$MoC_6[CF_3]_6S_6$	*hP*110	(176) $P6_3/m$ – i^9d

$Mo[(CF_3)_2C_2S_2]_3$ [1]
Structural features: $Mo(C_4S_2F_6)_3$ units (a MoS_6 trigonal prism sharing atoms with three F_3C-C(S)-C(S)-CF_3 units; two-fold rotational disorder for CF_3) in a Mg-type (h.c.p.) arrangement.

Wang K. et al. (1999) [1]
$C_{12}F_{18}MoS_6$
a = 0.96795, c = 1.3951 nm, c/a = 1.441, V = 1.1320 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12*i*	1	0.0687	0.2837	0.0473	0.56	single atom F
F2	12*i*	1	0.0839	0.1926	0.1291	0.44	single atom F
C3	12*i*	1	0.1273	0.3366	0.1363		7-vertex polyhedron F_6C
F4	12*i*	1	0.1321	0.3995	0.0554	0.44	single atom F
F5	12*i*	1	0.168	0.2318	0.1697	0.56	single atom F
F6	12*i*	1	0.2624	0.4707	0.136	0.56	
F7	12*i*	1	0.2655	0.4205	0.175	0.44	
C8	12*i*	1	0.3387	0.0001	0.201		non-coplanar triangle C_2S
S9	12*i*	1	0.5013	0.1357	0.1393		single atom C
Mo10	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		trigonal prism S_6

Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, diffractometer, X-rays, R = 0.104, T = 294 K

Remarks: Tris[cis-1,2-di(trifluoromethyl)ethylene-1,2-disulfato] molybdenum. Short interatomic distances for partly occupied site(s).

References: [1] Wang K., McConnachie J.M., Stiefel E.I. (1999), Inorg. Chem. 38, 4334-4341.