

Cd<sub>5</sub>[VO<sub>4</sub>]<sub>3</sub>I

hP58

(176)  $P6_3/m - ih^4fe^4a$ **Cd<sub>5</sub>(VO<sub>4</sub>)<sub>3</sub>I** [1], apatite family

Structural features: Infinite columns of base-linked CdO<sub>6</sub> trigonal prisms share vertices with VO<sub>4</sub> tetrahedra to form a 3D-framework; I in infinite columns of face-linked Cd<sub>6</sub> octahedra (partial vacancies ignored) parallel to [001] (high degree of disorder).

Sudarsanan K. et al. (1977) [1]

Cd<sub>4.64</sub>I<sub>0.74</sub>O<sub>12</sub>V<sub>3</sub> $a = 1.0307$ ,  $c = 0.6496$  nm,  $c/a = 0.630$ ,  $V = 0.5976$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.343	0.0733	0.0413		single atom V
O2	6h	<i>m</i> ..	0.1571	0.5223	<sup>1</sup> / <sub>4</sub>		single atom V
Cd3	6h	<i>m</i> ..	0.2894	0.2458	<sup>1</sup> / <sub>4</sub>	0.899	non-coplanar triangle O <sub>3</sub>
V4	6h	<i>m</i> ..	0.4113	0.0263	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O5	6h	<i>m</i> ..	0.6076	0.1478	<sup>1</sup> / <sub>4</sub>		single atom V
Cd6	4f	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0037	0.97	trigonal prism O <sub>6</sub>
I7	4e	3..	0	0	0.05	0.049	
I8	4e	3..	0	0	0.1	0.076	
I9	4e	3..	0	0	0.15	0.08	
I10	4e	3..	0	0	0.2	0.118	
I11	2a	-6..	0	0	<sup>1</sup> / <sub>4</sub>	0.09	

Transformation from published data: *y*,*x*,*-z*

Experimental: single crystal, diffractometer, X-rays, R = 0.043

Remarks: No significant electron density was detected in Wyckoff position 2*b* (occ.(I) < 0). Short interatomic distances for partly occupied site(s).

References: [1] Sudarsanan K., Young R.A., Wilson A.J.C. (1977), Acta Crystallogr. B 33, 3136-3142.