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$Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ(Mg–O) = 0.003 Å; disorder in main residue; R factor = 0.021; wR factor = 0.053; data-to-parameter ratio = 13.3.

The title compound, lithium/aluminium dimagnesium tetrakis[orthomolybdate(VI)], was prepared by a solid-state reaction route. The crystal structure is built up from MgO_6 octahedra and MoO_4 tetrahedra sharing corners and edges, forming two types of chains running along [100]. These chains are linked into layers parallel to (010) and finally linked by MoO_4 tetrahedra into a three-dimensional framework structure with channels parallel to [001] in which lithium and aluminium cations equally occupy the same position within a distorted trigonal–bipyramidal coordination environment. The title structure is isotypic with $LiMgIn(MoO_4)_3$, with the In site becoming an Mg site and the fully occupied Li site a statistically occupied Li/Al site in the title structure.

Related literature

For complex oxides containing lithium ions, see: Whittingham & Silbernagel (1976); Mizushima *et al.* (1980); Kanno *et al.* (1994). For details of chemically and/or structurally related compounds, see: Efremov & Trunov (1972); Ozima & Zoltai (1976); Klevtsov (1970); Kolitsch & Tillmanns (2003); Tsyrenova *et al.* (2001, 2004); Gicquel-Mayer *et al.* (1981); Klevtsova & Magarill (1970); Klevtsov & Zolotova (1973); Klevtsova *et al.* (1979); Nord & Kierkegaard (1984); Solodovnikov *et al.* (1997). For the isotypic structure of $LiMgIn(MoO_4)_3$, see: Khazheeva *et al.* (1985).

Experimental

Crystal data

$Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$
M_r = 545.40
Triclinic, $P\overline{1}$
a = 6.8555 (7) Å
b = 8.2910 (9) Å
c = 9.5760 (9) Å
α = 96.032 (7)°
β = 106.743 (8)°
γ = 101.824 (9)°
V = 502.27 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.92 mm^{-1}
T = 298 K
0.20 × 0.18 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.520, T_{max} = 0.648
3450 measured reflections
2187 independent reflections
2150 reflections with $I > 2s\sigma(I)$
R_{int} = 0.014
2 standard reflections every 120 min intensity decay: 1.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.053
S = 1.29
2187 reflections
164 parameters
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—O5^{i}	1.721 (3)	Mg1—O4	1.992 (3)
Mo1—O12	1.745 (3)	Mg1—O10^{iii}	2.033 (3)
Mo1—O1	1.781 (3)	Mg1—O2^{v}	2.104 (3)
Mo1—O2	1.812 (3)	Mg2—O12^{vi}	2.042 (3)
Mo2—O3	1.738 (3)	Mg2—O1^{vii}	2.045 (3)
Mo2—O6	1.743 (3)	Mg2—O9	2.046 (3)
Mo2—O11^{ii}	1.763 (3)	Mg2—O5	2.049 (3)
Mo2—O10^{iii}	1.807 (3)	Mg2—O6^{viii}	2.049 (3)
Mo3—O9	1.718 (3)	Mg2—O7^{vi}	2.121 (3)
Mo3—O4	1.736 (3)	Li1—O3^{ix}	1.974 (4)
Mo3—O7	1.777 (3)	Li1—O7^{ix}	2.009 (4)
Mo3—O8	1.812 (3)	Li1—O1	2.044 (4)
Mg1—O2^{iv}	1.968 (3)	Li1—O8	2.070 (4)
Mg1—O11	1.974 (3)	Li1—O10^{vi}	2.076 (4)
Mg1—O8^{v}	1.983 (3)		

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

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2760).

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supporting information

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$Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$

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S1. Comment

In recent years, great attention has been devoted to the examination of metal oxides containing mobile lithium ions due to their potential application in the fields of energy and electronics, such as Li*M*O_2 materials (*M*= Mn, Fe, Co, Ni) (Whittingham & Silbernagel, 1976; Mizushima *et al.*, 1980; Kanno *et al.*, 1994) which allowed to construct electrochemical generators with a high energy density. In our field of research we are interested especially to doubles molybdates of alkali and divalent metals, and we tried to explore systems like Li_2O—*M*O—MoO_3. For such systems, the compounds $Li_3Fe(MoO_4)_3$ and $Li_2Fe_2(MoO_4)_3$ are already known, the crystal structures of which have been determined by Klevtsova & Magarill (1970) and the structural similarity to $NaCo_{2.31}(MoO_4)_3$ and to other framework oxides is noted. These compounds include $Li_2M_2(MoO_4)_3$ (*M* = Mg, Mn, Co, Ni, Cu, Zn) (Efremov & Trunov, 1972; Ozima & Zoltai, 1976), $Li_3M^{3+}(MoO_4)_3$ (*M*=Al, Cr, Ga, Sc, In, Co) (Klevtsov, 1970; Kolitsch & Tillmanns, 2003) and $Li_2M^{4+}(MoO_4)_3$ (*M* = Ti, Zr, Hf) (Klevtsov & Zolotova, 1973; Klevtsova *et al.*, 1979). During our examinations we now have serendipitously obtained a new molybdenum oxide crystal with composition $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$, (I).

