Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: MU1154). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-Chloromethylbis(triphenylarsine)platinum(II)

ANDREAS ROODT, STEFANUS OTTO AND
JOHANN G. LEIPOLDT†

Department of Chemistry, University of the Orange Free State, Bloemfontein 9300, South Africa

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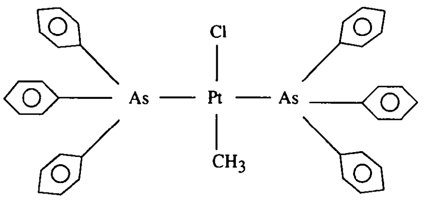
Abstract

The title compound, *trans*-chloromethylbis(triphenylarsine)platinum(II), *trans*-$[PtCl(CH_3)(C_{18}H_{15}As)_2]$, is isomorphous and isostructural with one of the two known crystalline forms of the corresponding triphenylphosphine analogue.

Comment

trans-Bis(triphenylarsine)chloromethylplatinum(II), (I), is one of the few bis(AsX_3)–platinum(II) complexes (where X is alkyl or aryl) isolated to date. It is isomorphous and isostructural with the analogous bis(triphenylphosphine) complex described by Bardi & Piazzesi (1981). However, a second crystalline form of the bis(triphenylphosphine) complex has recently been shown to exist (Otto, Roodt & Leipoldt, 1995).



[†] Deceased.

The *trans* influence of the methyl group is marginally less pronounced in (I) than it is in the bis(PPh_3) complex; Pt—Cl bond distances of 2.431 (3) and 2.415 (5) Å found in the above mentioned studies of the bis(PPh_3) complex may be compared with the slightly shorter distance of 2.410 (2) Å obtained from this study. This is in agreement with the electronic influence PPh_3 > $AsPh_3$ (Cheeseman, Odell & Raethel, 1968). The Pt—Cl bond is shorter than that of 2.437 (2) Å found in *trans*-$[PtClMe(AsMe_3)_2(\eta^2\text{-}F_3CC_2CF_3)]$ (Davies, Puddephatt & Payne, 1972). The larger steric demand of the methyl group (C1) compared with that of the chloro ligand is illustrated both by the As1—Pt—As2 angle [176.30 (3)°], which deviates significantly from 180°, and by the C11—As1—Pt and C41—As2—Pt angles, which are *ca* 10° greater than the ideal tetrahedral angle of 109.5°.

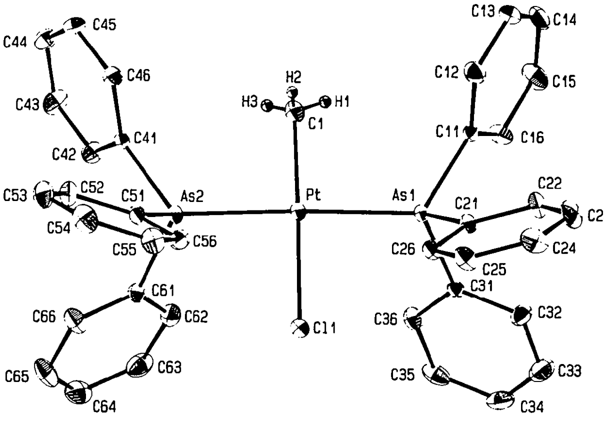


Fig. 1. *ORTEPII* (Johnson, 1976) view of the title structure showing the atom-numbering scheme and 30% displacement ellipsoids. The phenyl H atoms are omitted for clarity.

Experimental

The title complex was prepared by the addition of an excess of $[As(C_6H_5)_3]$ (1.0 g, 3.3 mmol) in acetone (20 ml) to *trans*-$[PtCl(CH_3)\{S(CH_3)_2\}_2]$ (500 mg, 1.35 mmol) (Scott & Puddephatt, 1983) in acetone (10 ml). The solution was stirred for 30 min at room temperature. Filtration and recrystallization from benzene gave the desired product (1.05 g, yield >90%). ^1H NMR ($CDCl_3$): $\delta(CH_3)$ 0.07 p.p.m., $^2J(PtH)$ 78 Hz. IR (KBr): $\nu(Pt—Cl)$ 324 cm^{-1}. The density D_m was measured by flotation in NaI/H_2O

Crystal data

$[PtCl(CH_3)(C_{18}H_{15}As)_2]$
$M_r = 858.01$
Monoclinic
$P2_1/n$
$a = 11.749\ (1)$ Å
$b = 23.342\ (2)$ Å
$c = 12.644\ (2)$ Å
$\beta = 111.32\ (1)°$

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 17–20°$
$\mu = 6.484$ mm^{-1}
$T = 293\ (2)$ K
Diamond shape

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$V = 3230.3$ (6) Å^3
$Z = 4$
$D_x = 1.764$ Mg m^{-3}
$D_m = 1.744$ Mg m^{-3}

0.29 × 0.28 × 0.27 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical (Akselrud, Grin, Zavalii, Pecharsky & Fundamuntsky, 1989)
$T_{\min} = 0.397$, $T_{\max} = 0.577$
2833 measured reflections
2833 independent reflections

2653 observed reflections [$I > 2\sigma(I)$]
$\theta_{\max} = 24.94°$
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 27$
$l = 0 \rightarrow 15$
3 standard reflections monitored every 100 reflections intensity decay: <1%

Refinement

Refinement on F^2
$R(F) = 0.0275$
$wR(F^2) = 0.0696$
$S = 1.066$
2833 reflections
373 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$ where $P = [\max(0,F_o^2) + 2F_c^2]/3$

