Verfeinerung

Verfeinerung auf F^2
$R[F^2 > 2\sigma(F^2)] = 0,0405$
$wR(F^2) = 0,1201$
$S = 0,980$
1343 Reflexe
76 Parameter
Ein gemeinsamer Wert für
$\quad U(H)$
$w = 1/[\sigma^2(F_o^2) + (0,1000P)^2]$
$\quad$ mit $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = -0,023$
$\Delta\rho_{max} = 0,717$ e Å^{-3}
$\Delta\rho_{min} = -0,769$ e Å^{-3}
Extinktionskorrektur: keine
Atomformfaktoren aus
International Tables for
Crystallography (1992,
Bd. C, Tabellen 4.2.6.8
und 6.1.1.4)

Tabelle 3. *Atomkoordinaten und Parameter für den äquivalenten isotropen Temperaturfaktor (Å^2) von PPh$_4$[SnCl$_5$.H$_2$O]*

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

	x	y	z	$U_{\text{äq}}$
Sn	1/4	1/4	0,17383 (9)	0,0403 (3)
Cl1	1/4	1/4	0,4841 (4)	0,0692 (10)
Cl2	0,1905 (2)	0,07952 (15)	0,1495 (3)	0,0900 (8)
O	1/4	1/4	−0,1216 (18)	0,181 (9)
P	3/4	1/4	0	0,0369 (6)
C1	0,7072 (4)	0,3506 (4)	0,1422 (7)	0,0391 (12)
C2	0,6104 (4)	0,3891 (4)	0,1334 (8)	0,0447 (13)
C3	0,5811 (5)	0,4636 (5)	0,2519 (10)	0,059 (2)
C4	0,6475 (6)	0,4984 (5)	0,3755 (9)	0,062 (2)
C5	0,7442 (6)	0,4600 (6)	0,3863 (9)	0,063 (2)
C6	0,7747 (5)	0,3847 (5)	0,2717 (8)	0,0506 (15)

Tabelle 4. *Bindungsabstände (Å) und -winkel (°) im PPh$_4$[SnCl$_5$.H$_2$O]*

Sn—Cl1	2,355 (3)	Sn—O	2,24 (1)
Sn—Cl2	2,386 (2)	P—C1	1,800 (5)
Cl1—Sn—Cl2	94,44 (6)	O—Sn—Cl2	85,56 (6)
Cl2^i—Sn—Cl2	171,12 (13)	C1—P—C1^{iii}	106,3 (3)
Cl2^{ii}—Sn—Cl2	89,656 (10)	C1—P—C1^{iv}	111,1 (2)
O—Sn—Cl1	180,0		

Symmetriebezeichnungen: (i) $\frac{1}{2} - x, \frac{1}{2} - y, z$; (ii) $\frac{1}{2} - y, x, z$; (iii) $\frac{1}{2} - x, \frac{1}{2} - y, z$; (iv) $\frac{1}{2} + y, 1 + x, -z$.

Für beide Verbindungen gilt, Datensammlung und Zellverfeinerung: *CAD-4 Software* (Enraf–Nonius, 1989). Datenreduktion: *XCAD4* (Harms, 1987). Programm zur Strukturlösung von PPh$_4$[SnCl$_5$]: *SHELXS86* (Sheldrick, 1985). Strukturlösung von PPh$_4$[SnCl$_5$.H$_2$O]: Isotypie zu AsPh$_4$[ReOCl$_4$.H$_2$O] (Müller, 1984). Strukturverfeinerung beider Verbindungen: *SHELXL93* (Sheldrick, 1993). Graphik: *ORTEX* (McArdle, 1994), *ATOMS* (Dowty, 1993). Programm zur Aufbereitung des Datenmaterials: *SHELXL93*.

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(±)-*cis*-Dichloro[*P*-(isopropylamino)-dinaphtho[2,1-*d*:1′,2′-*f*][1,3,2]dioxaphosphepine](triethylphosphine)platinum(II) Dichloromethane Solvate

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Abstract

In the racemic title compound, [PtCl$_2$(C$_{23}$H$_{20}$NO$_2$P)-(C$_6$H$_{15}$P)].CH$_2$Cl$_2$, the platinum(II) ion, which has approximately square-planar coordination geometry, is coordinated to two different monophosphorus ligands in a *cis* arrangement along with two chloride ions. A significant shortening of the P—N bond [1.604 (7) Å] relative to that in phosphinoamines and their complexes was observed.

