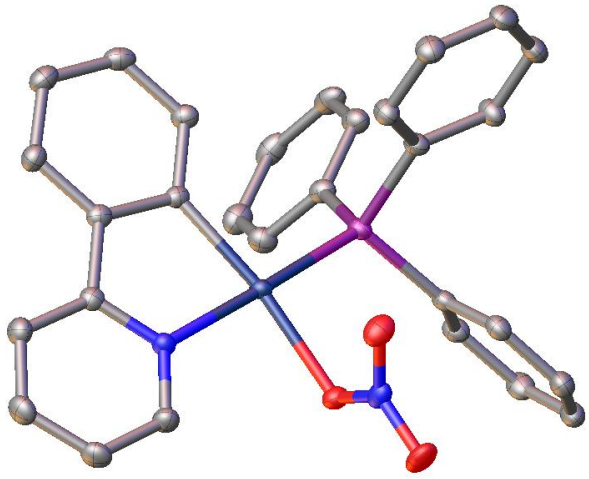

Table 1 Crystal data and structure refinement for Compound 26

Identification code	
Empirical formula	$C_{29}H_{23}N_2O_3PPd$
Formula weight	584.86
Temperature/K	110.00(14)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.43313(15)
b/Å	15.07499(18)
c/Å	17.3486(2)
α/°	90.00
β/°	90.1549(13)
γ/°	90.00
Volume/Å^3	2467.04(6)
Z	4
ρ_{calc}mg/mm^3	1.575
m/mm^{-1}	0.852
F(000)	1184.0
Crystal size/mm^3	0.4233 × 0.154 × 0.1148
2Θ range for data collection	5.62 to 64.46°
Index ranges	$-14 \leq h \leq 14$, $-22 \leq k \leq 21$, $-25 \leq l \leq 22$
Reflections collected	18360
Independent reflections	7871[R(int) = 0.0274]
Data/restraints/parameters	7871/0/325
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0303, wR_2 = 0.0672
Final R indexes [all data]	R_1 = 0.0381, wR_2 = 0.0716
Largest diff. peak/hole / e Å^{-3}	0.68/-0.73