$(\Delta/\sigma)_{\max} = 0.118$
$\Delta\rho_{\max} = 1.69$ e Å^{-3}
$\Delta\rho_{\min} = -1.41$ e Å^{-3}
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

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

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Pt	0.17280 (3)	0.346516 (13)	0.49556 (2)	0.03648 (13)
As1	0.16095 (8)	0.37062 (3)	0.30849 (6)	0.0364 (2)
As2	0.17871 (8)	0.32829 (3)	0.68258 (6)	0.0384 (2)
Cl1	0.1978 (2)	0.44693 (9)	0.5426 (2)	0.0492 (6)
C1	0.1610 (8)	0.2595 (3)	0.4603 (6)	0.041 (2)
C11	0.1486 (8)	0.3098 (3)	0.2012 (6)	0.033 (2)
C12	0.0408 (9)	0.2809 (4)	0.1531 (8)	0.059 (3)
C13	0.0296 (11)	0.2367 (4)	0.0755 (8)	0.066 (3)
C14	0.1262 (12)	0.2221 (4)	0.0463 (8)	0.067 (3)
C15	0.2344 (11)	0.2498 (5)	0.0948 (9)	0.073 (3)
C16	0.2458 (10)	0.2940 (4)	0.1720 (8)	0.057 (3)
C21	0.0217 (8)	0.4174 (3)	0.2196 (6)	0.042 (2)
C22	−0.0143 (9)	0.4198 (4)	0.1036 (7)	0.055 (3)
C23	−0.1118 (10)	0.4543 (5)	0.0416 (8)	0.072 (3)
C24	−0.1728 (9)	0.4847 (4)	0.0969 (9)	0.068 (3)
C25	−0.1386 (9)	0.4827 (4)	0.2097 (8)	0.055 (3)
C26	−0.0402 (8)	0.4486 (4)	0.2725 (7)	0.045 (2)
C31	0.3000 (7)	0.4145 (3)	0.3119 (6)	0.037 (2)
C32	0.2986 (9)	0.4494 (4)	0.2223 (8)	0.059 (3)
C33	0.3984 (12)	0.4812 (4)	0.2298 (11)	0.077 (3)
C34	0.5012 (11)	0.4799 (4)	0.3229 (11)	0.069 (3)
C35	0.5058 (9)	0.4452 (5)	0.4108 (9)	0.066 (3)
C36	0.4063 (8)	0.4127 (4)	0.4066 (7)	0.052 (2)
C41	0.1975 (8)	0.2503 (3)	0.7400 (6)	0.037 (2)
C42	0.3084 (9)	0.2305 (4)	0.8125 (8)	0.053 (2)
C43	0.3217 (10)	0.1757 (4)	0.8535 (9)	0.065 (3)
C44	0.2251 (10)	0.1393 (4)	0.8248 (8)	0.058 (3)
C45	0.1131 (10)	0.1584 (4)	0.7527 (8)	0.058 (3)
C46	0.0977 (9)	0.2135 (4)	0.7097 (7)	0.053 (2)
C51	0.0351 (8)	0.3550 (3)	0.7087 (6)	0.043 (2)
C52	0.0011 (10)	0.3329 (4)	0.7952 (7)	0.056 (3)
C53	−0.1018 (12)	0.3530 (5)	0.8098 (9)	0.072 (3)
C54	−0.1699 (10)	0.3957 (5)	0.7425 (9)	0.068 (3)
C55	−0.1368 (9)	0.4180 (4)	0.6587 (8)	0.059 (3)
C56	−0.0339 (9)	0.3986 (4)	0.6416 (7)	0.047 (2)
C61	0.3182 (9)	0.3631 (3)	0.7984 (7)	0.045 (2)
C62	0.4254 (11)	0.3660 (4)	0.7780 (8)	0.061 (3)
C63	0.5322 (10)	0.3830 (4)	0.8666 (10)	0.075 (3)
C64	0.5264 (12)	0.3984 (5)	0.9691 (9)	0.080 (4)
C65	0.4203 (8)	0.3980 (3)	0.9860 (6)	0.082 (4)
C66	0.3159 (8)	0.3792 (3)	0.9005 (6)	0.065 (3)

Table 2. *Selected geometric parameters* (Å, °)

Pt—C1	2.073 (8)	As1—C11	1.933 (7)
Pt—As2	2.3786 (9)	As1—C21	1.948 (8)
Pt—As1	2.3856 (9)	As2—C61	1.935 (9)
Pt—Cl1	2.410 (2)	As2—C51	1.936 (9)
As1—C31	1.915 (8)	As2—C41	1.942 (8)
C1—Pt—As2	90.8 (2)	C31—As1—Pt	111.2 (2)
C1—Pt—As1	92.4 (2)	C11—As1—Pt	119.0 (2)
As2—Pt—As1	176.30 (3)	C21—As1—Pt	116.0 (3)
C1—Pt—Cl1	177.0 (2)	C61—As2—Pt	112.8 (3)
As2—Pt—Cl1	88.38 (5)	C51—As2—Pt	113.6 (2)
As1—Pt—Cl1	88.46 (5)	C41—As2—Pt	119.8 (2)

H atoms were positioned assuming a C—H distance of 0.96 Å and were constrained to ride on their parent C atoms. A single orientation parameter was refined for the methyl group and the refined H-atom $U_{\rm iso}$ was 0.062 (5) Å^2.

Data collection: CAD-4 diffractometer software. Cell refinement: CAD-4 diffractometer software. Data reduction: *PROFIT* (Streltsov & Zavodnik, 1989). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1156). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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