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ORIGINAL RESEARCH PAPER

SYNTHESIS, CRYSTAL STRUCTURE OF A NOVEL 1D CHAINED Na(I) COORDINATION POLYMER MATERIALS BASED ON SCHIFF-BASE LIGAND

Li-Hua Wang

College of Information and Engineering, Weifang University, Weifang 261061, P. R. China

*Corresponding author: wanglihua929@163.com

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Abstract: A novel 1D chained Na(I) coordination polymer materials has been obtained by reaction of 2-hydrazinobenzoic acid with 2-formyl-benzenesulfonic acid sodium salt in CH_3CH_2OH/H_2O. It was characterized X-ray single crystal diffraction analysis. The crystal of the Na(I) coordination polymer belongs to triclinic, space group *P-1* with a = 6.0354(12) Å, b = 8.1922(16) Å, c = 18.729(4) Å, α = 93.70(3)º, β = 95.68(3)º, γ = 97.03(3)º, V = 911.8(3) Å^3, Z = 2, Dc = 1.444 μg·m^{-3}, μ= 0.245 mm^{-1}, F(000)= 412, and final R_1 = 0.0833, ωR_2 = 0.2867. X-ray analysis reveals that each Na(I) center is six-coordination with a O_6 distorted octahedron coordination environment. The Na(I) ions are linked through the O atoms of sodium 2-{(*E*)-[2-(2-carboxyphenyl) hydrazinylidene]methyl}benzenesulfonate to form 1D chain coordination polymer.

Keywords: *sodium 2-{(E)-[2-(2-carboxyphenyl)hydrazinylidene] methyl}benzenesulfonate, Na(I) coordination polymer, structural characterization, synthesis*

INTRODUCTION

Investigating on the inorganic-organic hybrid materials with carboxylate ligands have gained considerable attention during the last decade due to their attractive structures and promising potential applications for catalysis, gas storage, magnetic, luminescence materials [1-9]. Structural studies have shown that the organic ligands containing multi-oxygen atoms can coordinate with metal ions in different ways, resulting in the formations of various metal-organic frameworks with specific topologies and useful properties [10-17]. We have been exploring the preparation of inorganic-organic hybrid materials by combining metal ions and organic ligands containing multi-oxygen atoms. In this paper, A novel 1D chained Na(I) coordination polymer has been obtained and characterized by X-ray single crystal diffraction analysis.

EXPERIMENTAL

Materials and methods

The following A. R. grade chemicals and other solvents were used for the preparation of the studied compound without further purifications: 2-hydrazinobenzoic acid, 2-formyl-benzenesulfonic acid sodium salt. The crystal data was collected on a Bruker smart CCD Area Detector.

Synthesis of the Na(I) coordination polymer

1.0 mmol (0.152 g) of 2-hydrazinobenzoic acid and 1.0 mmol (0.2081 g) of 2-formyl-benzenesulfonic acid sodium salt were added to the 15 mL of CH_3OH/H_2O (v:v = 2:1) solution. The mixture was continuously stirred for 3 h at refluxing temperature. The mixture was cooled at room temperature, and was collected by filtration. By evaporation in air at room temperature, the single crystal suitable for X-ray determination was obtained from methanol solution after several days. Yield: 56%.

X-ray Crystallography

A colourless block single crystal with dimensions of 0.24 mm×0.22 mm×0.20 mm was selected for measurement. Diffraction data of the single crystal were collected by φ~ω scan mode using a graphite-monochromatic Mo Kα radiation (λ = 0.71073 Å) at 293 (2) K on a Bruker Smart Apex CCD diffractometer. A total of 8756 reflections were collected in the range 3.20-27.48°, of which 4152 were unique (Rint = 0.0408) and 3165 were observed with I>2σ(I). The data were corrected for Lp factors. The structure was solved by direct methods and refined by full-matrix least-squares techniques on F2. The structure was solved by direct methods [18] using SHELXL-97 and expanded using Fourier techniques. All of the non-hydrogen atoms and hydrogen atoms were refined anisotropically and isotropically, respectively. The final refinement by full-matrix least squares method was converged at R = 0.0833, and wR = 0.2867 (w = 1/[δ2(Fo2)+(0.1358P)2+2.1280P], P = (Fo2+2Fc2)/3, S = 1.102, (Δ/σ)max = 0.000). The largest peak in the final difference Fourier map is 0.844 $e \cdot Å^{-3}$ and the minimum peak is –0.500 $e \cdot Å^{-3}$. Molecular graphics were drawn with the program package

