Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1,3-Propanediamine-κ^2N,N')bis(thiocyanato-κN)copper(II)

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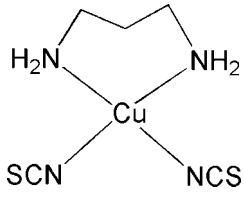
Received 20 July 2007; accepted 10 August 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(N–C) = 0.005 Å; disorder in main residue; R factor = 0.023; wR factor = 0.066; data-to-parameter ratio = 13.3.

The title compound, $[Cu(NCS)_2(C_3H_{10}N_2)]$, synthesized from the reaction of propane-1,3-diamine, ammonium thiocyanate and copper acetate monohydrate in anhydrous methanol solution, is a mononuclear copper(II) complex which lies on a mirror plane. The Cu^{II} ion is four-coordinated by the two N atoms of the propane-1,3-diamine ligand and by two N atoms from two thiocyanate ligands, forming a square-planar geometry. The propane-1,3-diamine ligand is disordered over four orientations, two symmetry-independent and two related by mirror symmetry, each with an occupancy of 0.25. The refinement results indicate inversion twinning.

Related literature

For related structures, see: Ye & You (2007); You *et al.* (2004); You, Han *et al.* (2006); You, Wang & Han (2006); You & Niu (2006); You & Zhu (2004).



Experimental

Crystal data

$[Cu(NCS)_2(C_3H_{10}N_2)]$
M_r = 253.83
Orthorhombic, $Cmc2_1$
a = 5.9505 (17) Å
b = 20.478 (6) Å
c = 8.475 (2) Å
V = 1032.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.47 mm^{-1}
T = 295 (2) K
0.32 × 0.30 × 0.27 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.505, T_{max} = 0.555
(expected range = 0.467–0.513)
4393 measured reflections
1287 independent reflections
1264 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.066
S = 1.04
1287 reflections
97 parameters
63 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 593 Friedel pairs
Flack parameter: 0.50 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—N4	1.963 (3)	Cu1—N2	1.999 (3)
Cu1—N3	1.984 (3)	Cu1—N1	2.001 (3)
N4—Cu1—N3	89.57 (16)	N4—Cu1—N1	88.87 (16)
N4—Cu1—N2	178.10 (16)	N3—Cu1—N1	178.44 (16)
N3—Cu1—N2	88.53 (15)	N2—Cu1—N1	93.03 (14)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Scientific Research Foundation of the Education Office of Liaoning Province (project No. 20060495). We also thank the University of Malaya for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2424).

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 doi:10.1107/S1600536807039645

supplementary materials

Acta Cryst. (2007). E**63**, m2347 [**doi:10.1107/S1600536807039645**]

(1,3-Propanediamine-κ^2N,N')bis(thiocyanato-κN)copper(II)

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Comment

Recently, we have reported the crystal structures of a few Schiff base metal complexes (You, Han *et al.*, 2006; You, Wang & Han, 2006; You & Niu, 2006). As an extension of the work on the structural characterization of such complexes, the title copper(II) complex is reported here.

The complex is a mononuclear copper(II) complex, which lies on a mirror plane. The Cu^{II} ion is four-coordinated by two N atoms of the propane-1,3-diamine ligand and by two N atoms from two thiocyanate ligands, forming a square planar geometry (Table 1). The coordination bond lengths are within normal ranges and comparable to the values observed in other copper(II) complexes reported by us recently (You & Zhu, 2004; You *et al.*, 2004; Ye & You, 2007).

Experimental

All the reagents used were of commercial grade and used without further purification. Propane-1,3-diamine (0.1 mmol, 7.4 mg), ammonium thiocyanate (0.2 mmol, 15.2 mg) and copper acetate monohydrate (0.1 mmol, 20.0 mg) were mixed in an anhydrous methanol solution (10 ml). The mixture was stirred at room temperature for 30 min to give a clear blue solution. After keeping the solution in air for a week, blue block-shaped crystals were formed.

Refinement

All non-hydrogen atoms except the C atoms of the 1,3-propanediamine ligand lie on a mirror plane. The 1,3-propanediamine ligand is disordered over four orientations, two symmetry independent and two related by mirror symmetry, each with an occupancy of 0.25. The N—C bond distances were restrained to 1.45 (1) Å and the C–C distances to 1.54 (1) Å. The 1,3-related N···C distances were restrained to 2.35 (1) Å and the 1,3-related C···C distances to 2.51 (1) Å. Additionally, the displacement parameters of the primed atoms were set to those of the unprimed ones; the anisotropic displacement parameters of the entire ligand were restrained to be nearly isotropic. C– and N-bound H atoms were generated geometrically (C–H = 0.97 and N–H = 0.86 Å), and were included in the refinement in the riding model approximation. The refined Flack parameter of 0.50 (2) indicates that the crystal is an inversion twin.

