

CsCrF<sub>4</sub>*hP18*(189) *P-62m-jg<sup>2</sup>f<sup>2</sup>***CsCrF<sub>4</sub>** [1]Structural features: Triple infinite chains of vertex-linked CrF<sub>6</sub> octahedra.

Babel D., Knoke G. (1978) [1]

CrCsF<sub>4</sub> $a = 0.965$ ,  $c = 0.3857$  nm,  $c/a = 0.400$ ,  $V = 0.3111$  nm<sup>3</sup>,  $Z = 3$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	6 <i>j</i>	<i>m.</i>	0.15968	0.43654	0		single atom Cr
F2	3 <i>g</i>	<i>m2m</i>	0.2201	0	<sup>1</sup> / <sub>2</sub>		non-colinear Cr <sub>2</sub>
Cs3	3 <i>g</i>	<i>m2m</i>	0.57237	0	<sup>1</sup> / <sub>2</sub>		trigonal prism F <sub>6</sub>
Cr4	3 <i>f</i>	<i>m2m</i>	0.22382	0	0		octahedron F <sub>6</sub>
F5	3 <i>f</i>	<i>m2m</i>	0.83493	0	0		non-colinear Cr <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.023

Remarks: Supersedes a report on CsCrF<sub>4</sub> with an orthorhombic cell in [2]. The authors state that the hexagonal cell with double *c*-parameter proposed in [3] is probably also wrong.

References: [1] Babel D., Knoke G. (1978), Z. Anorg. Allg. Chem. 442, 151-162. [2] Babel D., Wall F., Heger G. (1974), Z. Naturforsch. B 29, 139-148. [3] De Kozak A. (1971), Rev. Chim. Miner. 8, 301-337.