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**Di- μ -bromo-1:2 κ^4 Br-bis(quinoline)-
1 κ N,2 κ N-bis(triphenylphosphine)-
1 κ P,2 κ P-dicopper(I)**

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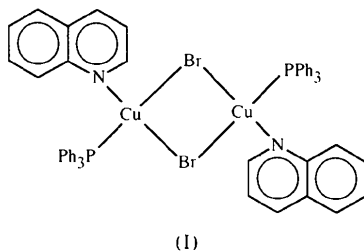
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Abstract

The crystal structure of the title complex, [Cu₂Br₂(C₉H₇N)₂(C₁₈H₁₅P)₂], has been determined by X-ray diffraction. The molecule possesses a crystallographic centre of symmetry in which the four-membered Cu₂(μ -Br)₂ ring is planar, as required by the symmetry, with a Br—Cu—Br angle of 95.83 (2)° and two Cu—Br distances of 2.520 (1) and 2.573 (1) Å. The long Cu···Cu distance [3.414 (1) Å] indicates the absence of direct bonding between the two Cu atoms. The coordination sphere of copper is a distorted tetrahedron, with the six angles around copper ranging from 95.83 (2) to 118.1 (1)°. The Cu—N and Cu—P distances are 2.065 (3) and 2.216 (1) Å, respectively.

Comment

In the course of our work on syntheses of Mo(W)—Cu—S compounds, we obtained a series of complexes containing phosphorus and nitrogen ligands (Lang, Bao *et al.*, 1993; Lang, Zhou *et al.*, 1993; Lang *et al.*, 1994; Hou *et al.*, 1995). Recently, in a similar system, we acquired a halogen-bridged dicopper complex, (I), which contains phosphino and heterocyclic ligands.



As depicted in Fig. 1, [Cu(PPh₃)(C₉H₇N)(μ -Br)]₂ is centrosymmetric and the four-membered Cu₂(μ -Br)₂ ring is planar, as required by the symmetry, with a Br—

Cu—Br angle of 95.83 (2)°. The long Cu···Cu distance [3.414 (1) Å] indicates the absence of direct bonding between the two Cu atoms. The Cu atom has a distorted tetrahedral coordination geometry and is bonded to two bridging Br atoms, an N atom of quinoline and a P atom of triphenylphosphine. The geometry of (I) is similar to that of the copper complexes [Cu(PPh₃)(C₇H₅NS₂)(μ -Cl)]₂ (Shibahara *et al.*, 1997) and [Cu(PPh₃)Br(μ -Py-SH)]₂ (Karagiannidis *et al.*, 1989). In the latter case, the pyridinethione ligand bridges two Cu atoms. The bond distances between the Cu and bridging Br atoms [Cu—Br 2.520 (1) and Cu—Brⁱ 2.573 (1) Å; symmetry code: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, 2 - z$] are normal for a bridging Cu—Br bond (Dyason *et al.*, 1985), but longer than the terminal Cu—Br bond [2.462 (2) Å] in [Cu(PPh₃)Br(μ -PysH)]₂ (Karagiannidis *et al.*, 1989). The smaller Br—Cu—Brⁱ angle (95.83°) in the planar Cu₂(μ -Br)₂ ring causes the transannular Br···Brⁱ distance of 3.780 (5) Å, which is shorter than the sum of the van der Waals radius of Br atoms (1.95 Å; Dean, 1985).

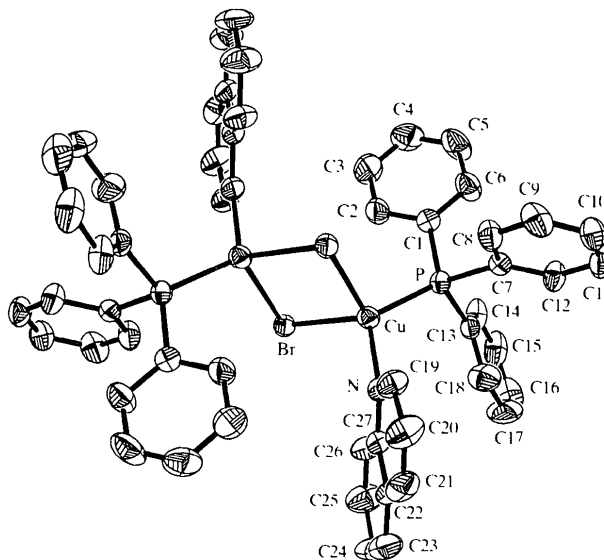


Fig. 1. The title complex with displacement ellipsoids shown at the 30% probability level. H atoms have been omitted for clarity.

Experimental

[Cu(C₉H₇N)(PPh₃)Br]₂ was obtained as a by-product of the reaction of equimolar CuBr, PPh₃ and C₉H₇N in the presence of (NH₄)₂MoO₄·2H₂O in DMF solution for 4 h at 373 K. Yellow crystals of the complex were obtained by slow evaporation of the DMF solution.

Crystal data

[Cu₂Br₂(C₉H₇N)₂(C₁₈H₁₅P)₂] Mo K α radiation
M_r = 1069.76 λ = 0.71073 Å

Monoclinic

 $C2/c$ $a = 24.823 (4) \text{ \AA}$ $b = 18.170 (2) \text{ \AA}$ $c = 11.429 (2) \text{ \AA}$ $\beta = 110.61 (1)^\circ$ $V = 4825 (2) \text{ \AA}^3$ $Z = 4$ $D_x = 1.473 \text{ Mg m}^{-3}$ D_m not measured

Cell parameters from 30 reflections

 $\theta = 4.92\text{--}14.95^\circ$ $\mu = 2.64 \text{ mm}^{-1}$ $T = 293 (2) \text{ K}$

Prism

 $0.5 \times 0.4 \times 0.3 \text{ mm}$

Yellow

Data collection: *XSCANS* (Fait, 1991). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *SHELXL93*.

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Data collection

Siemens P4 diffractometer

 θ - 2θ scans

Absorption correction:

 ψ scan (North *et al.*, 1968) $T_{\min} = 0.258$, $T_{\max} = 0.453$

4909 measured reflections

4270 independent reflections

2575 reflections with

 $I > 2\sigma(I)$ $R_{\text{int}} = 0.045$ $\theta_{\text{max}} = 25^\circ$ $h = -29 \rightarrow 27$ $k = 0 \rightarrow 21$ $l = 0 \rightarrow 13$

3 standard reflections

every 97 reflections

intensity decay: none

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.036$ $wR(F^2) = 0.072$ $S = 1.051$

4270 reflections

281 parameters

H atoms: see below

 $w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$

Extinction correction:

SHELXL93

Extinction coefficient:

0.00197 (8)

Scattering factors from

International Tables for Crystallography (Vol. C)

The data were corrected for Lorentz and polarization effects. The structure was solved by direct methods (*SHELXS86*; Sheldrick, 1990) and expanded using Fourier techniques. H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding ($U_{\text{iso}} = 0.078 \text{ \AA}^2$).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1096). Services for accessing these data are described at the back of the journal.

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