Supplementary Material (ESI) for Dalton Transactions

STRUCTURE DETERMINATION SUMMARY

Crystal Data for 211031

Empirical Formula	C 36 H 46 I 4 O 4 P 2 Pd 2
Crystal System	Monoclinic
Space Group	$P2_1/n$
Unit Cell Dimensions	a = 10.5171(14) Δ
	b = 10.7549(12) Δ
	c = 19.5756(14) Δ
	β = 97.973(8) °
Volume	2192.8(11) Δ^3
Z	2
Formula weight	1325.1
Density(calc.)	2.007 Mg/m 3
Absorption Coefficient	3.742 mm -1
F(000) 1256	

Data Collection

Diffractometer Used	Enraf Nonius CAD4
Radiation	MoK_α (λ = 0.71073 Δ)
Temperature (K)	298
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 45.0°
Index Ranges	0 < h < 11, -11 < k < 11, -21 < l < 20
Reflections Collected	5898
Independent Reflections	2865 (R_{int} = 2.68 %)
Observed Reflections	2865 (F > 0.3σ(F))
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.0981/0.1623

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Refinement on	F^2
Absolute Structure	N/A
Extinction Coefficient	0.00013(2
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma 2(F) + 0.0005F^2$
Number of Parameters Refined	218
Final R Indices (obs. data)	R = 4.74 %, wR = 4.51 %
R Indices (all data)	R = 4.74 %, wR = 4.51 %
Goodness-of-Fit	1.01
Largest and Mean shift/error	0.000, 0.000
Data-to-Parameter Ratio	13.1:1
Largest Difference Peak	0.93 eΔ^{-3}
Largest Difference Hole	-0.92 eΔ^{-3}

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Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($\Delta^2 x10^3$)

	x	y	z	U(eq)
I(1)	820(1)	1441(1)	93(1)	64(1)
I(2)	-677(1)	2171(1)	1677(1)	82(1)
Pd(1)	-739(1)	281(1)	845(1)	49(1)
P(1)	-2021(2)	-701(2)	1505(1)	51(1)
O(1)	604(4)	-1597(5)	2067(3)	69(2)
O(6)	2007(6)	-3405(7)	1488(3)	98(3)
C(1)	-1337(7)	-865(8)	2423(3)	62(3)
C(2)	113(7)	-850(8)	2563(4)	68(3)
C(4)	1960(8)	-1561(8)	2123(5)	83(4)
C(5)	2378(9)	-2153(9)	1513(5)	96(4)
C(7)	2155(12)	-3999(11)	875(6)	122(6)
C(8)	1821(12)	-5236(10)	866(6)	125(6)
C(11)	-3533(7)	100(7)	1500(4)	60(3)
C(12)	-4076(9)	733(10)	913(5)	94(4)
C(13)	-5258(9)	1296(11)	887(5)	109(5)
C(14)	-5904(9)	1279(9)	1443(6)	88(4)
C(15)	-5361(8)	677(8)	2028(5)	76(3)
C(16)	-4204(7)	99(7)	2062(4)	63(3)
C(21)	-2517(7)	-2272(7)	1243(3)	54(2)
C(22)	-3762(8)	-2564(9)	984(5)	82(4)
C(23)	-4092(10)	-3772(11)	778(5)	104(5)
C(24)	-3209(10)	-4702(9)	847(4)	86(4)
C(25)	-1971(9)	-4416(8)	1092(4)	79(4)
C(26)	-1624(8)	-3239(7)	1287(4)	64(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U ij tensor

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Table 2. Bond lengths (Δ)

I(1)-Pd(1)	2.661 (1)
I(1)-Pd(1A)	2.601 (1)
I(2)-Pd(1)	2.601 (1)
Pd(1)-P(1)	2.256 (2)
Pd(1)-I(1A)	2.601 (1)
P(1)-C(1)	1.849 (6)
P(1)-C(11)	1.807 (7)
P(1)-C(21)	1.821 (7)
O(1)-C(2)	1.412 (10)
O(1)-C(4)	1.415 (9)
O(6)-C(5)	1.401 (12)
O(6)-C(7)	1.387 (14)
C(1)-C(2)	1.512 (10)
C(4)-C(5)	1.473 (14)
C(7)-C(8)	1.375 (16)
C(11)-C(12)	1.390 (11)
C(11)-C(16)	1.386 (11)
C(12)-C(13)	1.378 (14)
C(13)-C(14)	1.360 (15)
C(14)-C(15)	1.369 (13)
C(15)-C(16)	1.360 (11)
C(21)-C(22)	1.373 (10)
C(21)-C(26)	1.397 (10)
C(22)-C(23)	1.390 (15)
C(23)-C(24)	1.358 (15)
C(24)-C(25)	1.358 (14)
C(25)-C(26)	1.358 (11)

Table 3. Bond angles (E)