Figures

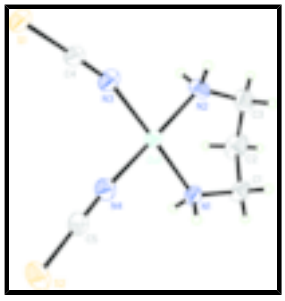

Fig. 1. The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Only one of the four disorder components is shown.

(1,3-Propanediamine-κ^2*N*,*N*')bis(thiocyanato-κ*N*)\ copper(II)

Crystal data

$[Cu(NCS)_2(C_3H_{10}N_2)]$	F_{000} = 516
M_r = 253.83	D_x = 1.633 Mg m^{-3}
Orthorhombic, *Cmc*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2c -2	Cell parameters from 4527 reflections
a = 5.9505 (17) Å	θ = 2.7–27.5º
b = 20.478 (6) Å	μ = 2.47 mm^{-1}
c = 8.475 (2) Å	*T* = 295 (2) K
V = 1032.7 (5) Å^3	Block, blue
Z = 4	0.32 × 0.30 × 0.27 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1287 independent reflections
Radiation source: fine-focus sealed tube	1264 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 295(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −7→7
T_{min} = 0.505, T_{max} = 0.555	*k* = −26→26
4393 measured reflections	*l* = −11→11

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.023	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.1407P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.066	$(\Delta/\sigma)_{max} < 0.001$

S = 1.04	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
1287 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
97 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
63 restraints	Extinction coefficient: 0.010 (1)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 593 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.50 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.5000	0.701275 (15)	0.5000	0.04011 (15)	
S1	0.5000	0.80305 (4)	0.0035 (2)	0.0479 (2)	
S2	0.5000	0.92135 (5)	0.6725 (2)	0.0766 (4)	
N3	0.5000	0.72640 (19)	0.2739 (4)	0.0501 (7)	
N4	0.5000	0.79405 (14)	0.5584 (5)	0.0516 (8)	
C4	0.5000	0.75676 (17)	0.1619 (4)	0.0404 (7)	
C5	0.5000	0.84648 (18)	0.6040 (5)	0.0481 (8)	
N1	0.5000	0.67852 (16)	0.7296 (4)	0.0495 (7)	
H11	0.6242	0.6940	0.7656	0.059*	0.25
H12	0.3953	0.7021	0.7703	0.059*	0.25
H13	0.5656	0.7100	0.7786	0.059*	0.25
H14	0.3623	0.6783	0.7603	0.059*	0.25
N2	0.5000	0.60769 (14)	0.4330 (4)	0.0529 (9)	
H21	0.3721	0.6005	0.3890	0.064*	0.25
H22	0.5999	0.6040	0.3603	0.064*	0.25
H23	0.3616	0.5964	0.4224	0.064*	0.25
H24	0.5587	0.6065	0.3403	0.064*	0.25
C1	0.477 (2)	0.6158 (3)	0.8026 (9)	0.052 (2)	0.25
H1A	0.3715	0.6191	0.8896	0.063*	0.25
H1B	0.6209	0.6025	0.8453	0.063*	0.25
C2	0.396 (2)	0.5649 (4)	0.6890 (11)	0.072 (3)	0.25
H2A	0.2458	0.5770	0.6544	0.086*	0.25
H2B	0.3826	0.5239	0.7453	0.086*	0.25
C3	0.539 (3)	0.5537 (6)	0.5448 (12)	0.064 (3)	0.25
H3A	0.6960	0.5521	0.5743	0.077*	0.25
H3B	0.5000	0.5125	0.4959	0.077*	0.50
C1'	0.6032 (17)	0.6171 (4)	0.7849 (11)	0.052 (2)	0.25
H1'1	0.5751	0.6111	0.8967	0.063*	0.25
H1'2	0.7644	0.6181	0.7680	0.063*	0.25

C2'	0.497 (4)	0.5609 (4)	0.6903 (10)	0.072 (3)	0.25
H2'1	0.3377	0.5690	0.6767	0.086*	0.25
H2'2	0.5147	0.5202	0.7476	0.086*	0.25
C3'	0.611 (3)	0.5552 (6)	0.5270 (12)	0.064 (3)	0.25
H3'1	0.7717	0.5626	0.5348	0.077*	0.25
H3'2	0.5848	0.5126	0.4807	0.077*	0.25

