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A new chain-like polyoxometallate based on B-Anderson-type building blocks and rare earth metal ion linkers

Da-Peng Zhou and Dong Yang*

Institute of Molecular and Crystal Engineering, School of Chemistry and Chemical Engineering, Henan University, Kaifeng, Henan 475001, People's Republic of China

Correspondence e-mail: yangdong8049@163.com

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Key indicators

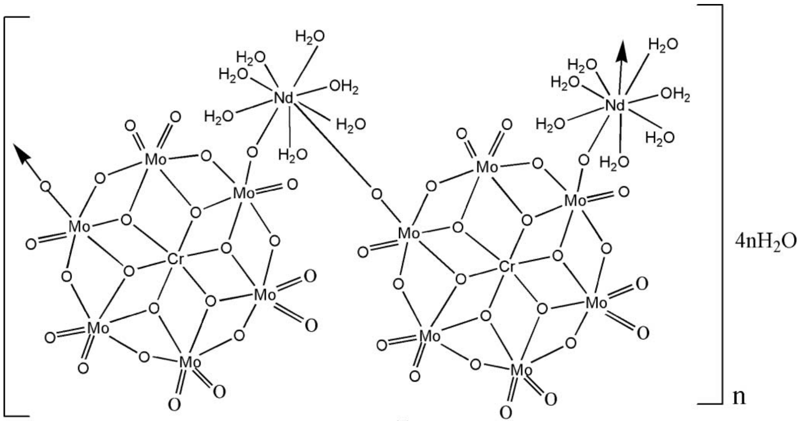
Single-crystal X-ray study
T = 294 K
Mean σ(Cr–O) = 0.004 Å
R factor = 0.022
wR factor = 0.059
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title polymer chain, *catena*-poly[[[hexa-μ_2-hydroxido-hexa-μ_3-oxido-decaoxido-chromium(III)hexamolybdenum(IV)]-μ_2-oxido-[heptaaquaneodymium(III)]- μ_2-oxido] tetrahydrate], $[NdCrMo_6O_{18}(OH)_6(H_2O)_7]\cdot 4H_2O$, the Nd atom has a tricapped trigonal-prismatic environment, being coordinated by two terminal O atoms from different $[Cr(OH)_6Mo_6O_{18}]^{3-}$ units, and by seven water molecules. In the crystal structure, hydrogen bonds result in the formation of a three-dimensional network and may be effective in the stabilization of the structure.

Comment

Polyoxometallate compounds have attracted considerable attention due to their variety of structures and their potential applications in catalysis, biochemical analysis, medicinal chemistry and magnetism (Pope & Müller, 1991; Shivaiah & Das, 2005; Shivaiah *et al.*, 2003; Khan *et al.*, 2003). Most of them have discrete cluster-like structures containing arrays of edge-, corner- and face-sharing octahedral $\{MO_6\}$ coordinated $\{MO_6\}$ units (where *M* is Mo, W, V *etc.*), and they play an important role in forming new classes of materials with potentially useful electronic and magnetic properties (Gimenez-Saiz *et al.*, 1995; Lopez *et al.*, 2002; Müller *et al.*, 1998). Taking advantage of the ability of polyanions to act as ligands, it is possible to form cation–polyanion complexes which may exhibit low-dimensional, or even high-dimensional, structures. We report here a new example, the title extended polyoxometallate, $[Nd(H_2O)_7Cr(OH)_6Mo_6O_{18}]_n\cdot 4nH_2O$, (I), which contains an Anderson anion acting as a bidentate ligand and coordinating to two Nd ions.



