Crystal structure of *trans*-bis-thiocyanato-di(bis(pyrazolyl)methane)-copper(II), $C_{16}H_{16}CuN_{10}S_2$

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the complex. The major distortion from the ideal octahedral geometry is manifested in the N21–Cu–N3 angle of 93.4(1)°. The Cu–N3–C3 angle is 153.0(3)° and the thiocyanate anion is linear as seen in the N3–C3–S3 angle of 179.0(3)°.

Table 1. Data collection and handling.

Crystal:	green block, size 0.16 × 0.24 × 0.24 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	13.17 cm ⁻¹
Diffractometer, scan mode:	Rigaku AFC6R, $\omega/2\theta$
$2\theta_{\max}$:	55.2°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2572, 2324
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1531
$N(\text{param})_{\text{refined}}$:	134
Programs:	SIR92 [2], teXsan [3], SHELXL-97 [4], PLATON [5], DIBABS [6], ORTEPII [7]

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

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1a)	4e	0.4390	−0.1454	0.1481	0.060(4)
H(1b)	4e	0.3632	−0.0664	0.2116	0.060
H(11)	4e	0.0841	0.0527	−0.3445	0.048(3)
H(12)	4e	0.3213	−0.0102	−0.3993	0.048
H(13)	4e	0.4745	−0.1053	−0.1427	0.048
H(21)	4e	−0.1610	−0.1825	0.0734	0.048
H(22)	4e	−0.0103	−0.3221	0.1161	0.048
H(23)	4e	0.2753	−0.288	0.1344	0.048

Abstract

$C_{16}H_{16}CuN_{10}S_2$, monoclinic, $P12_1/c1$ (No. 14), $a = 8.670(1)$ Å, $b = 15.4307(9)$ Å, $c = 8.230(2)$ Å, $\beta = 113.76(1)^\circ$, $V = 1007.7$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.039$, $wR_{\text{ref}}(F^2) = 0.101$, $T = 293$ K.

Source of material

The complex was prepared by reaction of [(bis(pyrazolyl)methane)₂Cu(H₂O)₂](NO₃)₂, which was made by reacting bis(pyrazolyl)methane with Cu(NO₃)₂·3H₂O in water [1], with KSCN (2 mole equivalents) in methanol. Dark green crystals were deposited from the solution upon standing.

Discussion

The Cu atom in the title complex is situated on a centre of symmetry and exists in a N₆ donor set defined by two bidentate bis(pyrazolyl)methane ligands and two N-bound thiocyanate anions. The Cu–N bond distances involving the thiocyanate (2.433(3) Å) are significantly longer than those involving the bis(pyrazolyl)methane ligand, i.e. 2.033(2) Å and 2.031(2) Å. This is ascribed, in part, to the Jahn–Teller distortion operating in

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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	2a	0	0	0	0.0420(3)	0.0373(2)	0.0440(3)	0.0057(2)	0.0201(2)	0.0082(2)
S(3)	4e	0.4363(1)	0.19091(7)	0.4561(1)	0.0603(5)	0.0743(6)	0.0583(6)	−0.0092(5)	0.0182(5)	−0.0069(5)
N(3)	4e	0.2231(4)	0.0597(2)	0.2639(4)	0.066(2)	0.062(2)	0.062(2)	0.000(2)	0.021(2)	−0.007(2)
N(11)	4e	0.1669(3)	−0.0128(1)	−0.1151(3)	0.042(1)	0.044(1)	0.032(1)	0.004(1)	0.012(1)	0.005(1)
N(12)	4e	0.3013(3)	−0.0667(1)	−0.0495(3)	0.035(1)	0.040(1)	0.037(1)	−0.001(1)	0.013(1)	−0.001(1)
N(21)	4e	0.0508(3)	−0.1241(2)	0.0874(4)	0.038(1)	0.040(1)	0.054(2)	0.001(1)	0.018(1)	0.003(1)
N(22)	4e	0.1995(3)	−0.1623(1)	0.1093(3)	0.035(1)	0.039(1)	0.044(2)	0.004(1)	0.012(1)	0.008(1)
C(1)	4e	0.3396(3)	−0.1094(2)	0.1188(4)	0.035(2)	0.046(2)	0.036(2)	0.002(1)	0.007(1)	0.004(1)
C(3)	4e	0.3109(4)	0.1140(2)	0.3417(4)	0.047(2)	0.057(2)	0.038(2)	0.011(2)	0.019(2)	0.009(2)
C(11)	4e	0.1641(4)	0.0148(2)	−0.2686(4)	0.055(2)	0.053(2)	0.036(2)	−0.003(1)	0.014(2)	0.006(1)
C(12)	4e	0.2958(5)	−0.0202(2)	−0.3014(5)	0.068(2)	0.060(2)	0.041(2)	−0.014(2)	0.030(2)	−0.007(2)
C(13)	4e	0.3797(4)	−0.0721(2)	−0.1598(4)	0.045(2)	0.048(2)	0.053(2)	−0.007(1)	0.027(2)	−0.011(2)
C(21)	4e	−0.0498(4)	−0.1890(2)	0.0871(5)	0.044(2)	0.051(2)	0.061(2)	−0.003(1)	0.023(2)	0.003(2)
C(22)	4e	0.0326(4)	−0.2675(2)	0.1098(5)	0.063(2)	0.040(2)	0.073(3)	−0.006(1)	0.032(2)	0.009(2)
C(23)	4e	0.1901(4)	−0.2484(2)	0.1211(5)	0.057(2)	0.041(2)	0.064(2)	0.009(1)	0.029(2)	0.013(2)

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