بررسی ساختار بلوری پلیمر $[Co(dipic)_2MnO_2]_n$

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چکیده :

ساختار بلوری پلیمر $[Co(dipic)_2MnO_2]_n$ که dipic عبارت است از لیگاند ۲و۶-پیریدین دی کربوکسیلیک اسید، به وسیله روش کریستالو گرافی X-Ray مورد شناسایی قرار گرفت. بلورهای قرمز این پلیمر که مناسب برای کریستالوگرافی بوده اند از واکنش نیترات منگنز (II)، نیترات کبالت (II) در حضور نیترات اهن (III) به عنوان کاتالیزور بدست امد. داده های X-Ray در دمای K (2) 200 مورد پردازش قرار گرفت. سیستم بلوری این پلیمر منوکلینیک بوده و گروه فضایی ان Cc می باشد. در این پلیمر Co(II) دارای عدد کوردیناسیون ٦ است و به دو لیگاند دایپیک که هر کدام به صورت لیگاند سه دندانه عمل می کنند کوئوردینه شده و منگنز (II) دارای عدد کئوردیناسیون ٤ می باشد و به چهار پل اکسو متعلق به گروههای دایپیک کوئوردینه شده به چهار Co(II) متصل است. مقادیر ابعاد سلول واحد این پلیمر به صورت مقادیر زیر است.

a (A^o) =14.948(3)	α (^{o}) = 90
b (A^o) = 12.460(3)	β (^{o}) = 93.18(3)
c. (A^o) = 8.6697(17)	λ (^{o})=90

کلمات کلیدی: ساختار بلوری، پلیمر دو هسته ای، سیستم بلوری منوکلینیک:

Crystal Structure of New Supramolecular Polymer $[Co(dipic)_2MnO_2]_n$

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Abstract

The crystal structure of $[Co(dipic)_2Mn(O)_2]_n$, where dipic is Pyridine-2,6-dicarboxylic acid, was characterized using single-crystal X-ray diffraction method, (SC-XRD). The red crystals of this polymer, which are suitable for X-ray crystallography, was synthesized via simple mixing of precursors. This polymer has a monoclinic crystal system (Z=4) and space group of Cc with a = 14.948(3) *Å*, b =12.460(3) *Å*, c = 8.6697(17) *Å*, β = 93.18(3) °, and V= 1612.3(6)Å3.

Keywords: Crystal structure, Binuclear polymer, Monoclinic crystal system

1. Introduction

Pyridine-2,6-dicarboxylic acid (dipicolinic acid, H_2dipic) is a water-soluble, commercially available, cheap and versatile N,O-chelator possessing diverse coordination modes [1], with a recognized biological function in the body metabolism, namely as a major component of bacterial spores [2, 3], and in a variety of processes as an enzyme inhibitor [4–6], plant preservative [7], food sanitizer [8], etc. Although a high number of dipicolinate complexes of almost all transition metals is known [9], heterometallic complexes with this ligand are rather scant and appear to be limited to only a few examples based on lanthanide metals i.e. La/(Eu, Cr or Co) and Y/(Cr or Co) species. Some composite crystals comprising mixtures of different 3d metal dipicolinate complexes located in separated regions of the crystals have also been reported.

2. Experimental

In this study, we report the synthesis and crystal structure of $[Co(dipic)_2Mn(O)_2]_n$, where dipic is Pyridine-2,6-dicarboxylic acid. The X-ray data were collected on an STOE-IPDS 2T diffractometer, equipped with a graphite monochromator and thus Mo K_α radiation (λ=0.71073) was used. The reaction of pyridine-2,6-dicarboxylic acid as ligand and aqueous solution of NaOH with cobalt (II) nitrate hexahydrate and manganese (II) nitrate tetrahydrate results in the formation of $[Co(dipic)_2Mn(O)_2]_n$. In

this study role Fe is catalyst and association for nuclear Co and Mn for preparation polymer structure. The single crystals of this polymer that suitable for X-ray crystallography, were synthesized by reflux approach.

3. Result and Discussion

The Crystallography data collections and structure refinement are listed in Table 1. Bond lengths, bond angles are listed in Table 2. Figure. 1 shows the ORTEP diagram of unit part of $[Co(dipic)_2Mn(O)_2]_n$. The X-ray single crystal, showed that in the structure of polymer $[Co(dipic)_2Mn(O)_2]_n$, the Mn^{II} ion is tetra-coordination with four μ-carboxylate oxygen O from $[Co(dipic)_2]^{2-}$. The cobalt ion in $[Co(dipic)_2]^{2-}$ achieves six-coordination by coordinating with two deprotonated dipicolinate groups, acting as tridentate chelating ligands. The title polymer, crystallized in the monoclinic space group Cc.

