

*hP*48

(180) $P6_222 - k^2j^2hca$

$\text{NH}_4[\text{In}(\text{C}_2\text{O}_4)_2] \cdot 2\text{H}_2\text{O}$ [1]; $\text{NH}_4[\text{Ti}(\text{C}_2\text{O}_4)_2] \cdot 2\text{H}_2\text{O}$ [2]

Structural features: InO_8 square antiprisms share edges (of the square faces) with planar $\text{O}_2\text{C}-\text{CO}_2$ (oxalate) units to form a 3D-framework; NH_4 and H_2O in channels parallel to $[001]$. See Fig. IV.45.

Bulc N. et al. (1983) [1]

$\text{C}_4\text{H}_8\text{InNO}_{10}$

$a = 0.9025$, $c = 1.1343$ nm, $c/a = 1.257$, $V = 0.8001$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.3117	0.5531	0.22207		single atom C
O2	12 <i>k</i>	1	0.3468	0.0787	0.10527		single atom C
C3	6 <i>j</i>	$\bar{2}$	0.2109	0.4219	$\frac{1}{2}$		non-colinear O ₂
C4	6 <i>j</i>	$\bar{2}$	0.3097	0.6195	$\frac{1}{2}$		non-colinear O ₂
(OH ₂)5	6 <i>h</i>	$\bar{2}$	0.248	0	$\frac{1}{2}$		tetrahedron O ₂ (NH ₄) ₂
In6	3 <i>c</i>	222	$\frac{1}{2}$	0	0		square antiprism O ₈
(NH ₄)7	3 <i>a</i>	222	0	0	0		8-vertex polyhedron (OH ₂) ₄ O ₄

Experimental: single crystal, diffractometer, X-rays, $R = 0.024$, $T = 293$ K

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

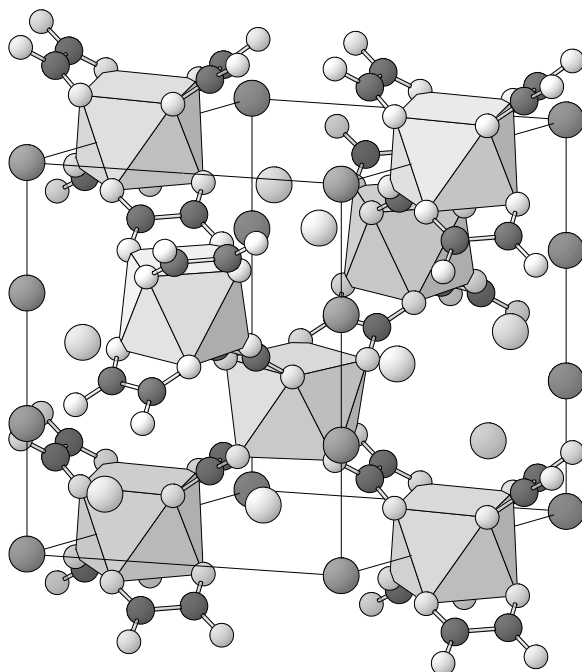


Fig. IV.45. **$\text{NH}_4[\text{In}(\text{C}_2\text{O}_4)_2] \cdot 2\text{H}_2\text{O}$**

Arrangement of InO_8 square antiprisms, C_2O_4 units (C atoms small dark, O atoms small light), NH_4 units (N atoms large dark) and H_2O molecules (O atoms large light).

References: [1] Bulc N., Golic L., Siftar J. (1983), *Acta Crystallogr. C* 39, 176-178. [2] English R.B., Eve D.J. (1993), *Inorg. Chim. Acta* 203, 219-222.