Table 2. *Selected bond lengths (Å) and angles (°)*

(I)

Mn1—P1	2.370 (1)	Mn1—P1A	2.374 (1)
P1—Mn1—P1A	77.0 (1)	Mn1—P1—Mn1A	103.0 (1)

(II)

Mn1—P1	2.408 (1)	Mn1—P1A	2.408 (1)
P1—Mn1—P1A	79.0 (1)	Mn1—P1—Mn1A	101.0 (1)

Compound (I) was obtained by the reaction of $Mn_2(CO)_{10}$ with cyclohexylphosphine in xylene solution in a glass tube at 443 K for 36 h and compound (II) by the reaction of $Mn_2(CO)_{10}$ with dicyclohexylphosphine dissolved in xylene in a glass tube at 433 K for 15 h. In both cases, the product was recrystallized from dichloromethane/pentane.

Scattering factors, structure solution, refinement, and all calculations for both stuctures: *SHELXTL-Plus* (Sheldrick, 1990). Other programs used: *PARST* (Nardelli, 1983).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55723 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: NA1017]

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inversion centres. Both the Pt atoms have square-planar coordination with Pt—S distances 2.313 (2) and 2.309 (2) Å and Pt—Cl distances 2.299 (2) and 2.300 (2) Å. In both molecules, benzothiophene C atoms are almost planar [maximum deviations 0.05 (1) and 0.04 (1) Å] with S atoms lying 0.434 (7) and 0.329 (6) Å out of the planes comprising C atoms.

Comment

Formation of coordination complexes between transition-metal species and organosulfur compounds could be employed as a means of removing sulfur compounds from effluents produced by pulp mills and other industrial facilities. Such complexes are also of intrinsic interest because of the fluxional behaviour of the sulfur ligand around the metal centre (Abel, 1990). The title compound (I) is an example of such a complex and was prepared by the interaction of 1,3-dihydrobenzo[c]thiophene with platinum(II) chloride in hot ethanolic solution. The crude product was purified by crystallization from ethanol. Full details of the preparative method have been published previously (Clark, Fait, Jones & Kirk, 1991).
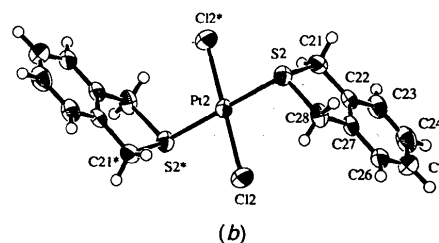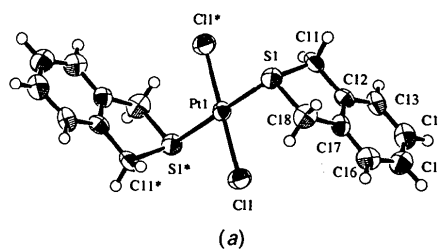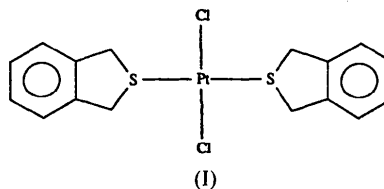

(I)

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trans-Dichlorobis(1,3-dihydrobenzo[c]thiophene-S)platinum(II)

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(*Received* 21 *April* 1992; *accepted* 8 *September* 1992)

Abstract

The asymmetric unit consists of two centrosymmetric half molecules of the title compound lying on

(a)

(b)

Fig. 1. Perspective views of the two independent molecules (a) and (b) of the title compound with crystallographic numbering scheme plotted by *ORTEP*II (Johnson, 1976).

Experimental

Crystal data

[Pt(C$_8$H$_8$S)$_2$Cl$_2$]
M_r = 538.43
Triclinic
$P\bar{1}$
a = 8.722 (1) Å
b = 10.240 (1) Å
c = 10.997 (1) Å
α = 109.38 (1)°
β = 96.64 (1)°
γ = 109.02 (1)°
V = 847.9 (2) Å^3
Z = 2

D_x = 2.110 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 10–16°
μ = 8.855 mm^{-1}
T = 295 K
Prism
0.30 × 0.30 × 0.24 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
Variable speed $\omega/2\theta$ scans
Absorption correction:
  DIFABS (Walker & Stuart, 1983)
  T_{min} = 0.764, T_{max} = 1.254
11050 measured reflections
4942 independent reflections

3900 observed reflections
  $[I > 3\sigma(I)]$
R_{int} = 0.023
θ_{max} = 30°
h = 0 → 12
k = −14 → 13
l = −15 → 15
3 standard reflections
  frequency: 60 min
  intensity variation: none

Refinement

Refinement on F
Final R = 0.037
wR = 0.037
S = 3.854
3900 reflections
193 parameters
H-atom parameters not refined
w = 1/σF

$(\Delta/\sigma)_{max}$ = 0.04
$\Delta\rho_{max}$ = 1.4 e Å^{-3}
$\Delta\rho_{min}$ = −2.3 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

Atoms Pt(1) and Pt(2) are on special positions with 0.5 occupancy factors.
U_{eq} = 1/3(trace of the orthogonalized U_{ij} tensor).

