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Bromido[(1,2,5,6-η)-1,3,5,7-cyclooctatetraene]methylplatinum(II)

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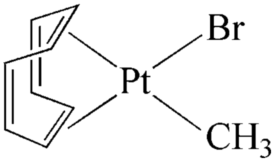
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.032 Å; R factor = 0.057; wR factor = 0.176; data-to-parameter ratio = 19.9.

In the title complex, $[PtBr(CH_3)(C_8H_8)]$, the Pt^{II} centre lies in a square-planar environment defined by the Br and methyl C atoms and the midpoints of the two π-coordinated double bonds of 1,3,5,7-cyclooctatetraene. Because of the different *trans* influences of the Br atom and the methyl group, the Pt—C bonds *trans* to the methyl group are longer than those *trans* to the Br atom.

Related literature

For related literature, see: Song *et al.* (2007).



Experimental

Crystal data

$[PtBr(CH_3)(C_8H_8)]$	V = 979.0 (2) Å^3
M_r = 394.18	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 8.3637 (12) Å	μ = 18.35 mm^{-1}
b = 10.1098 (15) Å	T = 293 (2) K
c = 11.6897 (17) Å	0.12 × 0.10 × 0.08 mm
β = 97.928 (3)°	

Data collection

Bruker SMART 1000 CCD diffractometer	5568 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	2009 independent reflections
T_{min} = 0.095, T_{max} = 0.230	1435 reflections with $I > 2\sigma(I)$
	R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057	101 parameters
$wR(F^2)$ = 0.176	H-atom parameters constrained
S = 1.04	$\Delta\rho_{max}$ = 3.68 e Å^{-3}
2009 reflections	$\Delta\rho_{min}$ = −2.52 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2159).

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supplementary materials

Acta Cryst. (2007). E**63**, m2484   [**doi:10.1107/S1600536807043279**]

Bromido[(1,2,5,6-η)-1,3,5,7-cyclooctatetraene]methylplatinum(II)

A.-R. Song, I.-C. Hwang and K. Ha

Comment

In the title complex, [Pt(CH_3)Br(C_8H_8)], the central Pt^{II} ion lies in an essentially square-planar environment defined by the Br and methyl C atoms and by the two mid-points (M1, M2) of the π-coordinated double bonds of the 1,3,5,7-cyclooctatetraene (cot) ligand (M1 and M2 denote the mid-points of the olefinic bonds C1—C2 and C5—C6, respectively). The Pt, Br, C9 atoms and the mid-points lie in a coordination plane with the largest deviation of 0.031 Å (M2) from the least-squares plane, and with bond angles in the range 88.0°–92.9°.

Owing to the different *trans* influences of the Br atom and methyl group, the Pt—C bonds *trans* to C9 are on average 0.173 Å longer than those *trans* to Br (mean lengths: Pt—C1/C2 = 2.314 Å, Pt—C5/C6 = 2.141 Å). The distances between the Pt atom and the mid-points are 2.227 Å (M1) and 2.027 Å (M2). The cot ligand coordinates symmetrically to the Pt atom in the "tub" conformation. The four coordinating C atoms (C1, C2, C5 and C6) and the four non-coordinating C atoms (C3, C4, C7 and C8) lie on respective planes, with the torsion angles C1—C2—C5—C6 = 0.2 (16)° and C3—C4—C7—C8 = −0.7 (18)°. The Pt atom is displaced by 1.524 (9) Å from the plane C1/C2/C5/C6, and by 2.503 (9) Å from the plane C3/C4/C7/C8. In the complex, the cot ring angles lie in the range 118 (2)° − 126 (2)°.

Experimental

To a solution of cyclooctatetraenedimethylplatinum(II) (0.2035 g, 0.618 mmol) in CH_2Cl_2 (30 ml) was added hydrobromic acid (48%; 0.1120 g, 0.664 mmol), and stirred for 5 h at room temperature. The solvent was removed under vacuum, the residue was washed with pentane, dissolved in ether, and filtered through a plug of Al_2O_3 (1 cm *x* 2 cm). Evaporation of the solvent gave a yellow powder (0.0763 g). Large plates were obtained by slow evaporation from a $CDCl_3$ solution.

Refinement

H atoms were positioned geometrically and allowed to ride on their respective carrier atoms, with C—H = 0.98, 0.93 or 0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

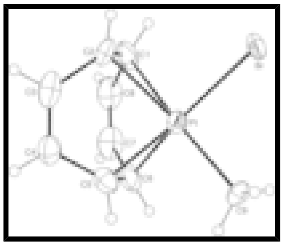

Fig. 1. The structure of the title compound with displacement ellipsoids drawn at the 30% probability level for non-H atoms. Hydrogen atoms are shown as spheres of arbitrary radii.