SHELXTL-97 crystallographic software package [19]. The most relevant crystal data for complex are quoted in Table 1, and the selected bond distances and angles are listed in Table 2.

Table 1. *Crystallographic data for Na(I) coordination polymer*

Formula	$C_{14}H_{17}N_2NaO_8S$
Formula weight	396.35
Cell setting, space group	Triclinic
a [Å]	P-1
b [Å]	6.0354(12)
c [Å]	8.1922(16)
β [°]	18.729(4)
Volume [Å^3]	911.8(3)
Z	2
Dc [μg m^{-3}]	1.444
μ [mm^{-1}]	0.245
Crystal size [mm]	0.24×0.22×0.20
Radiation [Å]	0.71073
Limiting indices	$-7 \leq h \leq 7$; $-10 \leq k \leq 10$; $-24 \leq l \leq 24$
Theta min–max [°]	3.20-27.48
Tot., uniq. data, R(int)	8756, 4152, 0.0408
Observed data [I > 2 sigma(I)]	3165
F (000)	412
Goodness-of-fit on F^2	1.102
R_1 [I > 2 sigma(I)]	0.0833
ωR_2 [I > 2 sigma(I)]	0.2867
R_1 (all data)	0.0947
ωR_2 (all data)	0.2917
Min. and max. resd. dens. [e·Å^{-3}]	0.844-0.500
CCDC	1008953

Table 2. *Selected bond lengths and angles for Na(I) coordination polymer*

Bond	**Distance [Å]**	**Bond**	**Distance [Å]**
S1-O1	1.446(4)	S1-O3	1.451(3)
S1-O2	1.464(4)	S1-C4	1.786(4)
O6-Na1	2.337(4)	O5-Na1	2.393(4)
O3-Na1	2.312(4)	O7-Na1	2.458(4)
N2-C7	1.261(6)	N2-N1	1.361(6)
N1-C8	1.369(6)	Na1-O8	2.498(5)
Angle	**[°]**	**Angle**	**[°]**
O3-Na1-O6	173.25(15)	O3-Na1-O5A	86.61(15)
O5A-Na1-O6	89.24(15)	O3-Na1-O7	90.31(15)
O7-Na1-O6	94.18(16)	O5A-Na1-O7	79.66(15)
O3-Na1-O8	90.32(17)	O8-Na1-O6	85.50(18)
O5A-Na1-O8	103.81(15)	O7-Na1-O8	176.51(16)
O3-Na1-O8B	99.11(17)	O8B-Na1-O6	85.57(18)
O7-Na1-O8B	94.45(16)	O8-Na1-O8B	82.06(16)
O1-S1-O3	111.6(2)	O1-S1-O2	112.8(2)
O2-S1-O3	111.0(2)		

Symmetry code: $-x+1, -y, -z$

RESULTS AND DISCUSSION

Structure Description

Perspective view of the molecule in a unit cell and molecular packing arrangement are shown in Figure 1 and Figure 2, respectively. It can be seen that the coordination environment of each Na(I) atom consists of two oxygen atoms from the two sodium 2-{(*E*)-[2-(2-carboxyphenyl)hydrazinylidene]methyl}benzenesulfonate ligands and four oxygen atoms from the four coordinated water molecules, making up a distorted octahedral environment. The coordination atoms (O5, O7, O8, O8A) are situated equatorial place, and the coordination atoms (O3, O6) are situated axial place. In the complex molecule, the organic ligand acts as bridge between two Na atoms. It is coordinated through O from sulfonate group to one Na atom and O from carboxylato group to another Na atom. Each sodium atom environment is completed by four water molecules.
The distances of the Na1-O bonds are in the range of 2.312-2.559 Å, which are similar to the Na-O bond lengths reported previously [20, 21].