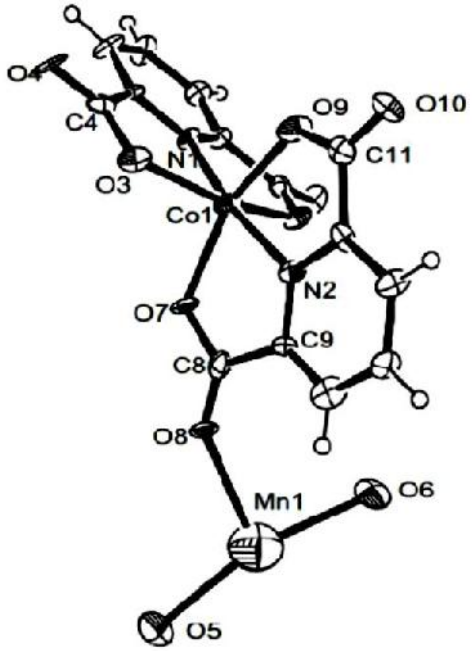

Fig. 1.ORTEP representation of unit part $[Co(dipic)_2MnO_2]_n$ polymer

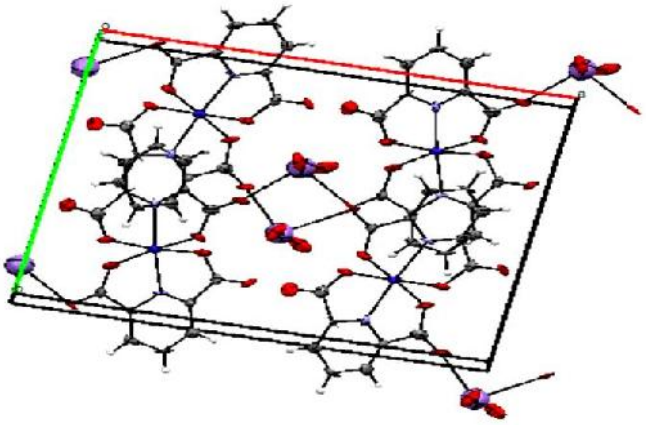

Fig. 2. Unit cell of $[Co(dipic)_2MnO_2]_n$

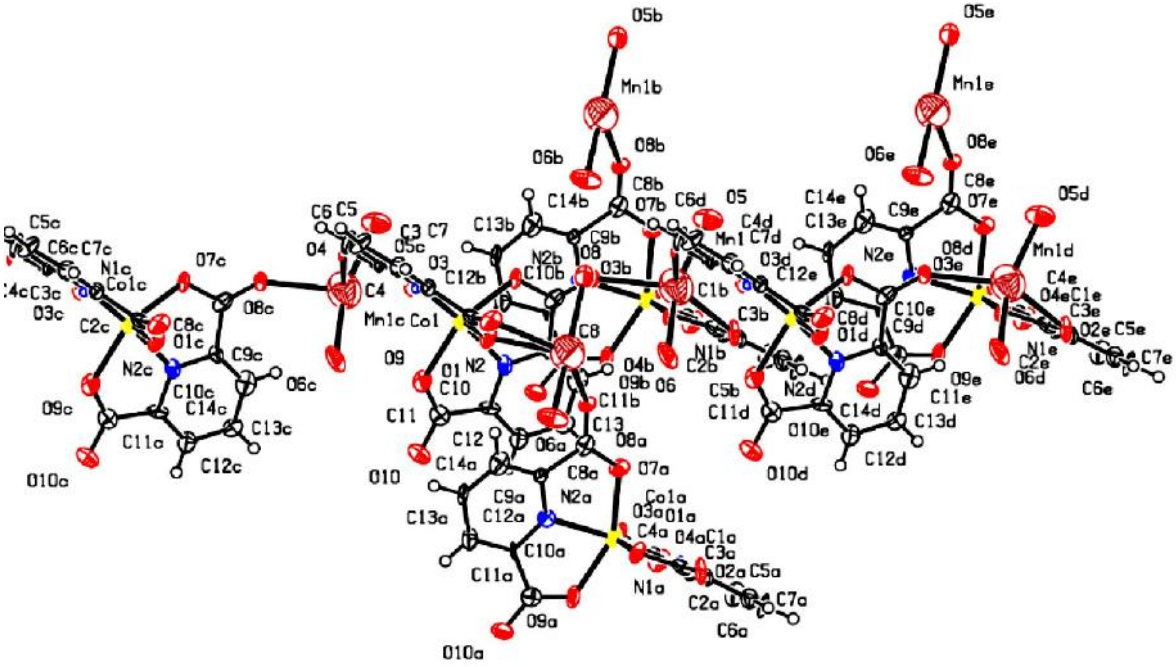

Fig. 3. A fragment of the environmental of $[Co(dipic)_2MnO_2]_n$

Table 1
Cystallographic data and data-collection parameters for $[Co(dipic)_2Mn(O)_2]_n$