Pd(1)-I(1)-Pd(1A)	95.4(1)
I(1)-Pd(1)-I(2)	90.9(1)
I(1)-Pd(1)-P(1)	178.5(1)
I(2)-Pd(1)-P(1)	88.4(1)
I(1)-Pd(1)-I(1A)	84.6(1)
I(2)-Pd(1)-I(1A)	174.0(1)
P(1)-Pd(1)-I(1A)	96.2(1)
Pd(1)-P(1)-C(1)	114.8(2)
Pd(1)-P(1)-C(11)	111.7(3)
C(1)-P(1)-C(11)	105.9(3)
Pd(1)-P(1)-C(21)	116.3(2)
C(1)-P(1)-C(21)	104.0(3)
C(11)-P(1)-C(21)	102.9(3)
C(2)-O(1)-C(4)	113.0(6)
C(5)-O(6)-C(7)	114.2(8)
P(1)-C(1)-C(2)	114.9(5)
O(1)-C(2)-C(1)	109.0(6)
O(1)-C(4)-C(5)	109.6(7)
O(6)-C(5)-C(4)	109.4(8)
O(6)-C(7)-C(8)	113.4(11)
P(1)-C(11)-C(12)	119.9(6)
P(1)-C(11)-C(16)	122.7(5)
C(12)-C(11)-C(16)	117.5(7)
C(11)-C(12)-C(13)	120.7(9)
C(12)-C(13)-C(14)	120.9(9)
C(13)-C(14)-C(15)	118.6(9)
C(14)-C(15)-C(16)	121.5(9)
C(11)-C(16)-C(15)	120.8(7)
P(1)-C(21)-C(22)	122.5(6)
P(1)-C(21)-C(26)	120.6(5)
C(22)-C(21)-C(26)	116.8(7)
C(21)-C(22)-C(23)	120.6(8)
C(22)-C(23)-C(24)	121.3(9)
C(23)-C(24)-C(25)	118.5(9)
C(24)-C(25)-C(26)	121.1(8)
C(21)-C(26)-C(25)	121.7(7)

Table 4. Anisotropic displacement coefficients (Δ^2 x10^3)

	U11	U22	U33	U12	U13	U23
I(1)	87(1)	56(1)	53(1)	-21(1)	27(1)	-9(1)
I(2)	126(1)	49(1)	78(1)	-6(1)	43(1)	-14(1)
Pd(1)	64(1)	43(1)	44(1)	-2(1)	17(1)	0(1)
P(1)	57(1)	53(1)	46(1)	2(1)	14(1)	2(1)
O(1)	57(3)	73(3)	78(3)	-7(3)	15(2)	-10(3)
O(6)	98(4)	104(5)	94(5)	2(4)	17(4)	-22(4)
C(1)	75(5)	70(5)	39(4)	0(4)	5(3)	5(3)
C(2)	65(5)	67(5)	69(5)	2(4)	-4(4)	0(4)
C(4)	65(5)	86(6)	99(7)	-11(4)	16(5)	-18(5)
C(5)	82(6)	96(8)	112(8)	-10(5)	26(6)	-13(6)
C(7)	129(9)	107(9)	143(11)	-7(7)	65(8)	-21(8)
C(8)	150(10)	112(9)	114(9)	-31(8)	27(8)	-26(7)
C(11)	60(4)	63(5)	61(5)	8(4)	16(4)	6(4)
C(12)	88(6)	127(8)	71(6)	25(6)	27(5)	13(6)
C(13)	89(7)	154(11)	83(7)	47(7)	4(6)	28(7)
C(14)	67(5)	89(7)	110(8)	4(5)	16(6)	-17(6)
C(15)	62(5)	82(6)	86(6)	-8(4)	20(4)	-20(5)
C(16)	66(5)	66(5)	61(5)	4(4)	15(4)	-1(4)
C(21)	56(4)	62(4)	47(4)	-10(4)	18(3)	0(3)
C(22)	65(5)	90(6)	90(6)	-8(5)	10(5)	-15(5)
C(23)	87(7)	111(9)	112(8)	-27(6)	10(6)	-33(7)
C(24)	107(7)	72(6)	81(6)	-28(6)	22(5)	-1(5)
C(25)	108(7)	55(5)	77(6)	-10(5)	18(5)	-3(4)
C(26)	74(5)	58(5)	60(5)	-3(4)	9(4)	6(4)

3The anisotropic displacement exponent takes the form:
$-2\pi^2(h^2a^{*2}U11 + ... + 2hka^*b^*U12)$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($\Delta^2 x10^3$)

	x	y	z	U
H(1A)	-1622	-1643	2588	62
H(1B)	-1675	-213	2681	62
H(2A)	406	-10	2524	68
H(2B)	414	-1144	3020	68
H(4A)	2313	-2049	2515	83
H(4B)	2271	-724	2189	83
H(5A)	1940	-1733	1116	95
H(5B)	3286	-2069	1513	95
H(7A)	3025	-3912	786	121
H(7B)	1605	-3610	504	121
H(8A)	1927	-5620	435	123
H(8B)	2379	-5631	1232	123
H(8C)	946	-5326	947	123
H(12)	-3633	752	516	94
H(13)	-5613	1738	479	110
H(14)	-6745	1638	1416	88
H(15)	-5796	690	2428	76
H(16)	-3844	-322	2476	64
H(22)	-4395	-1916	934	82
H(23)	-4970	-3950	600	104
H(24)	-3455	-5538	718	85
H(25)	-1341	-5067	1129	79
H(26)	-745	-3059	1463	65