Asian Journal of Chemistry; Vol. 27, No. 2 (2015), 777-778

ASIAN JOURNAL OF CHEMISTRY

http://dx.doi.org/10.14233/ajchem.2015.17425

NOTE

Hydrothermal Synthesis and Crystal Structure of Neodymium(III) formate

Y.X. He

College of Chemical Engineering and Pharmaceutics, Henan University of Science and Technology, Henan, P.R. China

Corresponding author: Fax: +86 379 64232193; Tel: +86 379 64231914; E-mail: zhanglihxx@126.com

Received: 20 Februray 2014; *Accepted*: 21 May 2014; *Published online*: 10 January 2015; AJC-16669

One new neodymium compound *i.e.*, neodymium(III) formate with the m.f. $Nd(HCOO)_3$ was synthesized by reaction of $Nd(NO_3)_3{\cdot}6H_2O$, thiophene-2,5-dicarboxylic acid and formic acid. The compound has been characterized by X-ray single-crystal diffraction, compound shows a one-dimensional framework. The 3D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Neodymium(III) formate.

Metal organic frameworks (MOFs) have received much attention in the field of crystal engineering and supramolecular chemistry because of their diverse structures and promising applications in functional materials such as luminescent materials, gas adsorption and magnetism[1-4]. Hydrogen bonds are well suited for the design of polymeric arrangement and crystal engineering because of their important directional interactions and because they can interlink 1-D, or 3-D structures into higher-dimensionality systems[5,6].

All the reagents and solvents employed were commercially available and used as received without further purification.

A mixture of $Nd(NO_3)_3{\cdot}6H_2O$ (0.25 mmol), thiophene-2,5-dicarboxylic acid (0.05 mmol) and formic acid (0.25 mmol) and distilled water (8 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 423 K for 36 h, followed by slow cooling to room temperature. Colourless crystals of the compound formed (Fig. 1).

Detection method: Diffraction intensity data of the single crystal of the five compounds were collected on a Bruker SMART APEX-II CCD diffractometer equipped with a graphite monochromated MoK_α radiation ($\lambda = 0.71073$ Å) by using a ω-scan mode. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[7]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement. The crystallographic data and experimental details of structural analyses for coordination polymers are summarized in Table-1. Selected bond and angle parameters are listed in Table-2.

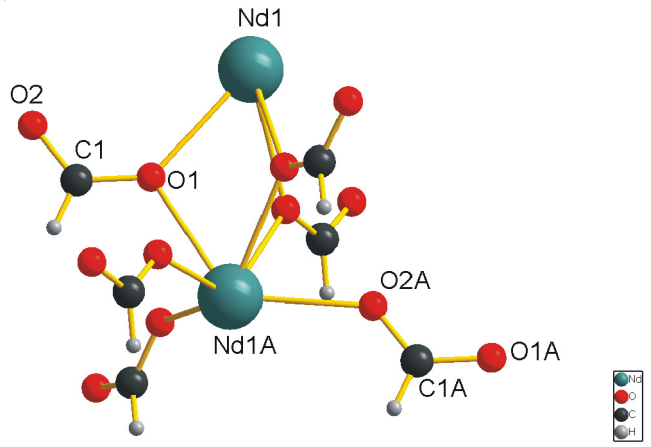

Fig. 1. Molecular structure of $Nd(HCOO)_3$ at 30 % probability displacement ellipsoids

X-ray diffraction analysis revealed that the fundamental building unit consists of metal neodymium ion and formic acid as bridging ligands to construct a new coordination polymer. On the formic acid ligands, the hydrogen atoms were assigned with Uiso(H) = 1.2 Ueq(C) and included in the final refinement by using geometrical restraints, with d(C-H) = 0.93 Å, the coordination geometry of neodymium atom is $[NdO_9]$ in a distorted octahedral manner and two oxygen atoms (O1 and O2) from formic acid ligands. The Nd-O bond lengths are 2.533 (12) Å and 2.470 (11) Å, respectively. The chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 3D framework (Fig. 2).

