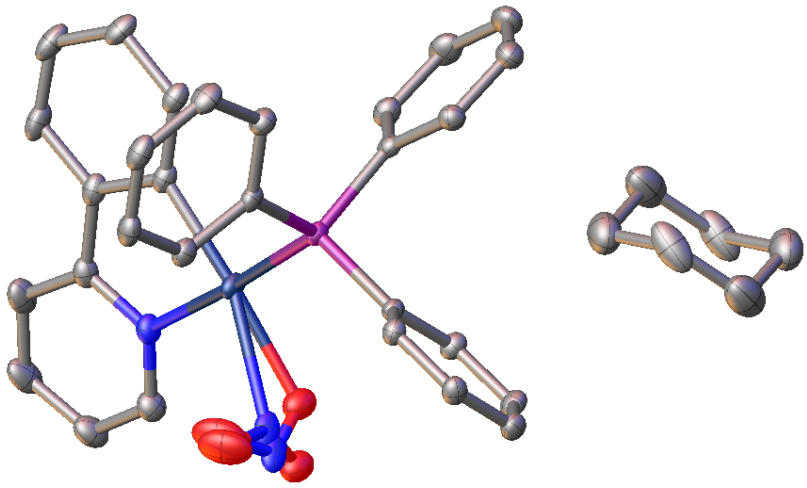

Table 1 Crystal data and structure refinement for Compound 26

Identification code	ijsf1306
Empirical formula	$C_{32}H_{29}N_2O_2PPd$
Formula weight	610.94
Temperature/K	110.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	17.0574(7)
b/Å	9.4203(3)
c/Å	17.4240(6)
α/°	90.00
β/°	109.393(4)
γ/°	90.00
Volume/Å^3	2640.94(17)
Z	4
ρ_{calc}mg/mm^3	1.537
m/mm^{-1}	0.797
F(000)	1248.0
Crystal size/mm^3	0.2239 × 0.173 × 0.0852
2Θ range for data collection	5.8 to 64.32°
Index ranges	$-25 \leq h \leq 24$, $-11 \leq k \leq 13$, $-25 \leq l \leq 12$
Reflections collected	14958
Independent reflections	8322[R(int) = 0.0237]
Data/restraints/parameters	8322/0/353
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0393, wR_2 = 0.0821
Final R indexes [all data]	R_1 = 0.0490, wR_2 = 0.0871
Largest diff. peak/hole / e Å^{-3}	1.56/-1.68

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for ijsf1306. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	3129.1(15)	4579(2)	3939.9(13)	17.8(4)
C2	2474.9(16)	5443(2)	3954.0(13)	19.8(4)
C3	2391.1(18)	5907(3)	4682.3(14)	23.4(5)
C4	2987.6(19)	5539(3)	5419.1(14)	28.1(6)
C5	3651.0(18)	4707(3)	5427.4(14)	26.0(5)
C6	3727.5(15)	4209(3)	4698.6(13)	19.9(4)
C7	4386.6(15)	3238(3)	4686.6(13)	20.1(4)
C8	5025.2(16)	2736(3)	5360.6(14)	28.5(6)
C9	5582.9(17)	1765(4)	5255.5(16)	33.0(6)
C10	5506.1(16)	1295(3)	4483.1(16)	29.1(6)
C11	4876.1(15)	1846(3)	3832.4(14)	23.7(5)
C12	1160.3(16)	3505(3)	2478.6(14)	21.2(5)
C13	349.4(18)	3086(3)	2373.5(16)	28.8(6)
C14	-305.9(17)	3630(3)	1737.3(16)	28.7(5)
C15	-151.1(16)	4587(3)	1200.3(15)	25.0(5)
C16	654.5(14)	4996(3)	1299.4(13)	19.0(4)
C17	1319.8(14)	4467(2)	1943.7(13)	15.7(4)
C18	2523.0(14)	6827(2)	2205.3(12)	16.2(4)
C19	1885.5(15)	7764(3)	2175.2(14)	20.5(4)
C20	2058.5(17)	9198(3)	2352.2(15)	24.7(5)
C21	2860.2(17)	9700(3)	2542.7(14)	24.4(5)
C22	3499.4(16)	8770(3)	2571.7(14)	23.1(5)
C23	3332.5(15)	7343(3)	2410.4(13)	20.0(4)
C24	2364.1(13)	4631(2)	1003.0(12)	14.5(4)
C25	2445.1(14)	5721(2)	501.4(13)	16.7(4)
C26	2418.0(15)	5425(3)	-291.9(13)	19.3(4)
C27	2309.9(15)	4049(3)	-578.5(13)	20.0(4)
C28	2213.5(15)	2959(3)	-84.6(13)	20.2(4)
C29	2246.4(15)	3245(2)	705.5(13)	18.5(4)
N1	4334.5(12)	2799(2)	3929.1(11)	19.7(4)
N2	4245(3)	3220(5)	1915(2)	23.7(8)
N2A	4130(20)	3350(40)	2060(20)	23.7(8)
O1	3766.2(14)	2604(3)	2133.3(12)	30.2(5)
O1A	4216(10)	2224(18)	1964(9)	30.2(5)
O2A	4480(50)	4510(80)	1980(40)	50.3(12)
O2	4449(6)	4418(10)	2125(5)	50.3(12)
P1	2388.4(4)	4922.5(6)	2043.0(3)	13.95(10)
Pd1	3399.47(11)	3753.45(19)	2998.07(9)	17.18(5)

