$Zn_2Mo_3O_8$	*hP*26	(186) $P6_3mc$ – c^3b^3a

$Zn_2Mo_3O_8$ [2]

Structural features: Close-packed O layers in hc stacking; Mo in octahedral, Zn in octahedral and tetrahedral voids. Infinite slabs of edge-linked MoO_6 octahedra are interconnected via ZnO_6 octahedra and ZnO_4 tetrahedra to form a 3D-framework. Ordering variant of tohdite, $Al_2O_3 \cdot 0.2H_2O$. See Fig. IV.27.

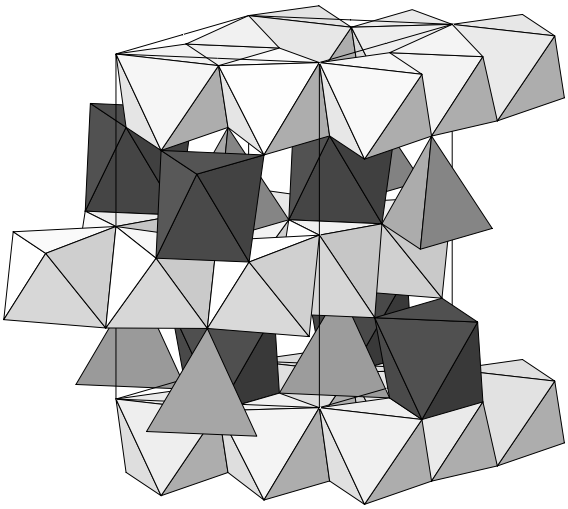

Fig. IV.27. **$Zn_2Mo_3O_8$**

Arrangement of ZnO_4 tetrahedra (medium), ZnO_6 (dark) and MoO_6 (light) octahedra.

Ansell G.B., Katz L. (1966) [1]

$Mo_3O_8Zn_2$

$a = 0.5759$, $c = 0.9903$ nm, $c/a = 1.720$, $V = 0.2844$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Mo1	6*c*	.*m*.	0.1461	0.8539	0.3614		octahedron O_6
O2	6*c*	.*m*.	0.4861	0.5139	0.4753		tetrahedron Zn_2Mo_2
O3	6*c*	.*m*.	0.8353	0.1647	0.2468		non-coplanar triangle Mo_2Zn
Zn4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0579		tetrahedron O_4
O5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2584		tetrahedron $ZnMo_3$
Zn6	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.6246		octahedron O_6
O7	2*a*	3*m*.	0	0	0.0		non-coplanar triangle Mo_3

Transformation from published data: origin shift 0 0 0.8886

Experimental: single crystal, diffractometer, X-rays, R = 0.069

Remarks: A refinement on powder neutron diffraction data collected at 13 K is reported in [3].

References: [1] Ansell G.B., Katz L. (1966), Acta Crystallogr. 21, 482-485. [2] McCarroll W.H., Katz L., Ward R. (1957), J. Am. Chem. Soc. 79, 5410-5414. [3] Hibble S.J., Cooper S.P., Patat S., Hannon A.C. (1999), Acta Crystallogr. B 55, 683-697.