Study on novel structure of Mn complex, $C_{24}H_{18}CrMnN_4O_5$

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Abstract. The novel Mn complex $C_{24}H_{18}CrMnN_4O_5$ was investigated by hydrothermal and its crystal structure was characterized using X-ray diffraction technology. The Mn atom is six coordinated by four N atom from two 1,10-phenanthroline and two O atoms from CrO_4^-. The hydrogen bonding O-H...O had central effect for crystal stability.

1 Introduction

The diversity of metal-organic coordination structures will have certain advantages in photochemistry, catalysis, absorptivity, biological properties, magnetism and electrical properties [1-3]. Because manganese (II) complexes often exist in the center of the activity of enzymes (superoxide dismutase, peroxidase, aminopeptidase, sialyl and fucosyl transferase), the investigation of manganese (II) complexes is a very meaningful work [4-7]. The Mn (II) biological activity may be related to the interaction of carboxylate ligands and manganese. The carboxylate ligands are easy to form binuclear, trinuclear and high nuclear compounds [8]. 1,10-phenanthroline is major chelating agent for the formation of various supramolecular structures. Yang Hongli et al [9] synthesized two silver and cadmium compounds of Ag(1,2,4-benzenetricarboxylic acid)(2,2'-bipyridine) and Cd(1,2,4-benzenetricarboxylic acid)(2,2'-bipyridine)$(H_2O)_2]_n$ by hydrothermal and studied their structure and property by X-ray single crystal diffraction, thermal gravimetric analysis, IR spectra and fluorescence spectroscopy. The three Co metal-organic frameworks compounds ([Co(2,6-di(1H-imidazol-1-yl)naphthalene)(5-aminoisophthalic acid)]·2DMF, [Co(2,6-di(1H-imidazol-1-yl)naphthalene)(5-aminoisophthalic acid)]·DMF, [Co(2,6-di(1H-imidazol-1-yl)naphthalene)(4,4'-iminodibenzoic acid)$(H_2O)_2$]·0.5(2,6-di(1H-imidazol-1-yl)naphthalene)·H_2O) were synthesized by Liu et al [10] using solvothermal method. The compounds were analysized again with powder X-ray diffraction analyses, infrared spectra, single-crystal and elemental analyses. Zhang Li et al [11] explored new cobalt compound [Co(pyridine-2,6-dicarboxylic acid)(2,2′-bipyridine)Cl]·C_2H_5OH using hydrothermal condition and characterized by X-ray single crystal diffraction and infrared spectroscopy. The material charge distribution, electrostatic potential and relevant electronic properties were analyzed by density functional theory calculations method. In this paper, the novel Mn complex is reported.

2 Experimental

The mixture of $MnSO_4$ (0.1 mmol, 0.015g), 1,10-phenanthroline (0.1mmol, 0.02g), K_2CrO_4 (0.1mmol, 0.02g) and $Na_2B_4O_710H_2O$ (0.1mmol, 0.04g) were added into 10 mL water (containing methanol(4/10, v/v)) with heated for 8h at 414K. The solution was obtained by filtration after cooling the reaction to room temperature. Black block single crystals was got for X-ray analysis after weeks.

3 Results and discussions

Fig.1 is novel compound crystal sketch map. It composed of Mn cation, 1,10-phenanthroline, chromate anion and water molecular. The Table 1 lists the crystal compound refinement data. The Mn atom is six coordinated by four N atom from two 1,10-phenanthroline and two O atoms from CrO_4^-. The bond lengths d(Mn-N) are in the range of 2.266-2.355 Å. The d(Mn-O) are 2.067 and 2.108 Å. The bond angles of O1-Mn1-O2#, O1-Mn1-N2, N1-Mn1-N3 are 90.1, 94.5, 88.7°, respectively. The torsion angles of O2#-Mn1-O1-Cr1, N3-Mn1-O1-Cr1, O4-Cr1-O1-Mn1 are 38.4, 129.5, 78.3°, respectively. The Table 2 lists the section bond lengths and angles.
The crystal packing is stabilized by hydrogen bond interaction.

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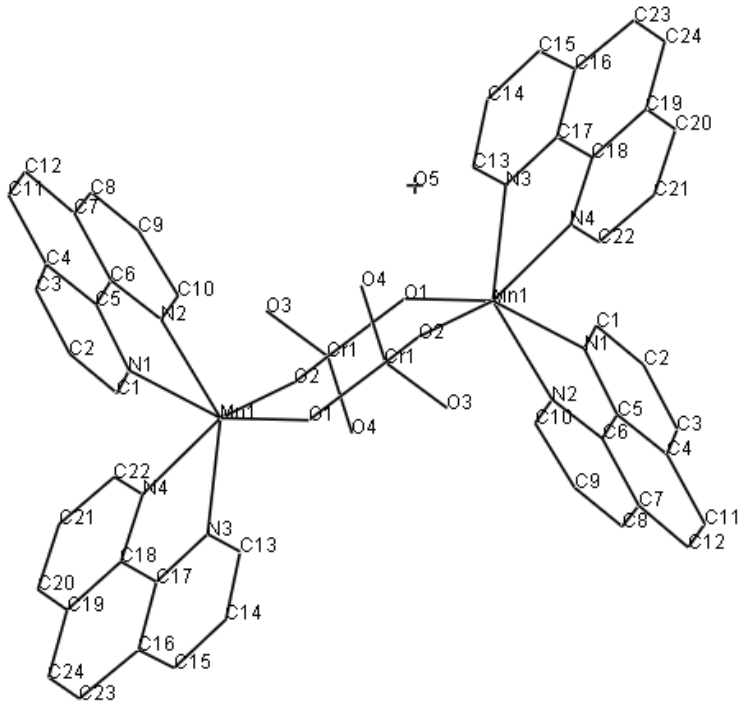