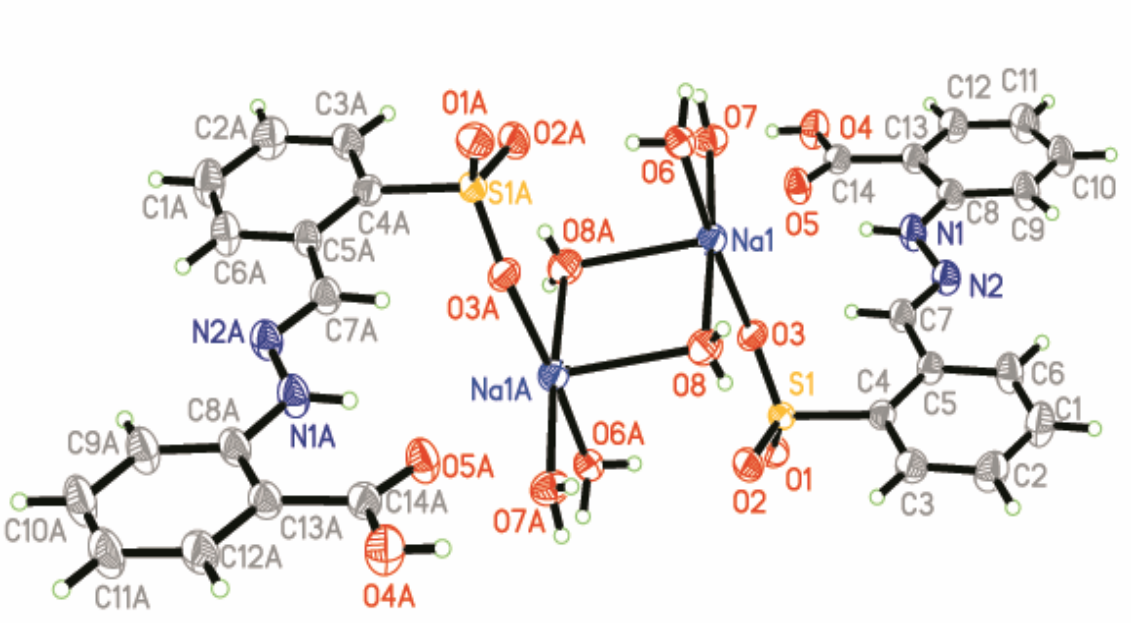

Figure 1. *Molecular structure of the Na (I) coordination polymer, where the thermal ellipsoids were drawn at 30% possibility*

The complex forms one dimensional chain coordination polymer structure by bridging oxygen atoms of sodium 2-{(*E*)-[2-(2-carboxyphenyl)hydrazinylidene]methyl} benzenesulfonate ligands and π-π stacking (Figure 3).

