

Christian Näther,* Tobias
Steinhoff and Inke JeßInstitut für Anorganische Chemie,
Christian-Albrechts-Universität Kiel,
Olshausenstraße 40, D-24098 Kiel,
GermanyCorrespondence e-mail:
cnaether@ac.uni-kiel.de

Key indicators

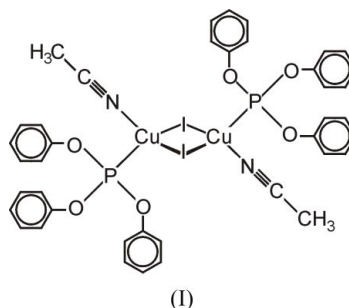
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.026
 wR factor = 0.066
Data-to-parameter ratio = 16.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Di- μ -iodo-bis[(acetonitrile- κN)(triphenyl-
phosphite- κP)copper(I)]

In the title compound, $[\text{Cu}_2\text{I}_2(\text{C}_2\text{H}_3\text{N})_2(\text{C}_{18}\text{H}_{15}\text{O}_3\text{P})_2]$, $(\text{CuI})_2$ rings are found in which each Cu atom is coordinated by one triphenylphosphite ligand and one acetonitrile ligand within a slightly distorted tetrahedron. All atoms are located in general positions and the $(\text{CuI})_2$ rings are located on centres of inversion. In the crystal structure, the Cu and I atoms are packed in a layer-like arrangement.

Received 1 October 2003
Accepted 15 October 2003
Online 23 October 2003

Comment

We are interested in the synthesis, crystal structure and thermal properties of coordination polymers built up of copper(I) halides and aromatic N-donor ligands. For one specific copper(I) halide and one specific N-donor ligand several compounds of different stoichiometry are observed. We have found that most of the amine-rich coordination polymers can be transformed into new amine-poorer coordination polymers by a well directed thermal decomposition (Näther & Jeß, 2002, 2003; Näther, Greve & Jeß, 2002; Näther, Wriedt & Jeß, 2002). To continue this work, we have started investigations on ternary coordination polymers based on copper(I) halides, N-donor ligands and triphenylphosphite. Some of these compounds with CuCl and CuBr have been investigated (Graham *et al.*, 2000; Pike *et al.*, 1999, 2002), but with copper(I) iodide, no compounds have been structurally characterized. During our own investigations on such coordination polymers we have isolated crystals of the title compound, (I).



In the structure of (I), $(\text{CuI})_2$ -four-membered coplanar rings are found in which the copper cations are connected by the iodide anions *via* μ_2 coordination. Each Cu atom is coordinated by two I atoms, one P atom of the triphenylphosphite ligand and one N atom of the acetonitrile ligand, forming discrete molecular complexes. All atoms are located in general positions and the $(\text{CuI})_2$ rings are located on centres of inversion. The Cu—I bond lengths of 2.6427 (4) and 2.6477 (4) Å, the Cu—N bond length of 2.018 (2) Å and the

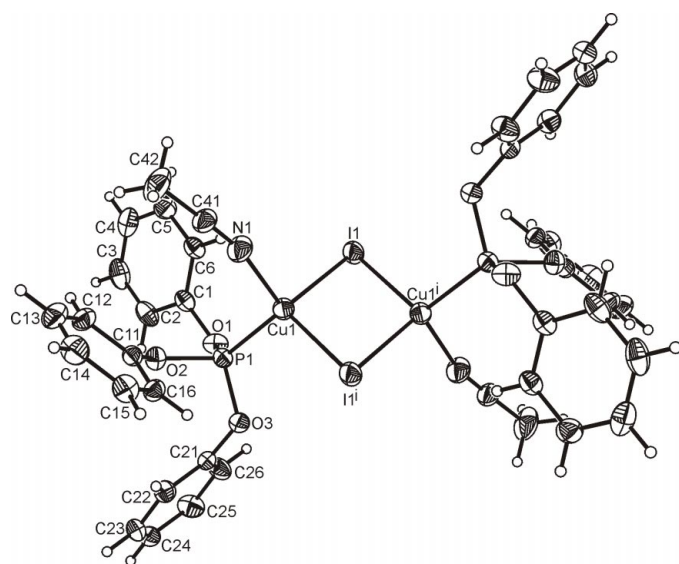


Figure 1
The crystal structure of the title compound with the atom labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $-x, -y, 1 - z$.]

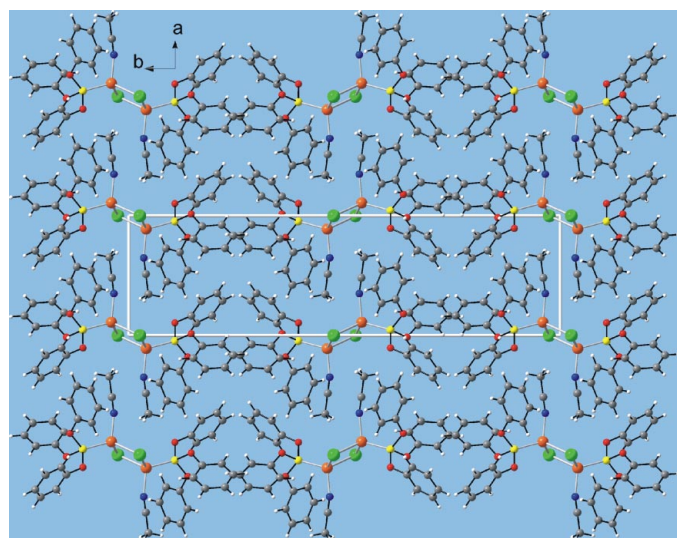


Figure 2
The crystal structure of the title compound, viewed along the crystallographic c axis.