	x	y	z	U_{eq}
Pt(1)	0.0000	0.0000	0.5000	0.0370 (2)
Pt(2)	0.5000	0.0000	0.0000	0.0317 (1)
S(1)	0.0496 (2)	−0.0281 (2)	0.2925 (2)	0.0458 (7)
S(2)	0.4359 (2)	0.2101 (2)	0.0433 (2)	0.0367 (6)
Cl(1)	0.1201 (2)	0.2582 (2)	0.5933 (2)	0.0541 (8)
Cl(2)	0.7864 (2)	0.1238 (2)	0.0746 (2)	0.0564 (8)
C(11)	0.2265 (9)	−0.0860 (8)	0.2867 (7)	0.047 (3)
C(12)	0.3801 (8)	0.0599 (7)	0.3398 (6)	0.037 (3)
C(13)	0.5404 (9)	0.0706 (8)	0.3796 (7)	0.046 (3)
C(14)	0.6714 (10)	0.2092 (9)	0.4144 (7)	0.054 (3)
C(15)	0.6403 (10)	0.3280 (9)	0.4103 (7)	0.056 (3)
C(16)	0.4788 (10)	0.3182 (8)	0.3746 (7)	0.050 (3)
C(17)	0.3491 (8)	0.1822 (8)	0.3381 (6)	0.040 (3)
C(18)	0.1682 (9)	0.1547 (8)	0.2896 (7)	0.052 (3)
C(21)	0.3919 (8)	0.2221 (6)	−0.1187 (6)	0.037 (3)
C(22)	0.5497 (8)	0.3324 (6)	−0.1252 (6)	0.032 (2)
C(23)	0.5790 (9)	0.3552 (7)	−0.2389 (6)	0.043 (3)
C(24)	0.7279 (11)	0.4654 (9)	−0.2283 (8)	0.056 (4)
C(25)	0.8460 (9)	0.5541 (8)	−0.1058 (9)	0.054 (4)
C(26)	0.8163 (8)	0.5271 (7)	0.0034 (8)	0.043 (3)
C(27)	0.6707 (8)	0.4177 (6)	−0.0053 (6)	0.034 (2)
C(28)	0.6255 (9)	0.3838 (6)	0.1119 (6)	0.040 (3)

Table 2. *Geometric parameters* (Å, °)

Pt(1)—Cl(1)	2.299 (2)	Pt(2)—Cl(2)	2.300 (2)
Pt(1)—S(1)	2.313 (2)	Pt(2)—S(2)	2.309 (2)
S(1)—C(11)	1.826 (9)	S(2)—C(21)	1.831 (8)
S(1)—C(18)	1.833 (8)	S(2)—C(28)	1.836 (5)
C(11)—C(12)	1.518 (8)	C(21)—C(22)	1.496 (9)
C(12)—C(17)	1.369 (12)	C(22)—C(23)	1.383 (11)
C(12)—C(13)	1.374 (11)	C(22)—C(27)	1.389 (8)
C(13)—C(14)	1.397 (10)	C(23)—C(24)	1.378 (11)
C(14)—C(15)	1.344 (15)	C(24)—C(25)	1.400 (10)
C(15)—C(16)	1.379 (13)	C(25)—C(26)	1.354 (14)
C(16)—C(17)	1.370 (9)	C(26)—C(27)	1.360 (9)
C(17)—C(18)	1.506 (11)	C(27)—C(28)	1.505 (11)
Cl(1)—Pt(1)—S(1)	96.45 (7)	Cl(2)—Pt(2)—S(2)	97.25 (7)
C(11)—S(1)—C(18)	93.5 (4)	C(21)—S(2)—C(28)	93.6 (3)
Pt(1)—S(1)—C(11)	106.0 (3)	Pt(2)—S(2)—C(21)	104.8 (2)
Pt(1)—S(1)—C(18)	110.8 (2)	Pt(2)—S(2)—C(28)	111.6 (3)
C(12)—C(11)—S(1)	104.7 (5)	C(22)—C(21)—S(2)	106.5 (4)
C(17)—C(12)—C(13)	121.2 (6)	C(23)—C(22)—C(27)	119.8 (6)
C(17)—C(12)—C(11)	114.7 (7)	C(23)—C(22)—C(21)	124.9 (5)
C(13)—C(12)—C(11)	124.0 (7)	C(27)—C(22)—C(21)	115.3 (6)
C(12)—C(13)—C(14)	117.8 (8)	C(24)—C(23)—C(22)	118.2 (6)
C(15)—C(14)—C(13)	120.7 (8)	C(23)—C(24)—C(25)	121.3 (8)
C(14)—C(15)—C(16)	121.4 (7)	C(26)—C(25)—C(24)	119.4 (7)
C(17)—C(16)—C(15)	118.5 (8)	C(25)—C(26)—C(27)	120.2 (6)
C(12)—C(17)—C(16)	120.4 (7)	C(26)—C(27)—C(22)	121.1 (7)
C(12)—C(17)—C(18)	115.9 (6)	C(26)—C(27)—C(28)	123.6 (6)
C(16)—C(17)—C(18)	123.7 (8)	C(22)—C(27)—C(28)	115.3 (5)
C(17)—C(18)—S(1)	104.7 (6)	C(27)—C(28)—S(2)	106.1 (4)

Space group P or $P\bar{1}$; the latter was chosen and confirmed by successful analysis. Lorentz–polarization and absorption corrections; no extinction correction. Structure solved by direct methods using *Xtal2.6* (Hall & Stewart, 1989) and refined by full-matrix least-squares calculations. Non-H atoms allowed to refine with anisotropic temperature factors. H atoms included at geometrically idealized positions (C—H 0.95 Å).

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