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Chloro[1-(diphenylphosphinoyl)-2-(diphenylphosphino)ethane-κP^2](1,10-phenanthroline-$\kappa^2 N,N'$)copper(I) dichloromethane solvate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
Disorder in solvent or counterion
R factor = 0.036
wR factor = 0.102
Data-to-parameter ratio = 19.4

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

In the structure of the title complex, $[CuCl(C_{12}H_8N_2)(C_{26}H_{24}OP_2)]\cdot CH_2Cl_2$, the coordination polyhedron about the Cu atom is a distorted tetrahedron, with two 1,10-phenanthroline N atoms, one Cl ion and one P atom of the 1-(diphenylphosphinoyl)-2-(diphenylphosphino)ethane ligand occupying the four vertices.

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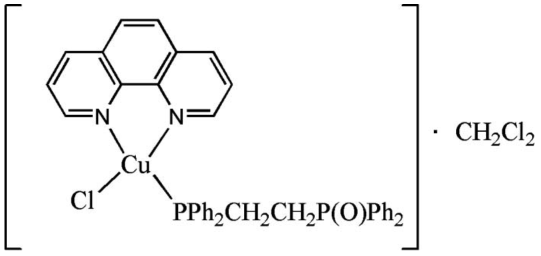
Comment

Bis(phosphine) monoxides (BPMOs) are an important class of hemilabile ligands, and their transition metal complexes are sometimes capable of catalyzing various reactions under uncommonly mild conditions with high selectivities (Grushin, 2004). Owing to the presence of both soft (phosphorus) and hard (oxygen) donor sites in the same molecule, BPMOs can serve as monodentate, bidentate or bridging ligands with different kinds of metal ions (Brassat *et al.*, 1998). It is well known that the soft donor phosphino group is favoured to bond to low-valent late transition metals such as copper(I) (Saravanabharathi *et al.*, 2002). On the contrary, the hard donor P═O group has a strong coordination ability for lanthanide ions such as Eu^{3+} (Montalti *et al.*, 2001). We envision that BPMOs could be used as briging ligands to construct heteronuclear complexes containing both 3d and 4f metals. If such materials could be prepared, the magnetic superexchange interaction or energy transfer process between the bridged metals would be of interest.



(I)

As a part of this approach, we report the synthesis and structure of the mononuclear title compound, (I) (Fig. 1), which crystallizes as a dichloromethane solvate. The free P═O group in (I) suggests that it could serve as an intermediate in the synthesis of heteronuclear complexes.

Compound (I) can be regarded as being analogous to Cu(bpy)(PPh3)X (bpy is 2,2′-bipyridine; X = I, Br, Cl) (Barron *et al.*, 1988), Cu(phen)(PPh_3)I (phen is 1,10-phenanthroline; Jin *et al.*, 1998) and Cu(phen)(PPh_2CH_2OH)Cl (Cao *et al.*, 2004). The copper(I) centre in (I) adopts a distorted tetrahedral geometry, with two N atoms provided by the chelating phen molecule, one P atom from the BPMO moiety and one Cl ion.

The two Cu—N distances in (I) are almost identical (Table 1) and the N—Cu—N angle is more acute than the equivalent angles in the analogous complexes noted above. The Cu—Cl and Cu—P distances in (I) are within normal ranges.

Experimental

The ligand $PPh_2CH_2CH_2P(O)Ph_2$ was prepared according to the literature method of Amenta *et al.* (2002). The reaction of equimolar quantities of CuCl, phen and $PPh_2CH_2CH_2P(O)Ph_2$ in dichloromethane under a dinitrogen atmosphere afforded an orange solution. Yellow single crystals of (I) suitable for X-ray analysis were obtained by vapor diffusion of diethyl ether into a dichloromethane solution.

Crystal data

$[CuCl(C_{12}H_8N_2)(C_{26}H_{24}OP_2)]\cdot CH_2Cl_2$
$M_r = 778.51$
Triclinic, $P\overline{1}$
$a = 11.7313$ (5) Å
$b = 12.5460$ (6) Å
$c = 14.2184$ (7) Å
$\alpha = 107.319$ (1)°
$\beta = 95.294$ (1)°
$\gamma = 108.767$ (1)°
$V = 1850.20$ (15) Å^3
$Z = 2$
$D_x = 1.397$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 947 reflections
$\theta = 2.66$–$24.18°$
$\mu = 0.93$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.30 × 0.25 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.768$, $T_{\max} = 0.801$
22495 measured reflections
8933 independent reflections
6332 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 28.2°$
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 16$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.103$
$S = 1.09$
8933 reflections
461 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.021$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.1013 (15)	Cu1—P1	2.1817 (5)
Cu1—N1	2.1020 (16)	Cu1—Cl1	2.3366 (6)
N2—Cu1—N1	79.34 (6)	N2—Cu1—Cl1	97.80 (5)
N2—Cu1—P1	123.40 (4)	N1—Cu1—Cl1	105.20 (5)
N1—Cu1—P1	127.45 (5)	P1—Cu1—Cl1	115.61 (2)

All H atoms were positioned geometrically and treated as riding (C—H = 0.97 Å for methylene and 0.93 Å otherwise) with the constraint $U_{\rm iso}(H) = 1.2U_{\rm eq}$(carrier) applied. The dichloromethane solvent molecule is disordered over two positions with roughly equal occupancies [0.586 (8) and 0.414 (8)].

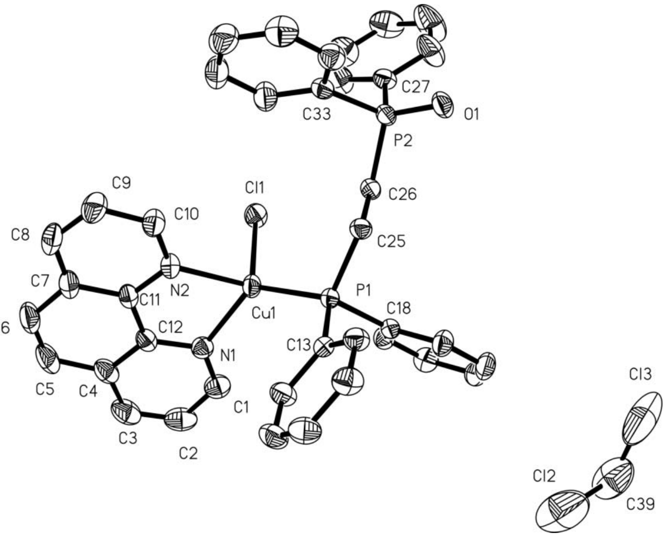


Figure 1
View of (I), showing 30% displacement ellipsoids. All H atoms have been omitted for clarity and only one orientation of the dichloromethane solvent molecule is shown.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2005). E**61**, m1744–m1745 Cao *et al.* • $[CuCl(C_{12}H_8N_2)(C_{26}H_{24}OP_2)]\cdot CH_2Cl_2$ **m1745**