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0494 (2)	0.0383 (2)	0.0327 (2)	0.000	0.000	0.00364 (17)
S1	0.0423 (4)	0.0641 (5)	0.0374 (4)	0.000	0.000	0.0121 (5)
S2	0.0979 (8)	0.0411 (5)	0.0909 (9)	0.000	0.000	−0.0032 (5)
N3	0.0439 (15)	0.065 (2)	0.0419 (17)	0.000	0.000	0.0092 (15)
N4	0.0581 (19)	0.0427 (15)	0.0541 (17)	0.000	0.000	0.0009 (12)
C4	0.0317 (13)	0.0519 (19)	0.0375 (16)	0.000	0.000	0.0009 (14)
C5	0.0492 (16)	0.0446 (17)	0.0506 (19)	0.000	0.000	0.0086 (16)
N1	0.0533 (16)	0.0577 (19)	0.0374 (16)	0.000 (11)	0.000 (11)	0.0062 (14)
N2	0.068 (2)	0.0428 (16)	0.0475 (17)	−0.007 (7)	−0.017 (6)	−0.0033 (15)
C1	0.059 (7)	0.055 (3)	0.042 (3)	−0.002 (4)	0.000 (4)	0.012 (2)
C2	0.077 (7)	0.062 (3)	0.077 (4)	−0.025 (5)	−0.010 (5)	0.021 (3)
C3	0.078 (8)	0.044 (2)	0.072 (5)	−0.001 (4)	0.001 (4)	0.000 (2)
N1'	0.0533 (16)	0.0577 (19)	0.0374 (16)	0.000 (11)	0.000 (11)	0.0062 (14)
N2'	0.068 (2)	0.0428 (16)	0.0475 (17)	−0.007 (7)	−0.017 (6)	−0.0033 (15)
C1'	0.059 (7)	0.055 (3)	0.042 (3)	−0.002 (4)	0.000 (4)	0.012 (2)
C2'	0.077 (7)	0.062 (3)	0.077 (4)	−0.025 (5)	−0.010 (5)	0.021 (3)
C3'	0.078 (8)	0.044 (2)	0.072 (5)	−0.001 (4)	0.001 (4)	0.000 (2)

Geometric parameters (Å, °)

Cu1—N4	1.963 (3)	C1—H1A	0.97
Cu1—N3	1.984 (3)	C1—H1B	0.97
Cu1—N2	1.999 (3)	C2—C3	1.507 (9)
Cu1—N1	2.001 (3)	C2—H2A	0.97
S1—C4	1.644 (4)	C2—H2B	0.97
S2—C5	1.639 (4)	C3—H3A	0.97
N3—C4	1.134 (5)	C3—H3B	0.97
N4—C5	1.141 (5)	C1'—C2'	1.537 (10)
N1—C1	1.432 (7)	C1'—H1'1	0.97
N1—H11	0.86	C1'—H1'2	0.97
N1—H12	0.86	C2'—C3'	1.545 (10)
N2—C3	1.473 (9)	C2'—H2'1	0.97
N2—H21	0.86	C2'—H2'2	0.97
N2—H22	0.86	C3'—H3'1	0.97
C1—C2	1.499 (9)	C3'—H3'2	0.97
N4—Cu1—N3	89.57 (16)	C2—C1—H1B	109.2
N4—Cu1—N2	178.10 (16)	H1A—C1—H1B	107.9
N3—Cu1—N2	88.53 (15)	C1—C2—C3	116.4 (8)

N4—Cu1—N1	88.87 (16)	C1—C2—H2A	108.2
N3—Cu1—N1	178.44 (16)	C3—C2—H2A	108.2
N2—Cu1—N1	93.03 (14)	C1—C2—H2B	108.2
C4—N3—Cu1	161.8 (4)	C3—C2—H2B	108.2
C5—N4—Cu1	174.8 (4)	H2A—C2—H2B	107.3
N3—C4—S1	178.0 (4)	N2—C3—C2	108.6 (7)
N4—C5—S2	179.1 (4)	N2—C3—H3A	110.0
C1—N1—Cu1	129.0 (4)	C2—C3—H3A	110.0
C1—N1—H11	105.0	N2—C3—H3B	110.0
Cu1—N1—H11	105.0	C2—C3—H3B	110.0
C1—N1—H12	105.0	H3A—C3—H3B	108.3
Cu1—N1—H12	105.0	C2'—C1'—H1'1	110.2
H11—N1—H12	105.9	C2'—C1'—H1'2	110.2
C3—N2—Cu1	122.4 (5)	H1'1—C1'—H1'2	108.5
C3—N2—H21	106.7	C1'—C2'—C3'	110.1 (10)
Cu1—N2—H21	106.7	C1'—C2'—H2'1	109.6
C3—N2—H22	106.7	C3'—C2'—H2'1	109.6
Cu1—N2—H22	106.7	C1'—C2'—H2'2	109.6
H21—N2—H22	106.6	C3'—C2'—H2'2	109.6
N1—C1—C2	112.1 (6)	H2'1—C2'—H2'2	108.2
N1—C1—H1A	109.2	C2'—C3'—H3'1	111.1
C2—C1—H1A	109.2	C2'—C3'—H3'2	111.1
N1—C1—H1B	109.2	H3'1—C3'—H3'2	109.1
N4—Cu1—N3—C4	0	N1—Cu1—N2—C3	−10.6 (7)
N2—Cu1—N3—C4	180	Cu1—N1—C1—C2	−13.6 (13)
N4—Cu1—N1—C1	172.9 (7)	N1—C1—C2—C3	58.3 (14)
N2—Cu1—N1—C1	−7.1 (7)	Cu1—N2—C3—C2	46.8 (12)
N3—Cu1—N2—C3	169.4 (7)	C1—C2—C3—N2	−76.4 (13)

Fig. 1