The asymmetric unit of compound (I) is composed of two MgO_6 octahedra and three MoO_4 tetrahedra sharing corners, as well as a (li/Al) site (Fig. 1). The structure of (I) can be described as being composed of two types of infinite chains expanding parallel to [100]. The first chain is built up from Mg2O_6 octahedra and Mo1O_4 tetrahedra sharing corners, forming double chains with composition $(Mg_2Mo_2O_{14})_n$ and with a *cis* arrangement of the MoO_4 tetrahedra relative to the MgO_6 octahedra (Fig. 2a). The second type of chain is formed by Mg1O_6 octahedra and Mo2O_4 tetrahedra, also linked by corners but in a *trans* arrangement. Single chains of the second type are linked by sharing edges between two adjacent Mg1O_6 octahedra (Fig. 2b). The linkage between the two types of chains leads to a layer-like arrangement parallel to (010) (Fig. 3), whereas the linkage into a three-dimensional framework is provided by Mo3O_4 tetrahedra by sharing corners. In this framework channels are present where the mixed-occupied Li^+/Al^{3+} sites are located (Fig. 4). The Mg2O_6 octahedron has an almost regular coordination sphere with five nearly equal Mg—O distances (*d*(Mg—O) = 2.04 Å) with the sixth slightly longer. Each $Mg1_2O_{10}$ double octahedron is surrounded by ten MoO_4 tetrahedra forming $Mg1_2Mo_{10}O_{40}$ units. The Mg—O distances vary from 1.968 (3) Å to 2.104 (3) Å which are close to those found for related systems (Nord & Kierkegaard, 1984). The Mo—O distances vary from 1.719 (3) Å to 1.812 (3) Å with the average Mo—O distance of 1.762 Å, closed to literature values (Solodovnikov *et al.*, 1997). The (Li/Al) site has a distorted trigonal-bipyramidal coordination environment.

The structure of compound (I) is isotypic with $LiMgIn(MoO_4)_3$ (Khazheeva *et al.*, 1985). The In^{3+} site becomes Mg2 in the title structure, and the Li site in $LiMgIn(MoO_4)_3$ has full occupation, whereas in the title structure it is a mixed-occupied (Li/Al) site with half-occupancy for each of the metal ions. In fact, charge compensation can only be ensured by insertion of Al^{3+} in the same site as Li^+ ((Mg^{2+} + In^{3+} + Li^+) = ($2Mg^{2+}$ + (Al^{3+}/Li^+)) (Fig. 5).

The unit-cell parameters of triclinic $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$ indicate some resemblance to the structures of $Ag_2M_2(MoO_4)_3$ (M = Zn, Mg, Co) (Tsyrenova *et al.*, 2004, 2001; Gicquel-Mayer *et al.*, 1981), but a close comparison of the structures reveals some differences. The latter have mixed frameworks of MoO_4 tetrahedra and pairs of MO_6 octahedra sharing common edges, whereas in structure (I) MO_6 octahedra and also Mg_2O_{10} units surrounded by MoO_4 tetrahedra are present. A further comparison of the structure of compound (I) with the $Li_2M_2(MoO_4)_3$ family (M=Mg, Mn, Co, Ni, Cu, Zn) (Efremov & Trunov, 1972; Ozima & Zoltai, 1976) reveals that the substitution of some of the lithium ions by aluminium has changed the crystal structure. The latter family adopts the lyonsite structure type, space group *Pnma*, and their general formula can be written as $A_{16}B_{12}O_{48}$. Generally, the A site is statistically occupied by Li^+ and a M^{2+} ion.

