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Bis[2,2′-(butane-1,4-diyl)bis(1*H*-benzimidazolium)] *α*-octamolybdate(VI)

Li-Jun Wang,[a]* Hong Jiang,[a] Yong Wang,[b] Kui-Zhan Shao[b] and Zhong-Min Su[b]*

[a]Public and Basic Courses Department of Beihua University, Jilin 132013, People's Republic of China, and [b]Institute of Functional Materials Chemistry, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: wanglj649@yahoo.com.cn, zmsu@nenu.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.028
wR factor = 0.049
Data-to-parameter ratio = 16.2

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

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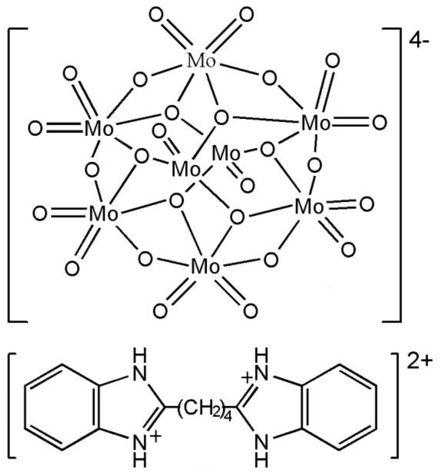
In the title compound, $(C_{18}H_{20}N_4)_2[\alpha\text{-}Mo_8O_{26}]$, the centrosymmetric α-octamolybdate anions are linked by 2,2′-(butane-1,4-diyl)bis(1*H*-benzimidazolium) cations through N—H⋯O hydrogen bonds, forming a three-dimensional network.

Comment

The rapid progress in exploring inorganic–organic hybrid materials has been driven by the interest in their fascinating structural diversity and promising potential applications in chemistry, biology and materials science (Pope & Müller, 1991; Moulton & Zaworotko, 2001). It is well known that polyoxometalate building blocks can be linked into extended structures *via* coordination bonds, π–π stacking, hydrogen bonds and combinations of these interactions (An *et al.*, 2006; Chen *et al.*, 2005; Lu *et al.*, 2004). The structures of many compounds containing octamolybdate anions and organic cations have been investigated (Gili *et al.*, 1992; Xu *et al.*, 1999; Feng *et al.*, 2005). The bis(2-benzimidazole) ligand and some substituted bis(2-benzimidazolyl)alkane ligands are attractive choices as multifunctional linking groups (Wang *et al.*, 2006). During our ongoing studies of related compounds, we obtained the title compound, (I), by a hydrothermal reaction of $Na_2MoO_4\cdot 2H_2O$, $Co(NO_3)_2\cdot 6H_2O$ and 2,2′-(butane-1,4-diyl)bis(1*H*-benzimidazole) (*L*) in water.



(I)

As illustrated in Fig. 1, compound (I) contains H_2L cations and centrosymmetric octamolybdate $[\alpha\text{-}Mo_8O_{26}]^{4-}$ anions. The anion is constructed from six MoO_6 octahedra and two MoO_4 tetrahedra. The Mo atoms in the six edge-sharing MoO_6 octahedra are coplanar, forming a six-membered ring with each side of the plane being capped by an MoO_4 tetrahedron

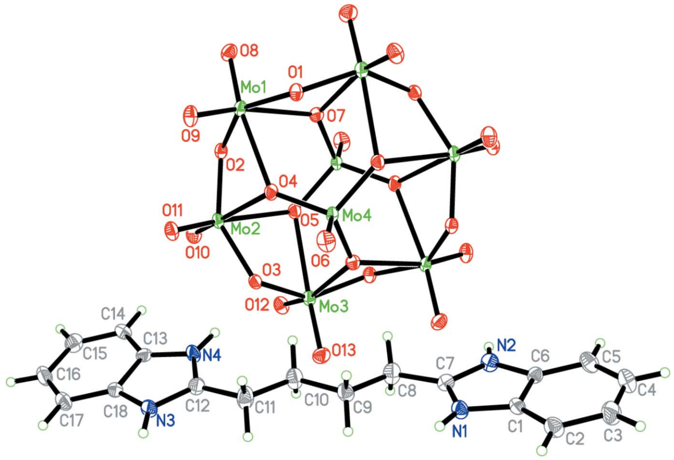


Figure 1

The structure of the anion and cation of (I). Displacement ellipsoids are drawn at the 30% probability level. The inversion center at the central point of the octamolybdate anion generates the unlabeled atoms by the symmetry operation $(1 - x, 2 - y, 1 - z)$.

