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NOTE

Crystal Structural of Phenanthroline and Thiocyanate Copper(II) Complex

JIAN-HONG BI* and HUA-ZE DONG

Deparment of Chemistry and Chemical Engineering, Hefei Normal University, Hefei, P.R. China

*Corresponding author: E-mail: bi010101@126.com

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A novel copper complex $[Cu(phen)_2(SCN)_2]$ has been synthesized, with the 1,10-phenanthroline (phen) and the thiocyanate (SCN^-) as ligands and characterized by IR spectra and single-crystal X-ray diffraction measurements. The crystal is orthorhombic, space group Pbcn with unit cell parameters: a =13.2449(15) Å, b = 10.0566(9) Å, c = 17.4257(16) Å, α = 90°, β = 90°, γ = 90°, V = 2321.1(4) $Å^3$, Z = 4, M_r = 540.11, D_c = 1.546 Mg/cm^3, μ = 1.150 mm^{-1}, $F_{(000)}$ =1100, T = 298(2) K, R = 0.0358, wR = 0.0803 for 8958 reflections with $I > 2\sigma(I)$. In the molecular structure unit, copper(II) cation is coordinated by six donor atoms.

Key Words: Copper(II) complex, Phenanthroline, Thiocyanate, Crystal structure.

Schiff bases copper complexes have great importance in many branch of chemistry due to their diversity of molecular structures[1-5] and a lot of application areas, such as catalysis, magnetism, biology and pharmacology[6-10].

Herein, the synthesis and crystal structure of a mononuclear complex $[Cu(phen)_2(SCN)_2]$ are reported.

All reagents were of AR grade and used without further purification. IR spectra were recorded on a Nexus-870 spectrophotometer. The x-ray structure was determined by Siemens SMART CCD area-detector diffractometer.

Synthesis: 10 mL ethanol solution of 1,10-phenanthroline (10 mmol) was respectively added to 20 mL H_2O solution of $Cu(CH_3COO)_2$ (5 mmol) and KSCN (10 mmol) under stirring for 4 h. After being filtered, the solution was stand at room temperature for one week, crystals were obtained. The product was blue cubic-shaped single crystals. Yield 30 %. IR spectrum (KBr, ν_{max}, cm^{-1}): 3450, 2089, 1621, 1512, 1421, 845, 723, 636.

Structure determination: A single crystal (0.4 6 mm × 0.45 mm × 0.23 mm) was selected for crystallographic data collection at 298(2) K and structure determinated with graphite monochromatic MoK_α radiation (λ = 0.71073 Å). A total of 8958 reflections were collected in the range of $2.43° \le \theta \le 25.04°$, of which 2051 reflections were unique with R_{int} = 0.0406 and R = 0.0358 and wR = 0.0803, where $w = 1/[s^2(F_0^2) + (0.0370P)^2 + 1.5691P]$, $P = (F_0^2 + 2F_0^2)/3$. The maximum and minimum peaks on the final difference Fourier map are corresponding to 0.335 and -0.431 e/$Å^3$ (CCDC No. 908533), respectively.

TABLE-1
NON-HYDROGEN ATOMIC COORDINATES (× 10^4)
AND THERMAL PARAMETERS (× 10^3 $Å^2$)

Atom	X	Y	Z	U (eq)
Cu(1)	5000	6602(1)	7500	41(1)
N(1)	6623(2)	6297(3)	7239(2)	45(1)
N(2)	4982(2)	5115(3)	6628(2)	45(1)
N(3)	5332(2)	7976(3)	8309(2)	63(1)
S(1)	6405(1)	9729(1)	9233(1)	73(1)
C(5)	6778(2)	5333(3)	6708(2)	41(1)
C(6)	5903(2)	4709(3)	6374(2)	41(1)
C(13)	5780(3)	8702(3)	8685(2)	48(1)

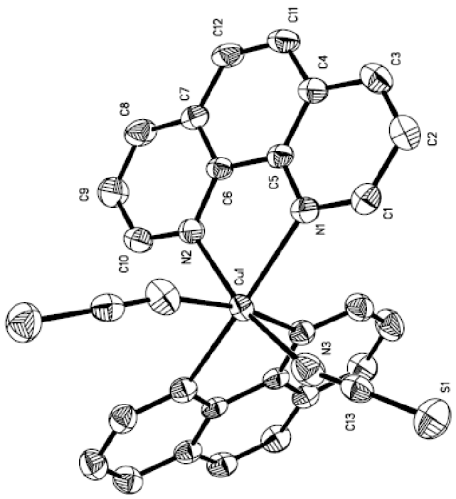

Fig. 1. Molecular structure of the complex $[Cu(phen)_2(SCN)_2]$

TABLE-2
SELECTED BOND LENGTHS (Å) AND BOND ANGLES (°)

Bond	Length	Angle	(°)	Angle	(°)
Cu(1)-N(1)	2.219(3)	N(2)- Cu(1)-N(1)	76.57(10)	N(1)- Cu(1)-N(1)#1	164.08(14)
Cu(1)-N(2)	2.133(3)	N(3)- Cu(1)-N(1)	91.54(12)	N(2)- Cu(1)-N(1)#1	92.17(10)
Cu(1)-N(3)	2.022(3)	N(3)- Cu(1)-N(2)	168.10(12)	N(2)- Cu(1)-N(2)#1	90.94(14)
N(3)-C(13)	1.147(4)	N(3)-C(13)-S(1)	179.1(4)	N(3)- Cu(1)-N(2)#1	88.85(12)
S(1)-C(13)	1.631(4)	C(5)-N(1)- Cu(1)	112.7(2)	N(3)- Cu(1)-N(3)#1	93.78(18)
C(5)-C(6)	1.440(5)	C(13)-N(3)- Cu(1)	161.1(3)	N(3)#1- Cu(1)-N(1)	99.35(11)

The atomic coordinates and thermal parameters are listed in Table-1 and the selected bond lengths and bond angles in Table-2, respectively. Fig. 1 shows diagram of the molecular structure of the complex $[Cu(phen)_2(SCN)_2]$. Fig. 2 shows a perspective view of the crystal packing in the unit cell. As shown in the Fig. 1, the center copper(II) cation is six-coordinated with four nitrogen atoms of the two phenanthroline ligands and two nitrogen atoms of the two thiocyanate anions.

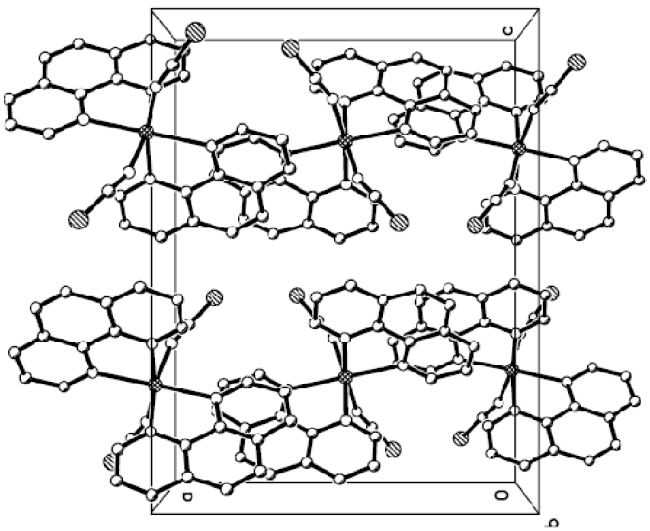

Fig. 2. Molecular packing arrangement in the unit cell

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