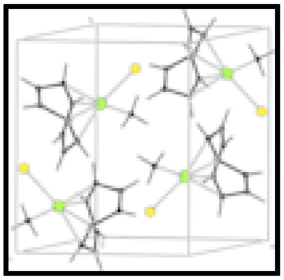

Fig. 2. View of the unit-cell contents of the title compound.

Bromido[(1,2,5,6-η)-1,3,5,7-cyclooctatetraene]methylplatinum(II)

Crystal data

$[PtBr(CH_3)(C_8H_8)]$

$M_r = 394.18$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.3637 (12)$ Å

$b = 10.1098 (15)$ Å

$c = 11.6897 (17)$ Å

$\beta = 97.928 (3)$°

$V = 979.0 (2)$ Å^3

$Z = 4$

$F_{000} = 712$

$D_x = 2.674$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 1512 reflections

$\theta = 2.8–24.2$°

$\mu = 18.35$ mm^{-1}

$T = 293 (2)$ K

Plate, yellow

0.12 × 0.10 × 0.08 mm

Data collection

Bruker SMART 1000 CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2)$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{min} = 0.095$, $T_{max} = 0.230$

5568 measured reflections

2009 independent reflections

1435 reflections with $I > 2\sigma(I)$

$R_{int} = 0.045$

$\theta_{max} = 26.4$°

$\theta_{min} = 2.7$°

$h = -10 \rightarrow 8$

$k = -12 \rightarrow 10$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.176$

$S = 1.04$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1039P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

2009 reflections	$\Delta\rho_{max} = 3.68$ e Å^{-3}
101 parameters	$\Delta\rho_{min} = -2.52$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The datum crystal was cut from a large plate of approximate dimensions 0.08 *X* 1.5 *X* 2.0 mm.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt	0.59256 (7)	0.30579 (7)	0.16610 (5)	0.0429 (3)
Br	0.36957 (17)	0.13420 (17)	0.12204 (16)	0.0469 (5)
C1	0.668 (2)	0.293 (2)	−0.0165 (17)	0.074 (7)
H1	0.5849	0.2611	−0.0775	0.088*
C2	0.749 (2)	0.2053 (18)	0.0419 (16)	0.050 (5)
H2	0.7231	0.1132	0.0207	0.060*
C3	0.923 (2)	0.234 (2)	0.106 (2)	0.068 (6)
H3	1.0085	0.1882	0.0819	0.081*
C4	0.956 (2)	0.320 (2)	0.1956 (18)	0.064 (6)
H4	1.0619	0.3357	0.2291	0.077*
C5	0.818 (2)	0.3893 (18)	0.2383 (17)	0.057 (5)
H5	0.8302	0.4016	0.3222	0.069*
C6	0.730 (2)	0.487 (2)	0.176 (2)	0.067 (6)
H6	0.6896	0.5572	0.2221	0.081*
C7	0.748 (3)	0.523 (3)	0.053 (2)	0.081 (7)
H7	0.7797	0.6088	0.0369	0.097*
C8	0.722 (3)	0.440 (3)	−0.028 (2)	0.084 (8)
H8	0.7352	0.4695	−0.1019	0.100*
C9	0.484 (2)	0.3641 (18)	0.3157 (12)	0.044 (4)
H9A	0.4693	0.2875	0.3617	0.066*
H9B	0.3808	0.4043	0.2910	0.066*
H9C	0.5527	0.4263	0.3607	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt	0.0398 (4)	0.0485 (5)	0.0418 (4)	0.0024 (3)	0.0102 (3)	0.0010 (3)

Br	0.0252 (7)	0.0412 (10)	0.0735 (11)	−0.0053 (6)	0.0036 (7)	0.0021 (8)
C1	0.051 (12)	0.13 (2)	0.042 (11)	−0.032 (12)	0.010 (9)	−0.001 (12)
C2	0.043 (9)	0.060 (13)	0.050 (10)	0.022 (8)	0.019 (8)	0.010 (9)
C3	0.055 (11)	0.059 (14)	0.096 (17)	0.014 (10)	0.035 (11)	0.040 (12)
C4	0.049 (11)	0.082 (16)	0.062 (13)	−0.001 (10)	0.014 (9)	0.009 (11)
C5	0.053 (11)	0.048 (12)	0.068 (12)	−0.005 (9)	−0.002 (9)	0.000 (9)
C6	0.047 (11)	0.065 (14)	0.091 (16)	−0.020 (10)	0.011 (10)	−0.004 (11)
C7	0.082 (16)	0.063 (16)	0.101 (19)	−0.004 (12)	0.030 (15)	0.041 (14)
C8	0.070 (14)	0.14 (3)	0.047 (13)	0.002 (15)	0.015 (11)	0.040 (14)
C9	0.051 (9)	0.053 (11)	0.029 (8)	0.008 (8)	0.015 (7)	0.010 (7)