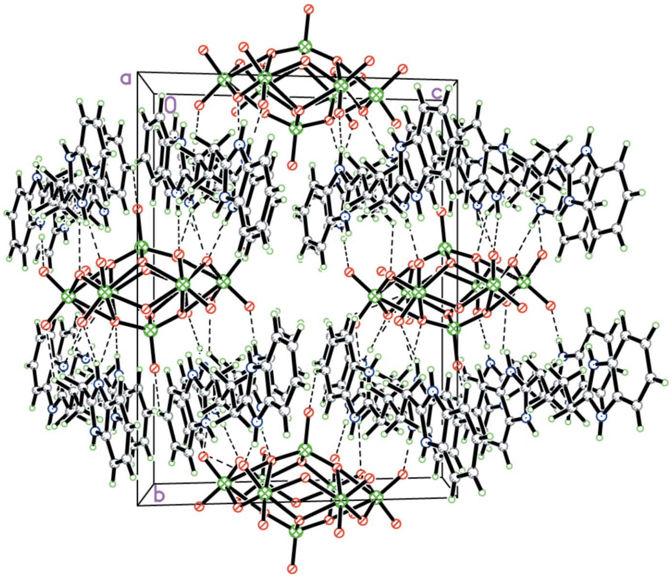


Figure 2

Crystal packing in (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds. Color scheme: C gray; H jade-green; Mo bottle-green; O red; N blue.

via corner sharing. There are three kinds of O atoms in the $[\alpha\text{-}Mo_8O_{26}]^{4-}$ anion: terminal O, μ_2-O and μ_3-O. The bond distances and angles in the anion fall within the expected ranges (Yang *et al.*, 2002). The α-octamolybdate anions and the H_2L cations are linked *via* N—H$\cdots$O hydrogen bonds to form a three-dimensional network structure (Fig. 2 and Table 1).

Experimental

A mixture of $Co(NO_3)_2\cdot 6H_2O$ (0.3 mmol, 0.087 g), $Na_2MoO_4\cdot 2H_2O$ (1 mmol, 0.242 g), *L* (0.3 mmol, 0.088 g) and water (10 ml) was adjusted to pH = 4 with 6 *M* HCl, with continuous stirring for 20 min in air. The mixture was then transferred to a 23 ml Teflon-lined reactor and kept at 443 K for 3 d under autogenous pressure. Upon cooling to room temperature at a rate of 5 K h^{-1}, colorless block-shaped crystals of (I) were obtained, washed with distilled water and dried at room temperature.

Crystal data

$(C_{18}H_{20}N_4)_2[Mo_8O_{26}]$
$M_r = 1768.28$
Monoclinic, $P2_1/c$
$a = 10.4046\ (4)$ Å
$b = 18.0223\ (7)$ Å
$c = 14.0282\ (5)$ Å
$\beta = 104.989\ (1)^\circ$
$V = 2540.99\ (17)$ Å^3
$Z = 2$
$D_x = 2.311$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.00$ mm^{-1}
$T = 293\ (2)$ K
Block, colorless
$0.25 \times 0.20 \times 0.17$ mm

Data collection

Bruker SMART APEX2 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.635$, $T_{max} = 0.727$
15487 measured reflections
5972 independent reflections
4246 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.3^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.049$
$S = 1.00$
5972 reflections
368 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0139P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

Table 1

Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1N$\cdots$O12^{i}	0.85 (1)	2.00 (2)	2.848 (4)	175 (3)
N2—H2N$\cdots$O11^{ii}	0.85 (1)	2.39 (2)	3.050 (4)	134 (3)
N2—H2N$\cdots$O8^{iii}	0.85 (1)	2.20 (2)	2.929 (4)	144 (3)
N3—H3N$\cdots$O9^{iv}	0.85 (1)	2.00 (2)	2.774 (4)	151 (3)
N4—H4N$\cdots$O3	0.86 (1)	1.97 (1)	2.819 (3)	172 (3)

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

H atoms attached to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) and 0.97 Å (CH_2) and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms attached to N atoms were located in a difference Fourier map and refined isotropically, with restraints of N—H = 0.86 (1) Å.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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m586 Wang *et al.* • $(C_{18}H_{20}N_4)_2[Mo_8O_{26}]$ *Acta Cryst.* (2007). E**63**, m584–m586