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NOTE

Synthesis and Crystal Structure of a New Complex: $[phen_2Co]_2 \cdot Mn(SCN)_6 \cdot 4H_2O$

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A novel cobalt(II) complex $[phen_2Co]_2 \cdot Mn(SCN)_6 \cdot 4H_2O$, where phen is 1,10-phenanthroline, was synthesized and characterized by IR spectra, elemental analysis and single-crystal X-ray. The crystal is monoclinic, space group P2(1)/n with unit cell parameters: a = 10.261(2) Å, b = 19.549(4) Å, c = 19.088(4) Å, $\alpha = 90^o$, $\beta = 95.743(3)^o$, $\gamma = 90^o$, V = 3809.7(13) $Å^3$, Z = 2, Mr = 761.06, Dc = 1.460Mg/cm^3, $\mu = 0.821$ mm^{-1}, F(000) = 1714, T = 293(2) K, R = 0.0676, wR = 0.2057 for 29078 reflections with $I > 2\sigma(I)$. The crystal structure analysis shows that the cobalt(II) is a six-coordinated in a slightly distorted octahedron environment.

Key Words: Crystal structure, 1,10-Phenanthroline, Cobalt(II) complex, π-π Interactions.

The transition metal complexes of phenanthroline and its derivatives have become an attractive research field[1,2]. These complexes has been widely used in molecular catalysis, self-assembly, antitumor drugs, and material chemistry field[3-6]. Here we will present a new phenanthroline complex $[phen_2Co]_2 \cdot Mn(SCN)_6 \cdot 4H_2O$ and describe its synthesis and crystal structure.

IR spectrum was recorded on an Nexus-870 spectromer. Elemental analyses on an Elementar Vario EL-III elemental analyzer.

Synthesis: An aqueous solution (50 mL) of $MnSO_4$ (1mmol) and KSCN (6 mmol) were mixed within 24 h, then diffused slowly into a mixed solution (50 mL) of $CoSO_4$ (2 mmol, 20 mL water) and 1,10-phenanthroline (6 mmol, 30 mL alcohol) in a cone bottle under normal atmospheric temperature and normal pressure for 2 weeks. The product was deep red rectangle-shaped crystals. IR spectrum (KBr, cm^{-1}): 3438, 2093, 2050, 1584, 1460, 846, 724. Elemental analysis (%) calcd. for $C_{78}H_{56}Co_2MnN_{18}O_4S_6$: C, 55.95; H, 3.37; N, 15.06. Found: (%) C, 55.73; H, 3.46; N, 15.18.

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Crystal structure determination: A deep red crystal (0.50 mm × 0.40 mm × 0.30 mm) was selected for crystallographic data collection at 293(2)K and structure determinated with graphite-monochromatic MoK_α radiation (λ = 0.71073 Å). A total of 29078 reflections were collected in the range of 2.34º≤θ≤27.48º, of which 8728 reflections were unique with Rint = 0.0267 and R = 0.0676, wR = 0.2057; where $w = 1/[\sigma^2(F_0^2) + (0.1182P)^2 + 4.2976P]$ and $P= (F_0^2 + 2F_C^2)/3$. The maximum and minimum peaks on the final difference Fourier map are corresponding to 1.176 and -0.879e/Å^3 (CCDC No.719397), 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 title compound. Fig. 2 shows the packing diagram of the title compound. From the Fig. 1, the cobalt(II) ion is coordinated with six nitrogen atoms and six Co-N bonds are varied. So it is obviously that cobalt(II) ion is in a slightly distorted octahedral geometry. Fig. 2 depicts the packing diagram in the unit cell, shows that the moleculars are linked to the neighbours by electrostatic interactions between $[phen_2Co]^{2+}$ and $[Mn(SCN)_6]^{4-}$ and the π-π stacking interactions. The title compound pack in a three-dimensional frameworks.

