595	5.17188
H	1.87971	2.29313	4.83964
H	-2.16533	2.24449	3.23746
H	2.01949	-1.08192	-0.84273
H	1.36673	-2.77567	-0.91052
H	0.63040	-2.40058	4.92106
H	2.92514	-2.45286	3.92541
H	3.26183	-2.14956	1.46513

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.41	0.54508	YES	YES
8	a	23.03	0.39672	YES	YES
9	a	28.19	0.11889	YES	YES
10	a	30.83	1.24478	YES	YES
11	a	31.54	2.17848	YES	YES
12	a	34.69	1.65554	YES	YES
13	a	40.42	2.24511	YES	YES
14	a	51.51	0.44497	YES	YES
15	a	54.31	0.81957	YES	YES
16	a	56.37	0.54768	YES	YES
17	a	59.76	1.31794	YES	YES
18	a	62.36	0.86335	YES	YES
19	a	64.12	0.94442	YES	YES
20	a	67.03	0.21535	YES	YES
21	a	72.37	0.19673	YES	YES
22	a	77.87	0.54969	YES	YES
23	a	112.51	0.22246	YES	YES
24	a	113.92	1.26125	YES	YES
25	a	122.62	0.56264	YES	YES
26	a	124.75	0.34585	YES	YES
27	a	133.44	1.66690	YES	YES
28	a	139.11	0.74327	YES	YES
29	a	141.16	5.00449	YES	YES
30	a	146.25	3.41674	YES	YES
31	a	153.37	0.75135	YES	YES
32	a	159.82	0.93765	YES	YES
33	a	162.42	7.01449	YES	YES
34	a	168.82	0.19355	YES	YES
35	a	182.46	1.08964	YES	YES
36	a	190.13	3.89008	YES	YES
37	a	192.28	1.52771	YES	YES
38	a	195.94	2.00366	YES	YES
39	a	215.38	23.41092	YES	YES
40	a	215.99	26.88761	YES	YES
41	a	231.07	5.25125	YES	YES
42	a	231.80	3.09749	YES	YES
43	a	240.84	1.62264	YES	YES
44	a	245.50	2.82022	YES	YES
45	a	253.17	11.76441	YES	YES
46	a	262.57	0.96942	YES	YES
47	a	265.14	2.42176	YES	YES
48	a	267.79	21.99010	YES	YES
49	a	286.02	2.02172	YES	YES
50	a	299.40	0.96418	YES	YES

Compound 59b

SCF Energy (au) (RI)BP86/SV(P) -2050.0934699510
SCF Energy (au) PBE0/def2-TZVPP -2049.717779082
Zero Point Energy (au) 0.5005397
Chemical potential (kJ mol^{-1}) 1110.97

xyz Coordinates

70

Pd	-0.14617	1.40208	-1.08148
Pd	-0.49564	-1.26000	-0.97009
O	-0.07758	3.44943	-1.82524
O	0.29633	5.57212	-2.24209
C	0.43632	4.60430	-1.48591
C	1.20278	4.74470	-0.17122
H	2.11914	4.11453	-0.18320
H	0.57795	4.42320	0.68978
H	1.50049	5.80376	-0.03104
O	-0.91106	-3.31556	-1.47526
O	-1.13099	-4.13434	0.64270
C	-1.14251	-4.24624	-0.58650
C	-1.43977	-5.59965	-1.26325
H	-1.77256	-6.32995	-0.49830
H	-0.51933	-5.97671	-1.76055
H	-2.21637	-5.48355	-2.04871
O	-1.81198	1.34387	-2.31607
O	-2.48601	-0.72993	-1.68857
C	-2.62201	0.34812	-2.33799
C	-3.83048	0.49325	-3.24546
H	-3.66499	-0.12890	-4.15269
H	-3.98120	1.54705	-3.55140
H	-4.73358	0.09805	-2.73502
O	1.11290	0.85767	-2.77438
O	0.17945	-1.20268	-2.93734
C	0.84955	-0.21067	-3.40073
C	1.34331	-0.34245	-4.82998
H	0.72545	0.31866	-5.47690
H	1.26369	-1.38635	-5.19152
H	2.39089	0.01836	-4.89988
N	1.39391	1.43576	0.25324
N	-1.02948	-1.31884	0.99672
C	-1.17035	1.95271	0.53138
C	-2.52017	2.32698	0.55963
H	-3.11123	2.33614	-0.36814
C	-3.10693	2.71931	1.77829
H	-4.16905	3.01696	1.79686
C	-2.34913	2.74855	2.96510
H	-2.81704	3.05740	3.91381
C	-0.99051	2.40796	2.93459
H	-0.39527	2.45999	3.86126
C	-0.38430	2.02002	1.71729
C	1.04033	1.73259	1.54516
C	2.04025	1.78172	2.53823
H	1.76272	2.01910	3.57578
C	3.37543	1.54349	2.19464
H	4.16038	1.58399	2.96719
C	3.70561	1.26136	0.85689
H	4.74349	1.07493	0.54394