S2. Experimental

The title compound, $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$, was obtained serendipitously by a solid state reaction from appropriate quantities of $LiNO_3$ (Fluka, 62575), $(NH_4)_2Mo_4O_{13}$ (Fluka, 69858) and $Mg(NO_3)_2{\cdot}6H_2O$ (Fluka, 63079) placed in a porcelain crucible, and slowly annealed in air at 623 K for 12 h, in order to eliminate volatile products. The resulting mixture was then heated to 853 K for 7 days before slowly cooling at 5 K/day to 773 K. Finally, the furnace was cooled at 50 K/day to room temperature. A qualitative EDX analysis of a selected crystal using a FEI Quanta 200 system revealed the presence of Al, Mo, Mg and O (Fig. 6). Aluminium was not present in the employed educts of the reaction mixture, but the incorporation of aluminium from the porcelain crucible is the most likely source of this element.

S3. Refinement

During the first stages of refinement the site in the channels was first attributed solely to Li. However, the refined composition did not satisfy electrical neutrality. After considering the presence of Al (see 'experimental part') on this site with an occupancy ratio of 1:1 for Li and Al, electrical neutrality was achieved. Both metals were refined with the same coordinates and the same anisotropic displacement parameters.

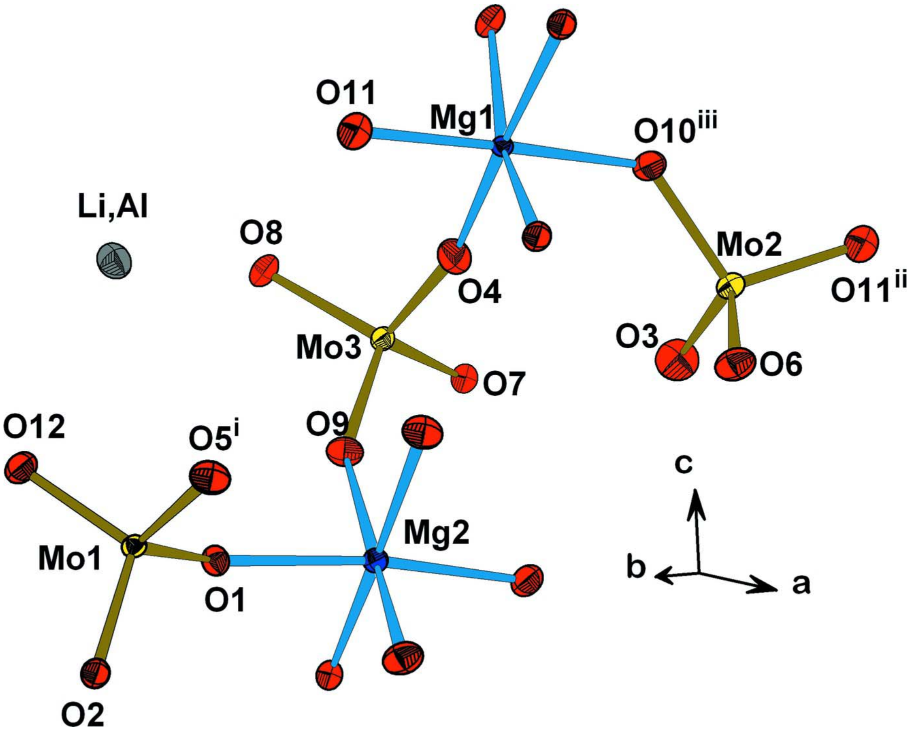

Figure 1

Expanded asymmetric unit of $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$ showing the main building units. All atoms are represented as displacement ellipsoids at the 50% probability level. [*Symmetry codes*: (i) *x*, *y+1*, *z*; (ii) *x+1*, *y*, *z*; (iii) *x*, *y*, *z*+1.]

