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The lanthanum(III) molybdate(VI)

La₄Mo₇O₂₇

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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{La-O}) = 0.006$ Å;
 R factor = 0.028; wR factor = 0.076; data-to-parameter ratio = 20.9.

Crystals of the orthorhombic phase La₄Mo₇O₂₇ (lanthanum molybdenum oxide) were obtained from a non-stoichiometric melt in the pseudo-ternary system La₂O₃–MoO₃–B₂O₃. In the crystal structure, distorted square-antiprismatic [LaO₈] and monocapped square-antiprismatic [LaO₉] polyhedra are connected *via* common edges and faces into chains along [010]. These chains are arranged in layers that alternate with layers of [MoO₄] and [MoO₅] polyhedra parallel to (001). In the molybdate layers, a distorted [MoO₅] trigonal bipyramid is axially connected to two [MoO₄] tetrahedra, forming a [Mo₃O₁₁] unit.

Related literature

The isoformular compounds Eu₄Mo₇O₂₇ (Naruke & Yamase, 2001) and Gd₄Mo₇O₂₇ (Naruke & Yamase, 2002) have a similar structure, but have monoclinic symmetry. Parameters needed to calculate bond-valence sums from bond lengths were taken from Brown & Altermatt (1985).

Experimental

Crystal data

La₄Mo₇O₂₇ $M_r = 1659.22$ Orthorhombic, $Pca2_1$ $a = 14.1443$ (14) Å $b = 7.2931$ (4) Å $c = 22.9916$ (13) Å $V = 2371.7$ (3) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 10.71$ mm⁻¹ $T = 295$ K $0.25 \times 0.23 \times 0.22$ mm

Data collection

Nonius MACH3 diffractometer

Absorption correction: ψ scan

(MolEN; Fair, 1990)

 $T_{\min} = 0.841$, $T_{\max} = 0.999$

(expected range = 0.080–0.095)

17773 measured reflections

7202 independent reflections

6225 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.042$

3 standard reflections

every 100 reflections

intensity decay: –4.1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.028$ $wR(F^2) = 0.076$ $S = 1.05$

7202 reflections

345 parameters

1 restraint

 $\Delta\rho_{\text{max}} = 2.27$ e Å⁻³ $\Delta\rho_{\text{min}} = -1.35$ e Å⁻³

Absolute structure: Flack (1983),

3515 Friedel pairs

Flack parameter: 0.039 (14)

Data collection: *MACH3* (Enraf–Nonius, 1993); cell refinement: *MACH3*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2242).

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