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NOTE

X-ray Single-Crystal Structure of Phenanthroline Manganese(II) Complex

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A new manganese(II) complex with molecular formula $C_{24}H_{32}N_4O_{12}SMn$ was synthesized and characterized by IR spectra and single-crystal X-ray. The crystal is triclinic, space group P-1 with unit cell parameters: a = 10.1775(12) Å, b = 12.2027(13) Å, c = 13.3829(15) Å, α = 109.329(2)°, β = 91.8970(10)°, γ = 110.846(2)°, V = 1444.1(3) Å^3, Z = 2, Mr = 655.54, Dc = 1.508 Mg/cm^3, μ = 0.598 mm^{-1}, F(000) = 682, T = 293(2) K, R = 0.0414, wR = 0.1000 for 7359 reflections with I > 2σ(I). The crystal structure analysis shows that manganese(II) is six coordinated in a slightly distorted octahedron environment.

Keywords: Manganese(II) complex, Single-crystal structure.

The metal complexes containing 1,10-phenanthroline (phen) have a lot of applications in chemistry, such as diversity of molecular structures, magnetism, catalytic and biological activities[1-4]. In an effort to bring these research areas, recently, in our laboratory, a series of metal complexes of phen have been synthesized and studied[5-8]. In this paper, we reported the synthesis and crystal structure of manganese (II) complex $[phen_2Mn(H_2O)_2]\cdot SO_4\cdot 6H_2O$.

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 diffracto-meter.

Synthesis: An aqueous solution (10 mL) of $MnSO_4$ (5 mmol) was respectively added to a mixed solution (20 mL) of 1,10-phenanthroline (10 mmol) and (10 mmol) sodium benzoate. Well-shaped yellow diamond single crystals grew within 2 weeks and were isolated in about a 36 % yield. IR spectrum (KBr, ν_{max}, cm^{-1}): 3552-3045, 1637, 1581, 1506, 1413, 1120, 847, 719, 621.

Crystal structure determination: A single crystal (0.45 mm × 0.40 mm × 0.37 mm) was selected for crystallographic data collection at 298(2) K and structure determinated with graphite monochromatic MoK$_\alpha$ radiation (λ = 0.71073 Å). A total of 7359 reflections were collected in the range of 2.94° ≤ θ ≤ 25.02°, of which 4989 reflections were unique with R_{int} = 0.0212 and R = 0.0414 and wR = 0.1000, where w = 1/[$s^2(F_0^2)$ + (0.0537 P)^2 + 0.6796 P], P = (F_0^2 + 2F_0^2)/3. The maximum and minimum peaks on the final difference fourier map are corresponding to 0.380 and -0.376 e/Å^3 (CCDC No. 985898), 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 $[phen_2Mn(H_2O)_2]\cdot SO_4\cdot 6H_2O$. Fig. 2 shows a perspective view of the crystal packing in the unit cell. From the Fig. 1, it is easy to see that the manganese(II) ion is six-coordinated with four nitrogen atoms of the two phen ligands and two oxygen atoms of the two coordinated water molecules.

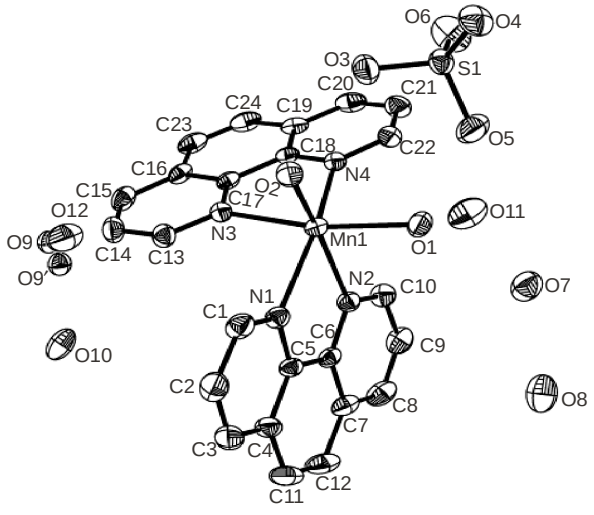

Fig. 1. Molecular structure of the complex $[phen_2Mn(H_2O)_2]\cdot SO_4\cdot 6H_2O$

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

Atom	X	Y	Z	U(eq)
Mn(1)	2467(1)	5620(1)	2540(1)	33(1)
N(1)	988(3)	4414(2)	3332(2)	38(1)
N(2)	3728(3)	6062(2)	4160(2)	37(1)
O(1)	2269(2)	7416(2)	3274(2)	51(1)
O(2)	784(2)	5162(2)	1315(2)	48(1)
S(1)	1326(1)	8180(1)	971(1)	42(1)
O(3)	767(3)	6819(2)	434(2)	60(1)
O(4)	433(3)	8688(2)	565(2)	65(1)

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

Bond	Length	Bond	Length
Mn(1)-N(1)	2.261(2)	Mn(1)-N(4)	2.249(2)
Mn(1)-N(2)	2.277(2)	Mn(1)-O(1)	2.170(2)
Mn(1)-N(3)	2.274(2)	Mn(1)-O(2)	2.112(2)
Angle	(°)	Angle	(°)
N(1)-Mn(1)-N(2)	73.52(9)	O(1)-Mn(1)-N(1)	102.32(9)
N(1)-Mn(1)-N(3)	90.97(9)	O(1)-Mn(1)-N(3)	166.44(9)
N(3)-Mn(1)-N(2)	94.97(9)	O(1)-Mn(1)-N(2)	86.34(9)
N(4)-Mn(1)-N(2)	89.92(9)	O(2)-Mn(1)-O(1)	87.22(8)
N(4)-Mn(1)-N(3)	73.50(9)	O(2)-Mn(1)-N(4)	106.82(9)
O(1)-Mn(1)-N(4)	93.03(9)	O(2)-Mn(1)-N(1)	91.88(9)

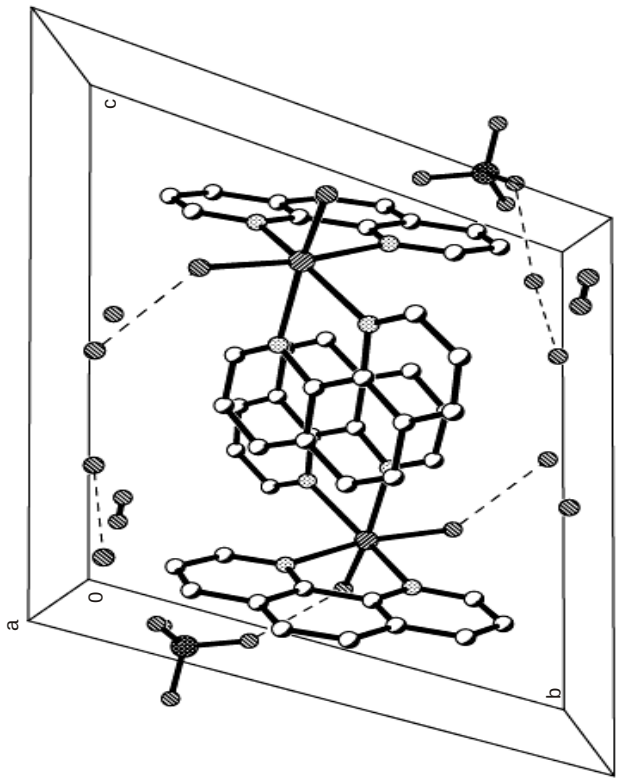

Fig. 2. Molecular packing arrangement in the unit cell

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