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## Key indicators

Single-crystal X-ray study

T = 180 K

Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$ 

R factor = 0.034

wR factor = 0.068

Data-to-parameter ratio = 16.8

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Di- $\mu$ -iodo-bis{[*N,N'*-bis(3,3-diphenylprop-2-enylidene)propane-1,3-diamine- $\kappa^2N,N'$ ]copper(I)}

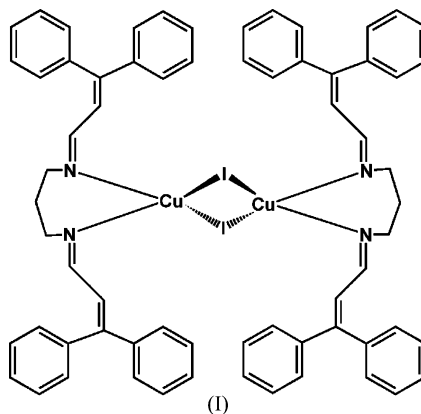
The title compound,  $[\text{Cu}_2\text{I}_2(\text{C}_{33}\text{H}_{30}\text{N}_2)_2]$ , is a centrosymmetric dinuclear copper(I) complex in which the Cu atom is coordinated by the bidentate *N,N'*-bis(3,3-diphenylprop-2-enylidene)propane-1,3-diamine ligands and bridged by two I atoms. The distance between the two Cu atoms is 3.372 (2) Å and the coordination geometry is distorted tetrahedral. Both coordinated diimine ligands adopt an *E,E* conformation.

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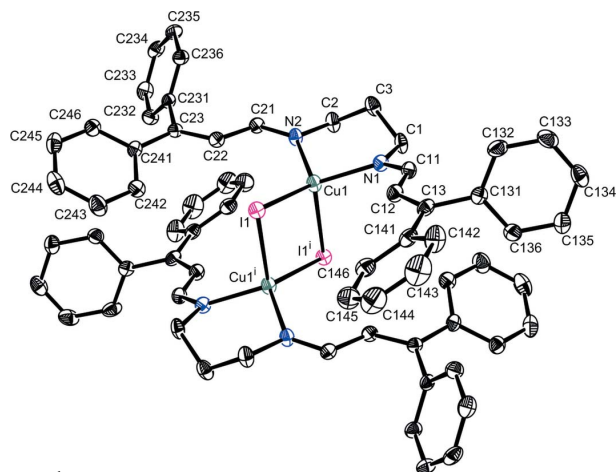
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## Comment

The reactions of CuI with nitrogen-based ligands have been investigated in recent years, due to their application in supramolecular (Amirnasr *et al.*, 2006) and photoluminescence chemistry (Li *et al.*, 2003). The number of ligands bound to the copper(I) ion is greatly influenced by both the chemical nature and the geometry of the ligand (Amirnasr *et al.*, 2006; Kickelbick *et al.*, 2002; Li *et al.*, 2003; Clarke *et al.*, 2003; Kickelbick *et al.*, 2003; Khalaji *et al.*, 2006) and the type of solvent (Gustafsson *et al.*, 2003, 2005). In this context, we decided to examine the nature of the title complex, (I), formed between an unconjugated diimine, *N,N'*-bis( $\beta$ -phenylcinnamaldehyde)propylenediimine (Phca<sub>2</sub>pn), and a copper(I) precursor.



The structure of (I) is consistent with the stoichiometry of a 1:1 copper(I) iodide ligand. This complex is a discrete halogen-bridged dinuclear molecule (Fig. 1), which has an inversion centre midway between the two Cu atoms. The geometry of (I) is in good agreement with that of several related compounds (Khalaji *et al.*, 2006; Kickelbick *et al.*, 2002). The coordination geometry around the copper(I) centre may be described as distorted tetrahedral. The chelate N1–Cu1–N2 angle [100.17 (12)°] is similar to the corresponding angle in related complexes (Amirnasr *et al.*, 2006). The N–Cu–I bond angles range from 100.53 (9) to 122.48 (9)° and are similar to the



**Figure 1**

A view of the molecular unit of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. [Symmetry code: (i)  $2 - x, 1 - z$ ]

corresponding bond angles in related complexes (Khalaji *et al.*, 2006; Kickelbick *et al.*, 2002), as is the I1—Cu1—I1<sup>i</sup> bond angle of 104.517 (17)<sup>o</sup> [symmetry code: (i)  $2 - x, -y, 1 - z$ ]. They are certainly larger than the usual tetrahedral value.

