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#### Key indicators

Single-crystal X-ray study  
T = 173 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
R factor = 0.033  
wR factor = 0.076  
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>.

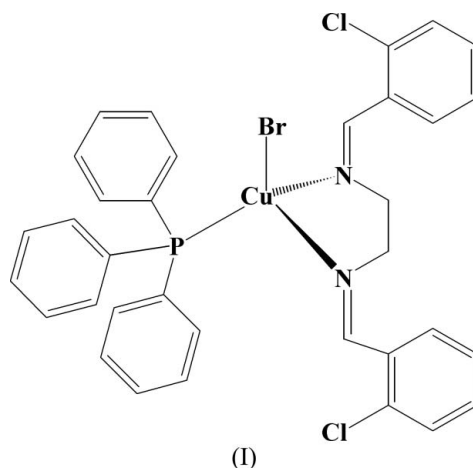
## [*N,N'*-Bis(2-chlorobenzylidene)ethylene-diamine]bromo(triphenylphosphine)copper(I)

In the title compound,  $[\text{CuBr}(\text{C}_{16}\text{H}_{14}\text{Cl}_2\text{N}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$ , the coordination polyhedron around the  $\text{Cu}^{\text{I}}$  centre is approximately tetrahedral, distorted by the restricted bite angle of the chelating ligand. Intra- and intermolecular  $\text{C}-\text{H} \cdots \pi$  and  $\pi-\pi$  stacking interactions are observed.

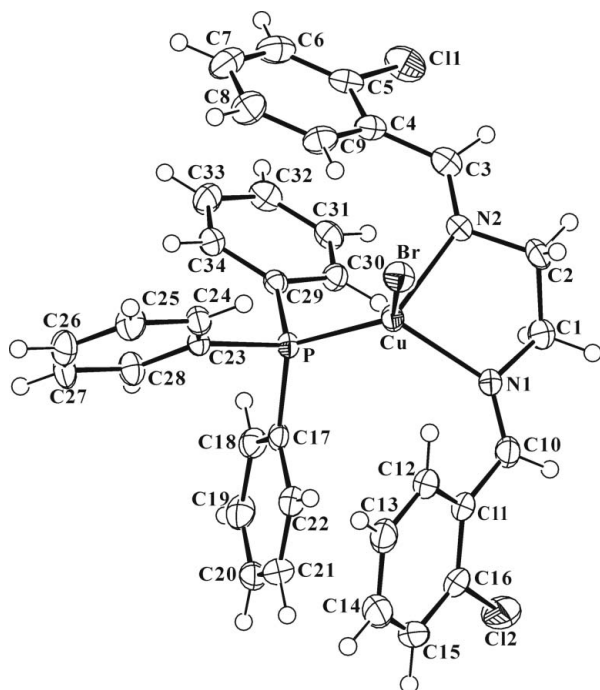
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#### Comment

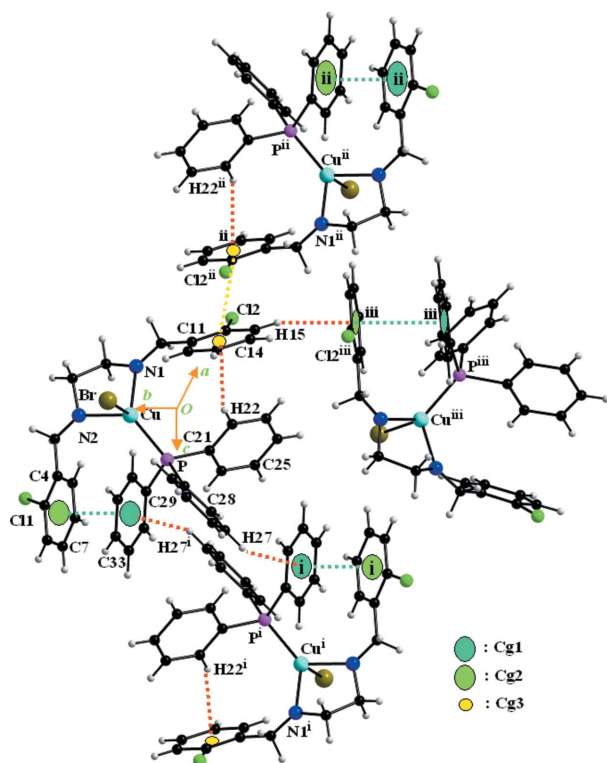
Transition metal compounds containing Schiff base ligands have been of interest for many years (Yamada, 1999; Archer & Wang, 1990; Chang *et al.*, 1998), since they play an important role in the development of coordination chemistry, particularly in relation to catalysis and enzymatic reactions, as well as molecular magnetism (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Bidentate ligands containing imine groups have also been used as modulators of the structural and electronic properties of transition metal centres (Miller *et al.*, 1999). The coordination environments and the structures of these complexes depend on the type of Schiff base and the associated anion. Bulky ligands and/or anions will generally force tetrahedral coordination (Butcher & Sinn, 1977; Tandon *et al.*, 2000).



