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Di-μ-iodo-bis{[bis(*trans*-cinnamaldehyde)-ethylenediimine-κ^2*N*,*N*′]copper(I)}

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Key indicators

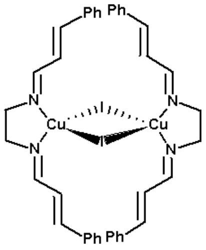
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.016 Å
R factor = 0.068
wR factor = 0.158
Data-to-parameter ratio = 18.2

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

The title complex, $[Cu(\mu\text{-}I)(ca_2en)]_2$ [ca$_2$en is *N*,*N*′-bis(*trans*-cinnamaldehyde)ethylenediimine, $C_{20}H_{20}N_2$], has a dimeric structure where two copper(I) ions are doubly bridged by iodine substituents. The inversion center is located midway between the two Cu atoms. The ca$_2$en acts as a bidentate ligand coordinating *via* two N atoms to the copper. The coordination geometry around the Cu atom is a distorted tetrahedron formed by two N atoms from a bidentate diimine ligand and two iodine substituents. The distance between the two Cu atoms is 2.635 (2) Å. The ca$_2$en ligand adopts a *Z*,*Z* configuration.

Comment

Reaction of copper(I) halides, Cu*X*, with nitrogen-based ligands yields adducts, Cu*LX*$_n$. The number of ligands bound to the monovalent copper seems to be influenced greatly by both the chemical nature and geometry of the ligand *L* and the type of halogen, *X*, used (Zubieta *et al.*, 1983; Kirchner *et al.*, 1987; Alyea *et al.*, 1990). The title complex, (I), was prepared by the reaction of CuI and the bidentate ligand, *N*,*N*′-bis(*trans*-cinnamaldehyde)ethylenediimine (*ca*$_2$en).



(I)

This complex is a halogen-bridged dinuclear discrete molecule (Fig. 1), which has an inversion center midway between the two Cu atoms. The coordination geometry around copper is that of a distorted tetrahedron. The N—Cu—N bond angle in the complex, [82.7 (3)°], is comparable to the corresponding angle in ethylendiimine chelate rings (Chowdhury *et al.*, 2000). The asymmetrically bridging iodine substituents are bonded to copper at distances of 2.5466 (13) and 2.6903 (14) Å. The Cu—I and Cu—N bond lengths are similar to the corresponding bond distances in related complexes (Oshio *et al.*, 1996). The ligand *L* adopts a *Z*,*Z* configuration. The C6—C7 and C16—C17 single-bond distances [1.441 (14) and 1.464 (13) Å, respectively] are slightly shorter than that for C11—C12 [1.516 (13) Å], indicating extended electron delocalization in this complex. The planarity of the conjugated chains C6—C7—C8—C9—N10 and C17—C16—C15—C14—

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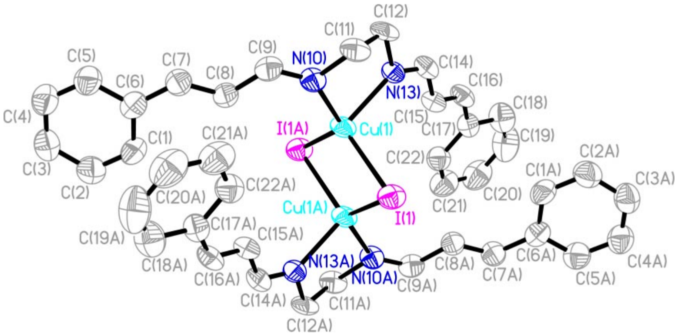

Figure 1
The molecular structure of the title complex, with probability ellipsoids drawn at the 50% level. H atoms have been omitted for clarity.

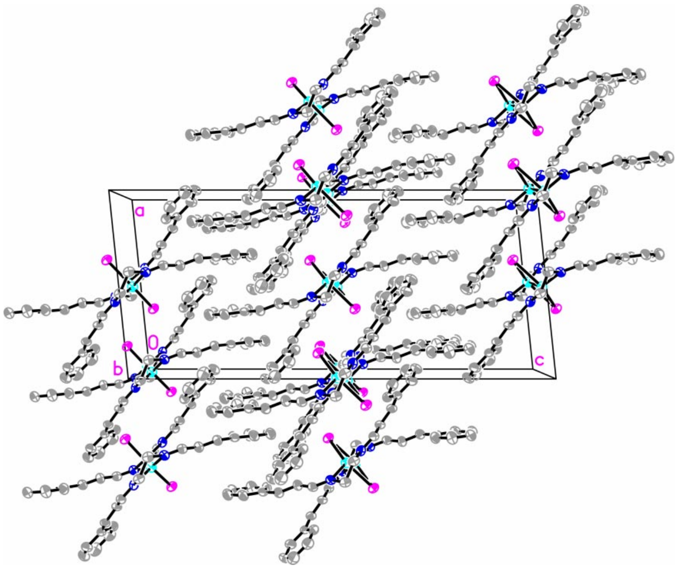

Figure 2
Projection of the structure along [010]. H atoms have been omitted for clarity.

N13 is evidenced by the mean value of the torsion angles in each chain, 179.3 and 174.4°, respectively. However, the two conjugated systems are not coplanar, but are bow-shaped. The rigidity of the ligands, together with the terminal phenyl groups, lead to a stacking arrangement in the crystal along the [010] axis (Fig. 2).

Experimental

The title complex was prepared by the reaction of CuI and ca$_2$en (molar ratio 1:1) in acetonitrile at room temperature under a nitrogen atmosphere. The solution was then concentrated under vacuum, and diffusion of diethyl ether vapor into the concentrated solution gave orange–red crystals of (I) in 78% yield.

Crystal data

$[Cu_2I_2(C_{20}H_{20}N_2)_2]$
$M_r = 957.64$
Monoclinic, $C2/c$
$a = 12.031\ (3)$ Å
$b = 11.926\ (3)$ Å
$c = 27.060\ (7)$ Å
$\beta = 95.877\ (4)°$
$V = 3862.2\ (16)$ Å^3
$Z = 4$
$D_x = 1.647$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3249 reflections
$\theta = 3.0$–$24.4°$
$\mu = 2.73$ mm^{-1}
$T = 294\ (2)$ K
Plate, orange
0.20 × 0.20 × 0.03 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω' scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.611$, $T_{max} = 0.923$
11236 measured reflections
3953 independent reflections
2614 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 26.4°$
$h = -15 \rightarrow 15$
$k = -14 \rightarrow 14$
$l = -33 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.158$
$S = 1.11$
3953 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 62.8396P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.72$ e Å^{-3}
$\Delta\rho_{min} = -1.01$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

I1—Cu1^i	2.5466 (13)	C8—C9	1.452 (13)
I1—Cu1	2.6903 (14)	C9—N10	1.268 (11)
Cu1—N10	2.069 (7)	N13—C14	1.269 (11)
Cu1—N13	2.085 (7)	C14—C15	1.436 (12)
C6—C7	1.441 (14)	C15—C16	1.325 (12)
C7—C8	1.341 (13)	C16—C17	1.464 (13)
Cu1^i—I1—Cu1	60.35 (4)	N13—Cu1—I1	103.8 (2)
N10—Cu1—N13	82.7 (3)	I1^i—Cu1—I1	119.65 (4)
N10—Cu1—I1^i	121.8 (2)	C9—N10—C11	118.7 (7)
N13—Cu1—I1^i	116.7 (2)	C14—N13—C12	117.7 (8)
N10—Cu1—I1	105.3 (2)		

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

H atoms were located in difference Fourier maps and were refined with a riding model.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL*97.

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