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Rerefinement of dichloro[3-(1,10-phenanthrolin-2-yl)-5,6-diphenyl-1,2,4-triazine]copper(II) as an anhydrous structure

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The crystal structure of $[CuCl_2(C_{27}H_{17}N_5)]$, which was reported as a 1/4 hydrate [Wang, Chao, Li, Hong, Ji & Li (2004). *J. Inorg. Biochem.* **98**, 423–429], has been rerefined as the anhydrous complex.

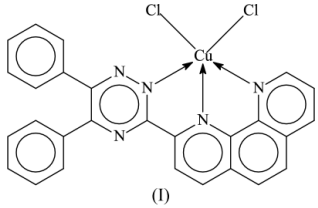
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.050
wR factor = 0.136
Data-to-parameter ratio = 17.0

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

Comment

The crystal structure of triclinic $[Cu(C_{27}H_{17}N_5)Cl_2]$ was reported as a 1/4 hydrate (Wang *et al.*, 2004). A check by *PLATON* (Spek, 2003) shows that the volume supposedly occupied partially by the water molecule is implausibly small, only 17 Å^3. The structure has now been rerefined without water. Although the rerefinement of the structure leads to no significant differences in bond dimensions, it nevertheless probably represents the correct formulation of the compound.



(I)

Experimental

Crystal data

$[CuCl_2(C_{27}H_{17}N_5)]$
M_r = 545.90
Triclinic, $P\overline{1}$
a = 10.320 (1) Å
b = 10.441 (1) Å
c = 11.793 (1) Å
α = 98.878 (1)°
β = 90.545 (2)°
γ = 107.244 (1)°
V = 1197.0 (2) Å^3
Z = 2
D_x = 1.515 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1900 reflections
θ = 2.5–22.6°
μ = 1.16 mm^{-1}
T = 298 (2) K
Prism, blue
0.20 × 0.15 × 0.15 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.472, T_{max} = 0.845
10453 measured reflections
5360 independent reflections
3445 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.5°
$h = -13 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.00
5360 reflections
316 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0702P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.100 (3)	Cu1—Cl1	2.396 (1)
Cu1—N2	1.963 (3)	Cu1—Cl2	2.208 (1)
Cu1—N3	2.116 (3)		
N1—Cu1—N2	79.3 (1)	N2—Cu1—Cl1	95.5 (1)
N1—Cu1—N3	154.5 (1)	N2—Cu1—Cl2	155.9 (1)
N1—Cu1—Cl1	93.9 (1)	N3—Cu1—Cl1	95.8 (1)
N1—Cu1—Cl2	98.8 (1)	N3—Cu1—Cl2	100.4 (1)
N2—Cu1—N3	76.3 (1)	Cl1—Cu1—Cl2	108.6 (1)

The diffraction data were obtained from one of the authors of the previous report (Wang *et al.*, 2004). Aromatic H atoms were placed at calculated positions in the riding model approximation [C—H 0.93 Å; U(H) = 1.2U_{eq}(C)]. The final difference Fourier map had a peak larger than 1 e Å^{-3} 2.5 Å from H11, H23 and H26, but was otherwise featureless.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from published structure; 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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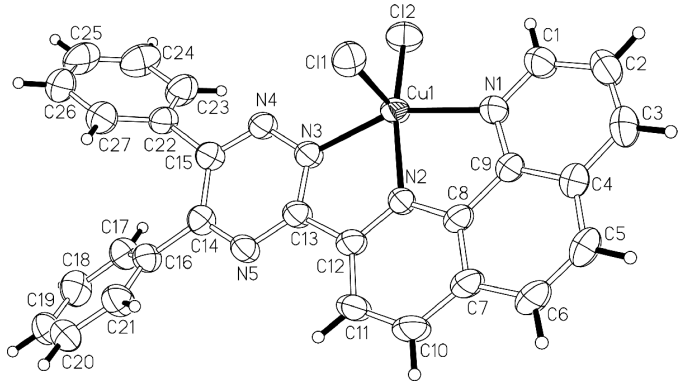

Figure 1
*ORTEP*II (Johnson, 1976) plot of [Cu($C_{27}H_{17}N_5$)Cl_2], with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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