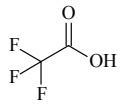
189 **$C_2HF_3O_2$** **Trifluoroacetic acid** **C_s**

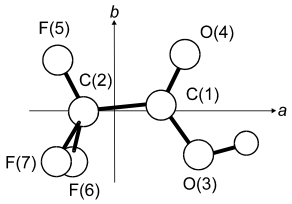
MW



r_s	Å [a])	θ_s	deg [a])
C(1)–O(3)	1.3215(20)	H–O(3)–C(1)	107.51(50)
H–O(3)	0.9684(50)	C(2)–C(1)–O(3)	110.81(20)
C(2)–C(1)	1.5225(20)	C(2)–C(1)=O(4)	122.95(20)
O(4)=C(1)	1.2167(20)		

r_0	Å [a])	θ_0	deg [a])
C(1)–O(3)	1.3294(20)	H–O(3)–C(1)	107.52(50)
H–O(3)	0.9713(50)	C(2)–C(1)–O(3)	110.90(20)
C(2)–C(1)	1.5210(20)	C(2)–C(1)=O(4)	122.60(20)
O(4)=C(1)	1.2219(20)	F(5)–C(2)–C(1)	111.24(30)
F(5)–C(2)	1.3309(30)	F(7)–C(2)–C(1)	111.01(30)
F(6)–C(2)	1.3445(30)	O(3)–C(1)–C(2)–F(6,7) [b])	±60.10(50)
F(7)–C(2)	1.3445(30)		

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1)	0.9827	0.1054	0.012
O(3)	1.5374	–1.0940	(0.028) [c])
H	2.4980	–0.9708	0.070
C(2)	–0.5362	(0.072) [c])	0.0
O(4)	1.5723	1.1698	(0.037) [c])
F(5)	(–1.095) [c])	(1.213) [c])	0.0
F(6)	(–0.973) [c])	(–0.649) [c])	(1.088) [c])
F(7)	(–0.973) [c])	(–0.649) [c])	(–1.088) [c])



[a]) Uncertainties were not estimated in the original paper.
[b]) Dihedral angle.
[c]) Calculated from the structure parameters.

Antolinez, S., Alonso, J.L., Dreizler, H., Hentrop, E., Sutter, D.H.: Z. Naturforsch. **54a** (1999) 524.

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