

Cd₃In₂[C₂O₄]₆[H₂O]₉

hP153

(180) *P*6₂22 – k⁹i²g³dcb**Cd₃In₂(C₂O₄)₆·9H₂O [1]**

Structural features: InO₈ square antiprisms and planar O₂C-CO₂ (oxalate) units share atoms to form infinite zigzag chains, which are interconnected via CdO₈ and Cd(O₄[OH₂]₄) polyhedra to form a 3D-framework; additional H₂O between the units.

Jeanneau E. et al. (2003) [1]

C₁₂Cd₃H_{18.04}In₂O_{33.02}*a* = 0.8566, *c* = 3.7811 nm, *c/a* = 4.414, *V* = 2.4027 nm³, *Z* = 3

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.1205	0.2897	0.1412		single atom C
O2	12 <i>k</i>	1	0.2052	0.0355	0.12603		single atom C
(OH ₂)3	12 <i>k</i>	1	0.2111	0.5183	0.20513		single atom Cd
C4	12 <i>k</i>	1	0.2261	0.3213	0.1162		coplanar triangle O ₂ C
O5	12 <i>k</i>	1	0.2438	0.3099	0.02183		single atom C
C6	12 <i>k</i>	1	0.2782	0.1775	0.1079		coplanar triangle O ₂ C
O7	12 <i>k</i>	1	0.2951	0.4606	0.09723		single atom C
O8	12 <i>k</i>	1	0.3916	0.2141	0.08373		single atom C
O9	12 <i>k</i>	1	0.5785	0.3304	0.02143		single atom C
C10	6 <i>i</i>	..2	0.1928	0.3856	0		coplanar triangle O ₂ C
C11	6 <i>i</i>	..2	0.2952	0.5904	0		coplanar triangle O ₂ C
(OH ₂)12	6 <i>g</i>	.2.	0.244	0	0		single atom Cd
(OH ₂)13	6 <i>f</i>	2..	¹ / ₂	0	0.05743		single atom Cd
In14	6 <i>f</i>	2..	¹ / ₂	0	0.27804		square antiprism O ₈
(OH ₂)15	6 <i>f</i>	2..	¹ / ₂	0	0.38353	0.51	non-coplanar square C ₄
Cd16	3 <i>d</i>	222	¹ / ₂	0	¹ / ₂		square antiprism (OH ₂) ₄ O ₄
Cd17	3 <i>c</i>	222	¹ / ₂	0	0		coplanar square (OH ₂) ₄
Cd18	3 <i>b</i>	222	0	0	¹ / ₂		8-vertex polyhedron O ₈

Transformation from published data (*P*6₄22): new axes -a,-b,-c; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.036

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Jeanneau E., Audebrand N., Louer D. (2003), J. Solid State Chem. 173, 387-394.