Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Redetermination of bis{[(2-hydroxyphenylmethyl)bis(2-pyridylmethyl)aminato]copper(II)} diperchlorate

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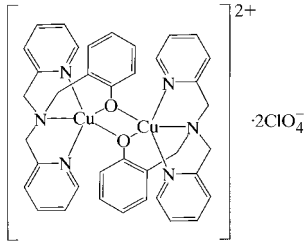
Received 5 April 2000
Accepted 11 April 2000

Data validation number: IUC0000114

The structure of the title compound, $[Cu_2(C_{19}H_{18}N_3O)_2](ClO_4)_2$, was reported with insufficient accuracy because of a twinning problem by Adams, Bailey, Campbell, Fenton & He [*J. Chem. Soc. Dalton Trans.* (1996), pp. 2233–2237]. The dinuclear phenolate-bridged Cu^{II} complex has an inversion centre.

Comment

The title copper(II) complex, $[Cu_2(phpy)_2](ClO_4)_2$ [phpy is (2-hydroxyphenylmethyl)bis(2-pyridylmethyl)aminate], (I), which has a long Cu–phenolic O atom bond, can be considered as a nobel model compound for galactose oxidase (Ito *et al.*, 1998).



(I)

Adams *et al.* (1996) noted that the structure was difficult to refine because of a twinning problem.

Experimental

In the present study, single crystals of (I) were grown from an acetonitrile solution as needles elongated along **a**.

Crystal data

$[Cu_2(C_{19}H_{18}N_3O)_2](ClO_4)_2$	D_x = 1.642 Mg m^{-3}
M_r = 934.74	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
a = 11.380 (1) Å	θ = 10–15°
b = 9.877 (2) Å	μ = 1.334 mm^{-1}
c = 17.400 (2) Å	T = 298 K
β = 104.79 (1)°	Needle, green
V = 1891.0 (5) Å^3	0.70 × 0.15 × 0.10 mm
Z = 2	

Data collection

Rigaku AFC-5*S* diffractometer	R_{int} = 0.059
θ–2θ scans	θ_{max} = 27.5°
Absorption correction: by integration (Coppens *et al.*, 1965)	$h = 0 \rightarrow 15$
T_{min} = 0.662, T_{max} = 0.897	$k = 0 \rightarrow 13$
4819 measured reflections	$l = -23 \rightarrow 23$
4338 independent reflections	3 standard reflections every 100 reflections
2393 reflections with $I > 2\sigma(I)$	intensity decay: 5.5%

Refinement

Refinement on F^2	H-atom parameters not refined
$R(F)$ = 0.063	$w = 1/[\sigma^2(F_o^2) + \{0.1(F_o^2 + 2F_c^2)/3\}^2]$
$wR(F^2)$ = 0.185	$(\Delta/\sigma)_{max}$ = 0.009
S = 0.98	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
4338 reflections	$\Delta\rho_{min}$ = −0.63 e Å^{-3}
262 parameters	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	2.203 (4)	Cu1—N2	2.037 (4)
Cu1—O1^{i}	1.938 (3)	Cu1—N3	2.000 (5)
Cu1—N1	2.013 (5)		
O1—Cu1—O1^{i}	80.4 (2)	Cu1—O1—Cu1^{i}	99.6 (2)

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

Positional parameters of all the H atoms were calculated geometrically and fixed with U(H) = 1.2U_{eq}(parent atom).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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