

MoSe₆C₆[CF₃]₆*hP*74(176) *P*6₃/*m* – i⁶d**Mo[(CF₃)₂C₂Se₂]₃** [1]

Structural features: Mo(C₄Se₂F₆)₃ units (a MoSe₆ trigonal prism sharing atoms with three F₃C-C(Se)-C(Se)-CF₃ units) in a Mg-type (h.c.p.) arrangement.

Pierpont C.G., Eisenberg R. (1971) [1]

C₁₂F₁₈MoSe₆*a* = 1.003, *c* = 1.43 nm, *c/a* = 1.426, *V* = 1.2459 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	12 <i>i</i>	1	0.011	0.341	0.2018		non-coplanar triangle C ₂ Se
F2	12 <i>i</i>	1	0.104	0.333	0.055		single atom C
C3	12 <i>i</i>	1	0.129	0.333	0.138		tetrahedron F ₃ C
F4	12 <i>i</i>	1	0.148	0.218	0.157		single atom C
F5	12 <i>i</i>	1	0.264	0.445	0.15		single atom C
Se6	12 <i>i</i>	1	0.5019	0.1326	0.1341		single atom C
Mo7	2 <i>d</i>	-6..	² / ₃	¹ / ₃	¹ / ₄		trigonal prism Se ₆

Transformation from published data: *y*,*x*,*z*Experimental: single crystal, diffractometer, X-rays, *R* = 0.041

Remarks: Tris[*cis*-1,2-di(trifluoromethyl)ethylene-1,2-diselenato] molybdenum. Two-fold rotational disorder of the CF₃ groups was found for Mo[(CF₃)₂C₂S₂]₃ in [2].

References: [1] Pierpont C.G., Eisenberg R. (1971), J. Chem. Soc. A 1971, 2285-2289. [2] Wang K., McConnachie J.M., Stiefel E.I. (1999), Inorg. Chem. 38, 4334-4341.