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

Atom	*x*	*y*	*z*	U(eq)
C1	914.8(19)	3583.7(11)	2382(1)	14.6(3)
C2	540(2)	3314.1(11)	3123.7(10)	18.4(3)
C3	-751(2)	2904.4(12)	3274.5(11)	20.9(4)
C4	-1724(2)	2751.4(12)	2688.6(11)	21.4(4)
C5	-1390(2)	3013.0(12)	1945.2(11)	19.7(3)
C6	-93(2)	3417.0(11)	1787.9(10)	15.9(3)
C7	317.7(19)	3662.0(11)	1002.7(10)	15.7(3)
C8	-545(2)	3600.6(12)	351.1(11)	20.2(4)
C9	-8(2)	3845.8(13)	-362.2(11)	22.2(4)
C10	1370(2)	4140.2(12)	-415.5(11)	22.0(4)
C11	2169(2)	4204.5(12)	252.9(10)	19.8(4)
C12	2567(2)	4923.5(11)	3864.2(10)	17.3(3)
C13	1697(2)	5599.8(12)	3588.2(11)	20.8(4)
C14	917(2)	6114.4(13)	4099.4(12)	23.5(4)
C15	996(2)	5951.7(13)	4882.0(12)	25.4(4)
C16	1836(2)	5276.6(14)	5160.0(11)	25.6(4)
C17	2626(2)	4762.1(13)	4655.1(10)	21.2(4)
C18	4382(2)	3364.4(11)	3621(1)	16.6(3)
C19	4026(2)	2544.4(11)	3309.4(11)	19.3(3)
C20	4577(2)	1765.9(12)	3620.5(11)	22.6(4)
C21	5478(2)	1807.5(13)	4251.1(11)	23.4(4)
C22	5838(2)	2622.9(13)	4565.9(11)	24.0(4)
C23	5308(2)	3399.3(12)	4251.9(11)	21.6(4)
C24	5257(2)	5075.4(11)	3138.8(10)	15.6(3)
C25	6467(2)	4746.4(11)	2781.7(10)	18.2(3)
C26	7676(2)	5257.7(12)	2712.7(11)	21.3(4)
C27	7686(2)	6118.2(13)	3010.3(11)	22.2(4)
C28	6509(2)	6444.9(12)	3384.1(11)	22.8(4)
C29	5285(2)	5934.2(11)	3446.8(10)	18.9(4)
N1	1658.6(17)	3974.0(9)	942.5(8)	15.5(3)
N2	5386.7(18)	4118.7(10)	1185.3(9)	19.3(3)
O1	4457.1(14)	4689.7(8)	1407.8(7)	18.9(3)
O2	5234.0(16)	3327.7(9)	1361.7(9)	26.3(3)
O3	6403.4(16)	4388.3(11)	807.8(8)	29.9(3)
P1	3693.3(5)	4361.9(3)	3170.8(3)	14.54(9)
Pd1	2699.97(14)	4124.59(8)	1993.86(7)	13.14(4)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	16.0(8)	12.3(6)	15.3(7)	-0.1(6)	1.7(6)	0.6(6)
C2	22.0(9)	18.0(7)	15.3(8)	-1.5(6)	1.4(7)	-1.8(7)
C3	27.2(10)	17.9(8)	17.7(8)	1.0(6)	5.5(7)	-0.2(7)
C4	20.0(9)	19.5(8)	24.8(9)	-1.2(7)	4.4(7)	-2.9(7)
C5	17.8(9)	21.1(8)	20.2(8)	-1.6(7)	0.3(7)	-2.1(7)
C6	17.9(9)	13.8(7)	16.0(7)	-1.4(6)	1.7(6)	1.0(6)
C7	18.0(9)	12.9(7)	16.1(8)	-1.2(6)	0.0(6)	0.6(6)
C8	19.8(9)	21.1(8)	19.7(8)	-1.5(7)	-2.8(7)	-3.1(7)
C9	26.9(10)	23.5(8)	16.0(8)	-2.2(7)	-5.8(7)	-0.9(8)
C10	28.6(11)	24.5(9)	12.8(8)	-0.1(7)	0.8(7)	-0.4(8)
C11	20.4(9)	23.7(8)	15.2(8)	0.7(7)	1.3(7)	-2.2(7)
C12	20.8(9)	17.1(7)	14.0(8)	-2.1(6)	0.3(6)	-3.5(7)
C13	25.7(10)	20.4(8)	16.3(8)	-0.9(7)	0.5(7)	0.1(7)
C14	22.7(10)	20.2(8)	27.7(10)	-4.3(7)	2.4(8)	0.5(7)
C15	23.3(10)	28.8(9)	24.2(9)	-12.0(8)	6.7(8)	-7.6(8)
C16	27.7(11)	35.6(10)	13.6(8)	-3.6(7)	2.7(7)	-10.8(9)
C17	23.8(10)	23.4(8)	16.5(8)	0.6(7)	-1.5(7)	-4.8(7)
C18	20.1(9)	14.1(7)	15.7(8)	1.5(6)	-0.7(6)	-0.3(6)
C19	21.4(9)	16.9(7)	19.4(8)	-0.9(6)	-3.5(7)	-1.3(7)
C20	25.5(10)	16.1(7)	26.1(9)	0.1(7)	-1.2(8)	-1.4(7)
C21	24.4(10)	20.4(8)	25.4(9)	7.0(7)	-0.7(8)	2.9(7)
C22	25.2(10)	25.3(9)	21.3(9)	5.6(7)	-6.3(7)	0.7(8)
C23	25.8(10)	19.0(8)	19.8(8)	0.5(7)	-6.9(7)	-2.0(7)
C24	20.4(9)	14.0(7)	12.4(7)	1.4(6)	-3.2(6)	-1.3(6)
C25	22.3(9)	15.9(7)	16.3(8)	0.3(6)	-4.1(7)	1.1(7)
C26	20.4(9)	23.9(8)	19.5(8)	2.9(7)	-3.6(7)	0.2(7)
C27	21.6(10)	20.1(8)	24.8(9)	5.5(7)	-6.5(7)	-3.5(7)
C28	28.1(11)	14.8(7)	25.4(9)	0.7(7)	-6.5(8)	-3.7(7)
C29	23.9(10)	14.9(7)	17.9(8)	0.0(6)	-2.5(7)	-0.1(7)
N1	16.3(7)	17.6(6)	12.7(6)	0.1(5)	0.1(5)	-0.6(6)
N2	17.2(8)	27.0(8)	13.6(7)	-2.1(6)	-0.4(6)	-5.8(6)
O1	18.6(7)	19.6(6)	18.3(6)	2.5(5)	1.3(5)	-3.5(5)
O2	24.4(8)	21.0(6)	33.6(8)	-3.5(6)	3.6(6)	-2.4(6)
O3	21.7(8)	46.2(9)	22.0(7)	1.4(6)	7.3(6)	-11.2(7)
P1	18.6(2)	12.65(18)	12.34(19)	0.33(15)	-1.98(16)	-0.63(16)
Pd1	15.50(7)	13.22(6)	10.69(6)	0.23(4)	-0.05(4)	-1.21(5)

