Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

[(1,2,5,6-η)-Cycloocta-1,5-diene]bis(4-methoxyphenyl)platinum(II)

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Received 26 April 2006
Accepted 24 May 2006

Key indicators

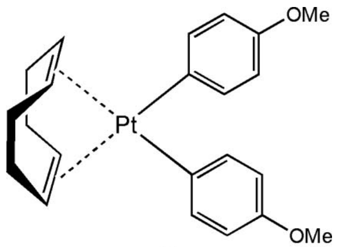
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.024
wR factor = 0.055
Data-to-parameter ratio = 17.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, [Pt(C_7H_7O)$_2$(C_8H_{12})], is a precursor to aryl Pt^{II} complexes containing N or P ligands, which are currently being investigated due to their possible role in C—H and C—C bond formation. The coordination geometry around the Pt atom is square planar, while the coordinated cycloocta-1,5-diene ligand adopts a twist-boat conformation.

Comment

Bis-hydrocarbyl–platinum(II) complexes are attracting increasing attention because of their involvement in C—H activations and in C—C bond formation. Within this latter research field, a kinetic study has recently evaluated the electronic effects on reductive elimination of the substituents of symmetrical and unsymmetrical bis-aryl–platinum complexes containing diphosphine ligands (Shekhar & Hartwig, 2004). Useful precursors of these compounds are the corresponding bis-aryl complexes containing COD as a bidentate ligand [COD = (1,2,5,6-η)-cycloocta-1,5-diene]. The molecular structure of a precursor used in this study, with a p-methoxyphenyl group as aryl substituent, is described here.



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1. The complex shows a square-planar geometry around the metal atom, with the coordination plane defined by atoms C9 and C16, and the mid-points of the coordinated double bonds (Ct1 and Ct2 lie at the mid-points of the C1═C2 and C5═C6 bonds, respectively) [Pt1—Ct1 = 2.152 (4)Å, Pt1—Ct2 = 2.150 (5)Å, Ct1—Pt1—Ct2 = 85.0 (2)°, Ct1—Pt1—C16 = 93.3 (2)° and Ct2—Pt1—C9 = 94.58 (2)°]. C9, C16, Ct1, Ct2 and Pt1 are coplanar (the maximum distance from the mean plane is within one standard uncertainty). The Pt—Ct1 and Pt—Ct2 distances are equivalent within the declared precision, showing a symmetrical coordination of the COD ligand. All bond distances and angles fall in the range reported for similar complexes (Debaerdemaeker, Stapp & Brune, 1987; Debaerdemaeker, Baumgartner & Brune, 1987; Deacon *et al.*, 1993). The coordinated COD molecule adopts a twist-boat conformation, as is commonly observed in most of its metal complexes (Rettig *et al.*, 1981).

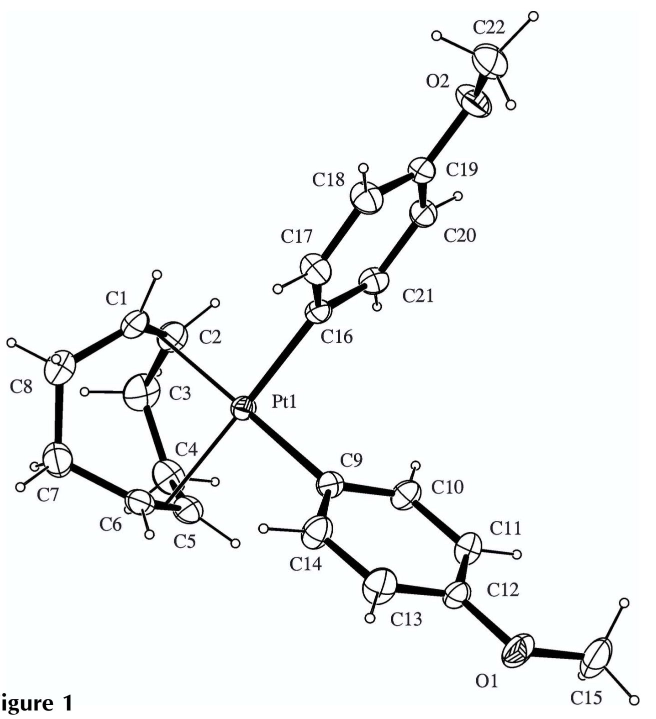


Figure 1
ORTEP-3 (Farrugia, 1997) view of compound (I). Displacement ellipsoids are drawn at the 30% probability level.

