$[NH_4]_2CdZr[C_2O_4]_4[H_2O]_{3.9}$	*hP*96	(180) $P6_222$ – k^7dcba

$(NH_4)_2CdZr(C_2O_4)_4 \cdot 3.9H_2O$ [1]
Structural features: CdO_8 and ZrO_8 square antiprisms share edges (of the square faces) with planar O_2C-CO_2 (oxalate) units to form a 3D-framework; NH_4 and H_2O in channels parallel to [001]. Substitution derivative of $NH_4[In(C_2O_4)_2] \cdot 2H_2O$.

Jeanneau E. et al. (2002) [1]
$C_8CdH_{15.89}N_2O_{19.94}Zr$
$a = 0.9061$, $c = 2.3394$ nm, $c/a = 2.582$, $V = 1.6634$ nm^3, $Z = 3$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*k*	1	0.0832	0.3488	0.21451		single atom C
C2	12*k*	1	0.2109	0.4193	0.24807		coplanar triangle O_2C
O3	12*k*	1	0.2209	0.5461	0.11243		single atom C
O4	12*k*	1	0.2435	0.2461	0.08287	0.986	tetrahedron O_2N_2
O5	12*k*	1	0.2629	0.343	0.27768		single atom C
C6	12*k*	1	0.3011	0.6157	0.24907		coplanar triangle O_2C
O7	12*k*	1	0.5646	0.2612	0.05797		single atom C
Zr8	3*d*	222	$^1/_2$	0	$^1/_2$		square antiprism O_8
Cd9	3*c*	222	$^1/_2$	0	0		square antiprism O_8
N10	3*b*	222	0	0	$^1/_2$		8-vertex polyhedron O_8
N11	3*a*	222	0	0	0		8-vertex polyhedron O_8
H12	12*k*	1	0.074	0.1002	0.14227		
H13	12*k*	1	0.1	0.079	0.02433		
H14	12*k*	1	0.256	0.357	0.08467	0.986	
H15	12*k*	1	0.358	0.085	0.24667	0.986	

Transformation from published data ($P6_422$): new axes -a,-b,-c
Experimental: single crystal, diffractometer, X-rays, R = 0.031

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

References: [1] Jeanneau E., Audebrand N., Louer D. (2002), Chem. Mater. 14, 1187-1194.