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Di- μ -iodo-bis[(1,10-phenanthroline- κ^2 N,N')]copper(I)] acetonitrile solvate

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Key indicators

Single-crystal X-ray study

$T = 295\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$

R factor = 0.041

wR factor = 0.107

Data-to-parameter ratio = 18.9

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

Di- μ -iodo-bis[(1,10-phenanthroline- κ^2N,N')-copper(I)] acetonitrile solvate

In the title complex, $[\text{Cu}_2\text{I}_2(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot \text{C}_2\text{H}_3\text{N}$, two Cu^{I} atoms are bridged by two I atoms and each Cu^{I} atom is chelated by a 1,10-phenanthroline ligand to give four-coordinate tetrahedral geometry.

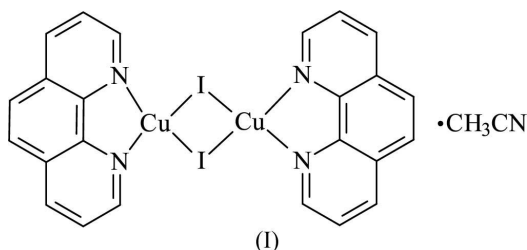
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Comment

The study of copper(I) complexes with the 1,10-phenanthroline (phen) ligand has attracted considerable attention (Healy *et al.*, 1985; Yu *et al.*, 2001). In our study of the preparation of copper(I) complexes, a binuclear compound, (I), was obtained and structurally characterized.



The crystallographic analysis reveals that (I) is a binuclear complex, in which each Cu^{I} atom is in an N_2I_2 four-coordinate environment with distorted tetrahedral geometry (Fig. 1). The structure is very similar to that of $[\text{Cu}_2(\mu\text{-I})_2(\text{phen})_2] \cdot \text{MeOH}$ (Healy *et al.*, 1985). The $\text{Cu}-\text{I}$, $\text{Cu}-\text{N}$ and $\text{Cu} \cdots \text{Cu}$ distances in both complexes are similar. In (I), the dihedral angle between the two Cu_2I planes is $16.74(2)^\circ$ and the two phen ligands are almost parallel, with a dihedral angle of $1.80(17)^\circ$. Interestingly, the $[\text{Cu}_2(\mu\text{-I})_2(\text{phen})_2]$ molecules form a simple

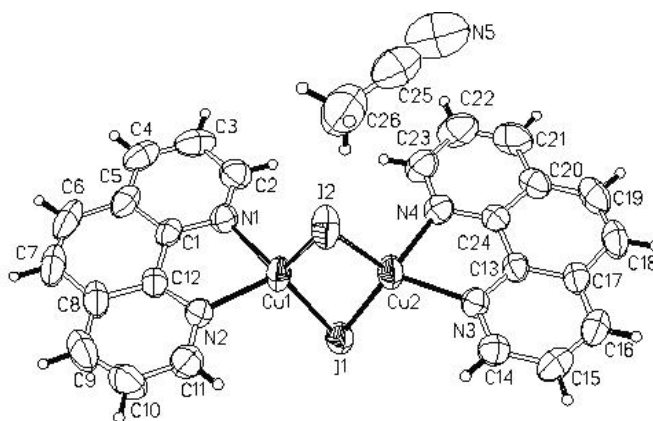


Figure 1
ORTEP plot (Johnson, 1976) of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms drawn as spheres of arbitrary radii.

one-dimensional chain *via* face-to-face π - π interactions between adjacent phen ligands. The distance between the parallel phen planes is 3.46 (4) Å.

Experimental

A mixture of CuI (0.019 g, 0.1 mmol) and 1,10-phenanthroline (0.018 g, 0.1 mmol) in CH₃CN (8 ml) in a 15 ml stainless steel reactor with a Teflon liner was heated to 453 K for 24 h. The reactor was cooled to room temperature at a rate of 10 K h⁻¹. Red crystals of the title complex were collected in 57% yield. Elemental analysis calculated for C₂₆H₁₉Cu₂I₂N₅: C 39.99, H 2.42, N 8.97%; found: C 39.9 5, H 2.44, N 8.96%. IR (KBr, cm⁻¹): 3054 (w), 2243 (w), 1957 (w), 1617 (m), 1581 (m), 1507 (m), 1421 (s), 1216 (w), 1152 (w), 1088 (w), 1053 (w), 988 (w), 837 (s), 713 (m), 735 (s), 627 (m), 417 (w).

Crystal data

[Cu₂I₂(C₁₂H₈N₂)₂].C₂H₃N
M_r = 782.36
 Monoclinic, *P*2₁/*n*
a = 10.4920 (6) Å
b = 23.6166 (13) Å
c = 10.6391 (6) Å
 β = 91.436 (1)°
V = 2635.4 (3) Å³
Z = 4

D_x = 1.972 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 4519 reflections
 θ = 2.6–26.0°
 μ = 3.98 mm⁻¹
T = 295 (2) K
 Prism, red
 0.25 × 0.16 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
T_{min} = 0.409, *T_{max}* = 0.550
 16 362 measured reflections

5991 independent reflections
 4466 reflections with *I* > 2σ(*I*)
R_{int} = 0.029
 θ_{\max} = 27.5°
h = -13 → 13
k = -30 → 30
l = -10 → 13

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.041
wR (*F*²) = 0.107
S = 1.03
 5991 reflections
 317 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.5635P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.57 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.06 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

I1—Cu1	2.5909 (6)	Cu1—N1	2.078 (3)
I1—Cu2	2.6297 (7)	Cu1—N2	2.085 (3)
I2—Cu1	2.5876 (7)	Cu2—N3	2.099 (4)
I2—Cu2	2.5953 (7)	Cu2—N4	2.080 (4)
I1—Cu1—I2	118.75 (2)	I2—Cu1—N2	108.9 (1)
I1—Cu1—N1	117.9 (1)	N1—Cu1—N2	80.6 (1)
I1—Cu1—N2	112.0 (1)	Cu1—I1—Cu2	59.78 (2)
I2—Cu1—N1	112.1 (1)	Cu1—I2—Cu2	60.26 (2)

The phenanthroline and acetonitrile H atoms were placed in calculated positions with C—H distances in the range 0.93–0.96 Å and treated as riding atoms with isotropic displacement parameters of 1.2*U*_{eq}(phen) or 1.5*U*_{eq}(Me) of the parent C atom. The largest peak and deepest hole in the final difference Fourier map were 0.935 and 0.745 Å from atom I2, respectively.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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