C30	545(2)	946(4)	603(2)	43.7(8)	
C31	132(2)	1393(3)	-280(2)	45.2(9)	
C32	-1(2)	163(5)	-824.3(19)	50.2(9)	

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for ijsf1306. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	25.0(11)	14.7(10)	13.8(9)	0.2(8)	6.4(8)	-3.6(9)
C2	28.6(12)	15.4(10)	15.7(9)	-0.8(8)	7.9(9)	-2.2(9)
C3	38.2(14)	15.4(10)	19.9(10)	-2.0(8)	13.8(10)	0.8(10)
C4	50.3(17)	19.3(11)	16.4(10)	-2.7(9)	13.3(11)	-1.0(11)
C5	39.8(14)	22.2(12)	12.9(9)	-0.7(9)	4.6(9)	-5.1(11)
C6	26.6(12)	16.4(10)	14.9(9)	0.7(8)	4.3(8)	-4.8(9)
C7	20.9(11)	21.7(11)	16.0(9)	3.4(8)	3.7(8)	-4.0(9)
C8	24.9(12)	41.5(15)	15.7(10)	6.8(10)	2.4(9)	-2.2(11)
C9	21.6(12)	50.3(18)	23.4(12)	14.1(12)	2.4(9)	4.5(12)
C10	21.0(12)	37.2(15)	27.2(12)	9.4(11)	5.8(9)	5.7(11)
C11	22.3(11)	25.7(12)	20.9(10)	3.5(9)	4.2(9)	2.1(10)
C12	26.6(12)	19.9(11)	18.1(10)	-0.2(8)	8.9(9)	-3.1(9)
C13	35.2(14)	29.2(13)	27.5(12)	-1.1(10)	18.0(11)	-8.5(11)
C14	23.0(12)	35.2(14)	31.8(13)	-5.7(11)	14(1)	-7.6(11)
C15	20.0(11)	28.8(13)	25.3(11)	-4.5(10)	6.3(9)	0.9(10)
C16	19.1(10)	19.1(10)	19.6(10)	0.3(8)	7.5(8)	-0.3(9)
C17	18.7(10)	13.9(9)	15.9(9)	-2.9(8)	7.6(8)	-1.0(8)
C18	21(1)	15.7(10)	10.8(8)	-0.6(7)	3.8(7)	0.2(8)
C19	22.8(11)	18.1(11)	20.4(10)	-2.0(8)	7.1(8)	0.7(9)
C20	33.8(13)	16.5(11)	23.9(11)	-1.4(9)	9.7(10)	4.1(10)
C21	38.0(14)	17.4(11)	17.1(10)	-2.4(8)	8.3(9)	-5.7(10)
C22	26.6(12)	22.6(11)	18.7(10)	-3.2(9)	5.8(9)	-9.2(10)
C23	23.7(11)	20.2(11)	15.3(9)	-1.1(8)	5.5(8)	-0.8(9)
C24	14.9(9)	15.7(9)	12.5(8)	-0.8(7)	4.2(7)	1.0(8)
C25	18.6(10)	15.6(9)	15.1(9)	-0.1(8)	4.5(8)	-0.9(8)
C26	20.8(11)	21.6(11)	15.5(9)	1.3(8)	6.0(8)	-3.5(9)
C27	20.7(11)	24.9(12)	14.3(9)	-1.6(8)	5.5(8)	-0.8(9)
C28	24.2(11)	17.3(10)	19(1)	-3.4(8)	7.1(8)	1.7(9)
C29	23.6(11)	15.2(10)	17.1(9)	-0.2(8)	7.5(8)	0.3(9)
N1	20.6(9)	20.2(9)	15.4(8)	2.5(7)	2.1(7)	-0.2(8)
N2	26.9(18)	16.2(14)	18.6(17)	3.9(12)	-4.8(11)	5.4(12)
N2A	26.9(18)	16.2(14)	18.6(17)	3.9(12)	-4.8(11)	5.4(12)
O1	31.3(12)	34.7(13)	23.2(10)	0.1(9)	7.2(8)	8.6(10)
O1A	31.3(12)	34.7(13)	23.2(10)	0.1(9)	7.2(8)	8.6(10)
O2A	47.5(17)	45(2)	74(4)	12(2)	41(2)	-0.2(15)
O2	47.5(17)	45(2)	74(4)	12(2)	41(2)	-0.2(15)

