

ORGANOMETALLICS

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Table 1. Crystal data and structure refinement for 1.

Identification code	sen04b
Empirical formula	$C_8H_{18}Cl_2Pt_2$
Formula weight	575.30
Temperature	265(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Crystal color	Pale yellow block
Unit cell dimensions	$a = 10.424(5)$ Å $\alpha = 90^\circ$ $b = 8.357(3)$ Å $\beta = 109.77(3)^\circ$ $c = 7.434(3)$ Å $\gamma = 90^\circ$
Volume, Z	$609.5(5)$ Å ³ , 2
Density (calculated)	3.135 g/cm ³
Absorption coefficient	23.318 mm ⁻¹
F(000)	512
Crystal size	0.40 x 0.40 x 0.30 mm
θ range for data collection	2.08 to 29.98°
Limiting indices	$-14 \leq h \leq 14$, $-1 \leq k \leq 11$, $-10 \leq l \leq 1$
Reflections collected	2410
Independent reflections	1776 ($R_{int} = 0.0806$)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1767 / 0 / 56
Goodness-of-fit on F^2	1.018
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0629$, $wR2 = 0.1592$
R indices (all data)	$R1 = 0.0934$, $wR2 = 0.2138$
Extinction coefficient	$0.013(2)$
Largest diff. peak and hole	3.042 and -3.889 eÅ ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt	1511.9(5)	-52.7(6)	2051.2(7)	26(1)
Cl	-793(4)	-1317(5)	885(6)	38(1)
C(1)	1829(21)	-702(29)	4934(22)	54(5)
C(2)	2393(18)	-1881(18)	4078(22)	41(4)
C(3)	3357(15)	1065(19)	2806(21)	35(3)
C(4)	4222(18)	465(23)	1771(28)	45(4)

Table 3. Bond lengths [Å] and angles [°] for 1.

Pt-C(3)	2.04(2)	Pt-C(1)	2.13(2)
Pt-C(2)	2.12(2)	Pt-Cl#1	2.352(4)
Pt-Cl	2.497(4)	Cl-Pt#1	2.352(4)
C(1)-C(2)	1.41(3)	C(3)-C(4)	1.46(2)
C(3)-Pt-C(1)	91.7(7)	C(3)-Pt-C(2)	89.6(6)
C(1)-Pt-C(2)	38.6(7)	C(3)-Pt-Cl#1	90.4(4)
C(1)-Pt-Cl#1	162.2(6)	C(2)-Pt-Cl#1	159.1(5)
C(3)-Pt-Cl	175.6(4)	C(1)-Pt-Cl	92.6(6)
C(2)-Pt-Cl	94.4(5)	Cl#1-Pt-Cl	85.22(13)
Pt#1-Cl-Pt	94.78(13)	C(2)-C(1)-Pt	70.7(9)
C(1)-C(2)-Pt	70.7(10)	C(4)-C(3)-Pt	113.0(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y, -z

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Pt	25(1)	28(1)	24(1)	3(1)	6(1)	2(1)
Cl	30(2)	44(2)	35(2)	16(2)	3(1)	-5(2)
C(1)	63(13)	81(13)	15(7)	1(8)	10(7)	-2(11)
C(2)	58(10)	28(7)	34(8)	7(6)	14(8)	-8(7)
C(3)	42(9)	33(7)	33(8)	-3(6)	16(7)	-1(6)
C(4)	27(8)	49(9)	50(11)	5(8)	0(7)	-2(7)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(1A)	2467(21)	-51(29)	5913(22)	64
H(1B)	1026(21)	-1005(29)	5234(22)	64
H(2A)	1939(18)	-2912(18)	3851(22)	49
H(2B)	3380(18)	-1958(18)	4530(22)	49
H(3A)	3213(15)	2203(19)	2565(21)	42
H(3B)	3825(15)	922(19)	4166(21)	42
H(4A)	5072(18)	1033(23)	2178(28)	68
H(4B)	3773(18)	621(23)	425(28)	68
H(4C)	4390(18)	-656(23)	2030(28)	68