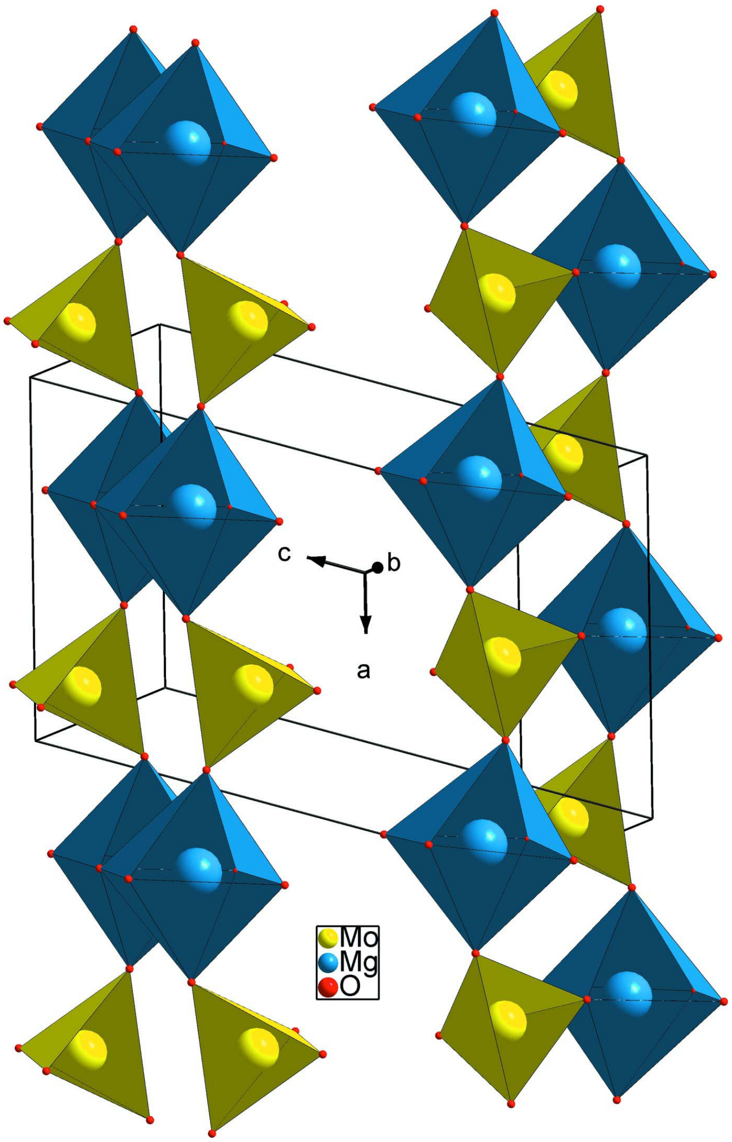

Figure 2

The two types of double chains with composition $(Mg_2Mo_2O_{14})_n$, (*a*) in *cis* arrangement, (*b*) in *trans* arrangement.

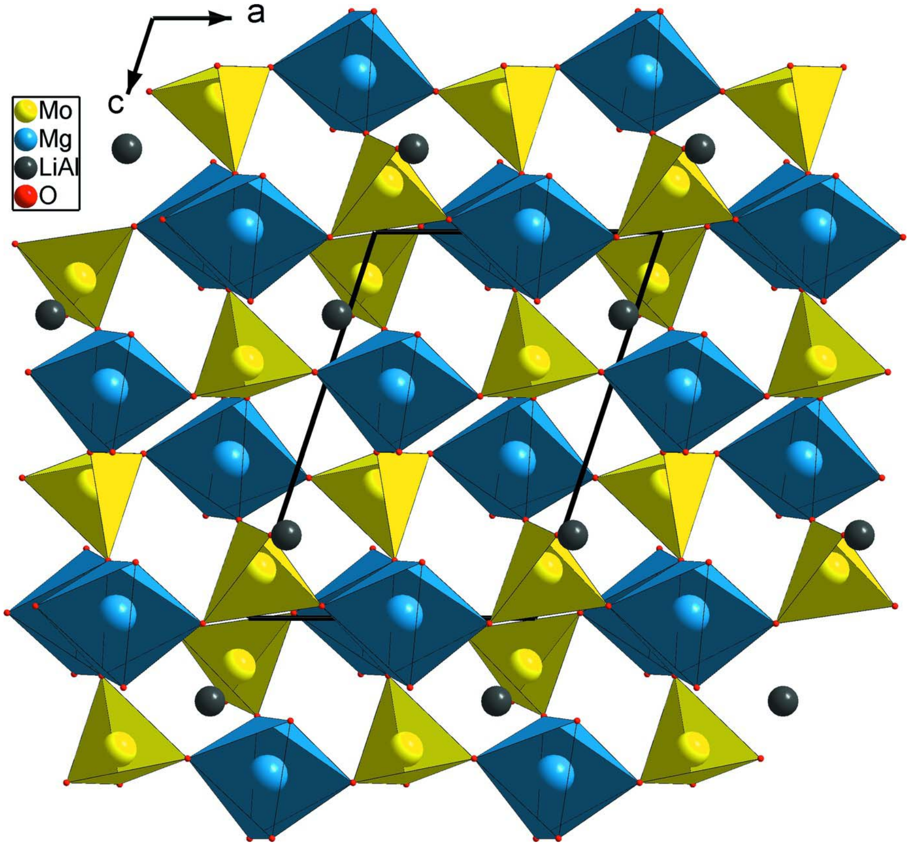

Figure 3

The projection of the $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$ structure showing the layer parallel to (010).