Comment

We performed the single-crystal X-ray diffraction study of the title compound, (I), as part of our continuing study of the synthesis and structures of phosphorus–nitrogen compounds and their transition metal complexes (Balakrishna, Reddy, Krishnamurthy, Nixon & Burckett St. Laurent, 1994; Krishnamurthy, 1994; Babu, Aparna, Krishnamurthy & Nethaji, 1995). Our recent studies on phosphazanes and their organometallic complexes (Murugavel, Krishnamurthy, Nethaji & Chandrasekhar, 1993; Murugavel, Kumaravel, Krishnamurthy, Nethaji & Chandrasekhar, 1994) have shown that 'negative hyperconjugation' plays a key role in determining the P—N bond distance. In the title compound, a very short P—N single bond [1.604 (7) Å] was observed; this is shorter than those in phosphinoamine complexes [1.68–1.75 Å (Balakrishna et al., 1994; Burrow, Farrar & Honeyman, 1994)] and close to the value observed for a P=N double bond [~1.57 Å (Corbridge, 1974)].

(I)
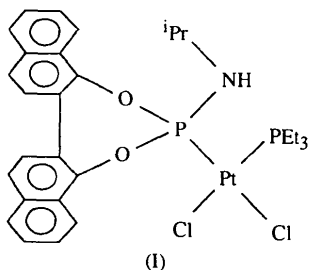
The Pt atom has approximately square-planar coordination geometry [cis Pt—Cl distances 2.362 (3) and 2.333 (2) Å, Cl—Pt—Cl angle 86.91 (9)°; cis Pt—P distances 2.190 (2) and 2.266 (3) Å, P—Pt—P angle 96.19 (9)°]. The molecular dimensions in the Et$_3$P [average P—C 1.817 (9) and C—C 1.51 (1) Å] and dioxybinaphthyl moieties [average C—O 1.41 (1) and C—C 1.40 (1) Å] are normal. The least-squares planes through the two naphthyl groups (which are essentially planar) are inclined at 120 (1)°. The seven-membered ring (P1, O1, C1, C10, C20, C11, O2) adopts a twist-helical conformation, as observed in PhP(O$_2$C$_{20}$H$_{12}$) (Tani, Yamagata & Nagata, 1994).

Short intermolecular N—H···Cl hydrogen bonds between molecules lying across inversion centres form a ten-membered ring [Cl1···N1^i 3.59 (1), Cl1···H1N1 2.67 Å, Cl1···H1N1—N1^i 165°; symmetry code: (i) 1−x, 1−y, 1−z]. The Cl2 atom is also involved in a C—H···Cl-type interaction [Cl2^{ii}···H302 2.79 (1), Cl2^{ii}···C30 3.50 (1) Å, Cl2^{ii}···H302—C30 133°; symmetry code: (ii) x, y, z−1]; in this case the Cl···H separation is less than the sum of the packing radii of the Cl and H atoms [1.77 and 1.17 Å, respectively (Gavezzotti, 1994)]. These interactions seem to have significant effects on the geometry of the complex as the Pt1—P1

distance where P is trans to Cl [2.190 (2) Å] is significantly shorter than the corresponding mean value in the literature of 2.246 Å (Orpen et al., 1994). These interactions may also be responsible for the shortening of the P—N bond.

The asymmetric unit also contains a molecule of dichloromethane which is not involved in any significant intermolecular interactions.
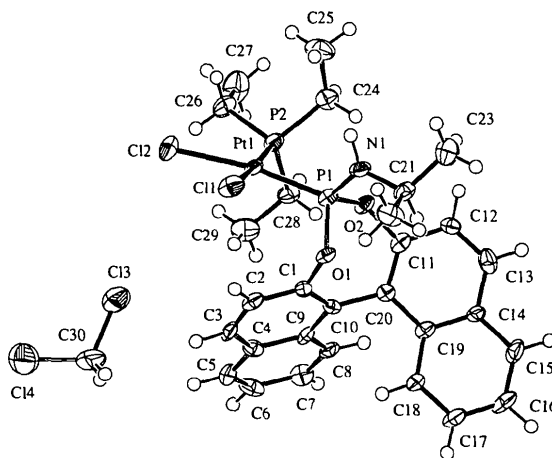

Fig. 1. An ORTEP (Johnson, 1976) drawing of the title compound showing the numbering scheme used. Displacement ellipsoids for the non-H atoms are plotted at the 50% probability level.

