

(NH₄)₂Cr₃O₁₀ hexagonal [1]

Structural features: Finite chains formed by three vertex-linked CrO₄ tetrahedra. See Fig. IV.82.

Blum D., Guitel J.C. (1980) [1]

Cr₃H₈N₂O₁₀

a = 1.1945, *c* = 1.2797 nm, *c/a* = 1.071, *V* = 1.5813 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.095	0.4237	0.1379		non-colinear Cr ₂
O2	12 <i>i</i>	1	0.2589	0.0894	0.092		single atom Cr
O3	12 <i>i</i>	1	0.3514	0.3929	0.0501		single atom Cr
Cr4	12 <i>i</i>	1	0.37193	0.05679	0.07129		tetrahedron O ₄
O5	12 <i>i</i>	1	0.5041	0.1703	0.1227		single atom Cr
O6	6 <i>h</i>	<i>m</i> ..	0.1437	0.2583	¹ / ₄		single atom Cr
Cr7	6 <i>h</i>	<i>m</i> ..	0.16219	0.39945	¹ / ₄		tetrahedron O ₄
O8	6 <i>h</i>	<i>m</i> ..	0.3128	0.5044	¹ / ₄		single atom Cr
(NH ₄)9	6 <i>h</i>	<i>m</i> ..	0.4281	0.3282	¹ / ₄		10-vertex polyhedron O ₁₀
(NH ₄)10	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0522		icosahedron O ₁₂
(NH ₄)11	2 <i>b</i>	-3..	0	0	0		octahedron O ₆

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.040

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the *z*-coordinate of former Cr(1) is misprinted as 0.007129 instead of 0.07129 (checked on interatomic distances).

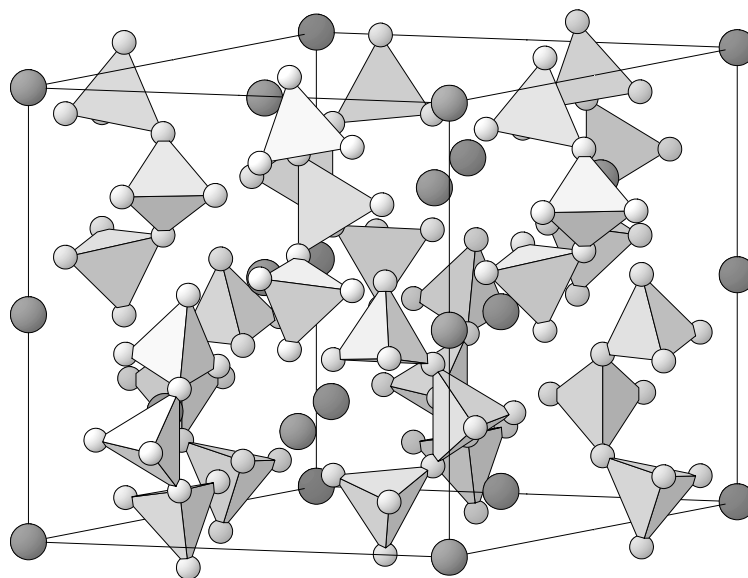


Fig. IV.82. (NH₄)₂Cr₃O₁₀ hexagonal

Arrangement of CrO₄ tetrahedra (O atoms small) and NH₄ units (N atoms large).

References: [1] Blum D., Guitel J.C. (1980), Acta Crystallogr. B 36, 135-137.

