$Ba_4(Ca_{0.9}Mn_{0.1})Mn_3O_{11.3}$	*hP*82	(187) *P*-6*m*2 – $n^7kji^5h^5g^6cb$

$Ba_4Ca_{0.9}Mn_{3.1}O_{11.3}$ [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 (one split O site) along [001]; (Ca,Mn) in octahedral, Mn in octahedral and tetrahedral voids. CaO_6 octahedra share vertices with units of four face-sharing MnO_6 octahedra and single MnO_4 tetrahedra.

Floros N. et al. (2002) [1]
$Ba_4Ca_{0.90}Mn_{3.10}O_{11.50}$
$a = 0.58005$, $c = 3.8954$ nm, $c/a = 6.716$, $V = 1.1350$ nm^3, $Z = 4$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*n*	.*m*.	0.14433	0.85567	0.062		non-colinear Mn_2
O2	6*n*	.*m*.	0.17933	0.82067	0.439		non-colinear Mn_2
O3	6*n*	.*m*.	0.29333	0.70667	0.251	0.333	
O4	6*n*	.*m*.	0.48933	0.51067	0.377		non-colinear MnCa
O5	6*n*	.*m*.	0.49133	0.50867	0.196		single atom Mn
O6	6*n*	.*m*.	0.84133	0.15867	0.308		non-colinear MnCa
O7	6*n*	.*m*.	0.84733	0.15267	0.121		non-colinear MnCa
O8	3*k*	*mm*2	0.48333	0.51667	$^1/_2$		non-colinear Mn_2
O9	3*j*	*mm*2	0.85733	0.14267	0		non-colinear Mn_2
Ba10	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.053		9-vertex polyhedron O_9
Ca11	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.154		octahedron O_6
Ba12	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.248		octahedron O_6
M13	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.345		octahedron O_6
Ba14	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.441		anticuboctahedron O_{12}
Ba15	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.108		9-vertex polyhedron O_9
Mn16	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.207		
Ba17	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.324		
Mn18	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.405		octahedron O_6
Mn19	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.467		octahedron O_6
Mn20	2*g*	3*m*.	0	0	0.03		octahedron O_6
Mn21	2*g*	3*m*.	0	0	0.097		octahedron O_6
Ba22	2*g*	3*m*.	0	0	0.18		10-vertex polyhedron O_{10}
O23	2*g*	3*m*.	0	0	0.248		single atom Mn
Mn24	2*g*	3*m*.	0	0	0.286		tetrahedron O_4
Ba25	2*g*	3*m*.	0	0	0.386		9-vertex polyhedron O_9
Ba26	1*c*	-6*m*2	$^1/_3$	$^2/_3$	0		anticuboctahedron O_{12}
Ba27	1*b*	-6*m*2	0	0	$^1/_2$		anticuboctahedron O_{12}

M13 = 0.8Ca + 0.2Mn
Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ $^1/_2$
Experimental: powder, diffractometer, neutrons, $R_B = 0.057$

Remarks: O vacancies not located. Short interatomic distances for partly occupied site(s). Ideal position for site O3 was found from a refinement on single-crystal neutron diffraction, as well as from a previous refinement on powder X-ray diffraction data in [3]. Preliminary data are reported in [2], where O vacancies are proposed for sites O4 and O5.

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