P1	17.0(3)	13.0(2)	11.4(2)	0.02(19)	4.05(19)	0.6(2)
Pd1	20.96(9)	17.77(8)	11.08(7)	0.50(6)	2.98(6)	4.10(7)
C30	38.8(17)	40.4(18)	45.7(18)	-9.8(15)	5.7(14)	-1.5(14)
C31	29.2(15)	30.7(15)	64(2)	22.8(15)	0.5(14)	-4.5(12)
C32	37.0(17)	81(3)	32.2(15)	7.8(17)	10.8(13)	-3.6(19)

Table 4 Bond Lengths for ijsf1306.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.388(3)	C19	C20	1.395(3)
C1	C6	1.419(3)	C20	C21	1.379(4)
C1	Pd1	2.003(2)	C21	C22	1.387(4)
C2	C3	1.394(3)	C22	C23	1.383(3)
C3	C4	1.391(4)	C24	C25	1.385(3)
C4	C5	1.373(4)	C24	C29	1.394(3)
C5	C6	1.400(3)	C24	P1	1.820(2)
C6	C7	1.455(4)	C25	C26	1.396(3)
C7	C8	1.393(3)	C26	C27	1.379(3)
C7	N1	1.358(3)	C27	C28	1.384(3)
C8	C9	1.375(4)	C28	C29	1.386(3)
C9	C10	1.381(4)	N1	Pd1	2.0653(19)
C10	C11	1.379(3)	N2	O1	1.163(6)
C11	N1	1.338(3)	N2	O2	1.201(11)
C12	C13	1.391(4)	N2A	O1A	1.09(4)
C12	C17	1.390(3)	N2A	O2A	1.27(8)
C13	C14	1.385(4)	N2A	Pd1	2.39(3)
C14	C15	1.386(4)	O1	Pd1	2.112(2)
C15	C16	1.381(3)	P1	Pd1	2.2473(6)
C16	C17	1.397(3)	C30	C31	1.524(5)
C17	P1	1.824(2)	C30	C32[1]	1.529(5)
C18	C19	1.388(3)	C31	C32	1.466(5)
C18	C23	1.394(3)	C32	C30[1]	1.529(5)
C18	P1	1.819(2)			

[1]-X,-Y,-Z

Table 5 Bond Angles for ijsf1306.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C6	117.5(2)	C25	C24	P1	122.85(17)
C2	C1	Pd1	130.34(16)	C29	C24	P1	117.67(16)
C6	C1	Pd1	112.18(17)	C24	C25	C26	120.0(2)
C1	C2	C3	121.7(2)	C27	C26	C25	120.2(2)
C4	C3	C2	119.8(2)	C26	C27	C28	120.1(2)