C	2.67817	1.21390	-0.09101
H	2.85283	0.99804	-1.15614
C	1.25533	-1.82474	-0.20959
C	2.39198	-2.17572	-0.94809
H	2.37045	-2.14862	-2.04770
C	3.55577	-2.59376	-0.27252
H	4.45049	-2.87165	-0.85523
C	3.57865	-2.67458	1.13244
H	4.49086	-3.00786	1.65351
C	2.42890	-2.35838	1.86967
H	2.44233	-2.45749	2.96763
C	1.25223	-1.94251	1.20765
C	-0.02886	-1.67276	1.86112
C	-0.31548	-1.79103	3.23422
H	0.48378	-2.07923	3.93267
C	-1.61946	-1.57410	3.69365
H	-1.85189	-1.67643	4.76617
C	-2.62815	-1.24074	2.77442
H	-3.66845	-1.07442	3.09111
C	-2.29003	-1.12402	1.42190
H	-3.02413	-0.87619	0.64055

Vibrational Spectrum (first 50 lines)

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.13	0.25546	YES	YES
8	a	27.07	1.68153	YES	YES
9	a	28.19	0.48483	YES	YES
10	a	34.02	0.26495	YES	YES
11	a	35.54	0.21357	YES	YES
12	a	41.00	4.30562	YES	YES
13	a	46.61	1.61641	YES	YES
14	a	47.52	1.60700	YES	YES
15	a	55.07	0.40950	YES	YES
16	a	58.62	0.61356	YES	YES
17	a	60.59	0.12163	YES	YES
18	a	63.24	0.87170	YES	YES
19	a	66.72	0.92855	YES	YES
20	a	68.37	0.35500	YES	YES
21	a	70.78	0.14070	YES	YES
22	a	78.12	0.32289	YES	YES
23	a	109.82	0.31181	YES	YES
24	a	115.09	0.17960	YES	YES
25	a	121.69	0.39358	YES	YES
26	a	125.46	0.38271	YES	YES
27	a	138.87	8.05994	YES	YES
28	a	140.12	0.23938	YES	YES
29	a	143.76	0.96080	YES	YES
30	a	145.73	0.61663	YES	YES
31	a	152.75	0.61853	YES	YES
32	a	157.20	5.49672	YES	YES
33	a	165.75	1.84869	YES	YES
34	a	166.79	0.02294	YES	YES
35	a	177.17	1.23210	YES	YES
36	a	183.54	4.08892	YES	YES
37	a	191.96	6.84905	YES	YES
38	a	203.73	2.67754	YES	YES
39	a	213.82	37.21573	YES	YES
40	a	215.33	1.81721	YES	YES
41	a	230.82	7.06231	YES	YES
42	a	232.42	6.81733	YES	YES
43	a	235.75	0.27698	YES	YES
44	a	239.71	12.64332	YES	YES
45	a	244.09	6.12174	YES	YES
46	a	261.25	5.38800	YES	YES
47	a	269.74	21.60068	YES	YES
48	a	273.97	2.93090	YES	YES
49	a	288.35	0.99382	YES	YES
50	a	295.90	0.44758	YES	YES