Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[(1,2,5,6-η)-1,3,5,7-Cyclooctatetraene]-iodido(methyl)platinum(II)

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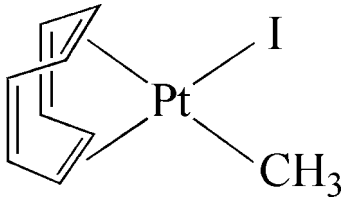
Received 30 May 2007; accepted 7 June 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.014 Å; R factor = 0.035; wR factor = 0.095; data-to-parameter ratio = 20.1.

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

Related literature

For a related structure, see: Song *et al.* (2006).



Experimental

Crystal data

$[Pt(CH_3)I(C_8H_8)]$
M_r = 441.17
Monoclinic, $P2_1/c$
a = 8.447 (2) Å
b = 10.181 (2) Å
c = 13.504 (2) Å
β = 120.901 (3)°
V = 996.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 17.12 mm^{-1}
T = 293 (2) K
0.18 × 0.17 × 0.10 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.063, T_{max} = 0.181
5241 measured reflections
2034 independent reflections
1824 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
S = 1.04
2034 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.04 e Å^{-3}
$\Delta\rho_{min}$ = −1.65 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*.

This study received financial support from Chonnam National University in 2006.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2192).

References

Bruker (2000). *SADABS* (Version 2.03), *SMART* (Version 5.618) and *SAINT* (Version 6.02a). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Song, A.-R., Hwang, I.-C. & Ha, K. (2006). *Z. Kristallogr. New Cryst. Struct.* **221**, 465–467.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E**63**, m1879 [**doi:10.1107/S1600536807028012**]

[(1,2,5,6-η)-1,3,5,7-Cyclooctatetraene]iodido(methyl)platinum(II)

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

Comment

In the title complex, [PtI(CH_3)(C_8H_8)], the central Pt^{II} ion lies in an essentially square-planar environment defined by the I and methyl C atoms and by the two midpoints (M1, M2) of the π-coordinated double bonds of the 1,3,5,7-cyclooctatetraene (cot) ligand (M1 and M2 denote the midpoints of the olefinic bonds C1—C2 and C5—C6, respectively). The Pt, I, C9 atoms and the midpoints lie in a coordination plane with the largest deviation of 0.024 Å (M2) from the least-squares plane, and with bond angles in the range 85.9–94.5°.

Owing to the different *trans* influence of the I atom and methyl group, the Pt—C bonds*trans* to C9 are on average 0.142 Å longer than those *trans* to I (mean lengths: Pt—C1/C2 = 2.280 Å, Pt—C5/C6 = 2.138 Å). The distances between the Pt atom and the midpoints are 2.174 Å (M1) and 2.019 Å (M2). The cot ligand coordinates symmetrically to the Pt atom in the "tub" conformation, and displays some increase in the coordinated double-bond distances (1.376 (12) Å and 1.401 (13) Å) compared to the non-coordinated double bonds (1.325 (13) Å and 1.289 (15) Å). 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 = 0.8 (7)° and C3—C4—C7—C8 = −1.6 (8)°. The Pt atom is displaced by 1.532 (5) Å from the plane C1/C2/C5/C6, and by 2.501 (5) Å from the plane C3/C4/C7/C8. The dihedral angle between these least-squares planes is 0.4 (7)°. In the complex, the cot ring angles lie in the range 121.2 (8)–123.7 (8)°.

Experimental

An aqueous solution of HI (57%; 0.1337 g, 0.596 mmol) was added to a solution of cyclooctatetraenedimethylplatinum(II) (0.2120 g, 0.644 mmol) in CH_2Cl_2 (20 ml) and MeOH (10 ml), and stirred for 10 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 × 2 cm). Evaporation of the solvent gave a yellow powder (0.0171 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a CH_2Cl_2 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

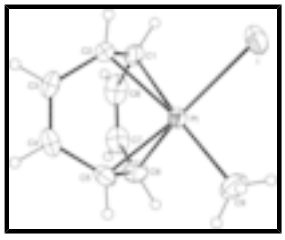


Fig. 1. The structure of the title compound, with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

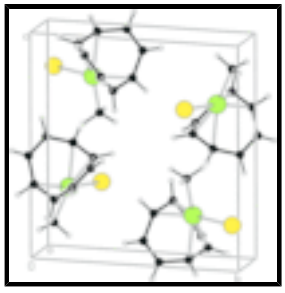


Fig. 2. View of the unit-cell contents of the title compound.

