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Diiodo(4′-phenyl-2,2′:6′,2″-terpyridine-κ^3N)-copper(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.009 Å
R factor = 0.040
wR factor = 0.111
Data-to-parameter ratio = 14.4

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

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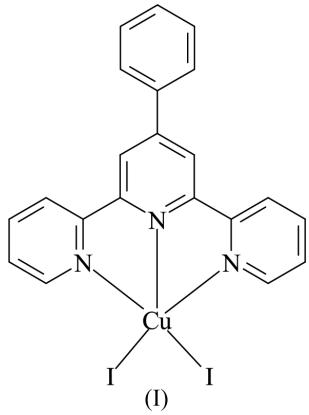
The Cu atom in the 1/1 adduct of copper(II) diiodide with 4′-phenyl-2,2′:6′,2″-terpyridine, $[CuI_2(C_{21}H_{15}N_3)]$, exists in a square-pyramidal environment. The Cu—I_{axial} bond [2.7872 (9) Å] is significantly longer than the Cu—I_{basal} bond [2.5394 (8) Å].

Comment

2,2′:6′,2″-Terpyridine, a commercially available chelating heterocyclic ligand, furnishes complexes with a large range of metal salts, and as the adducts are crystalline, the crystal structures of a plethora of such adducts have been authenticated. For the copper(II) iodide adduct in particular, the metal atom is chelated by the heterocycle in a five-coordinate environment; the geometry is that of a trigonal bipyramid and the N atoms of the outer pyridyl rings span the two apical positions. The Cu atom lies on a twofold axis and the two Cu—I bonds [2.647 (1) Å] are equivalent (Kutoglu *et al.*, 1991). With the 4-phenyl-substituted heterocycle, the corresponding copper iodide adduct, (I), which was the unexpected product from the reaction of the heterocycle with cuprous iodide, features a Cu atom in a square-pyramidal geometry (Fig. 1). The Cu—I_{axial} bond [2.7872 (9) Å] is significantly longer than the Cu—I_{basal} bond [2.5394 (8) Å].



(I)

Experimental

4′-Phenyl-2,2′:6′,2″-terpyridine was synthesized according to a published procedure (Constable *et al.*, 1990). This compound (0.031 g, 0.1 mmol) was dissolved in dichloromethane (3 ml) and the solution placed in a narrow glass tube. More dichloromethane (5 ml) was added as a buffer between a saturated potassium iodide solution containing copper(I) iodide (0.019 g, 0.1 mmol). Black crystals were formed at the interface in two weeks in about 50% yield.

Crystal data

$[CuI_2(C_{21}H_{15}N_3)]$	D_x = 2.086 Mg m^{-3}
M_r = 626.70	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2748 reflections
a = 13.855 (1) Å	θ = 2.7–23.2°
b = 14.995 (1) Å	μ = 4.20 mm^{-1}
c = 19.245 (1) Å	T = 295 (2) K
β = 93.571 (1)°	Prism, black
V = 3990.6 (5) Å^3	0.19 × 0.18 × 0.12 mm
Z = 8	

Data collection

Bruker SMART APEX area-detector diffractometer	3513 independent reflections
	2977 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.027
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	θ_{max} = 25.0°
	$h = -16 \rightarrow 16$
T_{min} = 0.454, T_{max} = 0.604	$k = -14 \rightarrow 17$
10302 measured reflections	$l = -22 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 14.3913P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	
$wR(F^2)$ = 0.111	
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
3513 reflections	$\Delta\rho_{max}$ = 1.18 e Å^{-3}
244 parameters	$\Delta\rho_{min}$ = −0.87 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

I1—Cu1	2.7872 (9)	Cu1—N2	1.959 (5)
I2—Cu1	2.5394 (8)	Cu1—N3	2.069 (5)
Cu1—N1	2.079 (5)		
N1—Cu1—N2	78.8 (2)	N2—Cu1—I1	100.3 (1)
N1—Cu1—N3	155.3 (2)	N2—Cu1—I2	154.7 (1)
N1—Cu1—I1	102.0 (1)	N3—Cu1—I1	92.0 (1)
N1—Cu1—I2	97.6 (1)	N3—Cu1—I2	98.4 (1)
N2—Cu1—N3	78.7 (2)	I1—Cu1—I2	104.96 (3)

H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}$(C)] and were included in the refinement in the riding-model approximation. The final difference map had a large peak at 0.5 Å from atom I1.

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.

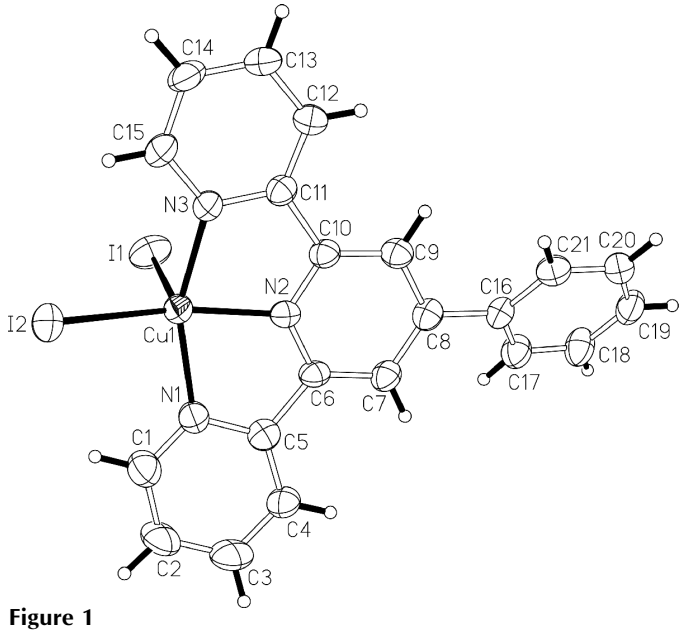


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

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