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Sodium barium hexahydrogenhexamolybdoaluminate(III) decahydrate

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The title compound, NaBa[$AlMo_6(OH)_6O_{18}$]·10H_2O, contains a B-type Anderson polyanion [$AlMo_6(OH)_6O_{18}$]$^{3-}$ having an inversion center with approximate D_{3d} symmetry. There are two uncoordinated water molecules per formula unit, the remaining eight being coordinated to the Na^+ and Ba^{2+} cations, which link the polyanions to form the three-dimensional structure. Hydrogen-bonding interactions exist to stabilize the structure.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(l–O) = 0.004 Å
R factor = 0.037
wR factor = 0.087
Data-to-parameter ratio = 17.2

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

Comment

The well known Anderson-type polyanions (Anderson, 1937) can be found in many compounds employing rare-earth cations and transition-metal cations or complexes as bridging linkers (Gao *et al.*, 2006; Shivaiah *et al.*, 2003). In contrast, the use of alkaline-earth cations as linkers remains rare, as in the title compound, NaBa[$AlMo_6(OH)_6O_{18}$]·10H_2O (I).

The structure consists of an Anderson polyanion, a sodium ion, a barium ion, eight coordinated waters, and two uncoordinated waters. The [$AlMo_6(OH)_6O_{18}$]$^{3-}$ polyanion adopts a B-type Anderson structure, consisting of seven edge-sharing octahedra, six of which are {MoO_6} octahedra arranged hexagonally around the central {$Al(OH)_6$} octahedron (Fig. 1). It has an inversion center and is close to D_{3d} symmetry, all bond lengths and angles being within the normal ranges (Lee *et al.*, 1991; Liu *et al.*, 2006). The Na^+ ion is six-coordinate and the Ba^{2+} ion is eight-coordinate. Not only do these cations

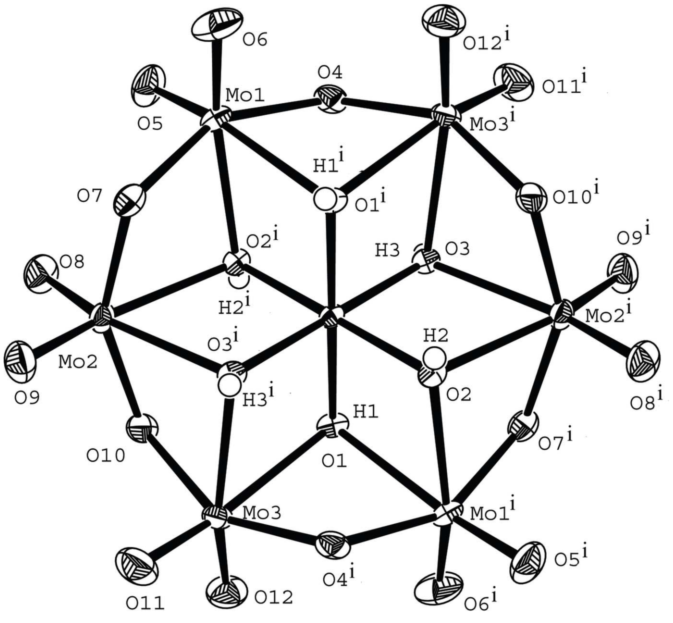

Figure 1
Structure of the polyanion in (I), showing 50% probability displacement ellipsoids. [Symmetry code: (i) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z$.]

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compensate for the polyanionic charge, they also act as linkers to form the three-dimensional structure (Fig. 2). It is believed that extensive hydrogen bonding interactions play an important role in stabilizing the structure.

Experimental

To a 30 ml aqueous solution of $AlCl_3{\cdot}6H_2O$ (0.36 g, 1.5 mmol) were added 10 ml aqueous solution of $Na_2MoO_4{\cdot}2H_2O$ (0.90 g, 3.7 mmol) and 5 ml of glacial acetic acid, followed by addition of 10 ml $BaCl_2{\cdot}2H_2O$ (0.15 g, 0.6 mmol). The pH of the resulting mixture was adjusted with dilute hydrochloric acid to about 2.6 and it was stirred for half an hour. The filtrate was allowed to evaporate at room temperature. After five days, colorless block-shaped crystals of (I) were collected in about 64% yield (0.53 g, based on Mo).