[(1,2,5,6-η^4)-1,3,5,7-Cyclooctatetraene]iodo(methyl)platinum(II)

Crystal data

[Pt(CH$_3$)I(C$_8$H$_8$)]	F_{000} = 784
M_r = 441.17	D_x = 2.941 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3200 reflections
a = 8.447 (2) Å	θ = 2.7–26.4º
b = 10.181 (2) Å	μ = 17.12 mm^{-1}
c = 13.504 (2) Å	T = 293 (2) K
β = 120.901 (3)º	Plate, yellow
V = 996.5 (3) Å^3	0.18 × 0.17 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	2034 independent reflections
Radiation source: fine-focus sealed tube	1824 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 293(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −5→10
T_{min} = 0.063, T_{max} = 0.181	k = −12→12
5241 measured reflections	l = −16→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.095$	$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.318P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2034 reflections	$\Delta\rho_{max} = 2.04$ e Å^{-3}
101 parameters	$\Delta\rho_{min} = -1.64$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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	−0.07706 (4)	0.19134 (3)	0.33127 (2)	0.03353 (14)
I	−0.25885 (8)	0.36453 (6)	0.37576 (6)	0.0554 (2)
C1	0.1744 (12)	0.1904 (9)	0.5146 (7)	0.048 (2)
H1	0.1547	0.2215	0.5761	0.058*
C2	0.2011 (11)	0.2851 (9)	0.4519 (8)	0.0438 (19)
H2	0.1965	0.3760	0.4743	0.053*
C3	0.3096 (11)	0.2642 (9)	0.3965 (7)	0.0456 (19)
H3	0.4196	0.3097	0.4233	0.055*
C4	0.2537 (12)	0.1815 (9)	0.3090 (8)	0.050 (2)
H4	0.3263	0.1694	0.2763	0.060*
C5	0.0784 (12)	0.1079 (9)	0.2621 (7)	0.048 (2)
H5	0.0101	0.0950	0.1783	0.057*
C6	0.0489 (13)	0.0121 (8)	0.3254 (8)	0.052 (2)
H6	−0.0371	−0.0580	0.2793	0.063*
C7	0.1911 (14)	−0.0256 (10)	0.4420 (10)	0.061 (2)
H7	0.2403	−0.1099	0.4550	0.073*
C8	0.2505 (14)	0.0547 (11)	0.5277 (9)	0.066 (3)
H8	0.3438	0.0272	0.6002	0.079*

C9	−0.3222 (14)	0.1393 (12)	0.1861 (8)	0.064 (3)
H9A	−0.3010	0.0683	0.1476	0.096*
H9B	−0.3711	0.2133	0.1350	0.096*
H9C	−0.4088	0.1122	0.2080	0.096*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt	0.0312 (2)	0.0354 (2)	0.0346 (2)	−0.00195 (10)	0.01736 (15)	−0.00058 (11)
I	0.0558 (4)	0.0487 (4)	0.0810 (4)	0.0069 (3)	0.0489 (3)	0.0041 (3)
C1	0.036 (4)	0.074 (7)	0.029 (4)	−0.008 (4)	0.013 (3)	−0.005 (4)
C2	0.037 (4)	0.051 (5)	0.045 (4)	−0.009 (3)	0.022 (4)	−0.015 (4)
C3	0.027 (4)	0.050 (5)	0.052 (5)	−0.003 (4)	0.015 (3)	0.010 (4)
C4	0.045 (5)	0.062 (6)	0.057 (5)	0.014 (4)	0.036 (4)	0.016 (4)
C5	0.052 (5)	0.052 (5)	0.048 (4)	0.004 (4)	0.032 (4)	−0.007 (4)
C6	0.063 (6)	0.028 (4)	0.067 (6)	−0.003 (4)	0.034 (5)	−0.007 (4)
C7	0.064 (6)	0.041 (5)	0.082 (7)	0.012 (4)	0.041 (5)	0.020 (5)
C8	0.053 (6)	0.076 (7)	0.062 (6)	0.013 (5)	0.025 (5)	0.041 (6)
C9	0.048 (5)	0.081 (7)	0.046 (5)	−0.014 (5)	0.012 (4)	−0.009 (5)