Table 4 Bond Lengths for .

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.396(2)	C18	C19	1.390(2)
C1	C6	1.423(2)	C18	C23	1.400(2)
C1	Pd1	1.9900(18)	C18	P1	1.8141(17)

C2	C3	1.391(3)	C19	C20	1.392(3)
C3	C4	1.387(3)	C20	C21	1.385(3)
C4	C5	1.386(3)	C21	C22	1.387(3)
C5	C6	1.395(3)	C22	C23	1.384(3)
C6	C7	1.465(2)	C24	C25	1.392(3)
C7	C8	1.394(2)	C24	C29	1.401(2)
C7	N1	1.354(2)	C24	P1	1.8262(18)
C8	C9	1.388(3)	C25	C26	1.382(3)
C9	C10	1.377(3)	C26	C27	1.396(3)
C10	C11	1.385(3)	C27	C28	1.379(3)
C11	N1	1.337(2)	C28	C29	1.392(3)
C12	C13	1.393(3)	N1	Pd1	2.0818(14)
C12	C17	1.395(2)	N2	O1	1.289(2)
C12	P1	1.8166(19)	N2	O2	1.240(2)
C13	C14	1.390(3)	N2	O3	1.232(2)
C14	C15	1.381(3)	O1	Pd1	2.1250(13)
C15	C16	1.376(3)	P1	Pd1	2.2725(4)
C16	C17	1.388(3)			

Table 5 Bond Angles for .

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C6	116.48(16)	C20	C21	C22	120.01(17)
C2	C1	Pd1	130.39(13)	C23	C22	C21	120.47(17)
C6	C1	Pd1	113.06(12)	C22	C23	C18	120.00(17)
C3	C2	C1	121.80(17)	C25	C24	C29	118.96(17)
C4	C3	C2	120.93(17)	C25	C24	P1	117.84(13)
C5	C4	C3	118.89(18)	C29	C24	P1	123.19(15)
C4	C5	C6	120.54(17)	C26	C25	C24	121.20(16)
C1	C6	C7	116.84(16)	C25	C26	C27	119.41(19)
C5	C6	C1	121.36(16)	C28	C27	C26	120.06(19)
C5	C6	C7	121.77(16)	C27	C28	C29	120.57(17)
C8	C7	C6	125.61(17)	C28	C29	C24	119.76(19)
N1	C7	C6	114.14(15)	C7	N1	Pd1	114.14(11)
N1	C7	C8	120.25(16)	C11	N1	C7	119.90(15)
C9	C8	C7	119.44(18)	C11	N1	Pd1	125.83(13)
C10	C9	C8	119.50(17)	O2	N2	O1	119.27(16)
C9	C10	C11	118.58(18)	O3	N2	O1	118.06(16)
N1	C11	C10	122.29(18)	O3	N2	O2	122.67(18)
C13	C12	C17	119.19(17)	N2	O1	Pd1	114.07(10)
C13	C12	P1	117.30(13)	C12	P1	C24	102.68(8)
C17	C12	P1	123.27(14)	C12	P1	Pd1	115.33(6)
C14	C13	C12	120.10(17)	C18	P1	C12	108.10(8)
C15	C14	C13	120.02(19)	C18	P1	C24	102.29(8)