Experimental

The title compound was synthesized by the bridge-splitting reaction of [PtCl$_2$(PEt$_3$)]$_2$ with the racemic aminophosphinite (isopropylamino)([1,1'-binaphthyl]-2,2'-dioxy)phosphane in dichloromethane.

Crystal data

[PtCl$_2$(C$_{23}$H$_{20}$NO$_2$P)-(C$_6$H$_{15}$P)].CH$_2$Cl$_2$	Mo Kα radiation
$M_r = 842.48$	$\lambda = 0.71069$ Å
Triclinic	Cell parameters from 25
$P\bar{1}$	reflections
$a = 10.856 (3)$ Å	$\theta = 15.0$–$22.5°$
$b = 15.051 (2)$ Å	$\mu = 4.753$ mm^{-1}
$c = 10.407 (2)$ Å	$T = 220$ K
$\alpha = 97.30 (2)°$	Prism
$\beta = 103.21 (2)°$	$0.25 \times 0.17 \times 0.08$ mm
$\gamma = 96.04 (2)°$	Colourless
$V = 1626.1 (7)$ Å^3	
$Z = 2$	
$D_x = 1.721$ Mg m^{-3}	

Data collection

AFC-6S diffractometer	3926 observed reflections
$\omega/2\theta$ scans	$[I > 3\sigma(I)]$

Absorption correction:
ψ scans (North, Phillips & Mathews, 1968)
$T_{min} = 0.599$, $T_{max} = 0.990$
6111 measured reflections
5747 independent reflections

$R_{int} = 0.028$
$\theta_{max} = 25°$
$h = 0 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -12 \rightarrow 12$
3 standard reflections
  frequency: 150 min
  intensity decay: 1.7%

Refinement

Refinement on F
$R = 0.039$
$wR = 0.037$
$S = 1.47$
3926 reflections
361 parameters
H atoms riding in geometrically idealized positions,
C—H and N—H 0.95 Å

$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} = 0.059$
$\Delta\rho_{max} = 1.24$ e Å^{-3}
  (peaks adjacent to Pt)
$\Delta\rho_{min} = -1.12$ e Å^{-3}
Atomic scattering factors
from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

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

	x	y	z	U_{eq}
Pt1	0.44549 (4)	0.33946 (3)	0.56426 (4)	0.0236 (2)
C11	0.5429 (2)	0.3873 (2)	0.3991 (2)	0.039 (1)
C12	0.6495 (2)	0.3227 (2)	0.6831 (3)	0.043 (1)
C13	0.8462 (3)	0.3242 (2)	0.0209 (3)	0.059 (1)
C14	1.0395 (3)	0.2188 (2)	−0.0475 (3)	0.069 (1)
P1	0.2638 (2)	0.3424 (2)	0.4215 (2)	0.025 (1)
P2	0.3595 (2)	0.3039 (2)	0.7332 (2)	0.028 (1)
O1	0.2482 (5)	0.2766 (4)	0.2806 (5)	0.023 (3)
O2	0.1412 (5)	0.2962 (4)	0.4675 (5)	0.027 (3)
N1	0.2318 (7)	0.4370 (5)	0.3761 (7)	0.031 (4)
C1	0.2603 (8)	0.1859 (6)	0.2942 (8)	0.024 (5)
C2	0.3795 (8)	0.1566 (6)	0.2941 (8)	0.027 (5)
C3	0.3954 (7)	0.0721 (6)	0.3132 (9)	0.032 (5)
C4	0.3009 (8)	0.0125 (6)	0.3414 (8)	0.025 (5)
C5	0.3200 (8)	−0.0729 (7)	0.3776 (9)	0.036 (5)
C6	0.2287 (10)	−0.1261 (6)	0.4147 (9)	0.035 (6)
C7	0.1098 (9)	−0.0978 (7)	0.4145 (9)	0.034 (6)
C8	0.0826 (8)	−0.0162 (6)	0.3773 (8)	0.027 (5)
C9	0.1766 (7)	0.0422 (6)	0.3414 (8)	0.024 (5)
C10	0.1569 (8)	0.1313 (5)	0.3103 (8)	0.019 (4)
C11	0.0288 (8)	0.2470 (6)	0.3814 (8)	0.025 (5)
C12	−0.0838 (8)	0.2843 (6)	0.3862 (9)	0.027 (5)
C13	−0.1971 (8)	0.2377 (7)	0.3094 (9)	0.035 (5)
C14	−0.2001 (8)	0.1567 (6)	0.2196 (8)	0.023 (5)
C15	−0.3159 (8)	0.1118 (7)	0.1310 (9)	0.035 (5)
C16	−0.3179 (9)	0.0365 (7)	0.0413 (9)	0.038 (5)
C17	−0.2050 (9)	0.0020 (7)	0.0380 (9)	0.036 (5)
C18	−0.0910 (8)	0.0432 (6)	0.1239 (9)	0.027 (5)
C19	−0.0846 (8)	0.1211 (6)	0.2171 (8)	0.023 (5)
C20	0.0329 (7)	0.1655 (6)	0.3047 (8)	0.021 (5)
C21	0.1301 (8)	0.4458 (6)	0.2586 (9)	0.031 (5)
C22	0.1830 (10)	0.4556 (7)	0.1407 (10)	0.048 (7)
C23	0.0543 (9)	0.5210 (7)	0.2952 (10)	0.045 (6)
C24	0.2550 (9)	0.3823 (7)	0.7774 (9)	0.032 (5)
C25	0.3193 (10)	0.4781 (7)	0.8254 (11)	0.054 (7)
C26	0.4764 (9)	0.3050 (7)	0.8892 (9)	0.040 (6)
C27	0.4255 (10)	0.2839 (8)	1.0077 (10)	0.058 (7)
C28	0.2662 (8)	0.1915 (6)	0.7015 (9)	0.031 (5)
C29	0.3429 (10)	0.1148 (7)	0.6851 (10)	0.046 (6)
C30	0.8767 (11)	0.2365 (8)	−0.0866 (11)	0.064 (7)

