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NOTE

Hydrothermal Synthesis and Structure of Zn(II) Thiocyanate Complex of Phenanthroline

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A new Zn(II) complex with m.f. $C_{26}H_{16}N_6S_2Zn$ has been synthesized by the hydrothermal reaction of 1,10-phenanthroline (phen) with $ZnSO_4$ and KSCN. The structure was characterized by IR spectra and single-crystal X-ray diffraction. The crystal is present in a orthorhombic system, space group Pbcn with a = 13.1988(15) Å, b = 10.0779(13) Å, c = 17.4640(19) Å, α = 90º, β = 90º, γ = 90º, V = 2323.0(5)Å^3, Z = 4, Mr = 541.94, Dc = 1.550 Mg/cm^3, μ = 1.266 mm^{-1}, F(000) = 1104, T = 298(2) K, R = 0.0524, wR = 0.1246 for 8916 reflections with I > 2σ(I). In the molecular structure unit, Zn(II) cation is coordinated by six N atoms.

Keywords: Zn(II) complex, Hydrothermal synthesis, Crystal structure.

Recently, there has been increasing interest of 1,10-phenanthroline complexes in the field of coordination chemistry[1-5]. In our laboratory, a series of 1,10-phenanthroline complexes were synthesized[6-10]. In this paper, we wish to report the synthesis and crystal structure of a new Zn(II) complex with m.f. $[Zn(phen)_2(SCN)_2]$.

All reagents were of AR grade and used without further purification. IR spectra were recorded on a Nicolet 380 FT-IR spectrophotometer. The crystal structure was determined by Siemens SMART CCD area-detector diffractometer.

Synthesis: 15 mL ethanolic solution of 1,10-phenanthroline (10 mmol) was respectively added to 25 mL H_2O solution of $ZnSO_4$ (5 mmol) and KSCN (10 mmol) in a autoclave and heated to 150 ºC for 72 h. After cooling, the colourless cubic-shaped single crystals were obtained. Yield 31 %. IR spectrum (KBr, ν_{max}, cm^{-1}): 3445, 2058, 1515 ,1420, 847, 725.

Structure determination: A single crystal (0.24 mm × 0.23 mm × 0.17 mm) was selected for crystallographic data collection at 298(2) K and structure determinated with graphite monochromatic MoK$_\alpha$ radiation (γ = 0.71073Å). A total of 5278 reflections were collected in the range of 2.54º ≤ θ ≤ 25.02º, of which 2047 reflections were unique with R_{int} = 0.0933 and R = 0.0524 and wR = 0.1246, where w = 1/[$s^2(F_0^2)$ + (0.0000P)^2 + 4.1934P], P = (F_0^2 + 2F_0^2)/3. The maximum and minimum peaks on the final difference Fourier map are corresponding to 0.545 and -0.623 e/Å^3, respectively.

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 $[Zn(phen)_2(SCN)_2]$. Fig. 2 shows a perspective view of the crystal packing in the unit cell. As shown in the Fig. 1, the center zinc(II) cation is six-coordinated with four nitrogen atoms from the two phen ligands and two nitrogen atoms form the two thiocyanate anions.

