Di-μ-iodo-bis[(3-cyanopyridine-κN)copper(I)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.023
wR factor = 0.060
Data-to-parameter ratio = 15.7

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

The Cu^I atom in the centrosymmetric title compound, $[Cu_2I_2(C_6H_5N)_4]$, shows tetrahedral coordination; the I atom functions as a μ_2 bridge.

Comment

Cuprous halide clusters display a wide variety of structural motifs in their complexes with nitrogen heterocycles, as well as in their nitrile complexes. Such complexes possess diverse photophysical properties (Ford *et al.*, 1999). Cuprous iodide forms a large number of adducts with substituted pyridine heterocycles in which one adduct molecule associates with another through iodide bridges, forming a dimeric entity, *e.g.* $[CuI(C_5H_5N)_2]_2$ (Dyason *et al.*, 1984). 3–Cyanopyridine is a heterocyclic ligand having both a Lewis-basic aromatic site and a cyano group; it does not cause steric crowding, unlike, for example, 2-methylpyridine (Habiyakare *et al.*, 1992; Healy *et al.*, 1983). This reagent also affords a dinuclear compound, (I), in which the Cu—I bonds are of nearly identical lengths [2.6450 (5) and 2.6496 (5) Å] (Fig. 1).

(I)
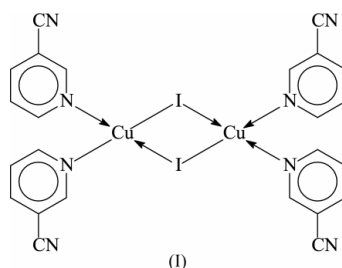
This centrosymmetric compound has a structure similar to that of the 3-cyanopyrazine adduct, with the Cu^I atom in a
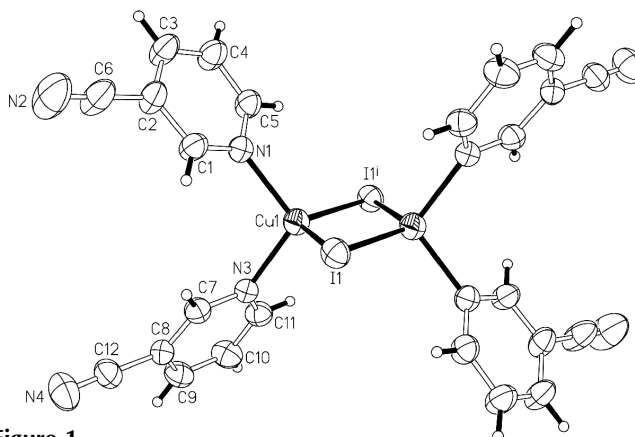
Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1 - x$, $1 - y$, $1 - z$.]

tetrahedral N_2I_2Cu geometry. The structure of the 3-cyano-pyrazine adduct has been described in detail (Rossenbeck & Sheldrick, 1999).

Experimental

A mixture of cuprous iodide (0.19 g, 1.0 mmol), 3-cyanopyridine (0.10 g, 1.0 mmol) and acetonitrile (10 ml) was sealed in a 23-ml Teflon-lined bomb, which was heated in an oven to 433 K for 80 h. The oven was cooled to room temperature at a rate of 5 K h^{-1}. Orange crystals were collected and washed with water. Elemental analysis calculated (%) for $C_{24}H_{16}Cu_2I_2N_8$: C 36.15, H 2.02, N 14.05; found: C 36.08, H 2.12, N 14.01.

Crystal data

$[Cu_2I_2(C_6H_5N)_4]$	$Z = 1$
$M_r = 797.33$	$D_x = 2.010$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.0880\ (6)$ Å	Cell parameters from 2924
$b = 8.9192\ (6)$ Å	reflections
$c = 9.7063\ (7)$ Å	$\theta = 2.4$–$28.3°$
$\alpha = 92.372\ (1)°$	$\mu = 3.99$ mm^{-1}
$\beta = 95.354\ (1)°$	$T = 293\ (2)$ K
$\gamma = 108.663\ (1)°$	Block, orange
$V = 658.60\ (8)$ Å^3	$0.28 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART APEX area-detector diffractometer	2565 independent reflections
	2382 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.014$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$\theta_{max} = 26.3°$
$T_{min} = 0.325$, $T_{max} = 0.450$	$h = -9 \rightarrow 10$
	$k = -11 \rightarrow 11$
4801 measured reflections	$l = -11 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$+ 0.0903P]$
$wR(F^2) = 0.060$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2565 reflections	$\Delta\rho_{max} = 0.42$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.50$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

I1—Cu1	2.6450 (5)	Cu1—N1	2.073 (2)
I1—Cu1^i	2.6496 (5)	Cu1—N3	2.082 (2)
Cu1—I1—Cu1^i	60.43 (2)	N3—Cu1—I1	106.07 (7)
N1—Cu1—N3	107.55 (9)	N3—Cu1—I1^i	107.96 (7)
N1—Cu1—I1	107.12 (7)	I1—Cu1—I1^i	119.57 (2)
N1—Cu1—I1^i	108.03 (7)		

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

H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$] and were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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