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

Xiao-Lin Zhang, Wen-Hong Wu, Qian-Yong Cao,* Yong-Xiu Li and Lai-Tao Luo

Department of Chemistry, Nanchang University, Nanchang 330047, People's Republic of China

Correspondence e-mail: cqyong@ncu.edu.cn

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Key indicators

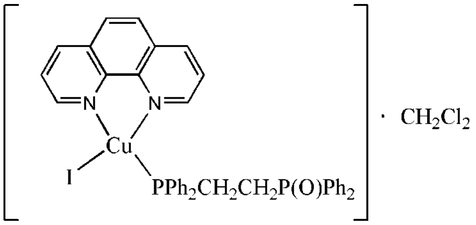
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.167
Data-to-parameter ratio = 21.0

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, $[\mathrm{CuI(C_{12}H_8N_2)\{Ph_2PCH_2CH_2P(O)Ph_2\}]\cdot CH_2Cl_2}$, the coordination polyhedron with copper as the central atom has a distorted tetrahedral geometry formed by two N atoms from 1,10-phenanthroline, one iodide anion and one P atom from 1-(diphenylphosphino)-2-(diphenylphosphinoyl)ethane.

Comment

Copper(I) complexes with the bidentate bridging ligand bis(diphenylphosphino)ethane (dppe) have received much attention for their various coordination geometries (Comba *et al.*, 1999; Cox *et al.*, 2000) and potential biological significance (Berners-Price *et al.*, 1987), but copper(I) complexes with its monoxide 1-(diphenylphosphinoyl)-2-(diphenylphosphino)ethane (dppeo) are rare (Saravanabharathi *et al.*, 2002; Cao *et al.*, 2005). Unlike dppe, dppeo is a semilabile ligand whose transition metal complexes often exhibit catalytic activity (Grushin, 2004). As part of our work in this area, we prepared a complex, (I), of copper(I) iodide with dppeo and 1,10-phenanthroline (phen) and present its structure here.



(I)

The molecular structure of (I) is shown in Fig. 1, and selected bond lengths and angles are given in Table 1. The coordination geometry of the Cu$^{\rm I}$ atom is distorted tetrahedral, with two N atoms provided by the chelating phen ligand, one P atom from the dppeo ligand and one I$^-$ anion. The bond distances (Cu—N, Cu—I and Cu—P) and the bond angles with the central Cu$^{\rm I}$ atom are within the normal ranges for analogous complexes, such as [Cu(phen)(PPh$_3$)I] (Jin *et al.*, 1998) and [Cu(phen)(dppeo)Cl] (Cao *et al.*, 2005).

Experimental

The ligand $\mathrm{PPh_2CH_2CH_2P(O)Ph_2}$ (dppeo) was prepared by a literature method (Amenta *et al.*, 2002). The reaction of CuI (50.0 mg, 0.26 mmol), phen (47.3 mg, 0.26 mmol) and dppeo (108.6 mg, 0.26 mmol) in dichloromethane (30 ml) under a dinitrogen atmosphere for 2 h afforded an orange solution. The solution was concentrated in vacuum to about 5 ml, and the product (175.0 mg, 0.22 mmol) precipitated by adding diethyl ether. Elemental analysis calculated for $C_{38}H_{32}CuIN_2OP_2$ (785.03): C 58.14, H 4.11, N 3.57%; found: C 58.02, H 4.23, N 3.60%. Yellow single crystals suitable for X-ray diffraction analysis were obtained by vapor diffusion of diethyl ether into a dichloromethane solution.

Crystal data

$[CuI(C_{12}H_8N_2)(C_{26}H_{24}OP_2)]\cdot CH_2Cl_2$
$M_r = 869.97$
Triclinic, $P\overline{1}$
$a = 11.1843\ (4)$ Å
$b = 12.1788\ (5)$ Å
$c = 15.0143\ (5)$ Å
$\alpha = 73.457\ (1)^\circ$
$\beta = 83.292\ (1)^\circ$
$\gamma = 74.132\ (2)^\circ$
$V = 1884.08\ (12)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.66$ mm^{-1}
$T = 293\ (2)$ K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.669$, $T_{max} = 0.720$
25497 measured reflections
8987 independent reflections
6232 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.167$
$S = 1.11$
8987 reflections
427 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 2.63$ e Å^{-3}
$\Delta\rho_{min} = -2.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

I1—Cu1	2.6418 (6)	Cu1—N1	2.101 (3)
Cu1—N2	2.072 (3)	Cu1—P2	2.1866 (10)
N2—Cu1—N1	80.57 (13)	N2—Cu1—I1	100.97 (10)
N2—Cu1—P2	129.13 (10)	N1—Cu1—I1	104.22 (9)
N1—Cu1—P2	114.93 (10)	P2—Cu1—I1	119.03 (3)

All H atoms were positioned geometrically and treated as riding (C—H = 0.97 Å for methylene and C—H = 0.93 Å otherwise); $U_{iso}(H) = 1.2U_{eq}(C)$. The highest peak and deepest hole in the final difference map were associated with atom Cl2 (at 0.57 and 0.56 Å, respectively).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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*.

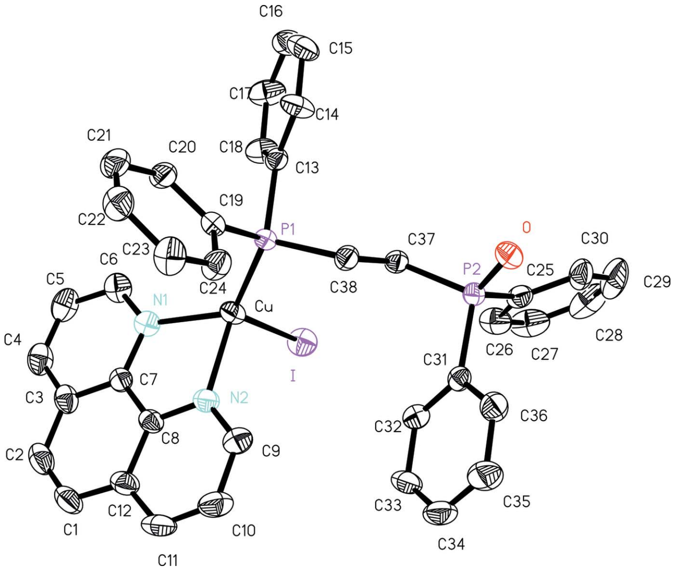


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dichloromethane molecule and all H atoms have been omitted for clarity.

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