C5	C4	C3	120.0(2)	C27	C28	C29	120.0(2)
C4	C5	C6	120.4(2)	C28	C29	C24	120.3(2)
C1	C6	C7	117.5(2)	C7	N1	Pd1	114.53(16)
C5	C6	C1	120.5(2)	C11	N1	C7	120.1(2)
C5	C6	C7	121.9(2)	C11	N1	Pd1	125.35(16)
C8	C7	C6	126.4(2)	O1	N2	O2	122.2(4)
N1	C7	C6	113.8(2)	O1A	N2A	O2A	136(5)
N1	C7	C8	119.8(2)	O1A	N2A	Pd1	113(3)
C9	C8	C7	119.7(2)	O2A	N2A	Pd1	108(3)
C8	C9	C10	119.8(2)	N2	O1	Pd1	112.5(2)
C11	C10	C9	118.5(3)	C17	P1	Pd1	116.86(7)
N1	C11	C10	122.1(2)	C18	P1	C17	108.52(10)
C17	C12	C13	120.3(2)	C18	P1	C24	105.29(10)
C14	C13	C12	120.2(2)	C18	P1	Pd1	110.00(7)
C13	C14	C15	119.8(2)	C24	P1	C17	100.27(10)
C16	C15	C14	120.1(2)	C24	P1	Pd1	114.93(7)
C15	C16	C17	120.7(2)	C1	Pd1	N1	81.57(9)
C12	C17	C16	118.9(2)	C1	Pd1	N2A	159.3(10)
C12	C17	P1	120.11(18)	C1	Pd1	O1	170.68(9)
C16	C17	P1	120.79(17)	C1	Pd1	P1	95.02(7)
C19	C18	C23	119.0(2)	N1	Pd1	N2A	91.6(9)
C19	C18	P1	124.37(18)	N1	Pd1	O1	90.16(8)
C23	C18	P1	116.55(17)	N1	Pd1	P1	175.99(6)
C18	C19	C20	120.1(2)	O1	Pd1	N2A	23.9(10)
C21	C20	C19	120.3(2)	O1	Pd1	P1	93.40(6)
C20	C21	C22	119.8(2)	P1	Pd1	N2A	90.9(9)
C23	C22	C21	120.0(2)	C31	C30	C32[1]	109.1(3)
C22	C23	C18	120.7(2)	C32	C31	C30	110.8(3)
C25	C24	C29	119.47(19)	C31	C32	C30[1]	110.7(3)

[1]-X,-Y,-Z

Table 6 Torsion Angles for ijsf1306.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	2.0(4)	C18	P1	Pd1	C1	58.52(10)
C1	C6	C7	C8	-179.4(2)	C18	P1	Pd1	N2A	-101.6(10)
C1	C6	C7	N1	-0.4(3)	C18	P1	Pd1	O1	-125.48(11)
C2	C1	C6	C5	-0.1(3)	C19	C18	C23	C22	-0.8(3)
C2	C1	C6	C7	176.5(2)	C19	C18	P1	C17	-5.7(2)
C2	C1	Pd1	N1	-175.8(2)	C19	C18	P1	C24	100.9(2)
C2	C1	Pd1	N2A	112(3)	C19	C18	P1	Pd1	-134.70(17)
C2	C1	Pd1	P1	6.4(2)	C19	C20	C21	C22	-1.1(4)

C2	C3	C4	C5	-0.8(4)	C20	C21	C22	C23	0.0(4)
C3	C4	C5	C6	-0.8(4)	C21	C22	C23	C18	1.0(3)
C4	C5	C6	C1	1.2(4)	C23	C18	C19	C20	-0.3(3)
C4	C5	C6	C7	-175.2(2)	C23	C18	P1	C17	171.13(16)
C5	C6	C7	C8	-2.8(4)	C23	C18	P1	C24	-82.22(18)
C5	C6	C7	N1	176.1(2)	C23	C18	P1	Pd1	42.15(18)
C6	C1	C2	C3	-1.5(3)	C24	C25	C26	C27	0.1(3)
C6	C1	Pd1	N1	5.31(16)	C24	P1	Pd1	C1	177.12(10)
C6	C1	Pd1	N2A	-66(3)	C24	P1	Pd1	N2A	17.0(10)
C6	C1	Pd1	P1	−172.57(16)	C24	P1	Pd1	O1	-6.88(11)
C6	C7	C8	C9	176.9(3)	C25	C24	C29	C28	0.2(3)
C6	C7	N1	C11	-176.5(2)	C25	C24	P1	C17	113.08(19)
C6	C7	N1	Pd1	5.0(3)	C25	C24	P1	C18	0.5(2)
C7	C8	C9	C10	0.0(4)	C25	C24	P1	Pd1	−120.72(17)
C7	N1	Pd1	C1	-5.84(17)	C25	C26	C27	C28	1.1(4)
C7	N1	Pd1	N2A	154.6(10)	C26	C27	C28	C29	-1.6(4)
C7	N1	Pd1	O1	178.46(18)	C27	C28	C29	C24	0.9(4)
C8	C7	N1	C11	2.5(4)	C29	C24	C25	C26	-0.7(3)
C8	C7	N1	Pd1	−176.01(19)	C29	C24	P1	C17	-65.99(19)
C8	C9	C10	C11	1.5(4)	C29	C24	P1	C18	−178.58(18)
C9	C10	C11	N1	-1.0(4)	C29	C24	P1	Pd1	60.21(19)
C10	C11	N1	C7	-1.0(4)	N1	C7	C8	C9	-2.0(4)
C10	C11	N1	Pd1	177.4(2)	N2	O1	Pd1	N1	-91.9(3)
C11	N1	Pd1	C1	175.7(2)	N2	O1	Pd1	N2A	2(2)
C11	N1	Pd1	N2A	-23.9(10)	N2	O1	Pd1	P1	86.3(3)
C11	N1	Pd1	O1	0.0(2)	O1A	N2A	Pd1	C1	133(2)
C12	C13	C14	C15	0.5(4)	O1A	N2A	Pd1	N1	63(3)
C12	C17	P1	C18	−120.97(18)	O1A	N2A	Pd1	O1	-24.2(15)
C12	C17	P1	C24	128.95(19)	O1A	N2A	Pd1	P1	-121(3)
C12	C17	P1	Pd1	4.1(2)	O2A	N2A	Pd1	C1	-31(6)
C13	C12	C17	C16	-0.4(3)	O2A	N2A	Pd1	N1	-101(4)
C13	C12	C17	P1	−175.92(19)	O2A	N2A	Pd1	O1	172(6)
C13	C14	C15	C16	0.1(4)	O2A	N2A	Pd1	P1	76(4)
C14	C15	C16	C17	-0.8(4)	O2	N2	O1	Pd1	-5.0(8)
C15	C16	C17	C12	0.9(3)	P1	C18	C19	C20	176.48(18)
C15	C16	C17	P1	176.43(19)	P1	C18	C23	C22	−177.86(17)
C16	C17	P1	C18	63.6(2)	P1	C24	C25	C26	−179.77(18)
C16	C17	P1	C24	-46.5(2)	P1	C24	C29	C28	179.32(18)
C16	C17	P1	Pd1	−171.41(16)	Pd1	C1	C2	C3	179.61(19)

