

BaMnO_{2.83}*hP40*(187) *P-6m2* – n³kji²h²g³da**BaMnO_{2.83} 8H** [1], perovskite 8HStructural features: Close-packed BaO₃ layers in hchch₄ stacking; Mn in octahedral (O₆) voids. Units of six and two face-linked MnO₆ octahedra share vertices to form a 3D-framework.

Gonzalez Calbet J.M. et al. (1993) [1]

BaMnO₃*a* = 0.57, *c* = 1.9 nm, *c/a* = 3.333, *V* = 0.5346 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>n</i>	. <i>m</i> .	0.16667	0.83333	0.125		colinear Mn ₂
O2	6 <i>n</i>	. <i>m</i> .	0.16667	0.83333	0.375		non-colinear Mn ₂
O3	6 <i>n</i>	. <i>m</i> .	0.83333	0.16667	0.25		non-colinear Mn ₂
O4	3 <i>k</i>	<i>mm</i> 2	0.83333	0.16667	¹ / ₂		non-colinear Mn ₂
O5	3 <i>j</i>	<i>mm</i> 2	0.5	0.5	0		non-colinear Mn ₂
Ba6	2 <i>i</i>	3 <i>m</i> .	² / ₃	¹ / ₃	0.125		cuboctahedron O ₁₂
Ba7	2 <i>i</i>	3 <i>m</i> .	² / ₃	¹ / ₃	0.375		anticuboctahedron O ₁₂
Mn8	2 <i>h</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.0625		octahedron O ₆
Ba9	2 <i>h</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.25		anticuboctahedron O ₁₂
Mn10	2 <i>g</i>	3 <i>m</i> .	0	0	0.1875		octahedron O ₆
Mn11	2 <i>g</i>	3 <i>m</i> .	0	0	0.3125		octahedron O ₆
Mn12	2 <i>g</i>	3 <i>m</i> .	0	0	0.4375		octahedron O ₆
Ba13	1 <i>d</i>	-6 <i>m</i> 2	¹ / ₃	² / ₃	¹ / ₂		anticuboctahedron O ₁₂
Ba14	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		anticuboctahedron O ₁₂

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

Experimental: polycrystalline sample, electron diffraction

Remarks: O vacancies not located. On page 102 of [1] the *z*-coordinates of former O1 and O2 are interchanged (checked on interatomic distances).

References: [1] Gonzalez Calbet J.M., Parras M., Alonso J.M., Vallet Regi M. (1993), J. Solid State Chem. 106, 99-110.