Crystal structure of copper(II) tetracyanamide dichloride, $Cu(NCNH_2)_4Cl_2$

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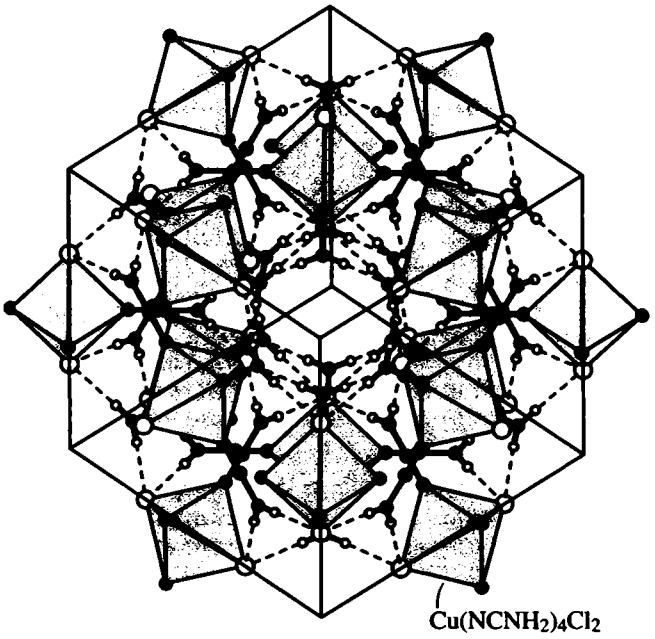

$Cu(NCNH_2)_4Cl_2$

Abstract

$C_4H_8Cl_2CuN_8$, cubic, $Im\bar{3}m$ (No. 229), $a = 12.443(2)$ Å, $V = 1926.3$ Å^3, $Z = 6$, $R_{gt}(F) = 0.051$, $wR_{ref}(F^2) = 0.179$, $T = 293$ K.

Source of material

Green-blue crystals were obtained from a mixture of aqueous 0.05 mol/l $CuCl_2$ and 0.5 mol/l H_2NCN by letting the solution evaporate at room temperature and become wax-like. The crystals precipitate from the solution and tend to decompose in dry air, changing into an unknown black powder.

Experimental details

Absorption correction on the intensity data was not justified, because the results did not improve.

Discussion

The crystal structure is isotypic with $Ni(NCNH_2)_4Cl_2$ and $Co(NCNH_2)_4Cl_2$ originally determined in [1]. Cu ions are octahedrally coordinated by four neutral cyanamide molecules and two chloride anions (see figure). Large white circles represent chloride anions, triple grey units cyanamide molecules, and small circles hydrogen atoms. The crystallographic symmetry (mirror plane) is higher than the molecular symmetry as reflected by the tilted N(1)–C2–N(2) angle (167°); consequently, the N(2) atom lies a bit above and below Wyckoff position 24*h*, with exactly 50% site occupancy. The interatomic distances are 2.04 Å for the Cu—N and 2.78 Å for the Cu—Cl combination. The latter distance is significantly longer than the sum of the ionic radii due to the Jahn-Teller effect, a common phenomenon for divalent copper.

Table 1. Data collection and handling.

Crystal:	green-blue cube, size 0.09 × 0.09 × 0.09 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	21.00 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, $\omega/2\theta$
$2\theta_{max}$:	69.86°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4612, 458
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 327
$N(param)_{refined}$:	24
Program:	SHELXL-97 [2]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H	48*j*	0.176(5)	0.0	0.260(3)	0.06(1)

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References

1. Liu, X.; Kroll, P.; Dronskowski, R.: Crystal Structure, Magnetic Properties, and Electronic Structure of $Ni(NCNH_2)_4Cl_2$ and $Co(NCNH_2)_4Cl_2$. Z. Anorg. Allg. Chem. **627** (2001) 1682-1686.
2. Sheldrick, G. M.: SHELXL-97, a program for refining crystal structures. University of Göttingen, Germany 1997.

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	6*b*		0	1/2	0	0.0376(4)	0.0862(9)	U_{11}	0	0	0
Cl	12*e*		0	0.2764(2)	0	0.0639(7)	0.100(2)	U_{11}	0	0	0
N(1)	24*h*		0.3843(3)	0	x	0.047(1)	0.088(3)	U_{11}	0	0.006(2)	0
C	24*h*		0.3248(3)	0	x	0.048(1)	0.110(4)	U_{11}	0	0.005(2)	0
N(2)	48*k*	0.50	0.2503(4)	0.024(3)	x	0.054(2)	0.17(4)	U_{11}	0.002(4)	-0.008(2)	U_{12}

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