The orientations of the two benzene rings with respect to the coordination plane are not equivalent [the angle with the C9–C14 mean plane is 69.8 (1)° and with C16–C21 is 86.2 (1)°]. One methoxy group is coplanar with the attached benzene ring, while a deviation from planarity is observed for the other one [C15—O1—C12—C13 = −178.7 (4)° and C22—O2—C19—C18 = −166.6 (4)°]. This effect could be due to a weak C—H···π interaction between one of the methoxy groups and the benzene ring of an adjacent molecule [C22—H22*b*···*Ct*3$^{\rm i}$ = 2.773 Å and 149°; *Ct*3 is the centroid of ring C9–C14; symmetry code: (i) $-x$, $-y + 1$, $-z + 1$].

Experimental

The title compound was obtained by reaction of [$PtCl_2$(COD)] (3.74 g, 10.0 mmol) with the aryl Grignard reagent 4-MeO-C_6H_4MgBr (100 mmol) in diethyl ether at room temperature, according to the literature procedure (Shekhar & Hartwig, 2004). After 2 h, the reaction mixture was hydrolysed with a saturated solution of NH_4Cl. The pure complex was extracted with diethyl ether (yield: 80%). Suitable crystals were obtained by slow evaporation of a diethyl ether solution of the complex at 278 K.

Crystal data

[$Pt(C_7H_7O)_2(C_8H_{12})$]
$M_r = 517.52$
Triclinic, $P\overline{1}$
$a = 9.0720$ (6) Å
$b = 10.359$ (2) Å
$c = 10.920$ (1) Å
$\alpha = 80.94$ (1)°
$\beta = 73.078$ (7)°
$\gamma = 76.924$ (8)°
$V = 951.7$ (2) Å^3
$Z = 2$
$D_x = 1.806$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 7.38$ mm^{-1}
$T = 295$ (2) K
Prism, white
0.40 × 0.40 × 0.30 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Thick–slice φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker–Nonius, 2002)
$T_{\rm min} = 0.079$, $T_{\rm max} = 0.109$
14434 measured reflections
4290 independent reflections
3782 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.041$
$\theta_{\rm max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.055$
$S = 1.03$
4290 reflections
240 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0221P)^2 + 0.4852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 1.01$ e Å^{-3}
$\Delta\rho_{\rm min} = -1.58$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—C1	2.252 (4)	Pt1—C9	2.034 (4)
Pt1—C2	2.264 (4)	Pt1—C16	2.027 (4)
Pt1—C5	2.244 (4)	C1—C2	1.370 (7)
Pt1—C6	2.267 (4)	C5—C6	1.359 (6)
C16—Pt1—C9	87.1 (1)		

All H atoms, except for the olefinic H atoms, were positioned geometrically and allowed to ride on their parent atoms (C—H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms), with $U_{\rm iso} = U_{\rm eq}$(C). The olefinic H atoms were located in a difference Fourier map and their coordinates were refined with isotropic displacement parameters equal to those of the carrier atoms. The highest peak is located 0.88 Å from atom Pt1 and the deepset hole 0.89 Å from the same atom.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the MIUR (PRIN 2004) for financial support. Thanks are also due to the 'Centro Regionale di Competenza, Regione Campania NTAP' and the 'Centro Interdipartimentale di Metodologie Chimico Fisiche' of University of Naples for X-ray equipment.

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