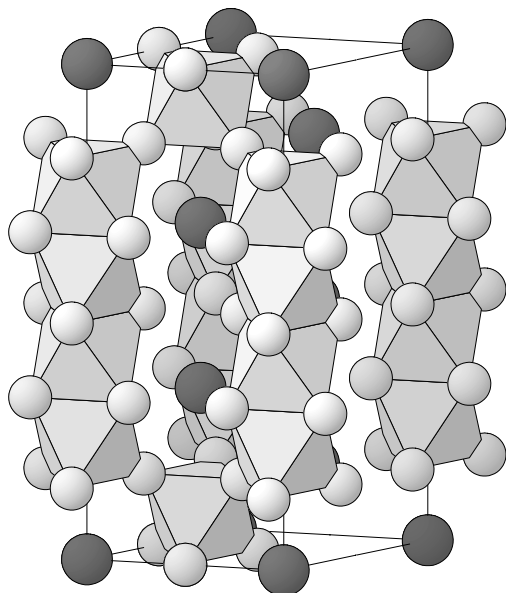


BaMnO₃ 6H [1], perovskite 6H

Structural features: Close-packed BaO₃ layers in hch₃c stacking; Mn in octahedral (O₆) voids. Units of four and two face-linked MnO₆ octahedra share vertices to form a 3D-framework. See Fig. IV.14.

Fig. IV.14. **BaMnO₃ 6H**

Arrangement of MnO₆ octahedra (O atoms light) and Ba atoms (dark).

Negas T., Roth R.S. (1971) [1]

BaMnO₃

$a = 0.5683$, $c = 1.4096$ nm, $c/a = 2.480$, $V = 0.3943$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6n	.m.	0.16667	0.83333	0.16667		colinear Mn ₂
O2	6n	.m.	0.83333	0.16667	0.33333		non-colinear Mn ₂
O3	3k	mm2	0.16667	0.83333	$\frac{1}{2}$		non-colinear Mn ₂
O4	3j	mm2	0.5	0.5	0		non-colinear Mn ₂
Ba5	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.16667		cuboctahedron O ₁₂
Mn6	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.08333		octahedron O ₆
Ba7	2h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.33333		anticuboctahedron O ₁₂
Mn8	2g	3m.	0	0	0.25		octahedron O ₆
Mn9	2g	3m.	0	0	0.41667		octahedron O ₆
Ba10	1f	-6m2	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		anticuboctahedron O ₁₂
Ba11	1a	-6m2	0	0	0		anticuboctahedron O ₁₂

Transformation from published data: $-x, -y, -z$

Experimental: powder, diffractometer, X-rays

Remarks: Phase stable at $1623 < T < 1748$ K in air; homogeneity range BaMnO_{3-x}, $0.10 < x < 0.15$. The cell parameters correspond to the O-poor boundary. Idealized coordinates. O vacancies not located.

References: [1] Negas T., Roth R.S. (1971), J. Solid State Chem. 3, 323-339.