(I)

The asymmetric unit of (I) is shown in Fig. 1. In the cluster, according to the manner of oxygen coordination, four kinds of

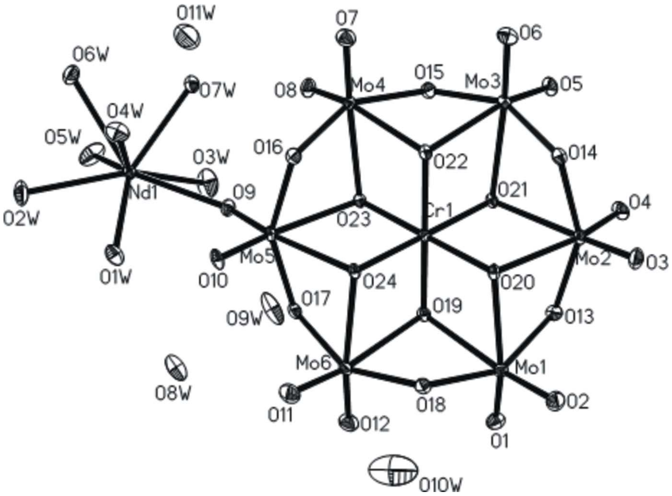


Figure 1
The asymmetric unit of (I). All H atoms are omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

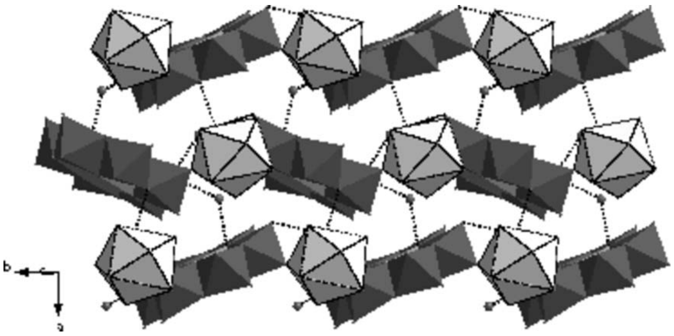


Figure 2
The two-dimensional layer of (I). Hydrogen bonds are shown as dashed lines. **AUTHOR: please provide a revised version of this Figure.**

O atoms exist, namely terminal (O*t*), terminal linked to Nd^{3+} (O*t*′), double-bridging (O*b*) and central (O*c*). Thus, the Mo—O distances can be grouped into four sets, Mo—O*t* [1.692 (6)–1.719 (5) Å], Mo—O*t*′ [1.722 (5) Å], Mo—O*b* [1.889 (5)–1.973 (5) Å] and Mo—O*c* [2.262 (5)–2.319 (5) Å]. Compound (I) is isostructural with $[La(H_2O)_7Cr(OH)_6Mo_6O_{18}]_n\cdot 4nH_2O$ (Shivaiah *et al.*, 2002).

In the title polymer chain, the coordination number of each Nd atom is 9 and they each exhibit a tricapped trigonal–prismatic environment, coordinated by two terminal O atoms from different $[Cr(OH)_6Mo_6O_{18}]^{3-}$ units and by seven water molecules. These coordination patterns result in slightly longer Mo—O*t*′ bonds than the unshared Mo—O*t* bonds. There are multi-point hydrogen bonds between the water molecules coordinated to the Nd ion, the coordinated hydroxide ions of the central {$Cr(OH)_6$} unit and the water molecules (Table 1).

As can be seen from the packing diagram (Fig. 2), the hydrogen bonds (Table 1) result in the formation of a three-dimensional network and may be effective in the stabilization of the crystal structure.

Experimental

$Na_3[CrMo_6O_{24}H_6]\cdot 8H_2O$ was prepared according to the literature method of Perloff (1970). $Na_3[CrMo_6O_{24}H_6]\cdot 8H_2O$ (1.00 g, 0.8 mmol) was dissolved in water (10 ml). A dilute hydrochloric acid solution (6 *M*, 10 ml) of Nd_2O_3 (0.34 g, 1 mmol) was then added to the above aqueous solution. The initial pH value of this mixture was adjusted to 3.3 with NaOH solution (2 *M*, 1 ml). The filtrate was kept for 38 d under ambient conditions and then the solution afforded purple–red block-shaped crystals of (I) (yield 0.18 g, 53%).

