

1036
MW

C₃HF₃

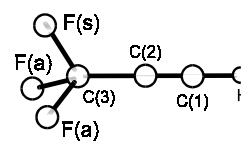
3,3,3-Trifluoro-1-propyne
(Trifluoromethyl)acetylene

C_{3v}
F₃C–C≡CH

r_{av}	Å	θ_{av}	deg
C≡C	1.2012(8)	F–C–F	108.27(20)

C–C	1.4742(45)
C–H	1.0510(17)
C–F	1.3372(22)

Atom	a_{av} [Å]	b_{av} [Å]
H	–3.44260	0.00
C(1)	–2.39162	0.00
C(2)	–1.19039	0.00
C(3)	0.28378	0.00
F(s)	0.75530	0.00
F(a)	0.75530	±1.08360



Cox, A.P., Ellis, M.C., Legon, A.C., Wallwork, A.: J. Chem. Soc. Farad. Trans. **89** (1993) 2937.