Sr_9Mg_{38}	*hP*94	(194) $P6_3/mmc$ – $k^5h^2gf^3e$

Sr_9Mg_{38} [1]
Structural features: Sr_6 octahedral clusters and Sr_3 trigonal clusters in a matrix of Mg atoms.

Merlo F., Fornasini M.L. (1982) [1]
$Mg_{38}Sr_9$
a = 1.0500, c = 2.8251 nm, c/a = 2.691, V = 2.6974 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sr1	12*k*	.*m*.	0.1362	0.2724	0.5621		7-capped pentagonal prism $Mg_{13}Sr_4$
Mg2	12*k*	.*m*.	0.1674	0.3348	0.1533		icosahedron Mg_8Sr_4
Mg3	12*k*	.*m*.	0.1743	0.3486	0.6898		icosahedron Mg_9Sr_3
Mg4	12*k*	.*m*.	0.2337	0.4674	0.0547		icosahedron Mg_9Sr_3
Mg5	12*k*	.*m*.	0.5037	0.0074	0.1170		pseudo Frank-Kasper $Mg_{10}Sr_3$
Mg6	6*h*	*mm*2	0.0989	0.1978	$^1/_4$		icosahedron $Mg_{10}Sr_2$
Sr7	6*h*	*mm*2	0.4688	0.9376	$^1/_4$		pseudo Frank-Kasper $Mg_{16}Sr_2$
Mg8	6*g*	.2/*m*.	$^1/_2$	0	0		icosahedron Mg_8Sr_4
Mg9	4*f*	3*m*.	$^1/_3$	$^2/_3$	0.1465		icosahedron Mg_9Sr_3
Mg10	4*f*	3*m*.	$^1/_3$	$^2/_3$	0.5378		pseudo Frank-Kasper $Mg_{10}Sr_3$
Mg11	4*f*	3*m*.	$^1/_3$	$^2/_3$	0.6426		7-vertex polyhedron Mg_7
Mg12	4*e*	3*m*.	0	0	0.1575		icosahedron Mg_9Sr_3

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.061

Remarks: Supersedes a structure proposal in [2] where site Mg8 was not detected ($SrMg_4$). In [2] the x-coordinate of former Sr(h) is misprinted as -0.478 instead of 0.0478 and the z-coordinate of former Mg(f2) as 0.1427 instead of -0.1427 (see [1] and [3]).

References: [1] Merlo F., Fornasini M.L. (1982), Acta Crystallogr. B 38, 1797-1798. [2] Wang F.E., Kanda F.A., Miskell C.F., King A.J. (1965), Acta Crystallogr. 18, 24-31. [3] (1975), Structure Reports 30A, 24.