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

Atom	x	y	z	U(eq)
Mn	5000	0	0	45(1)
Co	1962(1)	2508(1)	1823(1)	36(1)
N(1)	3351(4)	34(2)	692(2)	57(1)
N(12)	634(3)	3178(2)	1476(2)	42(1)
C(1)	2773(4)	-55(2)	1174(2)	48(1)
C(11)	4446(4)	3299(2)	1906(2)	56(1)
S(1)	1961(1)	-173(1)	1855(1)	71(1)
H(11A)	4879	2921	2112	67

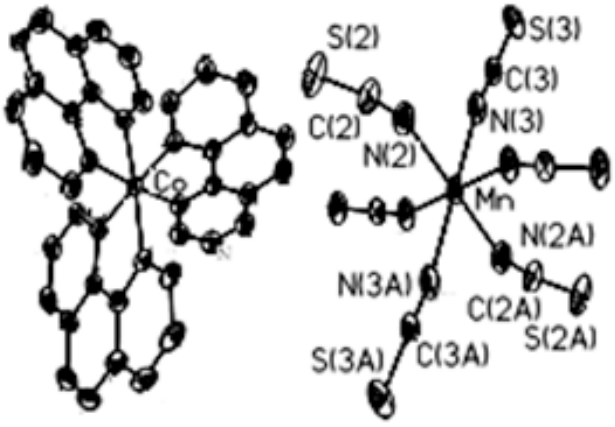

Fig. 1. Molecular structure of $[phen_2Co]_2{\cdot}Mn(SCN)_6{\cdot}4H_2O$

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

Bond	Length	Angle	(º)	Angle	(º)
Co-N(11)	1.958(2)	N(11)-Co-N(12)	71.0(5)	N(1)-Mn-N(2)	93.23(15)
Mn-N(1)	2.248(4)	N(21)-Co-N(12)	88.12(13)	N(3)-Mn-N(1)	88.93(14)
N(1)-C(1)	1.157(5)	N(31)-Co-N(11)	95.05(13)	C(11)-N(11)-Co	129.2(3)
S(1)-C(1)	1.630(4)	N(32)-Co-N(12)	95.16(13))	N(1)-C(1)-S(1)	179.4(4)
N(11)-C(11)	1.325(5)	N(21)-Co-N(11)	93.86(13)	C(1)-N(1)-Mn	159.8(4)

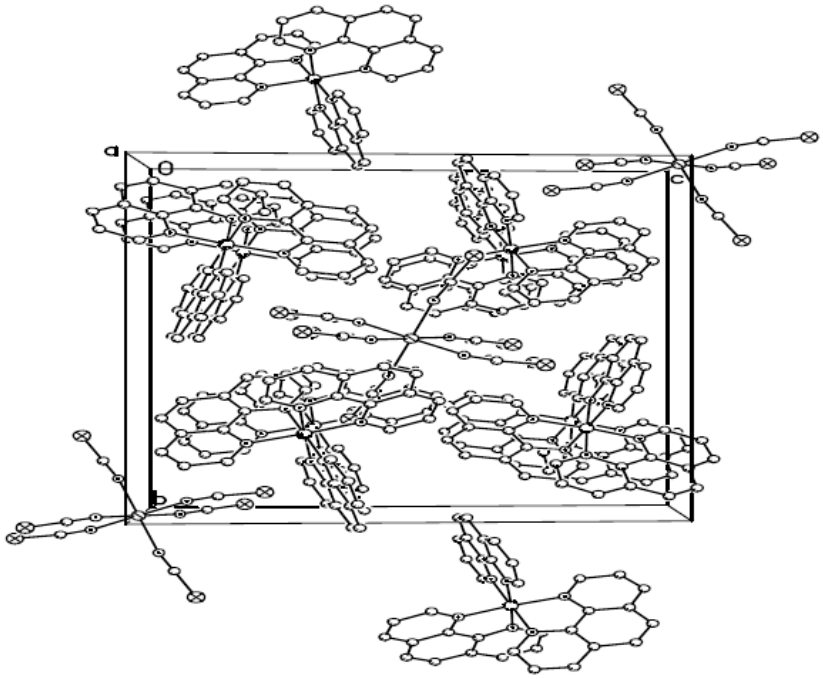

Fig. 2. Packing diagram of $[phen_2Co]_2{\cdot}Mn(SCN)_6{\cdot}4H_2O$

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