The phenyl rings are planar, as expected, and make dihedral angles to each other of 81.7 (2)<sup>o</sup> (C131—C136 and C141—C146) and 79.0 (1)<sup>o</sup> (C231—C236 and C241—C246). It is interesting to note that in each diimine group, one of the phenyl rings is only slightly twisted with respect to the double bond of the styryl group, by 24.0 (2)<sup>o</sup> for the plane of atoms C141—C146 and 23.9 (4)<sup>o</sup> for the plane of atoms C241—C246. These values indicate partial  $\pi$  delocalization along the carbon chains to the N atoms.

There are two intramolecular interactions, C12—H12 $\cdots$ I1 and C22—H22 $\cdots$ I1 (Table 2). In the crystal structure, there are also C—H $\cdots$  $\pi$  interactions (Table 1).

## Experimental

To a stirred solution of  $\beta$ -phenylcinnamaldehyde (416 mg, 0.2 mmol) in methanol (5 ml), in a beaker open to the atmosphere, was added 1,3-diaminopropane (74 mg, 0.1 mmol). A solution of CuI (190 mg, 0.1 mmol) in acetonitrile (10 ml) was then added, and the reaction mixture was stirred for an additional 30 min. The volume of the solvent was then reduced under vacuum to about 5 ml. The diffusion of diethyl ether vapour into the concentrated solution at 298 K gave the title compound, (I), as orange crystals suitable for X-ray studies (463 mg, 72%).

### Crystal data

[Cu<sub>2</sub>I<sub>2</sub>(C<sub>33</sub>H<sub>30</sub>N<sub>2</sub>)<sub>2</sub>]  
 $M_r = 1290.06$   
 Monoclinic,  $P2_1/n$   
 $a = 9.8335$  (7) Å  
 $b = 16.7979$  (15) Å  
 $c = 17.7501$  (13) Å  
 $\beta = 98.348$  (9)<sup>o</sup>  
 $V = 2900.9$  (4) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.477$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 1.84$  mm<sup>-1</sup>  
 $T = 180$  (2) K  
 Prism, orange  
 $0.27 \times 0.17 \times 0.1$  mm

### Data collection

Stoe IPDS diffractometer  
 $\varphi$  scans  
 Absorption correction: multi-scan  
 (Blessing, 1995)  
 $T_{\min} = 0.687$ ,  $T_{\max} = 0.745$   
 (expected range = 0.767–0.832)

28088 measured reflections  
 5626 independent reflections  
 3715 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.065$   
 $\theta_{\text{max}} = 26.0^{\circ}$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.068$   
 $S = 0.91$   
 5626 reflections  
 334 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0323P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.004$   
 $\Delta\rho_{\text{max}} = 0.54$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.62$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C241–C246 ring.

D—H $\cdots$ A	D—H	H $\cdots$ A	D $\cdots$ A	D—H $\cdots$ A
C132—H132 $\cdots$ Cg1 <sup>ii</sup>	0.95	2.93	3.877 (4)	173
C12—H12 $\cdots$ I1	0.95	3.04	3.950 (4)	161
C22—H22 $\cdots$ I1	0.95	2.99	3.906 (3)	163

Symmetry code: (ii)  $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ .

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (C<sub>aromatic</sub>) or 0.99 Å (C<sub>methylene</sub>), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *IPDS* (Stoe & Cie, 2000); cell refinement: *IPDS*; data reduction: *X-RED* (Stoe & Cie, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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