C16	C15	C14	120.37(19)	C18	P1	Pd1	113.75(6)
C15	C16	C17	120.09(18)	C24	P1	Pd1	113.36(6)
C16	C17	C12	120.22(18)	C1	Pd1	N1	81.61(6)
C19	C18	C23	119.16(16)	C1	Pd1	O1	171.11(6)
C19	C18	P1	118.94(13)	C1	Pd1	P1	96.18(5)
C23	C18	P1	121.85(13)	N1	Pd1	O1	89.50(5)
C18	C19	C20	120.64(16)	N1	Pd1	P1	175.42(4)
C21	C20	C19	119.72(17)	O1	Pd1	P1	92.66(4)

Table 6 Torsion Angles for .

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	-0.3(3)	C17	C12	P1	Pd1	147.46(14)
C1	C6	C7	C8	−176.07(16)	C18	C19	C20	C21	0.6(3)
C1	C6	C7	N1	3.6(2)	C18	P1	Pd1	C1	75.60(8)
C2	C1	C6	C5	0.6(2)	C18	P1	Pd1	O1	-105.25(8)
C2	C1	C6	C7	−177.38(15)	C19	C18	C23	C22	-1.1(3)
C2	C1	Pd1	N1	174.76(17)	C19	C18	P1	C12	117.22(16)
C2	C1	Pd1	P1	-9.28(16)	C19	C18	P1	C24	−134.87(16)
C2	C3	C4	C5	0.1(3)	C19	C18	P1	Pd1	-12.24(18)
C3	C4	C5	C6	0.5(3)	C19	C20	C21	C22	-0.6(3)
C4	C5	C6	C1	-0.9(3)	C20	C21	C22	C23	-0.4(3)
C4	C5	C6	C7	177.03(16)	C21	C22	C23	C18	1.2(3)
C5	C6	C7	C8	6.0(3)	C23	C18	C19	C20	0.2(3)
C5	C6	C7	N1	−174.38(16)	C23	C18	P1	C12	-65.54(18)
C6	C1	C2	C3	0.0(2)	C23	C18	P1	C24	42.37(18)
C6	C1	Pd1	N1	-2.03(12)	C23	C18	P1	Pd1	165.00(14)
C6	C1	Pd1	P1	173.92(11)	C24	C25	C26	C27	0.4(3)
C6	C7	C8	C9	−179.11(17)	C24	P1	Pd1	C1	-168.08(8)
C6	C7	N1	C11	178.74(15)	C24	P1	Pd1	O1	11.07(7)
C6	C7	N1	Pd1	-5.18(18)	C25	C24	C29	C28	0.7(2)
C7	C8	C9	C10	0.4(3)	C25	C24	P1	C12	166.94(13)
C7	N1	Pd1	C1	4.11(12)	C25	C24	P1	C18	54.92(15)
C7	N1	Pd1	O1	−175.66(12)	C25	C24	P1	Pd1	-67.97(14)
C8	C7	N1	C11	-1.6(2)	C25	C26	C27	C28	1.4(3)
C8	C7	N1	Pd1	174.50(13)	C26	C27	C28	C29	-2.1(3)
C8	C9	C10	C11	-1.7(3)	C27	C28	C29	C24	1.1(3)
C9	C10	C11	N1	1.4(3)	C29	C24	C25	C26	-1.4(2)
C10	C11	N1	C7	0.3(3)	C29	C24	P1	C12	-13.83(16)
C10	C11	N1	Pd1	-	C29	C24	P1	C18	-