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

Pt1—Cl1	2.362 (3)	P2—C24	1.809 (9)
Pt1—Cl2	2.333 (2)	P2—C26	1.815 (9)
Pt1—P1	2.190 (2)	P2—C28	1.827 (9)
Pt1—P2	2.266 (3)	O1—C1	1.407 (10)
P1—O1	1.626 (6)	O2—C11	1.408 (9)
P1—O2	1.632 (6)	N1—C21	1.48 (1)
P1—N1	1.604 (7)		
Cl1—Pt1—Cl2	86.91 (9)	Pt1—P2—C24	113.1 (3)
Cl1—Pt1—P1	85.87 (9)	Pt1—P2—C26	114.0 (3)
Cl1—Pt1—P2	175.5 (1)	Pt1—P2—C28	114.9 (3)
Cl2—Pt1—P1	169.59 (9)	C24—P2—C26	103.8 (4)
Cl2—Pt1—P2	91.56 (9)	C24—P2—C28	105.9 (4)
P1—Pt1—P2	96.19 (9)	C26—P2—C28	104.0 (5)
Pt1—P1—O1	112.6 (2)	P1—O1—C1	113.8 (5)
Pt1—P1—O2	112.7 (2)	P1—O2—C11	125.9 (5)
Pt1—P1—N1	118.7 (3)	P1—N1—C21	124.2 (6)
O1—P1—O2	99.4 (3)	O1—C1—C2	117.9 (8)
O1—P1—N1	103.3 (3)	O1—C1—C10	118.6 (7)
O2—P1—N1	108.1 (4)		

The space group was determined from statistical analysis of the intensity distribution and the successful solution and refinement of the structure.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1994). Program(s) used to solve structure: *DIRDIF* (Beurskens *et al.*, 1992). Program(s) used to refine structure: *TEXSAN*. Software used to prepare material for publication: *TEXSAN*.

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etc.) as well as to elucidate the mechanism of oxidative addition between iodomethane and Ir^I complexes (Theron, Purcell & Basson, 1995).

(I)

(η⁴-Cycloocta-1,5-diene)(2-pyridinethiolato N-oxide-κO,κS)iridium(I)

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(*Received 2 March 1995; accepted 28 June 1995*)

Abstract

The title compound, [Ir(C$_5$H$_4$NOS)(C$_8$H$_{12}$)], contains an Ir atom in an approximately square-planar environment if we consider the coordination plane formed by the midpoints of the double bonds of the cyclooctadiene ligand together with the S and O atoms [deviation from least-squares plane is 0.01 (5) Å]. The S,O-ligand is also planar and the five-membered chelate ring has a bite angle of 84.4 (3)° at the Ir atom. Bond distances are Ir—S = 2.270 (4), Ir—O = 2.031 (9) and average Ir—C(olefinic) = 2.11 (2) Å.