Geometric parameters (Å, °)

Pt—C5	2.129 (17)	C4—C5	1.50 (3)
Pt—C6	2.152 (19)	C4—H4	0.9300
Pt—C9	2.161 (15)	C5—C6	1.38 (3)
Pt—C1	2.31 (2)	C5—H5	0.9800
Pt—C2	2.318 (16)	C6—C7	1.52 (3)
Pt—Br	2.5472 (16)	C6—H6	0.9800
C1—C2	1.26 (3)	C7—C8	1.26 (3)
C1—C8	1.57 (3)	C7—H7	0.9300
C1—H1	0.9800	C8—H8	0.9300
C2—C3	1.57 (3)	C9—H9A	0.9600
C2—H2	0.9800	C9—H9B	0.9600
C3—C4	1.36 (3)	C9—H9C	0.9600
C3—H3	0.9300		

C5—Pt—C6	37.5 (7)	C2—C3—H3	117.8
C5—Pt—C9	91.1 (7)	C3—C4—C5	118.0 (18)
C6—Pt—C9	90.3 (8)	C3—C4—H4	121.0
C5—Pt—C1	92.8 (8)	C5—C4—H4	121.0
C6—Pt—C1	83.4 (8)	C6—C5—C4	122.8 (19)
C9—Pt—C1	164.0 (8)	C6—C5—Pt	72.1 (11)
C5—Pt—C2	83.0 (7)	C4—C5—Pt	111.4 (14)
C6—Pt—C2	93.7 (8)	C6—C5—H5	114.4
C9—Pt—C2	164.4 (6)	C4—C5—H5	114.4
C1—Pt—C2	31.6 (7)	Pt—C5—H5	114.4
C5—Pt—Br	158.9 (5)	C5—C6—C7	124 (2)
C6—Pt—Br	163.5 (6)	C5—C6—Pt	70.4 (11)
C9—Pt—Br	88.3 (5)	C7—C6—Pt	106.3 (15)
C1—Pt—Br	93.5 (5)	C5—C6—H6	115.4
C2—Pt—Br	92.0 (5)	C7—C6—H6	115.4
C2—C1—C8	125.5 (19)	Pt—C6—H6	115.4
C2—C1—Pt	74.5 (12)	C8—C7—C6	121 (2)
C8—C1—Pt	98.5 (14)	C8—C7—H7	119.3
C2—C1—H1	115.7	C6—C7—H7	119.3
C8—C1—H1	115.7	C7—C8—C1	126 (2)
Pt—C1—H1	115.7	C7—C8—H8	117.1
C1—C2—C3	121.6 (18)	C1—C8—H8	117.1
C1—C2—Pt	73.9 (12)	Pt—C9—H9A	109.5

C3—C2—Pt	100.6 (13)	Pt—C9—H9B	109.5
C1—C2—H2	116.8	H9A—C9—H9B	109.5
C3—C2—H2	116.8	Pt—C9—H9C	109.5
Pt—C2—H2	116.8	H9A—C9—H9C	109.5
C4—C3—C2	124.4 (18)	H9B—C9—H9C	109.5
C4—C3—H3	117.8		