Formula	$C_{14}\ H_6\ Co\ Mn\ N_2O_{10}$
Formula weight	476.03
Temperature (K)	293
Wavelength (A°)	0.71073
Crystal system	Monoclinic
Space group	Cc
a (A°)	14.948(3)
b (A°)	12.460(3)
c. (A°)	8.6697(17)
α (°)	90
β (°)	93.18(3)
λ (°)	90
V (A°)	1612.3(6)
Z	4
ρ_{calc} (g/m^3)	1.957
μ(Mo Kα) (mm^{-1})	2.011
F(000)	944
Theta range for data collection	2.7, 25.0
R(int)	0000
R_1, wR2	0.1157, 0.3086

Table 2
Selected bond lengths (A°) and angles (°)for $[Co(dipic)_2Mn(O)_2]_n$

Bond lengths		Bond lengths	
Co(1) –O(1)	2.035(16)	Co(1) –O(3)	2.016(13)
Co(1) –O(7)	2.014(13)	Co(1) –O(9)	2.040(17)
Co(1) –N(1)	2.051(12)	Co(1) –N(2)	2.078(15)
Mn(1) –O(5)	2.338(18)	Mn(1) –O(6)	2.366(18)
Mn(1) –O(2)_b	2.486(15)	Mn(1) –O(4)_d	2.454(15)
Bond angles		Bond angles	
O(1) –Co(1) –O(9)	95.6(6)	O(1) –Co(1) –N(1)	75.7(5)
O(1) –Co(1) -N(2)	93.4(5)	O(3) –Co(1) –O(7)	95.4(5)
O(5) –Mn(1) –O(8)	105.6(6)	O(1)_b –Mn(1) –O(5)	81.4(6
O(2)_b –Mn(1) –O(5)	86.5(6)	O(40_d –Mn(1) –O(5)	89.3(6)
O6 -Mn1 –O(8)	91.6(6)	O(1)_b –Mn(1) –O(6)	106.7(6
O(2)_b –Mn(1) –O(6)	86.3(6)	O(4)_d –Mn(1) –O(6)	84.5(6)
O(1)_b –Mn(1) –O(8)	84.1(5)	O(2)_b –Mn(1) –O(8)	131.9(6)
O(4)_d –Mn(1) –O(8)	90.7(5)	O(1)_b –Mn(1) –O(2)_b	51.2(4)

4. Conclusion

A new polymer of $[Co(dipic)_2Mn(O)_2]_n$, was synthesized using reflux method. The Crystalline structure was characterized using single-crystal X-ray diffraction. The crystalline structure of this compound was found to be a hetero binuclear coordination compound and shows that the coordination number for Mn(II) ion is four and for Co (II) center is six. In this structure cationic part was formed by a tetra-coordinated Mn center with four μ-carboxylate oxygen O from the anionic part Co $(dipic)_2^{-2}$. The cobalt ion achieves hexa-coordination by coordinating with to deprotonated dipicolinate groups, which acting as tridentate chelating ligands.

Acknowledgements

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References

[1] Chatterjee M., Maji M., Ghosh S.,and Mak T.C.W., 2000. *J. Chem. Soc., Dalton Trans*, 3641.
[2] Douki T., Setlow B., and Setlow P., 2005. *Photochem. Photobiol. Sci*, 4 , 591.
[3] Slieman T.A., and W.L. Nicholson., 2001. *Appl. Environ, Microbiol*, 67, 1274.
[4] K. Murakami., Y. Tanemura., and M. Yoshino., 2003. *J. Nutr. Biochem*, 14, 99.
[5] Couper L., Mckendrick J.E., Robins D.J., and Chrystal E.J.T., 1994. *Bioorg. Med. Chem. Lett*, 4 , 2267.
[6]. Griggs D.L., Hedden P., Templesmith K.E., and Rademacher W., 1991. *Phytochemistry*, 30, 2513.
[7] Kazuhiro Y., Noriko Y., and Tadayasu F., 1994. *Europ. Patent*, EP0603165.
[8] Burdock G.A., 1996. *Encyclopedia of Food and Color Additives*, vol. 3, CRC Press.
[9]. Allen F.H., 2002. *Acta Crystallogr*,B58 , 380.