Geometric parameters (Å, °)

Pt—C9	2.060 (9)	C4—C5	1.481 (13)
Pt—C6	2.135 (8)	C4—H4	0.930
Pt—C5	2.140 (8)	C5—C6	1.401 (13)
Pt—C2	2.270 (8)	C5—H5	0.980
Pt—C1	2.289 (8)	C6—C7	1.459 (14)
Pt—I	2.6029 (7)	C6—H6	0.980
C1—C2	1.376 (12)	C7—C8	1.289 (15)
C1—C8	1.495 (14)	C7—H7	0.930
C1—H1	0.980	C8—H8	0.930
C2—C3	1.466 (12)	C9—H9A	0.960
C2—H2	0.980	C9—H9B	0.960
C3—C4	1.325 (13)	C9—H9C	0.960
C3—H3	0.930		
C9—Pt—C6	91.2 (4)	C2—C3—H3	119.4
C9—Pt—C5	91.4 (4)	C3—C4—C5	121.6 (8)
C6—Pt—C5	38.3 (3)	C3—C4—H4	119.2
C9—Pt—C2	162.8 (4)	C5—C4—H4	119.2
C6—Pt—C2	92.0 (3)	C6—C5—C4	122.9 (8)
C5—Pt—C2	80.8 (3)	C6—C5—Pt	70.7 (5)
C9—Pt—C1	161.7 (4)	C4—C5—Pt	108.4 (6)
C6—Pt—C1	80.4 (3)	C6—C5—H5	115.4
C5—Pt—C1	91.9 (3)	C4—C5—H5	115.4
C2—Pt—C1	35.1 (3)	Pt—C5—H5	115.4
C9—Pt—I	88.3 (3)	C5—C6—C7	122.4 (8)
C6—Pt—I	162.2 (3)	C5—C6—Pt	71.1 (5)
C5—Pt—I	159.5 (2)	C7—C6—Pt	109.5 (7)

C2—Pt—I	93.7 (2)	C5—C6—H6	115.2
C1—Pt—I	94.8 (2)	C7—C6—H6	115.2
C2—C1—C8	121.6 (8)	Pt—C6—H6	115.2
C2—C1—Pt	71.7 (5)	C8—C7—C6	121.8 (9)
C8—C1—Pt	103.6 (6)	C8—C7—H7	119.1
C2—C1—H1	116.6	C6—C7—H7	119.1
C8—C1—H1	116.6	C7—C8—C1	122.3 (9)
Pt—C1—H1	116.6	C7—C8—H8	118.8
C1—C2—C3	123.7 (8)	C1—C8—H8	118.8
C1—C2—Pt	73.2 (5)	Pt—C9—H9A	109.5
C3—C2—Pt	105.1 (5)	Pt—C9—H9B	109.5
C1—C2—H2	115.3	H9A—C9—H9B	109.5
C3—C2—H2	115.3	Pt—C9—H9C	109.5
Pt—C2—H2	115.3	H9A—C9—H9C	109.5
C4—C3—C2	121.2 (8)	H9B—C9—H9C	109.5
C4—C3—H3	119.4		
C9—Pt—C1—C2	171.3 (12)	I—Pt—C5—C6	−179.1 (5)
C6—Pt—C1—C2	107.5 (6)	C9—Pt—C5—C4	150.5 (7)
C5—Pt—C1—C2	70.9 (6)	C6—Pt—C5—C4	−119.3 (8)
I—Pt—C1—C2	−89.7 (5)	C2—Pt—C5—C4	−14.1 (6)
C9—Pt—C1—C8	52.1 (15)	C1—Pt—C5—C4	−47.6 (6)
C6—Pt—C1—C8	−11.7 (6)	I—Pt—C5—C4	61.6 (10)
C5—Pt—C1—C8	−48.3 (6)	C4—C5—C6—C7	−1.8 (14)
C2—Pt—C1—C8	−119.2 (9)	Pt—C5—C6—C7	−101.6 (9)
I—Pt—C1—C8	151.1 (6)	C4—C5—C6—Pt	99.8 (8)
C8—C1—C2—C3	−2.2 (13)	C9—Pt—C6—C5	90.7 (6)
Pt—C1—C2—C3	−97.2 (8)	C2—Pt—C6—C5	−72.4 (5)
C8—C1—C2—Pt	95.0 (8)	C1—Pt—C6—C5	−105.7 (6)
C9—Pt—C2—C1	−170.8 (13)	I—Pt—C6—C5	178.9 (6)
C6—Pt—C2—C1	−70.2 (6)	C9—Pt—C6—C7	−150.6 (7)
C5—Pt—C2—C1	−106.9 (6)	C5—Pt—C6—C7	118.7 (9)
I—Pt—C2—C1	93.0 (5)	C2—Pt—C6—C7	46.3 (7)
C9—Pt—C2—C3	−49.5 (16)	C1—Pt—C6—C7	13.0 (6)
C6—Pt—C2—C3	51.1 (6)	I—Pt—C6—C7	−62.4 (11)
C5—Pt—C2—C3	14.3 (6)	C5—C6—C7—C8	66.5 (14)
C1—Pt—C2—C3	121.2 (9)	Pt—C6—C7—C8	−13.0 (12)
I—Pt—C2—C3	−145.8 (6)	C6—C7—C8—C1	1.9 (16)
C1—C2—C3—C4	66.9 (12)	C2—C1—C8—C7	−67.4 (13)
Pt—C2—C3—C4	−12.8 (10)	Pt—C1—C8—C7	9.3 (12)
C2—C3—C4—C5	0.9 (13)	C1—C2—C5—C6	0.8 (7)
C3—C4—C5—C6	−65.9 (12)	C3—C4—C7—C8	−1.6 (8)
C3—C4—C5—Pt	12.6 (10)	C3—C2—C1—C8	−2.2 (13)
C9—Pt—C5—C6	−90.2 (6)	C4—C5—C6—C7	−1.8 (14)
C2—Pt—C5—C6	105.2 (6)	C2—C3—C4—C5	0.9 (13)
C1—Pt—C5—C6	71.8 (5)	C6—C7—C8—C1	1.9 (16)