Fig.1 The crystal structure of $C_{24}H_{18}CrMnN_4O_5$

Table 1. Crystal compound refinement data

Empirical formula	$C_{24}H_{18}CrMnN_4O_5$
Weight	549.36
T	293(2) K
λ	0.71073 Å
System, group	Monoclinic, P2(1)/c
Cell	a = 9.3421(19) Å alpha = 90°.
	b = 13.021(3) Å beta = 93.388(3)°.
	c = 18.543(4) Å gamma = 90°.
Volume	2251.7(8) $Å^3$
Z, density	4, 1.621 Mg/m^3
Absorpting number	1.089 mm^{-1}
F	1116
Size	0.38 x 0.35 x 0.32 mm
Collecting range	3.01 to 25.01°.
Limiting indices	-10<=h<=11, -15<=k<=15, -22<=l<=22
Reflection collected (unique)	16157 / 3935 [R(int) = 0.1766]
Completeness to theta(25.02)	99.2 %
Correcting correction	Semi-empirical from equivalents
Transmissing	0.7220 and 0.6824
Refining	Full-matrix least-squares on F^2
Data / restraints / parameters	3935 / 0 / 317
GoF	1.285
Final R indices [I>2sigma(I)]	R1 = 0.1624, wR2 = 0.3920
R indices (all data)	R1 = 0.2515, wR2 = 0.4412
Extinction coefficient	0.007(4)
Largest diff. peak and hole	2.849 and -1.016 e.$Å^{-3}$

Table 2. The section bond lengths and angles ([Å], [°])

Mn(1)-O(1)	2.067(10)
Mn(1)-N(2)	2.266(13)
Mn(1)-N(3)	2.299(13)
Mn(1)-N(1)	2.344(12)
Mn(1)-N(4)	2.355(14)
Cr(1)-O(3)	1.580(10)

Cr(1)-O(4)	1.636(12)
Cr(1)-O(2)	1.651(11)
Cr(1)-O(1)	1.717(10)
N(1)-C(1)	1.36(2)
N(1)-C(5)	1.37(2)
O(2)-Mn(1)#1	2.108(11)
O(1)-Mn(1)-O(2)#1	90.1(4)
O(1)-Mn(1)-N(2)	94.5(5)
O(2)#1-Mn(1)-N(2)	111.8(4)
O(1)-Mn(1)-N(3)	110.2(4)
O(2)#1-Mn(1)-N(3)	90.9(5)
N(2)-Mn(1)-N(3)	146.6(4)
O(1)-Mn(1)-N(1)	159.9(4)
O(2)#1-Mn(1)-N(1)	82.6(4)
N(2)-Mn(1)-N(1)	71.2(5)
N(3)-Mn(1)-N(1)	88.7(5)
O(1)-Mn(1)-N(4)	93.3(4)
O(2)#1-Mn(1)-N(4)	162.1(5)
N(2)-Mn(1)-N(4)	85.4(5)
N(3)-Mn(1)-N(4)	71.4(5)
N(1)-Mn(1)-N(4)	99.3(4)
O(3)-Cr(1)-O(4)	111.1(8)
O(3)-Cr(1)-O(2)	110.7(6)
O(4)-Cr(1)-O(2)	107.5(7)
O(3)-Cr(1)-O(1)	108.3(5)
O(4)-Cr(1)-O(1)	110.9(6)
O(2)-Cr(1)-O(1)	108.3(5)
C(1)-N(1)-C(5)	118.2(13)
C(1)-N(1)-Mn(1)	126.4(10)
C(5)-N(1)-Mn(1)	114.1(11)
C(6)-N(2)-C(10)	119.9(14)
C(6)-N(2)-Mn(1)	117.2(11)
C(10)-N(2)-Mn(1)	122.7(10)
C(17)-N(3)-C(13)	117.1(14)
C(17)-N(3)-Mn(1)	118.6(11)
C(13)-N(3)-Mn(1)	123.3(10)
C(22)-N(4)-C(18)	118.8(14)
C(22)-N(4)-Mn(1)	126.7(11)
C(18)-N(4)-Mn(1)	114.2(12)
Cr(1)-O(1)-Mn(1)	132.8(5)
Cr(1)-O(2)-Mn(1)#1	161.2(6)

4 Conclusions

The novel Mn complex $C_{24}H_{18}CrMnN_4O_5$ was investigated by hydrothermal and its crystal structure was characterized using X-ray diffraction technology.

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