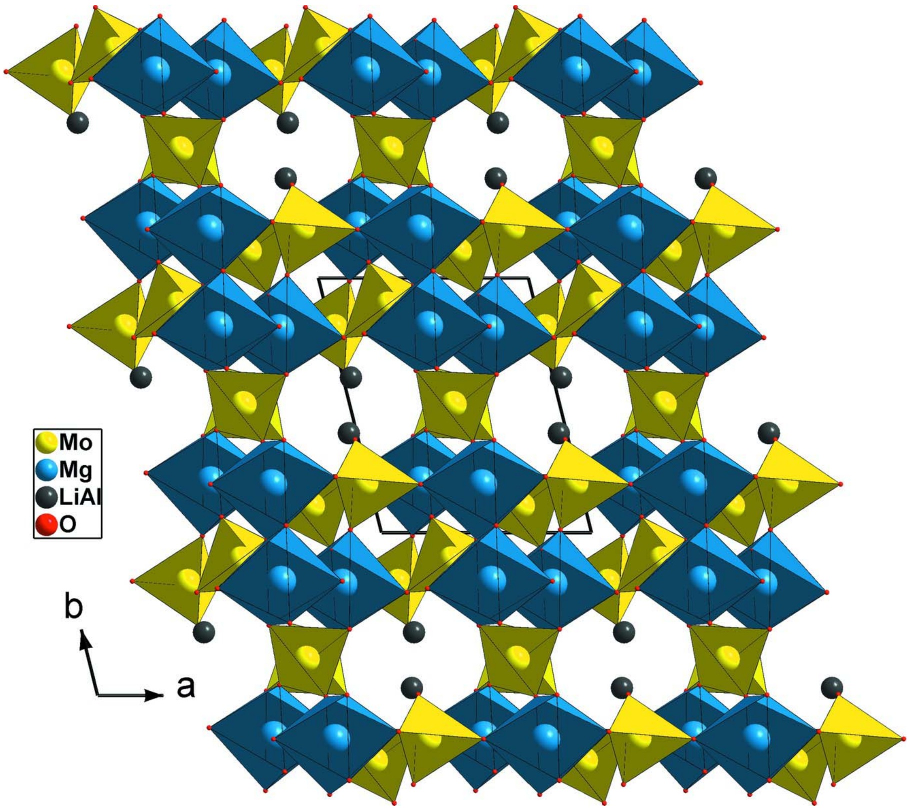

Figure 4

Projection of $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$ along [001].

