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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(C-C)$ = 0.008 Å
 Disorder in solvent or counterion
 R factor = 0.037
 wR factor = 0.095
 Data-to-parameter ratio = 14.6

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

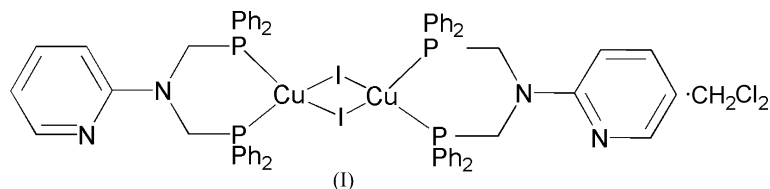
Di- μ -iodo-bis{[N,N-bis(diphenylphosphino-methyl)-2-pyridinamine- κ^2P,P']copper(I)} dichloromethane solvate

The title complex, $[Cu_2I_2(C_{31}H_{28}N_2P_2)_2] \cdot CH_2Cl_2$, has a dimeric structure where two Cu^I atoms are doubly bridged by two I atoms. An inversion center is located midway between the two Cu atoms. The coordination geometry around the Cu atom is distorted tetrahedral, formed by two P atoms from a bidentate N,N-bis(diphenylphosphinomethyl)-2-pyridinamine ligand and two iodine atoms. The complex has a metal-metal interaction with a $Cu \cdots Cu$ distance of 3.068 (3) Å.

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Comment

A large number of cuprous halide clusters with photoluminescence with different emissive behavior have been found (Ford *et al.*, 1999). Copper(I) complexes bridged by I atoms, forming a dimeric entity, have been widely studied (Kickelbick *et al.*, 2002; Huang & Ng, 2004). Recently, we have synthesized a new binuclear copper(I)-iodide complex, (I), with N,N'-bis[(diphenylphosphino)methyl]-2-pyridinamine as ligand.



The crystallographic analysis reveals that the title complex is a binuclear complex, in which each Cu^I atom is in a P_2I_2

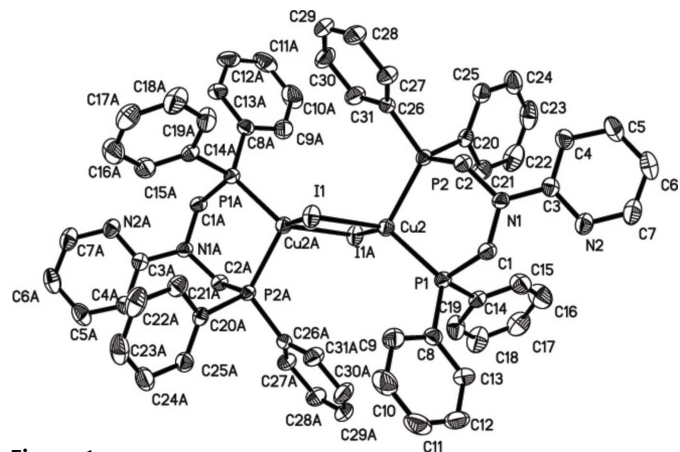


Figure 1
 The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms and the solvent molecule have been omitted. [Symmetry code: (A) 1 - x, 1 - y, -z.]

four-coordinate environment with distorted tetrahedral geometry (Fig. 1). There is an inversion center at the midpoint of the Cu_2I_2 ring. The structures of copper(I) halide compounds with bidentate ligands usually have tetrahedral coordination geometry (Zhou *et al.*, 2005).

Experimental

The ligand N,N' -bis[(diphenylphosphino)methyl]-2-pyridinamine (dpppa) was prepared according to the literature method (Balch *et al.*, 1990). A mixture of the dpppa ligand (49 mg, 0.1 mmol) and CuI (19 mg, 0.1 mmol) in 30 ml of dichloromethane was stirred for 6 h at room temperature. The resulting solution was filtered and concentrated to 5 ml. Addition of diethyl ether gave the product as a colorless solid. Recrystallization by slow diffusion of diethyl ether into a solution of the crude product in dichloromethane gave colorless crystals suitable for X-ray crystallography.

Crystal data

$[\text{Cu}_2\text{I}_2(\text{C}_{31}\text{H}_{28}\text{N}_2\text{P}_2)_2]\cdot\text{CH}_2\text{Cl}_2$	$V = 1517.6$ (9) \AA^3
$M_r = 1446.79$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.583$ Mg m^{-3}
$a = 10.510$ (4) \AA	Mo $K\alpha$ radiation
$b = 11.879$ (4) \AA	$\mu = 1.95$ mm^{-1}
$c = 12.935$ (4) \AA	$T = 298$ (2) K
$\alpha = 72.992$ (4) $^\circ$	Block, colorless
$\beta = 81.788$ (5) $^\circ$	$0.55 \times 0.47 \times 0.42$ mm
$\gamma = 81.119$ (5) $^\circ$	

Data collection

Bruker SMART APEX CCD diffractometer	7973 measured reflections
ω scans	5288 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	4019 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.343$, $T_{\max} = 0.444$	$R_{\text{int}} = 0.033$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.656P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.095$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.64$ e \AA^{-3}
5288 reflections	$\Delta\rho_{\text{min}} = -0.59$ e \AA^{-3}
362 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0052 (6)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu2—P1	2.2620 (13)	Cu2—I1 ⁱ	2.6313 (9)
Cu2—P2	2.2662 (13)	Cu2—I1	2.6597 (10)
P1—Cu2—P2	101.06 (5)	P1—Cu2—I1	114.38 (4)
P1—Cu2—I1 ⁱ	118.65 (4)	I1 ⁱ —Cu2—I1	109.13 (2)
P2—Cu2—I1 ⁱ	111.47 (4)		

Symmetry code: (i) $-x + 1, -y + 1, -z$.

All H atoms were placed in calculated positions. The H atoms were then constrained to an ideal geometry with C—H distances of 0.93–0.97 \AA ; $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The C—Cl and Cl—Cl distances were restrained to ensure a reasonable geometry. The refined displacement parameters were large, which may indicate partial solvent loss. The bond distances in the minor component were restrained to the corresponding bond distances in the major component; these refined to 1.72 (2) ($\text{C}32\text{—Cl}1$ and $\text{C}32\text{—Cl}2$) and 2.82 (2) \AA ($\text{Cl}1\text{—Cl}2$), and fixed in subsequent refinement cycles.

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: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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