

CdTh[MoO<sub>4</sub>]<sub>3</sub>*hP*34(176) *P*6<sub>3</sub>/*m* – ih<sup>3</sup>cb**CdTh(MoO<sub>4</sub>)<sub>3</sub>** [1]

Structural features: ThO<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms, CdO<sub>6</sub> octahedra (infinite columns of face-linked octahedra) and MoO<sub>4</sub> tetrahedra share atoms to form a 3D-framework. Filled-up derivative of ht-Yb(ReO<sub>4</sub>)<sub>3</sub>.

Launay S., Rimsky A. (1980) [1]

CdMo<sub>3</sub>O<sub>12</sub>Th*a* = 0.9803, *c* = 0.635 nm, *c/a* = 0.648, *V* = 0.5285 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.465	0.2159	0.0282		single atom Mo
O2	6 <i>h</i>	<i>m</i> ..	0.0478	0.4879	<sup>1</sup> / <sub>4</sub>		single atom Mo
O3	6 <i>h</i>	<i>m</i> ..	0.1818	0.0185	<sup>1</sup> / <sub>4</sub>		single atom Mo
Mo4	6 <i>h</i>	<i>m</i> ..	0.3883	0.0982	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
Th5	2 <i>c</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism O <sub>9</sub>
Cd6	2 <i>b</i>	-3..	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: *y*,*x*,*-z*Experimental: single crystal, diffractometer, X-rays, *R* = 0.040

References: [1] Launay S., Rimsky A. (1980), Acta Crystallogr. B 36, 910-912.