

SrMg₄

hP90

(194) $P6_3/mmc - k^5h^2gf^2e$

SrMg₄ [1]

Structural features: Sr₆ octahedral clusters and Sr₃ trigonal clusters in a matrix of Mg atoms.

Wang F.E. et al. (1965) [1]

Mg₄Sr

$a = 1.0511$, $c = 2.8362$ nm, $c/a = 2.698$, $V = 2.7137$ nm³, $Z = 18$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sr1	12k	.m.	0.1369	0.2738	0.0625		7-capped pentagonal prism Mg ₁₃ Sr ₄
Mg2	12k	.m.	0.1677	0.3354	0.654		11-vertex polyhedron Mg ₇ Sr ₄
Mg3	12k	.m.	0.1772	0.3544	0.1897		icosahedron Mg ₉ Sr ₃
Mg4	12k	.m.	0.2321	0.4642	0.5546		11-vertex polyhedron Mg ₈ Sr ₃
Mg5	12k	.m.	0.5	0.0	0.1177		icosahedron Mg ₉ Sr ₃
Sr6	6h	mm2	0.522	0.044	1/4		cuboctahedron Mg ₁₂
Mg7	6h	mm2	0.8989	0.7978	1/4		icosahedron Mg ₁₀ Sr ₂
Mg8	6g	.2/m.	1/2	0	0		icosahedron Mg ₈ Sr ₄
Mg9	4f	3m.	1/3	2/3	0.0373		pseudo Frank-Kasper Mg ₁₀ Sr ₃
Mg10	4f	3m.	1/3	2/3	0.1427		7-vertex polyhedron Mg ₇
Mg11	4e	3m.	0	0	0.158		icosahedron Mg ₉ Sr ₃

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.120

Remarks: An additional Mg site was detected in [2]. In table 3 of [1] the x-coordinate of former Sr(h) is misprinted as 0.0478 instead of -0.478, and the z-coordinate of former Mg(f2) as -0.1427 instead of 0.1427 (checked on interatomic distances).

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