

## Tricaesium dimolybdate(VI) bromide

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{Mo}-\text{O}) = 0.004$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.062; data-to-parameter ratio = 17.2.

The title compound,  $\text{Cs}_3(\text{Mo}_2\text{O}_7)\text{Br}$ , was synthesized by the reaction of  $\text{CsNO}_3$ ,  $\text{MoO}_3$  and 1-ethyl-3-methylimidazolium bromide. Its crystal structure is isotypic with  $\text{K}_3(\text{Mo}_2\text{O}_7)\text{Br}$  and contains  $(\text{MoO}_4)^{2-}$  tetrahedra which share an O atom to produce a  $[\text{Mo}_2\text{O}_7]^{2-}$  dimolybdate(VI) anion with a linear bridging angle and  $\bar{6}m2$  symmetry. The anions are linked by Cs atoms (site symmetry  $\bar{6}m2$ ), forming sheets parallel to (001). Br atoms (site symmetry  $\bar{6}m2$ ) are also part of this layer. Another type of Cs atom ( $3m$  site symmetry) is located in the interlayer space and connects the layers *via* Cs—O and Cs—Br interactions into a three-dimensional array.

### Related literature

For the isotypic compound  $\text{K}_3(\text{Mo}_2\text{O}_7)\text{Br}$ , see: Becher & Fenske (1978). For dimolybdates with similar condensed anions made up of  $\text{MoO}_4$  tetrahedra, see:  $\text{Ce}_2(\text{MoO}_4)_2(\text{Mo}_2\text{O}_7)$  (Fallon & Gatehouse, 1982);  $\text{Mg}_2\text{Mo}_2\text{O}_7$  (Stadnicka *et al.*, 1977).

### Experimental

#### Crystal data

$\text{Cs}_3(\text{Mo}_2\text{O}_7)\text{Br}$   
 $M_r = 782.52$

Hexagonal,  $P6_3/mmc$   
 $a = 6.3993$  (5) Å

$c = 16.4870$  (15) Å  
 $V = 584.71$  (8) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation

$\mu = 14.77$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.15 \times 0.15 \times 0.05$  mm

#### Data collection

Stoe IPDS-2 diffractometer  
Absorption correction: integration  
(*X-RED* and *X-SHAPE*; Stoe, 2005)  
 $T_{\min} = 0.153$ ,  $T_{\max} = 0.532$

5224 measured reflections  
344 independent reflections  
338 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.044$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.062$   
 $S = 1.18$   
344 reflections

20 parameters  
 $\Delta\rho_{\max} = 0.60$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.21$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Mo—O1	1.725 (4)	Mo—O2	1.8764 (7)
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Data collection: *X-AREA* (Stoe, 2007); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2275).

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