Crystal structure of *N,N'*-ethylene-bis(1,3-dimethyl-5-pyrazolethiolatoiminomethyl)copper(II), $C_{14}H_{18}CuN_6S_2$

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Table 1. Data collection and handling.

Crystal:	red-orange block, size 0.19 × 0.19 × 0.32 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	15.71 cm ⁻¹
Diffractionmeter, scan mode:	Rigaku AFC6R, $\omega/2\theta$
$2\theta_{\max}$:	55.2°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4089, 3829
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2987
$N(\text{param})_{\text{refined}}$:	209
Programs:	SHELXS-86 [5], teXsan [6], PLATON [7], ORTEPII [8]

Abstract

$C_{14}H_{18}CuN_6S_2$, triclinic, $P\bar{1}$ (No. 2), $a = 8.474(1)$ Å, $b = 12.417(1)$ Å, $c = 8.2077(9)$ Å, $\alpha = 99.115(7)^\circ$, $\beta = 102.094(9)^\circ$, $\gamma = 91.875(9)^\circ$, $V = 831.9$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.038$, $wR_{\text{ref}}(F^2) = 0.103$, $T = 293$ K.

Source of material

The title compound was crystallised and characterised as described in [1,2].

Discussion

The Cu(II) atom exists in a distorted square planar environment defined by a N_2S_2 donor set. The ethylenediamine portion of the ligand chelates the Cu atom and the thiolate S atoms derived from the side arms complete the coordination geometry. There are distortions from the ideal square planar geometry with the S1, S2, N1 and N2 donor atoms lying $-0.035(1)$ Å, $0.041(1)$ Å, $0.322(3)$ Å, and $-0.367(4)$ Å out of their least-squares plane, respectively. The Cu atom lies $0.0223(5)$ Å out of this plane. The Cu—S ($2.2696(9)$ Å & $2.2781(9)$ Å) bond distances are equal within experimental error as are the Cu—N bonds ($1.998(2)$ Å & $1.984(3)$ Å). In terms of angles subtended at Cu, the greatest deviation from the ideal geometry is manifested in the S1—Cu—N2 angle of $167.37(8)^\circ$. Whereas the five-membered chelate ring is puckered as expected, the two six-membered rings are planar to 0.037 Å and 0.059 Å, respectively and form a dihedral angle of $15.16(9)^\circ$. The near planar CuN_2S_2 chromophore is similar to the related *t*-salen Cu(II) complex [3]. These complexes were used to develop models for type 1 ("blue") copper sites in copper proteins and type A copper sites in cytochrome C oxidase enzyme, which have a more tetrahedral environment [4].

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1)	2i	-0.0713	0.1376	0.6704	0.064(3)
H(4a)	2i	-0.3741	-0.1076	0.4678	0.096(4)
H(4b)	2i	-0.3546	0.0062	0.5867	0.096
H(4c)	2i	-0.2093	-0.0692	0.5953	0.096
H(6a)	2i	-0.3300	-0.0464	-0.0793	0.096
H(6b)	2i	-0.1586	0.0067	-0.0753	0.096
H(6c)	2i	-0.3062	0.0797	-0.0760	0.096
H(7a)	2i	0.0437	0.3593	0.8063	0.080(3)
H(7b)	2i	0.1177	0.2489	0.8445	0.080
H(8a)	2i	0.3192	0.3965	0.8772	0.080
H(8b)	2i	0.3467	0.2919	0.7530	0.080
H(9)	2i	0.3848	0.5357	0.7695	0.064
H(12a)	2i	0.5341	0.8205	0.7089	0.096
H(12b)	2i	0.5789	0.7142	0.7837	0.096
H(12c)	2i	0.4159	0.7663	0.8007	0.096
H(14a)	2i	0.3262	0.7246	0.1160	0.096
H(14b)	2i	0.1656	0.6501	0.0796	0.096
H(14c)	2i	0.3279	0.5981	0.0595	0.096