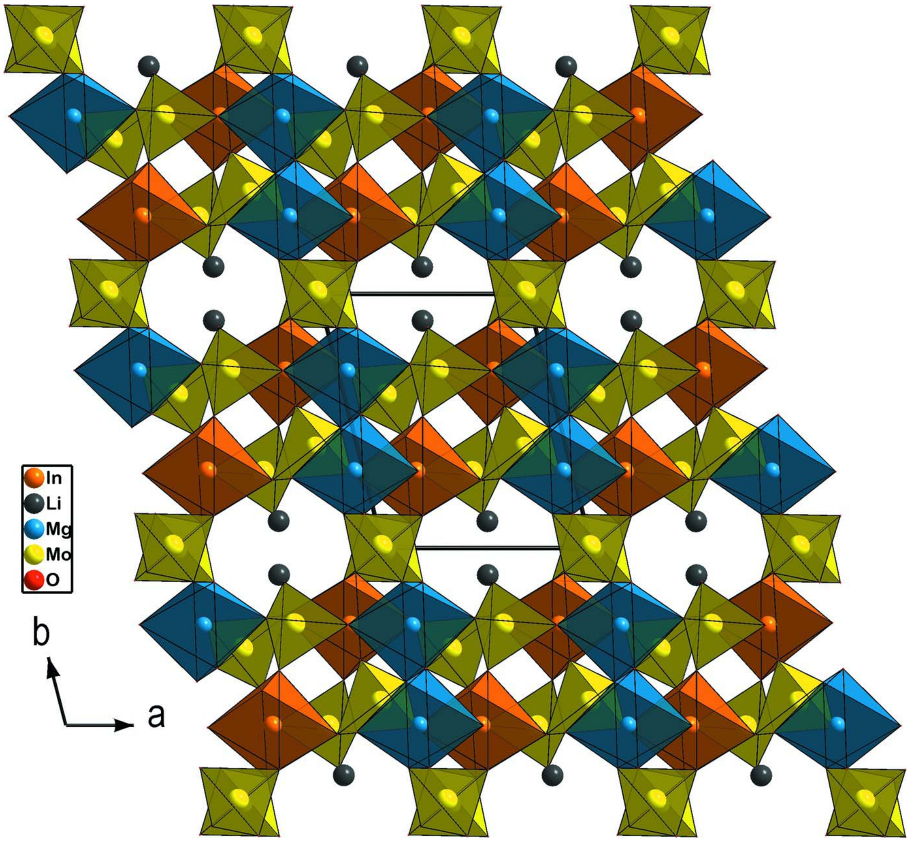

Figure 5

Projection of the isotypic structure of LiMgIn$(MoO_4)_3$ along [010].

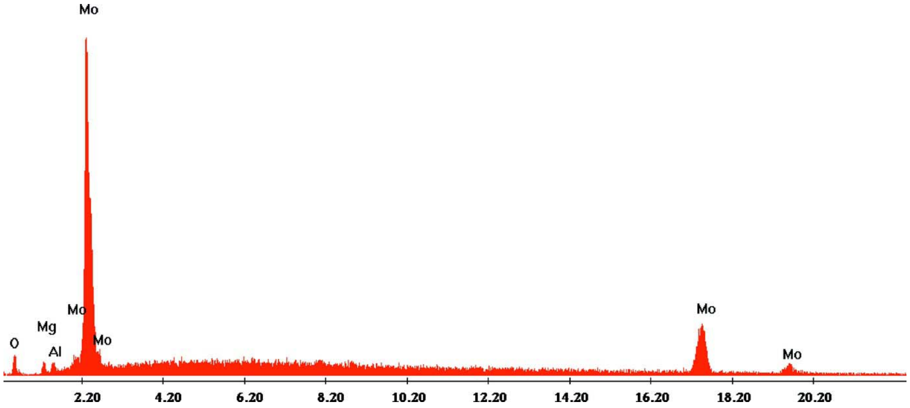

Figure 6

Qualitative EDX analysis of $Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$, showing the presence of Al.

Lithium aluminium dimagnesium tetrakismolybdate

Crystal data

$Li_{0.5}Al_{0.5}Mg_2(MoO_4)_3$	$a = 6.8555$ (7) Å
$M_r = 545.40$	$b = 8.2910$ (9) Å
Triclinic, $P\overline{1}$	$c = 9.5760$ (9) Å
Hall symbol: -P 1	$\alpha = 96.032$ (7)°

β = 106.743 (8)°
γ = 101.824 (9)°
V = 502.27 (9) Å^3
Z = 2
F(000) = 508
D_x = 3.606 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 25 reflections
θ = 10–15°
μ = 3.92 mm^{-1}
T = 298 K
Prism, colourless
0.2 × 0.18 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min}$ = 0.520, $T_{\max}$ = 0.648
3450 measured reflections

2187 independent reflections
2150 reflections with $I > 2s\sigma(I)$
R_{int} = 0.014
$\theta_{\max}$ = 27.0°, $\theta_{\min}$ = 2.3°
$h = -8 \rightarrow 4$
$k = -10 \rightarrow 10$
$l = -12 \rightarrow 12$
2 standard reflections every 120 min
intensity decay: 1.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.053
S = 1.29
2187 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0096P)^2 + 2.5823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.57 e Å^{-3}
$\Delta\rho_{\min}$ = −0.81 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0123 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Mo1	0.30272 (5)	0.89586 (4)	0.66046 (3)	0.00921 (10)	
Mo2	0.98153 (5)	0.19503 (4)	0.87863 (4)	0.01148 (10)	
Mo3	0.49457 (5)	0.50622 (4)	0.74760 (3)	0.00964 (10)	
Mg1	0.53871 (19)	0.19031 (15)	0.99366 (13)	0.0071 (2)	
Mg2	0.2478 (2)	0.20149 (16)	0.40750 (14)	0.0096 (2)	
Li1	0.0379 (4)	0.6097 (3)	0.7889 (3)	0.0200 (5)	0.50
Al1	0.0379 (4)	0.6097 (3)	0.7889 (3)	0.0200 (5)	0.50
O1	0.0505 (4)	0.7660 (3)	0.6386 (3)	0.0131 (5)	
O2	0.4454 (4)	0.9765 (4)	0.8546 (3)	0.0147 (6)	