			175.33(14)				125.85(15)
C11	N1	Pd1	C1	179.92(16)	C29	C24	P1	Pd1	111.26(14)
C11	N1	Pd1	O1	0.15(15)	N1	C7	C8	C9	1.2(3)
C12	C13	C14	C15	-0.4(3)	N2	O1	Pd1	N1	-89.25(11)
C12	P1	Pd1	C1	-50.11(8)	N2	O1	Pd1	P1	94.78(10)
C12	P1	Pd1	O1	129.03(7)	O2	N2	O1	Pd1	-4.07(19)
C13	C12	C17	C16	-0.7(3)	O3	N2	O1	Pd1	176.48(12)
C13	C12	P1	C18	−166.78(14)	P1	C12	C13	C14	−173.53(15)
C13	C12	P1	C24	85.57(15)	P1	C12	C17	C16	173.57(15)
C13	C12	P1	Pd1	-38.22(16)	P1	C18	C19	C20	177.53(16)
C13	C14	C15	C16	-0.6(3)	P1	C18	C23	C22	−178.35(17)
C14	C15	C16	C17	1.0(3)	P1	C24	C25	C26	177.87(13)
C15	C16	C17	C12	-0.3(3)	P1	C24	C29	C28	−178.53(14)
C17	C12	C13	C14	1.0(3)	Pd1	C1	C2	C3	−176.71(14)
C17	C12	P1	C18	18.89(18)	Pd1	C1	C6	C5	177.87(13)
C17	C12	P1	C24	-88.75(16)	Pd1	C1	C6	C7	-0.11(19)

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

Atom	*x*	*y*	*z*	U(eq)
H2	1184	3413	3537	22
H3	-969	2727	3786	25
H4	-2605	2472	2795	26
H5	-2051	2916	1539	24
H8	-1492	3393	395	24
H9	-587	3811	-810	27
H10	1764	4296	-900	26
H11	3114	4420	220	24
H13	1636	5710	3050	25
H14	329	6578	3910	28
H15	469	6308	5230	31
H16	1875	5162	5698	31
H17	3208	4299	4849	25
H19	3401	2515	2880	23
H20	4336	1208	3401	27
H21	5850	1277	4468	28
H22	6452	2649	5000	29
H23	5574	3956	4464	26
H25	6462	4160	2582	22
H26	8493	5026	2465	26
H27	8506	6479	2955	27

H28	6533	7023	3601	27
H29	4472	6167	3698	23

Experimental

Single crystals of $C_{29}H_{23}N_2O_3PPd$ **[]** 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(14) 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 **[]**

Crystal Data for $C_{29}H_{23}N_2O_3PPd$ (M =584.86): monoclinic, space group $P2_1/c$ (no. 14), a = 9.43313(15) Å, b = 15.07499(18) Å, c = 17.3486(2) Å, β = 90.1549(13)°, V = 2467.04(6) Å^3, Z = 4, T = 110.00(14) K, μ(Mo Kα) = 0.852 mm^{-1}, *Dcalc* = 1.575 g/mm^3, 18360 reflections measured ($5.62 \leq 2\Theta \leq 64.46$), 7871 unique ($R_{int}$ = 0.0274) which were used in all calculations. The final R_1 was 0.0303 (>2sigma(I)) and wR_2 was 0.0716 (all data).

This report has been created with Olex2, compiled on Dec 5 2012 16:17:34. Please let us know if there are any errors or if you would like to have additional featrues.