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NOTE

Hydrothermal Synthesis and Structure of 1,10-Phenanthroline Nickel(II) Complex

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A new nickel(II) complex with molecular formula $C_{26}H_{16}N_6S_2Ni$ has been synthesized by the reaction of 1,10-phenanthroline (phen) with $NiOAc_2$ and KSCN. The structure was characterized by IR spectra and single-crystal X-ray diffraction. The crystal is in a orthorhombic system, space group Pbcn with a =13.0276(14)Å, b = 10.1210(10)Å, c = 17.4717(19)Å, α = 90º, β = 90º, γ = 90º, V = 2303.7(4)Å^3, Z = 4, Mr = 535.28, Dc = 1.543 Mg/cm^3, μ = 1.052 mm^{-1}, F(000) = 1096, T = 298(2) K, R = 0.0428, wR = 0.0658 for 9652 reflections with I > 2σ(I). In the molecular structure unit, nickel(II) cation is coordinated by six donor atoms.

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

Nickel mixed ligand complexes containing 1,10-phenanthroline (phen) have great applications in many areas of chemistry due to their diversity of molecular structures, catalytic and biological activities, *etc*[1-9]. In this paper, the hydrothermal synthesis and crystal structure of a complex $[Ni(phen)_2(SCN)_2]$ are reported.

All reagents were of AR grade and used without further purification. IR spectra were recorded on a Nexus-870 spectrophotometer. The 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 nickel(II) acetate (5 mmol) and KSCN (10 mmol) were carried out in a autoclave and heated to 150 ºC for 72 h. After cooling, the well-shaped crystals were obtained. The product was blue cubic-shaped single crystals. Yield 40 %. IR spectrum (KBr, ν_{max}, cm^{-1}): 3430, 2112, 1620, 1550, 1420, 815, 729, 616.

Structure determination: A single crystal (0.26 mm × 0.16 mm × 0.12 mm) was selected for crystallographic data collection at 298(2) K and structure determinated with graphite monochromatic MoK$_\alpha$ radiation (λ = 0.71073Å). A total of 9652 reflections were collected in the range of 2.33º ≤ θ ≤ 25.01º, of which 2032 reflections were unique with Rint = 0.0691 and R = 0.0428 and wR = 0.0658, where w = 1/[s^2(F$_0^2$) + (0.0139P)^2 + 0.0000P], P = (F$_0^2$ + 2F$_0^2$)/3. The maximum and minimum peaks on the final difference Fourier map are corresponding to 0.653 and -0.317 e/Å^3 (CCDC No. 925323), 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 the molecular structure of the complex $[Ni(phen)_2(SCN)_2]$. Fig. 2 shows a perspective view of the crystal packing in the unit cell. As shown in the Fig. 1, the center nickel(II) cation is six-coordinated with four nitrogen atoms from the two 1,10-phenanthroline ligands and two nitrogen atoms form the two thiocyanate anions.

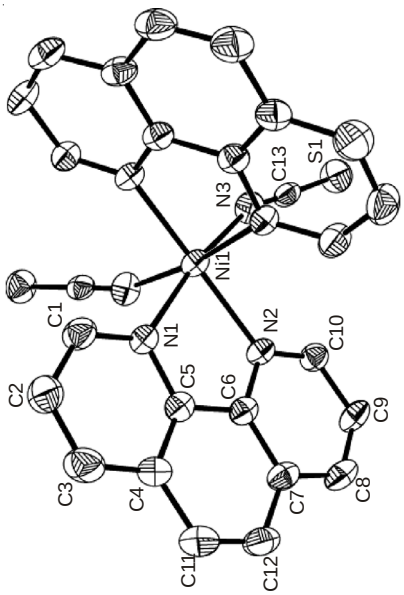

Fig. 1. Molecular structure of the complex $[Ni(phen)_2(SCN)_2]$

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

Atom	X	Y	Z	U(eq)
NI(1)	5000	6511(1)	7500	46(1)
N(1)	4924(2)	5058(3)	6639(1)	46(1)
N(2)	6566(2)	6277(3)	7234(2)	46(1)
N(3)	5303(2)	7903(3)	8304(2)	61(1)
S(1)	6338(1)	9709(1)	9227(1)	76(1)
C(5)	5859(3)	4682(4)	6367(2)	46(1)
C(6)	6739(3)	5331(3)	6697(2)	46(1)
C(13)	5739(3)	8647(4)	8684(2)	50(1)

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

BOND	LENGTH	ANGLE	(°)	ANGLE	(°)
NI(1)-N(3)	2.028(3)	N(2)-NI(1)-N(1)	79.02(11)	N(1)-NI(1)-N(1)#1	91.45(14)
NI(1)-N(2)	2.106(2)	N(3)-NI(1)-N(1)	171.43(11)	N(2)-NI(1)-N(1)#1	91.93(11)
NI(1)-N(1)	2.106(3)	N(3)-NI(1)-N(2)	92.42(11)	N(2)-NI(1)-N(2)#1	91.93(11)
N(3)-C(13)	1.154(4)	N(3)-C(13)-S(1)	179.0(4)	N(3)-NI(1)-N(1)#1	88.92(11)
S(1)-C(13)	1.632(4)	C(5)-N(1)-NI(1)	113.8(2)	N(3)-NI(1)-N(3)#1	91.99(17)
C(5)-C(6)	1.442(4)	C(13)-N(3)-NI(1)	161.4(3)	N(3)#1-NI(1)-N(1)	88.92(11)

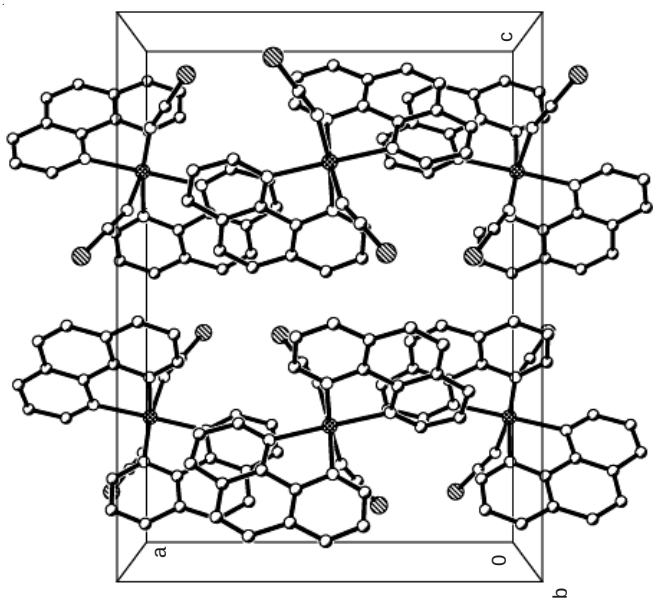

Fig. 2. Molecular packing arrangement in the unit cell

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