O3	0.9874 (5)	0.3666 (4)	0.7886 (4)	0.0252 (7)
O4	0.5435 (5)	0.3564 (4)	0.8579 (3)	0.0212 (6)
O5	0.2586 (5)	0.0618 (4)	0.5726 (3)	0.0197 (6)
O6	0.8558 (5)	0.0118 (4)	0.7493 (3)	0.0212 (6)
O7	0.7368 (4)	0.6232 (4)	0.7376 (3)	0.0138 (5)
O8	0.3563 (4)	0.6386 (4)	0.8234 (3)	0.0151 (6)
O9	0.3363 (5)	0.4040 (4)	0.5737 (3)	0.0165 (6)
O10	0.8481 (5)	0.2198 (4)	0.0140 (3)	0.0180 (6)
O11	0.2432 (5)	0.1911 (4)	0.9700 (4)	0.0226 (7)
O12	0.4468 (5)	0.7896 (4)	0.5776 (3)	0.0177 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.00817 (16)	0.01051 (16)	0.00822 (16)	0.00090 (12)	0.00288 (12)	0.00056 (11)
Mo2	0.01273 (17)	0.01071 (17)	0.01133 (17)	0.00244 (12)	0.00502 (12)	0.00086 (12)
Mo3	0.00894 (16)	0.01052 (16)	0.00917 (16)	0.00232 (12)	0.00293 (12)	0.00046 (11)
Mg1	0.0077 (6)	0.0069 (6)	0.0065 (5)	0.0020 (4)	0.0020 (4)	0.0006 (4)
Mg2	0.0088 (6)	0.0097 (6)	0.0094 (6)	0.0014 (5)	0.0027 (5)	0.0008 (5)
Li1	0.0172 (10)	0.0215 (11)	0.0203 (11)	0.0038 (9)	0.0046 (9)	0.0060 (9)
Al1	0.0172 (10)	0.0215 (11)	0.0203 (11)	0.0038 (9)	0.0046 (9)	0.0060 (9)
O1	0.0111 (13)	0.0137 (13)	0.0147 (13)	0.0028 (10)	0.0041 (11)	0.0044 (11)
O2	0.0121 (13)	0.0172 (14)	0.0128 (13)	0.0036 (11)	0.0025 (11)	−0.0018 (11)
O3	0.0305 (18)	0.0179 (15)	0.0298 (17)	0.0038 (13)	0.0127 (15)	0.0103 (13)
O4	0.0207 (15)	0.0250 (16)	0.0204 (15)	0.0089 (13)	0.0064 (13)	0.0084 (13)
O5	0.0244 (16)	0.0160 (14)	0.0180 (15)	0.0025 (12)	0.0064 (12)	0.0054 (12)
O6	0.0240 (16)	0.0198 (15)	0.0170 (15)	0.0020 (13)	0.0071 (13)	−0.0033 (12)
O7	0.0124 (13)	0.0158 (13)	0.0140 (13)	0.0050 (11)	0.0047 (11)	0.0024 (11)
O8	0.0136 (13)	0.0153 (14)	0.0175 (14)	0.0030 (11)	0.0081 (11)	−0.0004 (11)
O9	0.0187 (14)	0.0140 (14)	0.0126 (13)	0.0001 (11)	0.0028 (11)	−0.0011 (11)
O10	0.0222 (15)	0.0206 (15)	0.0150 (14)	0.0092 (12)	0.0084 (12)	0.0040 (12)
O11	0.0200 (15)	0.0275 (17)	0.0219 (16)	0.0080 (13)	0.0079 (13)	0.0031 (13)
O12	0.0147 (14)	0.0219 (15)	0.0157 (14)	0.0038 (12)	0.0056 (11)	−0.0016 (12)

Geometric parameters (Å, º)

Mo1—O5^{i}	1.721 (3)	Mg1—O4	1.992 (3)
Mo1—O12	1.745 (3)	Mg1—O10^{iii}	2.033 (3)
Mo1—O1	1.781 (3)	Mg1—O2^{v}	2.104 (3)
Mo1—O2	1.812 (3)	Mg2—O12^{vi}	2.042 (3)
Mo2—O3	1.738 (3)	Mg2—O1^{vii}	2.045 (3)
Mo2—O6	1.743 (3)	Mg2—O9	2.046 (3)
Mo2—O11^{ii}	1.763 (3)	Mg2—O5	2.049 (3)
Mo2—O10^{iii}	1.807 (3)	Mg2—O6^{viii}	2.049 (3)
Mo3—O9	1.718 (3)	Mg2—O7^{vi}	2.121 (3)
Mo3—O4	1.736 (3)	Li1—O3^{ix}	1.974 (4)
Mo3—O7	1.777 (3)	Li1—O7^{ix}	2.009 (4)
Mo3—O8	1.812 (3)	Li1—O1	2.044 (4)