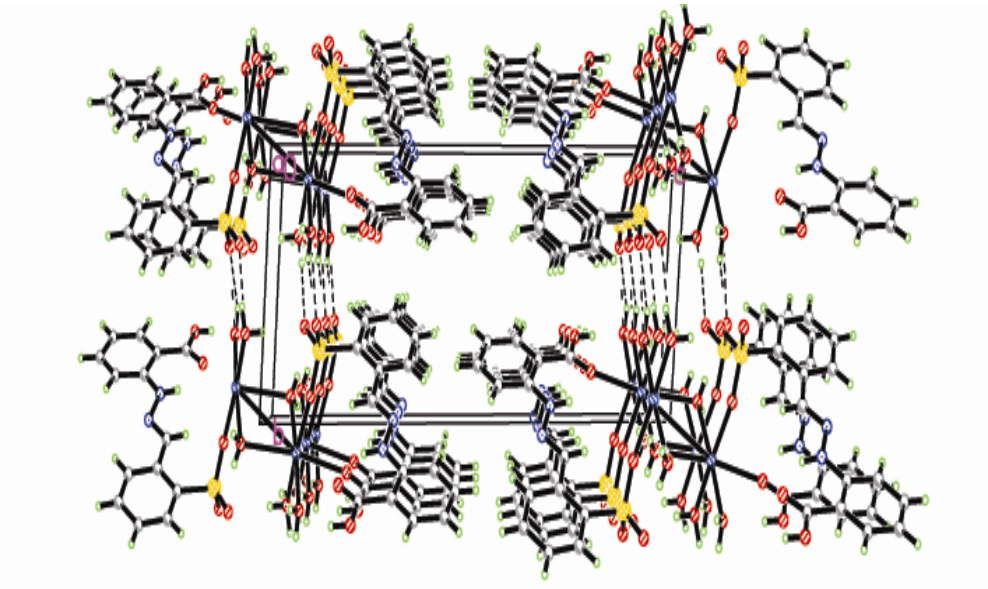

Figure 2. *Molecular packing of the Na (I) coordination polymer*

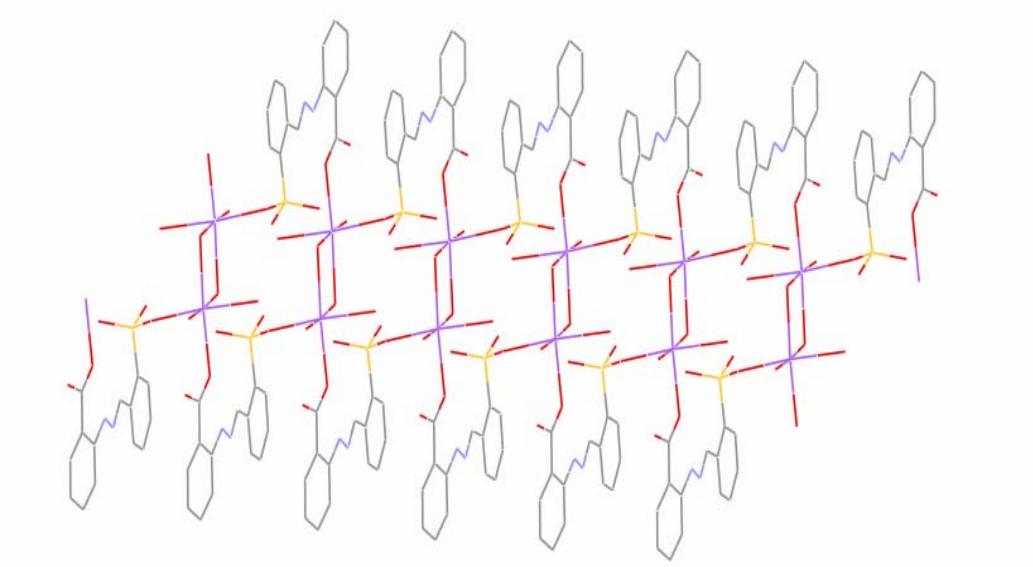

Figure 3. *One dimensional chain structure of the Na (I) coordination polymer*

CONCLUSIONS

In summary, a novel 1D chained Na(I) coordination polymer materials has been obtained by reaction of 2-hydrazinobenzoic acid with 2-formyl-benzenesulfonic acid sodium salt in CH_3CH_2OH/H_2O. X-ray analysis reveals that each Na(I) center is six-coordination with a O_6 distorted octahedron coordination environment. The Na(I) ions are linked through the O atoms of sodium 2-{(*E*)-[2-(2-carboxyphenyl)hydrazinylidene] methyl}benzenesulfonate to form 1D chain coordination polymer.

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