C5—Pt—C1—C2	71.8 (13)	Br—Pt—C5—C6	−177.3 (12)
C6—Pt—C1—C2	108.1 (14)	C6—Pt—C5—C4	−119 (2)
C9—Pt—C1—C2	176 (2)	C9—Pt—C5—C4	152.0 (14)
Br—Pt—C1—C2	−88.1 (12)	C1—Pt—C5—C4	−43.6 (15)
C5—Pt—C1—C8	−52.8 (14)	C2—Pt—C5—C4	−13.5 (14)
C6—Pt—C1—C8	−16.4 (13)	Br—Pt—C5—C4	64 (2)
C9—Pt—C1—C8	51 (3)	C4—C5—C6—C7	8(3)
C2—Pt—C1—C8	−124.6 (19)	Pt—C5—C6—C7	−97 (2)
Br—Pt—C1—C8	147.3 (12)	C4—C5—C6—Pt	104.4 (18)
C8—C1—C2—C3	−3(3)	C9—Pt—C6—C5	91.5 (13)
Pt—C1—C2—C3	−92.8 (18)	C1—Pt—C6—C5	−103.3 (14)
C8—C1—C2—Pt	90 (2)	C2—Pt—C6—C5	−73.4 (13)
C5—Pt—C2—C1	−107.1 (14)	Br—Pt—C6—C5	176.6 (16)
C6—Pt—C2—C1	−71.1 (14)	C5—Pt—C6—C7	121 (2)
C9—Pt—C2—C1	−175 (2)	C9—Pt—C6—C7	−147.5 (14)
Br—Pt—C2—C1	93.5 (12)	C1—Pt—C6—C7	17.7 (14)
C5—Pt—C2—C3	13.0 (11)	C2—Pt—C6—C7	47.6 (15)
C6—Pt—C2—C3	49.0 (12)	Br—Pt—C6—C7	−62 (3)
C9—Pt—C2—C3	−55 (3)	C5—C6—C7—C8	61 (3)
C1—Pt—C2—C3	120.1 (18)	Pt—C6—C7—C8	−16 (3)
Br—Pt—C2—C3	−146.5 (10)	C6—C7—C8—C1	0(4)
C1—C2—C3—C4	65 (3)	C2—C1—C8—C7	−63 (4)
Pt—C2—C3—C4	−12 (2)	Pt—C1—C8—C7	15 (3)
C2—C3—C4—C5	2(3)	C1—C2—C5—C6	0.2 (16)
C3—C4—C5—C6	−71 (3)	C3—C4—C7—C8	−0.7 (18)
C3—C4—C5—Pt	11 (2)	C3—C2—C1—C8	−3(3)
C9—Pt—C5—C6	−89.0 (13)	C4—C5—C6—C7	8(3)
C1—Pt—C5—C6	75.4 (14)	C2—C3—C4—C5	2(3)
C2—Pt—C5—C6	105.5 (13)	C6—C7—C8—C1	0(4)

Fig. 1

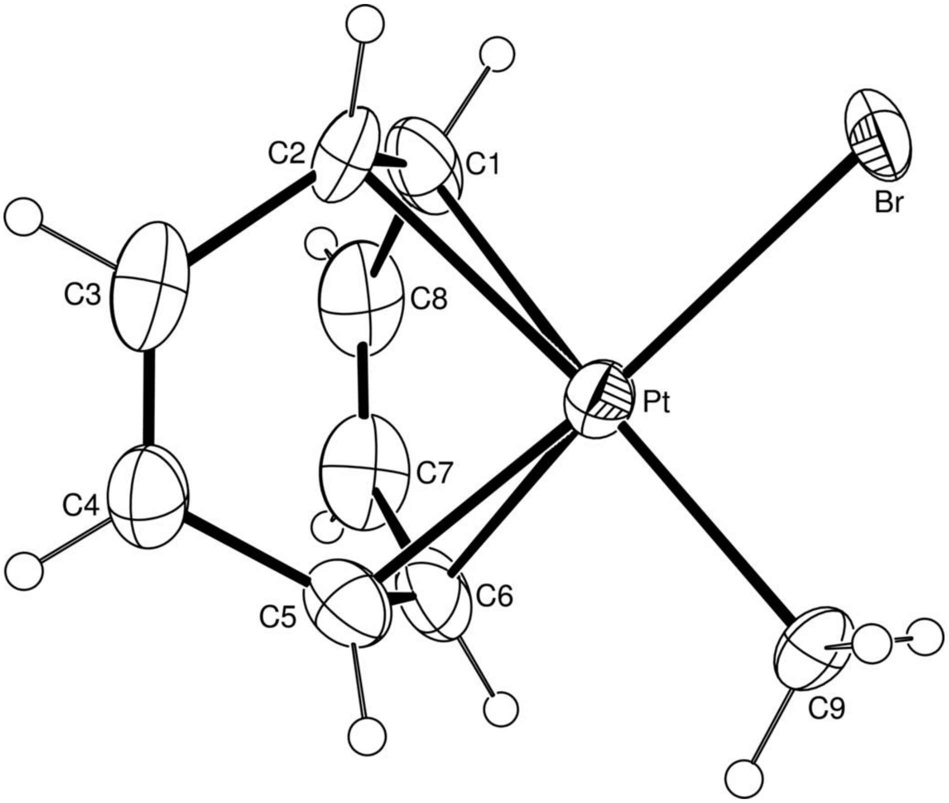

Fig. 2