C17	C12	C13	C14	-0.3(4)	Pd1	C1	C6	C5	179.00(19)
C17	P1	Pd1	C1	-65.75(10)	Pd1	C1	C6	C7	-4.4(3)
C17	P1	Pd1	N2A	134.1(10)	C30	C31	C32	C30[1]	58.8(4)
C17	P1	Pd1	O1	110.25(11)	C32[1]	C30	C31	C32	-57.9(4)
C18	C19	C20	C21	1.3(4)					

[1]-X,-Y,-Z

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for ijsf1306.

Atom	*x*	*y*	*z*	U(eq)
H2	2073	5725	3454	24
H3	1928	6473	4676	28
H4	2936	5863	5916	34
H5	4061	4468	5931	31
H8	5075	3063	5891	34
H9	6020	1419	5713	40
H10	5879	608	4402	35
H11	4825	1540	3298	28
H12	1607	3132	2918	25
H13	245	2425	2740	35
H14	-860	3349	1669	34
H15	-599	4963	764	30
H16	757	5643	926	23
H19	1330	7429	2034	25
H20	1622	9832	2342	30
H21	2974	10680	2654	29
H22	4052	9112	2702	28
H23	3774	6708	2440	24
H25	2519	6670	697	20
H26	2474	6173	-635	23
H27	2301	3850	-1116	24
H28	2125	2015	-287	24
H29	2188	2493	1046	22
H30A	615	1782	964	52
H30B	1101	542	678	52
H31A	-409	1850	-343	54
H31B	488	2095	-430	54
H32A	542	-265	-782	60
H32B	-273	476	-1394	60

Experimental

Single crystals of $C_{32}H_{29}N_2O_2PPd$ **[ijsf1306]** were **[DCM/cyclohexane]**. A suitable crystal was selected and **[oil on loop]** on a **Oxford Diffraction Supernova** diffractometer. The crystal was kept at 110.00(10) K

during data collection. Using Olex2 [1], the structure was solved with the Superflip [2] structure solution program using Charge Flipping and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.
2. SUPERFLIP, J. Appl. Cryst. (2007) 40, 786-790
3. SHELXL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122

Crystal structure determination of [ijsf1306]

Crystal Data for $C_{32}H_{29}N_2O_2PPd$ (M =610.94): monoclinic, space group $P2_1/c$ (no. 14), a = 17.0574(7) Å, b = 9.4203(3) Å, c = 17.4240(6) Å, β = 109.393(4)°, V = 2640.94(17) Å^3, Z = 4, T = 110.00(10) K, μ(Mo Kα) = 0.797 mm^{-1}, *Dcalc* = 1.537 g/mm^3, 14958 reflections measured ($5.8 \leq 2\Theta \leq 64.32$), 8322 unique ($R_{int}$ = 0.0237) which were used in all calculations. The final R_1 was 0.0393 (>2sigma(I)) and wR_2 was 0.0871 (all data).

This report has been created with Olex2, compiled on Mar 21 2013 11:17:50. Please let us know if there are any errors or if you would like to have additional featrues.