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$CsAl(MoO_4)_2$

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Al–O) = 0.002 Å
R factor = 0.015
wR factor = 0.043
Data-to-parameter ratio = 13.8

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

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The title compound, caesium aluminium dimolybdate(VI), $CsAl(MoO_4)_2$, belongs to the glaserite type family of double molybdates and tungstates. The crystal structure was studied by *in situ* X-ray single-crystal and powder diffraction at room temperature. The temperature dependence of the lattice parameters at low temperatures is also presented.

Comment

Double molybdates and tungstates with the general formula $M^{I}M^{III}(M^{VI}O_4)_2$, where M^{I} = alkali metal, M^{III} = Al, In, Cr, Bi, Fe, RE (rare earths), and M^{VI} = Mo or W, exhibit interesting structural and physicochemical properties, and are used as acousto-optic filters, second-harmonic generators and laser crystals. They exhibit ferroelectric, ferroelastic or even ferromagnetic properties and have been extensively studied for the last 40 years. $CsAl(MoO_4)_2$ belongs to this family.

The room temperature phase of $CsAl(MoO_4)_2$ was refined in the trigonal space group $P\bar{3}m1$ (No. 164), as for many other double molybdates and tungstates of the glaserite structure (Efremov *et al.*, 1971, Klevtsov *et al.*, 1972, Klevtsova & Klevtsov, 1970, Klevtsova *et al.*, 1995, Lii *et al.*, 1989, Tomaszewski *et al.* 2002). The structure consists of $[AlMo_2O_8^{-}]_n$ layers perpendicular to the trigonal c-axis, with the caesium cations between the layers. Each layer is built up from MoO_4 tetrahedra and AlO_6 octahedra; each octahedron shares its six corners with six MoO_4 tetrahedra.

The additional low-temperature experiments do not show any changes in the powder-diffraction diagram, thus indicating no symmetry changes and the absence of a phase transition. The low-temperature lattice parameters are as follows: a = 5.525 (2), c = 7.966 (3) Å at 110 K and a = 5.513 (3), c = 7.954 (4) Å at 40 K. The lattice parameter a changes linearly with temperature, while the temperature dependence of the parameter c is quadratic.

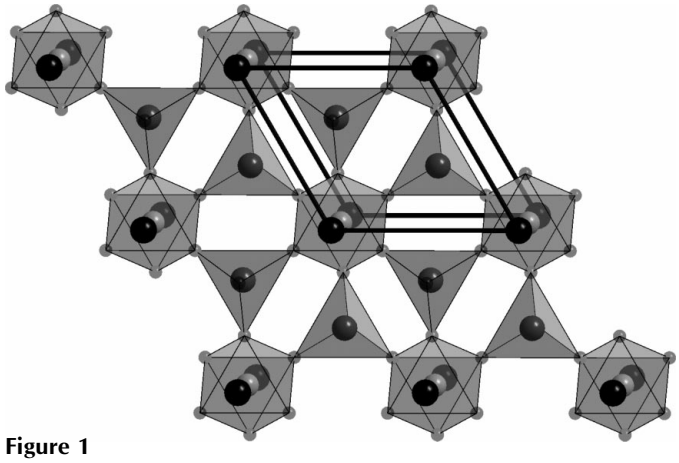

Figure 1
View of $CsAl(MoO_4)_2$, approximately down the c axis.

Experimental

Single crystals of $CsAl(MoO_4)_2$ were grown by cooling a molten mixture containing $CsAl(MoO_4)_2$ and solvent ($Cs_2Mo_2O_7$) in a 1:1 ratio. The cooling rate was 2 K h^{-1}. The resulting single crystals were colourless and of good optical quality.

Crystal data

$CsAl(MoO_4)_2$	Mo $K\alpha$ radiation
M_r = 479.77	Cell parameters from all reflections
Trigonal, $P\bar{3}m1$	θ = 4.2–29.0°
a = 5.551 (1) Å	μ = 7.21 mm^{-1}
c = 8.037 (2) Å	T = 293 (2) K
V = 214.47 (8) $Å^3$	Plate, colourless
Z = 1	0.20 × 0.20 × 0.10 mm
D_x = 3.715 Mg m^{-3}	

Data collection

KUMA Diffraction KM-4 CCD diffractometer	249 independent reflections
ω scans	248 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (*XEMP*; Sheldrick, 1991)	R_{int} = 0.045
T_{min} = 0.068, T_{max} = 0.155	θ_{max} = 29.0°
2447 measured reflections	$h = -7 \rightarrow 5$
	$k = -7 \rightarrow 7$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.017P)^2 + 0.22P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.015	$(\Delta/\sigma)_{max}$ = 0.027
$wR(F^2)$ = 0.043	$\Delta\rho_{max}$ = 0.65 e $Å^{-3}$
S = 1.37	$\Delta\rho_{min}$ = −0.36 e $Å^{-3}$
249 reflections	Extinction correction: *SHELXL*
18 parameters	Extinction coefficient: 0.253 (6)

Table 1
Selected geometric parameters (Å, °).

Cs—O1^{i}	3.2716 (9)	Mo—O1	1.721 (4)
Cs—O2^{ii}	3.287 (2)	Mo—O2	1.763 (2)
Al—O2	1.883 (2)		
O2—Al—O2^{iii}	88.98 (10)	O2—Mo—O2^{iv}	111.28 (7)
O1—Mo—O2	107.60 (8)		

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $x, y, z-1$; (iii) $-y, x-y, z$; (iv) $1-y, 1+x-y, z$.

The complementary studies on the temperature dependence of lattice parameters were performed on a Siemens D5000 diffractometer, working in θ–θ Bragg–Brentano geometry with Cu $K\alpha$ radiation. The powder diagrams were recorded at temperatures 295, 110 and 40 K in a 2θ range of 10–55°, with a step size of 0.02°. The temperature was set and stabilized by an Anton Paar circulated-gaseous-helium low-temperature attachment.

Data collection: *KM*-4 *CCD Software* (KUMA Diffraction, 1998); cell refinement: *KM*-4 *CCD Software*; data reduction: *KM*-4 CCD *Data Reduction Software* (KUMA Diffraction, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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