$Ba_4(Ca_{0.9}Mn_{0.1})Mn_3O_{11.3}$	*hP*78	(187) *P*-6*m*2 – $n^6kji^5h^6g^6da$

$Ba_4Ca_{0.9}Mn_{3.1}O_{11.3}$ [2]
Structural features: Perovskite-type slabs (seven close-packed BaO_3 layers in $c_2h_3c_2$ stacking) alternate with triangle-mesh BaO_2 layers along [001]; (Ca,Mn) in octahedral, Mn in octahedral and tetrahedral voids. Single $(Mn,Ca)O_6$ octahedra share vertices with units of four face-sharing $(Mn,Ca)O_6$ octahedra and single MnO_4 tetrahedra.

Floros N. et al. (2002) [1]
$Ba_4Ca_{0.90}Mn_{3.10}O_{11.50}$
$a = 0.5772$, $c = 3.86$ nm, $c/a = 6.687$, $V = 1.1137$ nm^3, $Z = 4$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*n*	.*m*.	0.14833	0.85167	0.439		non-colinear Mn_2
O2	6*n*	.*m*.	0.18633	0.81367	0.0625		non-colinear Mn_2
O3	6*n*	.*m*.	0.47833	0.52167	0.3051		single atom Mn
O4	6*n*	.*m*.	0.48733	0.51267	0.1242		non-colinear MnCa
O5	6*n*	.*m*.	0.83533	0.16467	0.1935		single atom Mn
O6	6*n*	.*m*.	0.84333	0.15667	0.3779		non-colinear MnCa
O7	3*k*	*mm*2	0.85633	0.14367	$^1/_2$		non-colinear Mn_2
O8	3*j*	*mm*2	0.48133	0.51867	0		non-colinear Mn_2
Ba9	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.05817		anticuboctahedron O_{12}
M10	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.1523		octahedron O_6
Ba11	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.2502		octahedron O_6
Ca12	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.3441		octahedron O_6
Ba13	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.4442		anticuboctahedron O_{12}
Mn14	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.0292		octahedron O_6
Mn15	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.0981		octahedron O_6
Ba16	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.17903		11-vertex polyhedron $O_{10}Mn$
O17	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.246		single atom Mn
Mn18	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.2871		tetrahedron O_4
Ba19	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.3891		9-vertex polyhedron O_9
Ba20	2*g*	3*m*.	0	0	0.1116		9-vertex polyhedron O_9
Mn21	2*g*	3*m*.	0	0	0.209		tetrahedron O_4
O22	2*g*	3*m*.	0	0	0.2501		single atom Mn
Ba23	2*g*	3*m*.	0	0	0.3183		10-vertex polyhedron O_{10}
Mn24	2*g*	3*m*.	0	0	0.4056		octahedron O_6
Mn25	2*g*	3*m*.	0	0	0.4659		octahedron O_6
Ba26	1*d*	-6*m*2	$^1/_3$	$^2/_3$	$^1/_2$		anticuboctahedron O_{12}
Ba27	1*a*	-6*m*2	0	0	0		anticuboctahedron O_{12}

M10 = 0.8Ca + 0.2Mn
Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ 0
Experimental: single crystal, diffractometer, X-rays, wR = 0.035, T = 294 K

Remarks: Splitting of the O site in the BaO_2 layer was found from a refinement on powder neutron diffraction data (see also [3]).

References: [1] Floros N., Hervieu M., Michel C., Perez O., Raveau B., Suard E. (2002), Solid State Sci. 4, 627-632. [2] Floros N., Michel C., Hervieu M., Raveau B. (2000), Chem. Mater. 12, 3197-3201. [3] Schuddinck W., Van Tendeloo G., Hervieu M., Floros N., Raveau B. (2001), Mater. Res. Bull. 36, 2689-2700.