Mg1—O2^{iv}	1.968 (3)	Li1—O8	2.070 (4)
Mg1—O11	1.974 (3)	Li1—O10^{vi}	2.076 (4)
Mg1—O8^{v}	1.983 (3)		
O5^{i}—Mo1—O12	108.83 (15)	O11—Mg1—O2^{v}	94.31 (13)
O5^{i}—Mo1—O1	106.36 (14)	O8^{v}—Mg1—O2^{v}	82.89 (12)
O12—Mo1—O1	111.36 (14)	O4—Mg1—O2^{v}	176.13 (14)
O5^{i}—Mo1—O2	108.44 (14)	O10^{iii}—Mg1—O2^{v}	91.76 (12)
O12—Mo1—O2	111.03 (13)	O12^{vi}—Mg2—O1^{vii}	166.46 (14)
O1—Mo1—O2	110.64 (13)	O12^{vi}—Mg2—O9	91.79 (13)
O3—Mo2—O6	109.58 (16)	O1^{vii}—Mg2—O9	86.88 (13)
O3—Mo2—O11^{ii}	108.05 (16)	O12^{vi}—Mg2—O5	92.20 (14)
O6—Mo2—O11^{ii}	109.67 (15)	O1^{vii}—Mg2—O5	101.11 (13)
O3—Mo2—O10^{iii}	108.85 (15)	O9—Mg2—O5	85.35 (13)
O6—Mo2—O10^{iii}	111.40 (15)	O12^{vi}—Mg2—O6^{viii}	91.25 (13)
O11^{ii}—Mo2—O10^{iii}	109.23 (14)	O1^{vii}—Mg2—O6^{viii}	91.06 (13)
O9—Mo3—O4	107.98 (15)	O9—Mg2—O6^{viii}	175.12 (14)
O9—Mo3—O7	109.75 (14)	O5—Mg2—O6^{viii}	90.72 (14)
O4—Mo3—O7	109.09 (14)	O12^{vi}—Mg2—O7^{vi}	85.67 (13)
O9—Mo3—O8	108.76 (14)	O1^{vii}—Mg2—O7^{vi}	80.80 (12)
O4—Mo3—O8	109.30 (14)	O9—Mg2—O7^{vi}	86.40 (12)
O7—Mo3—O8	111.88 (13)	O5—Mg2—O7^{vi}	171.41 (13)
O2^{iv}—Mg1—O11	90.13 (14)	O6^{viii}—Mg2—O7^{vi}	97.64 (13)
O2^{iv}—Mg1—O8^{v}	163.23 (14)	O3^{ix}—Li1—O7^{ix}	97.36 (16)
O11—Mg1—O8^{v}	92.29 (13)	O3^{ix}—Li1—O1	137.17 (18)
O2^{iv}—Mg1—O4	102.01 (14)	O7^{ix}—Li1—O1	83.58 (14)
O11—Mg1—O4	88.75 (14)	O3^{ix}—Li1—O8	93.03 (16)
O8^{v}—Mg1—O4	94.64 (14)	O7^{ix}—Li1—O8	168.56 (17)
O2^{iv}—Mg1—O10^{iii}	94.68 (13)	O1—Li1—O8	85.55 (14)
O11—Mg1—O10^{iii}	172.82 (15)	O3^{ix}—Li1—O10^{vi}	121.05 (17)
O8^{v}—Mg1—O10^{iii}	84.64 (13)	O7^{ix}—Li1—O10^{vi}	97.16 (15)
O4—Mg1—O10^{iii}	85.04 (13)	O1—Li1—O10^{vi}	101.10 (15)
O2^{iv}—Mg1—O2^{v}	80.38 (13)	O8—Li1—O10^{vi}	81.44 (14)

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*+1, *y*, *z*; (iii) *x*, *y*, *z*+1; (iv) *x*, *y*−1, *z*; (v) −*x*+1, −*y*+1, −*z*+2; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) −*x*, −*y*+1, −*z*+1; (viii) −*x*+1, −*y*, −*z*+1; (ix) *x*−1, *y*, *z*.