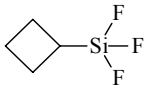
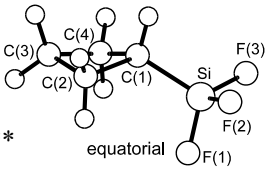
552 **$C_4H_7F_3Si$** **Cyclobutyltrifluorosilane** **C_s** assumed (equatorial)
ED, *ab initio* and DFT calculations **C_s** assumed (axial)

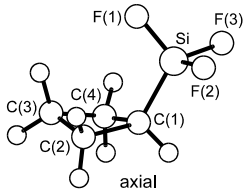


r_a	Å [a])
C(1)–C(2)	1.555(7)
C(2)–C(3)	1.538 [b])
Si–C	1.832(3)
Si–F(1)	1.579(1)
Si–F(2,3)	1.579(1)
C–H	1.142(5)

θ_a	deg [a])	
C(2)–C(1)–C(4)	89.3(28)	
C(2)–C(3)–C(4)	89.0 [c])	
H–C–H	108.6 [c])	
	equatorial	axial
Si–C(1)–H	113.8(60)	112.5 [c])
C(1)–Si–F(1)	110.7(16)	113.3(90)
C(1)–Si–F(2,3)	113.4(12)	113.3(90)
ϕ [d])	127.3(14)	124.0 [e])
φ [f])	24.4(50)	19.6(100)

The molecule was found to exist as a mixture of equatorial (81(15)%) and axial conformers. The structural parameters of both conformers were set equal to each other except for five angles (see table). The nozzle was at room temperature.





[a]) Three times the estimated standard errors.
[b]) Difference between the C(1)–C(2) and C(2)–C(3) bond lengths was assumed at the value from HF/6-31G** calculations.
[c]) Assumed at the values from HF/6-31G** or HF/3-21G* calculations.
[d]) Angle between the Si–C bond and the C(2)C(1)C(4) plane.
[e]) Assumed.
[f]) Ring puckering angle, *i.e.*, acute angle between the C(2)C(1)C(4) and C(2)C(3)C(4) planes.

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