Comment

Iridium complexes are known to serve as homogeneous catalysts in a wide variety of reactions, for example, in the oxidation of various organic compounds, isomerization of alkenes and alkynes, and hydrogenation of multiple C—C bonds (Dickson, 1985). Coordinative unsaturated square-planar Ir^I complexes are, in general, the best suited for these catalytic reactions owing to their capability to undergo addition reactions. The oxidative addition of specific substrates, for example, H$_2$, HI, I$_2$ and methyl halides, often form an intergal part in these catalytic cycles (Wilkinson, 1987). The isolation and characterization of the title complex, [Ir(C$_5$H$_4$NOS)(C$_8$H$_{12}$)], (I), forms part of our continued research to determine the different factors controlling the rate of oxidative addition (Lewis basicity of complex *via* ligand variation, solvents, addition of halides,
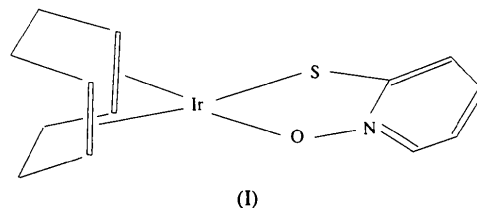
The olefinic bond lengths of 1.38 (2) Å obtained for the η⁴-cycloocta-1,5-diene are normal (Chaloner, Hitchcock & Reisinger, 1992; Abbassioun, Chaloner & Hitchcock, 1990) especially if these are compared with the abnormal metallocyclopropane ring distances in [Ir(C$_9$H$_{10}$NO$_2$S)(C$_8$H$_{12}$)] (Theron, Basson & Purcell, 1995) where a structurally similar substituted-thiohydroxamate ligand was used. The Ir—S bond distance in the title complex compares favourably with that of 2.279 (3) Å in the latter structure, which also contains a bidentate ligand with S and O 'bite' atoms. These Ir—S bond distances are, however, significantly longer than those of 2.215 (9) Å in [Ir(sacac)(cod)(CH$_3$)I] (sacac = thioacetylacetonato anion; cod = cycloocta-1,5-diene) (Terblans, Basson, Purcell & Lamprecht, 1995) and shorter than those of 2.338 (2) and 2.367 (3) Å in [(cod)Cl(SR)Ir(μ-SR)$_2$Ir(cod)] (R = C$_6$H$_5$) (Fonseca, Hernández, Sanz-Apiricio, Terreros & Torrens, 1994). The decrease in Ir—S bond length for the bidentate ligand which forms a six-membered chelate ring (sacac) is attributed to better orbital overlap compared with the five-membered ring systems. The bite angle of 84.4 (3)° obtained for the bidentate ligand (five-membered ring) in the title complex is significantly smaller than that of *ca* 90° observed for several six-membered chelate rings in Ir and Rh complexes (Botha, Basson & Leipoldt, 1987). The Ir—O bond distance of 2.031 (9) Å in the title complex compares favourably with the corresponding bond distance of 2.05 (2) Å in [Ir(acac)(cod)(CH$_3$)I] (acac = acetylacetonato anion) (Basson, Leipoldt, Purcell & Schoeman, 1989).
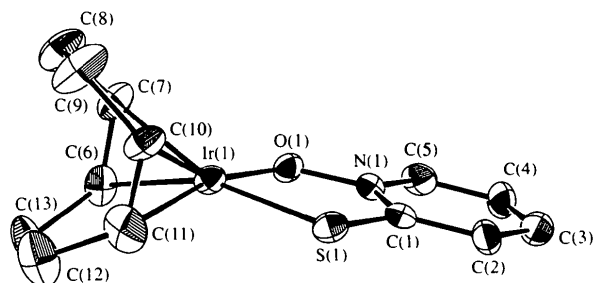

Fig. 1. Perspective view of [Ir(C$_5$H$_4$NOS)(C$_8$H$_{12}$)] indicating the atom labelling. Displacement ellipsoids are drawn at the 25% probability level.