Cu—P bond length of 2.2011 (7) Å are in the normal ranges for related compounds retrieved from the Cambridge Structural Database (Allen, 2002). The coordination of the Cu atoms can be described as slightly distorted tetrahedra, with X —Cu— X angles ($X = \text{I}, \text{N}, \text{P}$) between 106.68 (8) and 113.93 (2)°.

In the crystal structure, the (CuI)₂ rings are stacked in the direction of the crystallographic c axis. The Cu and I atoms are arranged in layers, which are parallel to the ac plane. In contrast to the previously reported compounds with CuBr, and 4,4'-bipyridine or pyrazine (Graham *et al.*, 2000), which are polymeric, the title compound forms only discrete molecular complexes because the acetonitrile ligand cannot bridge different Cu atoms.

Experimental

The title compound was prepared by the reaction of 189.9 mg (1 mmol) CuI and 0.263 ml (1 mmol) triphenylphosphite in about 2 ml acetonitrile in a glass container. After about 4 d, large colourless crystals had grown which decompose in air within a few hours.

Crystal data

[Cu₂I₂(C₂H₃N)₂(C₁₈H₁₅O₃P)₂]
 $M_r = 1083.53$
 Monoclinic, $P2_1/c$
 $a = 9.0239$ (6) Å
 $b = 30.1204$ (16) Å
 $c = 8.4220$ (5) Å
 $\beta = 112.139$ (7)°
 $V = 2120.4$ (2) Å³
 $Z = 2$

$D_x = 1.697$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 8000 reflections
 $\theta = 14$ –23°
 $\mu = 2.58$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 0.1 × 0.1 × 0.1 mm

Data collection

Stoe IPDS diffractometer
 φ scans
 Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
 $T_{\min} = 0.760$, $T_{\max} = 0.771$
 17645 measured reflections
 4082 independent reflections

3559 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\max} = 25.9^\circ$
 $h = -11 \rightarrow 11$
 $k = -36 \rightarrow 37$
 $l = -10 \rightarrow 9$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.066$
 $S = 1.04$
 4082 reflections
 246 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.0308P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.65$ e Å⁻³
 $\Delta\rho_{\min} = -0.66$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0043 (3)

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	2.018 (2)	Cu1—I1 ⁱ	2.6427 (4)
Cu1—P1	2.2011 (7)	Cu1—I1	2.6477 (4)
N1—Cu1—P1	109.56 (7)	P1—Cu1—I1	112.24 (2)
N1—Cu1—I1 ⁱ	108.07 (8)	I1 ⁱ —Cu1—I1	106.011 (12)
P1—Cu1—I1 ⁱ	113.93 (2)	Cu1 ⁱ —I1—Cu1	73.989 (12)
N1—Cu1—I1	106.68 (8)		

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

The aromatic H atoms were positioned with idealized geometry (C—H = 0.93 Å) and refined with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$], using a riding model. The positions of the methyl H atoms were idealized (C—H = 0.96 Å), then refined with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$] as rigid groups allowed to rotate but not tip.

Data collection: *IPDS* (Stoe & Cie, 1998); cell refinement: *IPDS*; data reduction: *IPDS*; 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: *CIFTAB* in *SHELXTL*.

This work is supported by the State of Schleswig-Holstein. We are very thankful to Professor Dr Wolfgang Bensch for financial support and the opportunity to use his experimental equipment.

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
- Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Graham, P. M., Pike, R. D., Sabat, M., Bailey, R. D. & Pennington, W. T. (2000). *Inorg. Chem.* **39**, 5121–5132.
- Näther, C., Greve, J. & Jeß, I. (2002). *Solid State Sci.* **4**, 813–820.
- Näther, C. & Jeß, I. (2002). *J. Solid State Chem.* **169**, 103–112.
- Näther, C. & Jeß, I. (2003). *Inorg. Chem.* **42**, 2968–2976.
- Näther, C., Wriedt, M. & Jeß, I. (2002). *Z. Anorg. Allg. Chem.* **628**, 394–400.
- Pike, R. D., Borne, B. D., Maeyer, J. T. & Rheingold, A. L. (2002). *Inorg. Chem.* **41**, 631–633.
- Pike, R. D., Starnes, W. H. & Carpenter, G. B. (1999). *Acta Cryst.* **C55**, 162–165.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Stoe & Cie (1998). *IPDS* (Version 2.89) and *X-SHAPE* (Version 1.03). Stoe & Cie, Darmstadt, Germany.