Crystal data

$NaBa[AlMo_6(OH)_6O_{18}]{\cdot}10H_2O$
$M_r = 1333.16$
Monoclinic, $C2/c$
$a = 23.553$ (5) Å
$b = 11.549$ (2) Å
$c = 11.227$ (2) Å
$\beta = 96.06$ (3)°
$V = 3037.0$ (10) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 3.84$ mm^{-1}
$T = 298$ (2) K
0.14 × 0.13 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.588$, $T_{max} = 0.632$
14015 measured reflections
3398 independent reflections
3082 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.087$
$S = 1.14$
3398 reflections
198 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max} = 1.75$ e Å^{-3}
$\Delta\rho_{min} = -0.89$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Al1—O1	1.902 (4)	Mo2—O7	1.959 (4)
Al1—O2	1.894 (4)	Mo2—O8	1.705 (4)
Al1—O3	1.896 (4)	Mo2—O9	1.708 (4)
Mo1—O4	1.936 (4)	Mo3—O10	1.935 (4)
Mo1—O5	1.704 (4)	Mo3—O11	1.702 (5)
Mo1—O6	1.713 (5)	Mo3—O12	1.712 (5)
O2—Al1—O3	84.38 (16)	O8—Mo2—O10	98.7 (2)
O3—Al1—O1	94.92 (16)	O10—Mo2—O7	150.75 (17)
O5—Mo1—O4	97.4 (2)	O11—Mo3—O12	105.7 (2)
O7—Mo1—O4	150.57 (17)	O11—Mo3—O1	160.56 (19)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯O8^{i}	0.85	1.95	2.790 (6)	169
O2—H2⋯O5W^{ii}	0.85	1.83	2.615 (6)	153
O3—H3⋯O5^{i}	0.85	1.88	2.718 (6)	169
O1W—H4⋯O6^{iii}	0.85	2.14	2.769 (7)	130
O1W—H5⋯O4W^{iv}	0.85	1.93	2.772 (7)	169
O2W—H6⋯O9^{v}	0.85	2.50	3.211 (7)	142
O2W—H7⋯O3W^{vi}	0.85	2.06	2.895 (8)	165
O3W—H8⋯O9^{vii}	0.85	2.43	3.114 (7)	139
O3W—H9⋯O10^{v}	0.85	1.90	2.738 (7)	167
O4W—H10⋯O9^{viii}	0.85	2.05	2.848 (7)	157
O4W—H11⋯O4^{ix}	0.85	1.91	2.747 (6)	170
O5W—H12⋯O7^{x}	0.85	2.07	2.810 (7)	145
O5W—H13⋯O7^{xi}	0.85	2.20	3.003 (6)	157

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

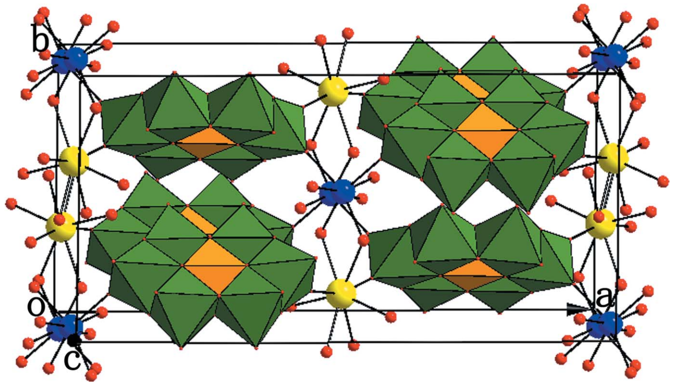

Figure 2
Polyhedral representation of the stacking of (I) in the unit cell. The uncoordinated waters and H atoms have been omitted for clarity. Blue circles are Na^+ and blue-gray circles are Ba^{2+}.

H atoms of the hydroxyl groups around the Al^{3+} ion and on water molecules were located in difference Fourier maps, idealized with O—H = 0.85 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2002); software used to prepare material for publication: *CrystalStructure*.

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References

Anderson, J. S. (1937). *Nature* (*London*), **140**, 850.
Gao, B., Liu, S. X., Xie, L. H., Yu, M., Zhang, C. D., Sun, C. Y. & Cheng, H. Y. (2006). *J. Solid State Chem.* **179**, 1681–1689.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Lee, H. Y., Park, K. M., Lee, U. & Ichida, H. (1991). *Acta Cryst.* C**47**, 1959–1961.
Liu, Y., Dou, J.-M., Wang, D.-Q., Zhang, X.-X. & Zhou, L. (2006). *Acta Cryst.* E**62**, i234–i235.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Version 3.00. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shivaiah, V., Nagaraju, M. & Das, S. K. (2003). *Inorg. Chem.* **42**, 6604–6606.