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cu	2i	0.10687(4)	0.33067(3)	0.42713(4)	0.0299(2)	0.0315(2)	0.0310(2)	0.0046(1)	0.0061(1)	0.0062(1)
S(1)	2i	−0.0162(1)	0.21405(7)	0.18916(9)	0.0556(5)	0.0438(4)	0.0311(4)	−0.0090(4)	0.0073(3)	0.0068(3)
S(2)	2i	0.1535(1)	0.44043(7)	0.2422(1)	0.0633(6)	0.0393(4)	0.0361(4)	−0.0064(4)	0.0041(4)	0.0095(3)
N(1)	2i	0.0374(3)	0.2494(2)	0.5945(3)	0.036(1)	0.039(1)	0.031(1)	0.002(1)	0.009(1)	0.004(1)
N(2)	2i	0.2558(3)	0.4131(2)	0.6314(3)	0.039(2)	0.041(1)	0.037(1)	−0.003(1)	0.006(1)	0.009(1)
N(3)	2i	−0.2972(3)	−0.0327(2)	0.2287(3)	0.038(2)	0.040(1)	0.044(1)	−0.005(1)	0.006(1)	0.006(1)
N(4)	2i	−0.2215(3)	0.0357(2)	0.1475(3)	0.042(2)	0.040(1)	0.033(1)	−0.002(1)	0.004(1)	0.003(1)
N(5)	2i	0.3981(3)	0.7216(2)	0.4213(4)	0.039(2)	0.036(1)	0.054(2)	0.001(1)	0.016(1)	0.007(1)
N(6)	2i	0.3121(3)	0.6398(2)	0.2995(3)	0.038(2)	0.038(1)	0.044(1)	0.005(1)	0.013(1)	0.012(1)
C(1)	2i	−0.0553(4)	0.1621(2)	0.5734(4)	0.031(2)	0.041(2)	0.033(1)	0.003(1)	0.010(1)	0.006(1)
C(2)	2i	−0.1353(3)	0.0997(2)	0.4167(3)	0.026(1)	0.032(1)	0.035(1)	0.005(1)	0.007(1)	0.006(1)
C(3)	2i	−0.1246(3)	0.1156(2)	0.2544(4)	0.029(2)	0.033(1)	0.036(1)	0.006(1)	0.006(1)	0.006(1)
C(4)	2i	−0.3005(4)	−0.0457(3)	0.5218(4)	0.036(2)	0.045(2)	0.048(2)	−0.003(1)	0.011(1)	0.011(1)
C(5)	2i	−0.2442(3)	0.0061(2)	0.3918(4)	0.025(1)	0.036(1)	0.040(2)	0.005(1)	0.007(1)	0.008(1)
C(6)	2i	−0.2571(5)	0.0174(3)	−0.0364(4)	0.069(3)	0.055(2)	0.035(2)	−0.009(2)	0.005(2)	0.002(2)
C(7)	2i	0.1099(4)	0.3021(3)	0.7689(4)	0.047(2)	0.052(2)	0.034(2)	−0.007(2)	0.008(1)	0.006(1)
C(8)	2i	0.2745(4)	0.3496(3)	0.7699(4)	0.047(2)	0.050(2)	0.038(2)	−0.001(2)	0.003(1)	0.012(1)
C(9)	2i	0.3286(4)	0.5094(2)	0.6595(4)	0.039(2)	0.041(2)	0.036(2)	−0.001(1)	0.008(1)	0.002(1)
C(10)	2i	0.3306(4)	0.5781(2)	0.5390(4)	0.033(2)	0.034(1)	0.040(2)	0.004(1)	0.013(1)	0.004(1)
C(11)	2i	0.2673(4)	0.5526(2)	0.3630(4)	0.031(2)	0.033(1)	0.041(2)	0.009(1)	0.011(1)	0.009(1)
C(12)	2i	0.4919(5)	0.7524(3)	0.7292(5)	0.050(2)	0.044(2)	0.055(2)	−0.008(2)	0.013(2)	−0.002(2)
C(13)	2i	0.4091(4)	0.6844(2)	0.5652(4)	0.030(2)	0.036(2)	0.047(2)	0.002(1)	0.015(1)	0.003(1)
C(14)	2i	0.2802(5)	0.6544(3)	0.1237(4)	0.057(2)	0.059(2)	0.051(2)	−0.003(2)	0.012(2)	0.022(2)

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