

Na<sub>2</sub>CdZr[C<sub>2</sub>O<sub>4</sub>]<sub>4</sub>[H<sub>2</sub>O]<sub>8.5</sub>

hP108

(180) *P*6<sub>2</sub>22 – k<sup>7</sup>f<sup>2</sup>dcba**Na<sub>2</sub>CdZr(C<sub>2</sub>O<sub>4</sub>)<sub>4</sub>·8.5H<sub>2</sub>O** [1]

Structural features: CdO<sub>8</sub> and ZrO<sub>8</sub> square antiprisms share edges (of the square faces) with planar O<sub>2</sub>C-CO<sub>2</sub> (oxalate) units to form a 3D-framework; Na and H<sub>2</sub>O in channels parallel to [001].

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

C<sub>8</sub>CdH<sub>16</sub>Na<sub>2</sub>O<sub>24</sub>Zr*a* = 0.8793, *c* = 2.453 nm, *c/a* = 2.790, *V* = 1.6425 nm<sup>3</sup>, *Z* = 3

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.0889	0.342	0.2134		single atom C
(OH <sub>2</sub> )2	12 <i>k</i>	1	0.206	0.187	0.08923		single atom Na
C3	12 <i>k</i>	1	0.211	0.416	0.2483		non-coplanar triangle O <sub>2</sub> C
O4	12 <i>k</i>	1	0.232	0.5487	0.11423		single atom C
O5	12 <i>k</i>	1	0.259	0.3398	0.2805		single atom C
C6	12 <i>k</i>	1	0.297	0.617	0.2495		non-coplanar triangle O <sub>2</sub> C
O7	12 <i>k</i>	1	0.564	0.258	0.05693		single atom C
(OH <sub>2</sub> )8	6 <i>f</i>	2..	<sup>1</sup> / <sub>2</sub>	0	0.16723		tetrahedron O <sub>2</sub> C <sub>2</sub>
(OH <sub>2</sub> )9	6 <i>f</i>	2..	<sup>1</sup> / <sub>2</sub>	0	0.33407		non-colinear O <sub>2</sub>
Zr10	3 <i>d</i>	222	<sup>1</sup> / <sub>2</sub>	0	<sup>1</sup> / <sub>2</sub>		square antiprism O <sub>8</sub>
Cd11	3 <i>c</i>	222	<sup>1</sup> / <sub>2</sub>	0	0		square antiprism O <sub>8</sub>
Na12	3 <i>b</i>	222	0	0	<sup>1</sup> / <sub>2</sub>		8-vertex polyhedron (OH <sub>2</sub> ) <sub>4</sub> O <sub>4</sub>
Na13	3 <i>a</i>	222	0	0	0		8-vertex polyhedron (OH <sub>2</sub> ) <sub>4</sub> O <sub>4</sub>

Transformation from published data (*P*6<sub>4</sub>22): new axes -a,-b,-c

Experimental: single crystal, diffractometer, X-rays, R = 0.098

Remarks: Part of H<sub>2</sub>O not located; we set the occupancy of site (OH<sub>2</sub>)9 equal to unity (published value 1.26(10)). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Jeanneau E., Audebrand N., Le Floch M., Bureau B., Louer D. (2003), J. Solid State Chem. 170, 330-338.