In the title complex, (I), the coordination geometry around  $\text{Cu}^{\text{I}}$  is approximately tetrahedral, but distorted by the restricted bite angle of the chelating ligand (Fig. 1). The  $\text{Cu}-\text{Br}$  distance (Table 1) is longer than the value of  $2.312 \text{ \AA}$  reported for  $[\text{Cu}(\text{bipyridine})(\text{PPh}_3)\text{Br}]$ , for example (Barron *et al.*, 1988; Green *et al.*, 1984), while the  $\text{Cu}-\text{P}$  distance (Table 1) is comparable with those in other tetrahedral copper(I) phosphine complexes (Balogh-Hergovich *et al.*, 1999; Barron *et al.*, 1988). Despite the fact that the donor N atoms in the Schiff base ligand are  $sp^2$ -hybridized, the chelate ring is significantly puckered, and the deviation from  $120^\circ$



**Figure 1**  
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.



**Figure 2**  
The  $\pi$ - $\pi$  and C-H $\cdots\pi$  interactions (dotted lines) in (I). Cg denotes ring centroids. [Symmetry codes: (i)  $1 - x, -y, 1 - z$ ; (ii)  $2 - x, -y, -z$ ; (iii)  $\frac{3}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ].

angles around N [Cu-N1-C10 = 134.4 (2) $^\circ$  and Cu-N1-C9 = 107.6 (2) $^\circ$ ] indicates some strain in the chelate ring. The

dihedral angles between the various benzene rings within the molecule are: C4-C9/C29-C34 = 1.25 (9) $^\circ$ , C29-C34/C17-C22 = 80.90 (9) $^\circ$ , C17-C22/C23-C28 = 82.41 (8) $^\circ$ , C23-C28/C29-C34 = 59.54 (8) $^\circ$  and C17-C22/C11-C16 = 54.58 (7) $^\circ$ .

In the crystal structure of (I),  $\pi$ - $\pi$  stacking interactions are observed between benzene rings, both within the molecule itself and between adjacent molecules (Fig. 2): Cg1 $\cdots$ Cg2 = 3.61 Å [where Cg1 and Cg2 are the centroids of the C17-C22 and C4-C9 rings, respectively] and Cg3 $\cdots$ Cg3<sup>ii</sup> = 3.65 Å [where Cg3 is the centroid of the C11-C16 ring; symmetry code: (ii)  $2 - x, -y, -z$ ]. C-H $\cdots\pi$  interactions are also observed within the molecule and between molecules (Fig. 2): C22-H22 $\cdots$ Cg3 = 2.72 Å, C27-H27 $\cdots$ Cg1<sup>i</sup> = 3.22 Å and C15-H15 $\cdots$ Cg1<sup>iii</sup> = 2.91 Å [symmetry codes: (i)  $1 - x, -y, 1 - z$ ; (iii)  $\frac{3}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z$ ].

## Experimental

A solution of PPh<sub>3</sub> (58 mg, 0.23 mmol) in acetonitrile (4 ml) was added dropwise to a solution of CuBr (31 mg, 0.23 mmol) in acetonitrile (5 ml). The mixture was stirred for 30 min and then bis[*N,N'*-(2-chlorobenzylidene)]ethylenediamine (70 mg, 0.23 mmol) in acetonitrile (2 ml) was added and stirred for an additional 20 min. Slow evaporation of the solvent under vacuum gave (I) as pale-blue crystals.

### Crystal data

[CuBr(C<sub>16</sub>H<sub>14</sub>Cl<sub>2</sub>N<sub>2</sub>)(C<sub>18</sub>H<sub>15</sub>P)]  
*M*<sub>r</sub> = 710.91  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 10.3050 (5) Å  
*b* = 21.671 (1) Å  
*c* = 14.0214 (7) Å  
 $\beta$  = 102.463 (1) $^\circ$   
*V* = 3057.6 (3) Å<sup>3</sup>

*Z* = 4  
*D*<sub>x</sub> = 1.544 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 2.28 mm<sup>-1</sup>  
*T* = 173 (2) K  
 Block, pale blue  
 0.32 × 0.24 × 0.22 mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 SADABS (Sheldrick, 1996)  
*T*<sub>min</sub> = 0.479, *T*<sub>max</sub> = 0.601

18624 measured reflections  
 6634 independent reflections  
 4939 reflections with *I* > 2σ(*I*)  
*R*<sub>int</sub> = 0.040  
 $\theta$ <sub>max</sub> = 27.0 $^\circ$

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.033  
*wR* (*F*<sup>2</sup>) = 0.077  
*S* = 0.99  
 6634 reflections  
 370 parameters

H-atom parameters constrained  
*w* = 1/[σ<sup>2</sup>(*F*<sub>o</sub><sup>2</sup>) + (0.0362*P*)<sup>2</sup>]  
 where *P* = (*F*<sub>o</sub><sup>2</sup> + 2*F*<sub>c</sub><sup>2</sup>)/3  
 (Δ/σ)<sub>max</sub> < 0.001  
 Δρ<sub>max</sub> = 0.70 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.36 e Å<sup>-3</sup>

**Table 1**

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

Cu-Br	2.4841 (4)	Cu-N2	2.126 (2)
Cu-N1	2.104 (2)	Cu-P	2.2014 (7)
N1-Cu-N2	83.31 (8)	N1-Cu-Br	107.68 (6)
N1-Cu-P	118.54 (6)	N2-Cu-Br	95.09 (6)
N2-Cu-P	117.61 (7)	P-Cu-Br	124.86 (2)

H atoms were placed in idealized positions, with C–H = 0.93 Å for aromatic H or 0.97 Å for methylene H, and refined as riding atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

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