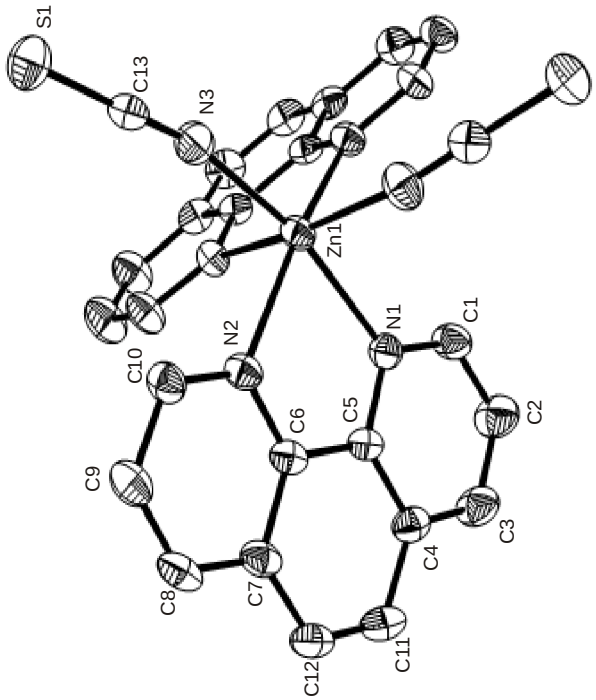

Fig. 1. Molecular structure of the complex $[Zn(phen)_2(SCN)_2]$

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

Atom	X	Y	Z	U(eq)
Zn(1)	10000	1668(1)	2500	41(1)
N(1)	10038(4)	95(5)	3396(3)	44(1)
N(2)	8400(4)	1292(5)	2763(3)	43(1)
N(3)	9616(5)	3051(6)	1677(3)	58(2)
S(1)	8578(2)	4770(2)	727(1)	69(1)
C(1)	10839(5)	-448(7)	3729(4)	58(2)
C(6)	8240(4)	311(6)	3286(3)	41(1)
C(13)	9177(5)	3764(6)	1288(4)	47(2)

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

BOND	LENGTH	ANGLE	(°)	ANGLE	(°)
Zn(1)-N(3)	2.065(6)	N(2)-Zn(1)-N(1)	75.61(19)	N(1)#1-Zn(1)-N(1)	89.3(3)
Zn(1)-N(2)	2.194(5)	N(3)-Zn(1)-N(1)	167.0(2)	N(2)-Zn(1)-N(1)#1	90.16(19)
Zn(1)-N(1)	2.227(5)	N(3)-Zn(1)-N(2)	91.5(2)	N(2)#1-Zn(1)-N(1)	90.16(18)
N(1)-C(5)	1.359(7)	C(1)-N(1)-Zn(1)	128.3(4)	N(3)-Zn(1)-N(1)#1	89.2(2)
S(1)-C(13)	1.616(7)	C(13)-N(3)-Zn(1)	163.7(6)	N(3)#1-Zn(1)-N(3)	95.1(3)
N(3)-C(13)	1.146(8)	N(3)-C(13)-S(1)	178.8(7)	N(3)-Zn(1)-N(2)#1	91.5(2)

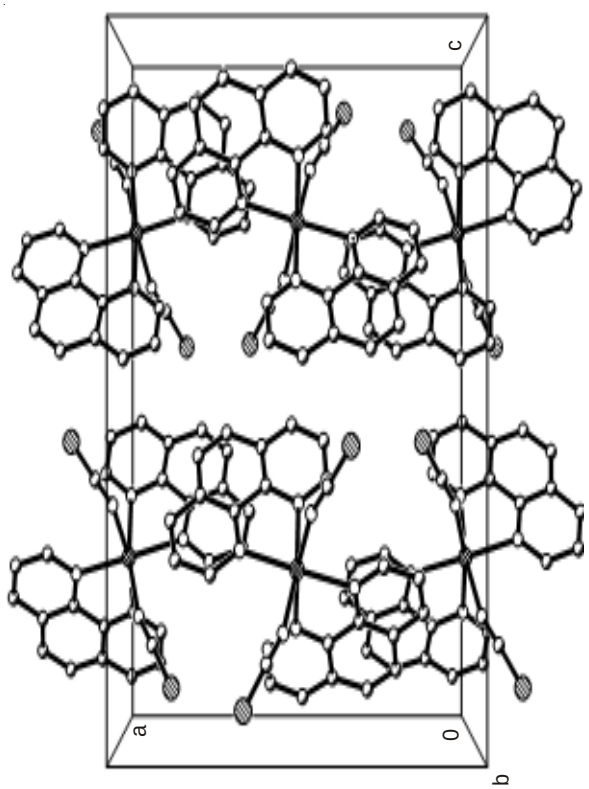

Fig. 2. Molecular packing arrangement in the unit cell

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