Hexamolybdenum Octatelluride, Mo$_6$Te$_8$

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Disciplines
Materials Chemistry | Other Chemistry | Physical Chemistry

Comments
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Hexamolybdenum Octatelluride, Mo$_6$Te$_8$

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Abstract

The title compound, isotypic with Mo$_6$Se$_8$, contains Mo$_6$Te$_8$ clusters. All eight faces of a distorted octahedral Mo cluster [Mo---Mo 2.699 (2), 2.785 (2) Å] are capped by Te atoms, six of which also provide bridges to neighboring clusters.

Comment

Mo$_6$Te$_8$ was reported in 1970 (Grandjean et al., 1970) to be isostructural with Mo$_6$Se$_8$ (Bars et al., 1973), based on photographically recorded diffraction patterns. Lattice constants were given. During the course of our studies on ternary molybdenum chalcogenide systems, crystals of Mo$_6$Te$_8$ were synthesized by chemical-transport reactions using a number of transport agents. The best crystals were grown using Sb or As at 1273 K. The material can be prepared in single-phase yield by direct combination of the elements at this temperature. Mo$_6$Te$_8$ obviously bears a close structural relationship to the important Chevrel phases M$_x$Mo$_6$Q$_8$ (M = alkali metal, alkaline earth, 3d transition metal, lanthanide, actinide or other cation; x < 4; Q = S, Se, Te), the superconducting and critical magnetic field properties of which have generated a great deal of synthetic and theoretical interest (see Etourneau, 1992). As such, Mo$_6$Te$_8$ warrants a complete structural determination.

The title compound contains interlinked Mo$_6$Te$_8$ clusters, the central metal cluster moiety of which is a distorted octahedral Mo$_6$ cluster. The distortion takes the form of an elongation of the cluster in the c direction, generating short [2.699 (2) Å] Mo—Mo distances in the crystallographic ab plane and long [2.785 (2) Å] Mo—Mo distances along the c direction. A distorted cube of Te atoms surrounds the Mo$_6$ cluster, with six Te2 atoms capping six of the faces of the Mo$_6$ cluster [Mo—Te2 2.711 (1), 2.777 (2) and 2.781 (2) Å] and Te1 atoms capping the other two faces, forming three bonds with Mo—Te1 2.732 (2) Å. The six Te2 atoms provide bridges to neighboring Mo$_6$Te$_8$ groups (Fig. 1) at the six cluster vertex sites. The distances from the vertex Mo to each bridging Te2 are equivalent [2.818 (1) Å].

Since the reactions that produced the crystals used for the present determination employed As or Sb, the possibility of incorporation of a ternary element must be addressed. In the Chevrel phases, the ternary M atom resides in the large eight-coordinate spaces formed by the chalcogens from eight different Mo$_6$Q$_8$ units. The corresponding position in Mo$_6$Te$_8$ is (0, 0, 1/2), but the Fourier map shows no significant features at this position (1.9 e Å$^{-3}$). Furthermore, qualitative energy-dispersive spectroscopy compositional analysis using a JEOL 6100 scanning electron microscope confirmed the presence of only Mo and Te in multiple crystal samples.

Experimental

Black reflective cubic crystals of Mo$_6$Te$_8$ formed as byproducts of reactions loaded according to the stoichiometry Mo$_3$X$_3$Te (X = As, Sb), and heated at 1273 K for 7 d in sealed evacuated fused-silica tubes. The compound can be synthesized in single-phase yield by stoichiometric reaction of the elements at 1273 K.

Crystal data

Mo$_6$Te$_8$
$M_r = 1596.44$
Hexagonal
$R$3
$a = 10.1790 (10) \ \text{Å}$
$c = 11.674 (2) \ \text{Å}$
$V = 1047.5 (2) \ \text{Å}^3$
$Z = 3$
$D_r = 7.592 \ \text{Mg} \ \text{m}^{-3}$
$D_m$ not measured

Data collection

Siemens $P4$ diffractometer
$\omega$ scans

$\theta_{\text{max}} = 25^\circ$

$R_{\text{int}} = 0.067$

Mo $K\alpha$ radiation
$\lambda = 0.71073 \ \text{Å}$

Cell parameters from 50 reflections
$\theta = 5.8-25.0^\circ$
$\mu = 21.560 \ \text{mm}^{-1}$
$T = 293 (2) \ \text{K}$
Block
$0.10 \times 0.07 \times 0.06 \ \text{mm}$

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Absorption correction:  
ψ scans (SHELXL93; Sheldrick, 1993)  
T_{min} = 0.234, T_{max} = 0.274  
604 measured reflections  
413 independent reflections  
398 reflections with  
I > 2σ(I)  

Refinement  
Refinement on F^2  
R[F > 4σ(F)] = 0.039  
wR(F^2) = 0.109  
S = 1.187  
413 reflections  
23 parameters  
Scattering factors from International Tables for Crystallography (Vol. C)  
Extinction correction:  
SHELXL93  
Extinction coefficient:  
0.00112 (13)  
(Δ/σ)_{max} < 0.001  

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)  

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>U_{eq}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo</td>
<td>-0.14367 (12)</td>
<td>0.01736 (13)</td>
<td>0.09888 (9)</td>
<td>0.0157 (5)</td>
</tr>
<tr>
<td>Te1</td>
<td>0</td>
<td>0</td>
<td>0.29112 (11)</td>
<td>0.0189 (5)</td>
</tr>
<tr>
<td>Te2</td>
<td>-0.36957 (10)</td>
<td>0.00200 (10)</td>
<td>0.24699 (7)</td>
<td>0.0181 (5)</td>
</tr>
</tbody>
</table>

A peak of 1.9 e Å^-3 remained in the final difference Fourier map. It is located 2.44 Å from Te1 at (0,0,1/2), but is small considering the heavy atoms in the structure.


Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1198). Services for accessing these data are described at the back of the journal.

References


