

Cs₅Mo₂₁Se₂₃

hP98

(176) $P6_3/m - i^6h^2f^2ea$ **Cs₅Mo₂₁Se₂₃** [1]

Structural features: Mo₂₁Se₂₃ units (a Mo₂₁ cluster formed by six face-sharing Mo₆ octahedra, one Se above each edge and the terminal faces) in a Mg-type (h.c.p.) arrangement.

Gougeon P. et al. (1990) [1]

Cs₅Mo₂₁Se₂₃
 $a = 0.96513$, $c = 2.9939$ nm, $c/a = 3.102$, $V = 2.4151$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	12 <i>i</i>	1	0.3342	0.2903	0.17533		4-vertex polyhedron Mo ₄
Se2	12 <i>i</i>	1	0.3376	0.2936	0.02958		4-vertex polyhedron Mo ₄
Se3	12 <i>i</i>	1	0.3764	0.0063	0.09918		4-vertex polyhedron Mo ₄
Mo4	12 <i>i</i>	1	0.4987	0.3153	0.10037		10-vertex polyhedron Se ₄ Mo ₆
Mo5	12 <i>i</i>	1	0.5184	0.1647	0.17488		10-vertex polyhedron Se ₄ Mo ₆
Mo6	12 <i>i</i>	1	0.5195	0.1653	0.02395		tricapped trigonal prism Se ₅ Mo ₄
Se7	6 <i>h</i>	<i>m</i> ..	0.0003	0.378	¹ / ₄		4-vertex polyhedron Mo ₄
Mo8	6 <i>h</i>	<i>m</i> ..	0.4981	0.3122	¹ / ₄		10-vertex polyhedron Se ₄ Mo ₆
Se9	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.04328		non-coplanar triangle Mo ₃
Cs10	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.16787		10-vertex polyhedron Se ₁₀
Cs11	4 <i>e</i>	3..	0	0	0.09476		tricapped trigonal prism Se ₉
Cs12	2 <i>a</i>	-6..	0	0	¹ / ₄		tricapped trigonal prism Se ₉

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.034, T = 295 K

References: [1] Gougeon P., Potel M., Sergent M. (1990), Acta Crystallogr. C 46, 2284-2287.