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Coordination polymer of Mn(II) based on triazol-ligand: Synthesis and crystal structure

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ABSTRACT

One new Mn(II) complex: $\{[MnL_2(H_2O)_2](BF_4)_2(CH_3COCH_3)_2\}_8$ [L = 2,3-bis(triazol-1-ylmethyl)quinoxaline] was prepared and structurally characterized. Single crystal X-ray diffraction analysis showed that the Mn(II) lies in distorted octahedron coordination geometry. Crystal data: Monoclinic, space group C2/c, α=32.905(7) Å, b=8.2749(17) Å, c=18.458(4) Å, β=118.53(3)°, V=4415.5(16) Å^3, Z=4, D=1.455 Mg·m^{-3}. © 2008 Trade Science Inc. - INDIA

KEYWORDS

Self-assembly;
Single crystal;
Mn(II) complex.

INTRODUCTION

The ration design and synthesis of novel coordination polymers have drawn much attention in the past decade, the motivation arising because of their intriguing topologies and their potential applications[1-2]. The structures of the coordination polymers are mainly dependent on the structure of organic ligand and the coordination geometry of metal ions, other factors such as the counterion, the solvent, and the reaction temperature can also affect the process of self-assembly[3]. Therefore, it is still a great challenge to design the exact structure for different systems, and systematic research is needed for understanding the roles of different factors. In contrast to the rigid ligands that show little or no conformational changes when they react with metal salts, the flexible ligands have many more possible coordination modes due to their flexibility and they can adopt different conformations according to the geometric requirements of different metal ions. More coordination architectures based on flexible ligands with interesting structures and properties have been reported in the recent years, especially those containing N-donor ligands. A series of imidazol-containing ligand have been synthesized, and their complexes have been studied by Sun and other researchers[4]. Su have reported the coordination networks based on the benzimidazol-containing ligands[5]. Hou and Li have reported a flexible ligand [1,4-bis(trizol-1-ylmethyl)benzene], the interesting structures and properties of the complexes have also been studied[6]. In order to explore the influence of ligand on the crystal structure, in the present work, one new complex: $\{[MnL_2(H_2O)_2](BF_4)_2(CH_3COCH_3)_2\}\infty$ [L = 2,3-bis(triazol-1-ylmethyl)quinoxaline] was synthesized and characterized.

EXPERIMENTAL

1. Synthesis of $\{[MnL_2(H_2O)_2](BF_4)_2(CH_3COCH_3)_2\}\infty$

L was synthesized by a modified procedure of the literature[4a]. A buffer layer of acetone and chloroform (4 mL, 1:1) was carefully layered over a chloroform (4 mL) solution of ligand (0.05 mmol). Then a acetone solution of $Mn(BF_4)_2$ (4 mL, 0.02 mmol) was layered over the buffer layer. After several weeks, colorless block crystals were obtained in 20% yield.

2. Structure determation

X-ray single-crystal diffraction data for the com-

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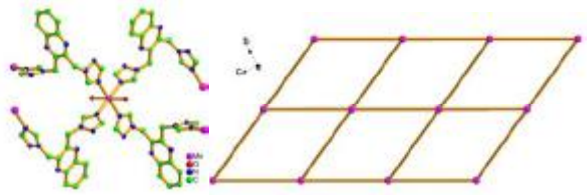

Figure 1: View of (a) the coordination environment of Mn (II); (b) 2D (4,4) grid

TABLE 1: Crystallographic data and structure refinement summary for the complex

Formula	$C_{34}H_{42}B_2F_8MnN_{16}O_4$		
Formula weight	967.40	V / Å^3	4415.5(16)
Crystal system	Monoclinic	Z	4
Space group	C2/c	D / g cm^{-3}	1.455
a (Å)	32.905(7)	μ / mm^{-1}	0.390
b (Å)	8.2749(17)	T / K	293(2)
c (Å)	18.458(4)	R(I>2σ)/wR(all data)	0.0699/0.2244
β / deg	118.53(3)	Total/unique/R_{int}	16818/4041/ 0.0857

TABLE 2 : Selected bond distances (Å) and angles (deg) for the complex

Mn(1)-O(13)	2.226(3)	Mn(1)-N(8)	2.229(4)
Mn(1)-N(1)	2.264(4)		
O(13)-Mn(1)-N(8)	88.00(14)	O(13)#1-Mn(1)-N(8)	92.00(14)
O(13)#1-Mn(1)-N(1)#1	91.09(14)	O(13)-Mn(1)-N(1)#1	88.91(14)
N(8)-Mn(1)-N(1)#1	92.34(14)	N(8)-Mn(1)-N(1)	87.66(14)
Symmetry codes: #1 -x+1/2,-y+1/2,-z+1			

plex was collected on a Bruker Smart 1000 CCD diffractometer at 293(2) K with Mo-*Kα* radiation (λ = 0.71073 Å) by ω scan mode. The program SAINT[7] was used for integration of the diffraction profiles. Semiempirical absorption corrections were applied using SADABS program. All the structures were solved by direct methods using the SHELXS program of the SHELXTL package and refined by full-matrix least-squares methods with SHELXL[8] Metal atoms in each complex were located from the E-maps and other non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on F^2. Hydrogen atoms of carbon were included in calculated positions and refined with fixed thermal parameters riding on their parent atoms. Crystallographic data and experimental details for structural analysis are summarized in TABLE 1. Selected bond lengths and angles are listed in TABLE 2.

RESULTS AND DISCUSSION

The compound was obtained as colorless block crystals by self-assembly of the organic ligand and the $Mn(BF_4)_2$ in the chloroform-cetone solvent system after several weeks days. Single-crystal analysis reveals that the complex is a coordination polymer with (4,4) topology (Figure 1b). As shown in figure 1a, the mental center adopts a distorted octahedron coordinate geometry, which coordinates to four N donors of four different L ligands, two O atoms of water molecules. The distance of Mn-N are 2.229(4) and 2.264(4) Å, the distance of and the distance of Mn–O is 2.226(3) Å,the angles around Mn(II) are between 87.66(14) and 92.34(14)°, all the distances and angles are in the normal range. In the complex, each metal center bridges four L ligands and each L Ligand coordinate to two metal ions, the whole molecular forms a 2D coordination network.

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