Crystal data

$[NdCrMo_6O_{18}(OH)_6(H_2O)_7]\cdot 4H_2O$
$M_r = 1354.06$
Orthorhombic, $Pca2_1$
$a = 11.8655\ (10)$ Å
$b = 10.9961\ (9)$ Å
$c = 22.5449\ (18)$ Å
$V = 2941.5\ (4)$ Å^3
$Z = 4$
Mo *Kα* radiation
$\mu = 4.68$ mm^{-1}
$T = 294\ (2)$ K
0.16 × 0.14 × 0.13 mm

Data collection

Rigaku R-AXIS IV diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.521$, $T_{max} = 0.581$ (expected range = 0.488–0.544)
20142 measured reflections
5150 independent reflections
5000 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.059$
$S = 1.08$
5150 reflections
389 parameters
1 restraint
1249 Friedel pairs
H-atom parameters constrained
$\Delta\rho_{max} = 1.28$ e Å^{-3}
$\Delta\rho_{min} = -0.85$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.531 (12)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H2···O10	0.85	2.39	3.060 (7)	137
O8*W*—H16···O1*W*	0.85	2.09	2.843 (4)	147
O1*W*—H1···O15^{i}	0.85	2.05	2.617 (7)	123
O8*W*—H15···O14^{ii}	0.85	2.15	2.771 (3)	129
O9*W*—H17···O14^{ii}	0.85	2.11	2.917 (4)	159
O2*W*—H4···O2^{iii}	0.85	2.11	2.855 (8)	146
O9*W*—H18···O24^{iv}	0.85	1.97	2.647 (3)	136
O4*W*—H8···O11*W*	0.85	1.90	2.697 (7)	155
O6*W*—H11···O3^{v}	0.85	2.23	2.883 (3)	133
O7*W*—H13···O12^{vi}	0.85	2.15	2.963 (9)	160
O11*W*—H22···O4*W*	0.85	2.17	2.697 (9)	120
O10*W*—H19···O5*W*^{vii}	0.85	2.14	2.751 (9)	129

Symmetry codes: (i) $x-\frac{1}{2}, -y+1, z$; (ii) $x, y-1, z$; (iii) $-x+1, -y+1, z-\frac{1}{2}$; (iv) $x+\frac{1}{2}, -y+1, z$; (v) $-x+\frac{3}{2}, y-1, z-\frac{1}{2}$; (vi) $-x+\frac{3}{2}, y, z-\frac{1}{2}$; (vii) $-x+1, -y+1, z+\frac{1}{2}$.

H atoms were located in difference syntheses and constrained to ride on their parent atoms, with O—H = 0.85 Å and $U_{iso}(H) = 1.2U_{eq}(O)$. The value of the Flack parameter indicates inversion twinning. The maximum electron-density peak is located 1.01 Å from atom Nd1.

Data collection: *PROCESS-AUTO* (Higashi, 1996); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1989); software used to prepare material for publication: *TEXSAN*.

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References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gimenez-Saiz, C., Galan-Mascaros, J. R., Triki, S., Coronado, E. & Ouahab, L. (1995). *Inorg. Chem.* **34**, 524–526.
Higashi, T. (1996). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Khan, M. I., Yohannes, E. & Doedens, R. J. (2003). *Inorg. Chem.* **42**, 3125–3129.
Lopez, X., Bo, C. & Poblet, J. M. (2002). *J. Am. Chem. Soc.* **124**, 12574–12582.
Molecular Structure Corporation (1989). *TEXSAN*. Version 1.11. MSC, The Woodlands, Texas, USA.
Müller, A., Peters, F., Pope, M. T. & Gatteschi, D. (1998). *Chem. Rev.* **98**, 239–272.
Perloff, A. (1970). *Inorg. Chem.* **9**, 2228–2239.
Pope, M. T. & Müller, A. (1991). *Angew. Chem. Int. Ed.* **30**, 34–48.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Shivaiah, V. & Das, S. K. (2005). *Inorg. Chem.* **44**, 8846–8854.
Shivaiah, V., Nagaraju, M. & Das, S. K. (2003). *Inorg. Chem.* **42**, 6604–6606.
Shivaiah, V., Reddy, P. V. N., Cronin, L. & Das, S. K. (2002). *J. Chem. Soc. Dalton Trans.* pp. 3781–3782.