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR $Nd(HCOO)_3$

Empirical formula	$C_3H_3O_6Nd$
Formula weight	279.29
Crystal system space group	Rhombohedral, R3m
Unit cell dimensions	a = 10.621(2) Å; b = 10.621(2)Å; c = 4.0657(16)Å
Volume ($Å^3$)	397.17(19)
θ range for data collection	3.84-25.42
Final R indices [I>2σ(I)]	R_1= 0.0239; wR_2= 0.0605
Z, calculated density (mg/m^3)	3, 3.503
Absorption coefficient (mm^{-1})	9.768
F(000)	387
Limiting indices	$-12 \le h \le 12$; $-11 \le k \le 12$; $-4 \le l \le 2$
Largest diff. peak and hole ($e/Å^3$)	0.359 and -1.403
Goodness-of-fit on F^2	1.177
R indices (all data)	R_1= 0.0239, wR_2= 0.0605

TABLE-2
SELECTED BOND LENGTHS (Å) AND ANGLES (°) FOR $Nd(HCOO)_3$

Nd(1)-O(2)	2.470(11)	Nd(1)-O(1)#3	4.0657(16)
Nd(1)-O(1)	2.533(12)	Nd(1)-Nd(1)#5	2.128(4)
O(2)-Nd(1)-O(1)#3	73.3(3)	O(2)-Nd(1)-Nd(1)#5	91.0(3)
O(1)-Nd(1)-O(1)#1	63.7(4)	O(1)#3-Nd(1)-O(1)#4	62.6(4)
O(2)#1-Nd(1)-O(1)	71.5(3)	O(1)#1-Nd(1)-O(1)#3	105.6(4)
O(2)-Nd(1)-O(1)	126.6(4)	O(1)-Nd(1)-O(1)#3	144.79(18)
O(2)-Nd(1)-O(2)#1	119.97(2)	O(2)#1-Nd(1)-O(1)#3	127.8(4)

Symmetry codes: #1 -y+2, x-y+1, z #3 -y+2, x-y+1, z-1 #4 -x+y+1, -x+2, z-1 #5 x, y, z-1

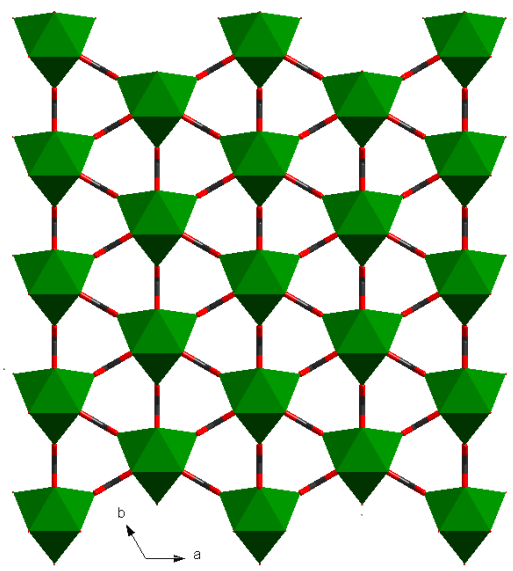

Fig. 2. 3D structure formed *via* hydrogen bonding interactions

REFERENCES

1. B.O. Patrick, C.L. Stevens, A. Storr and R.C. Thompson, *Polyhedron*, **24**, 2242 (2005).
2. Y.H. Wen, J.K. Cheng, Y.L. Feng, J. Zhang, Z.L. Li and Y.G. Yao, *Inorg. Chim. Acta*, **358**, 3347 (2005).
3. X.L. Wang, C. Qin, E.B. Wang and L. Xu, *J. Mol. Struct*., **749**, 45 (2005).
4. S.R. Batten and K.S. Murray, *Coord. Chem. Rev*., **246**, 103 (2003).
5. T.L. Hu, R.Q. Zou, J.R. Li and X.H. Bu, *J. Chem. Soc., Dalton Trans*., 1302 (2008).
6. J.F. Song, Y. Chen, Z.G. Li, R.S. Zhou, X.Y. Xu and J.Q. Xu, *J. Mol. Struct*., **842**, 125 (2007).
7. G.M. Sheldrick, SHELXTL97, Program for the Refinement of Crystal Structure, University of Gottingen, Germany (1997).