Fig. 1

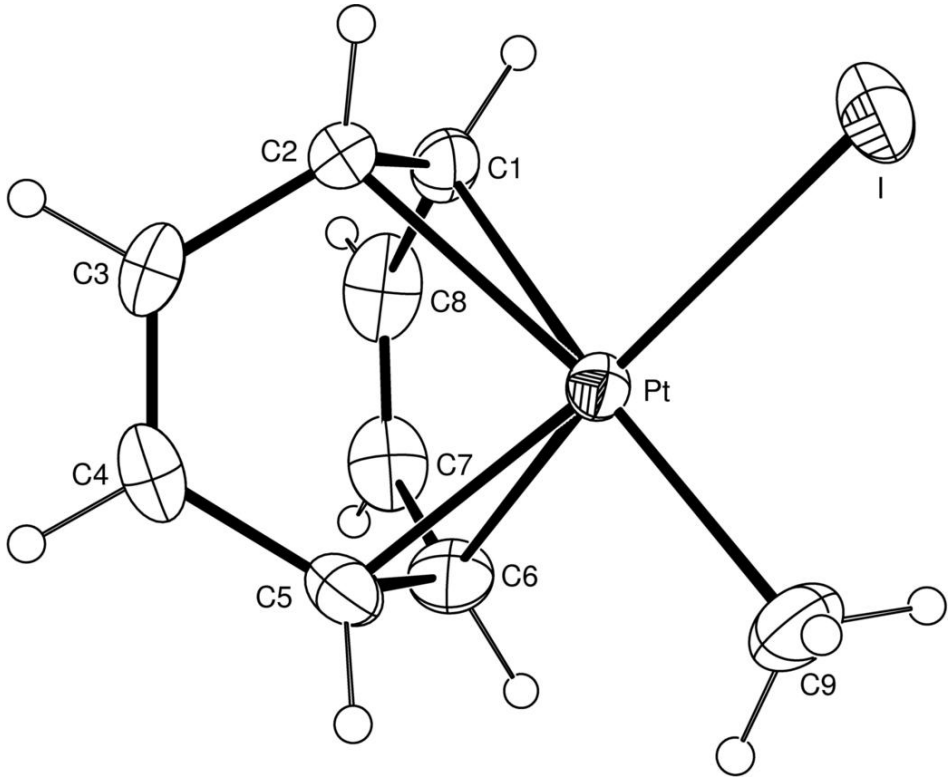


Fig. 2