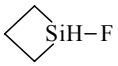
421 **C_3H_7FSi** **1-Fluorosilacyclobutane** **C_s** (equatorial)
ED, *ab initio* and DFT calculations **C_s** (axial)

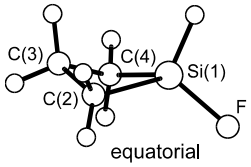


r_a	Å [a])
Si–C	1.855(1)
Si–F	1.592(2)
Si–H	1.472 [b])
C–C	1.586 [b])
C–H	1.089(3)

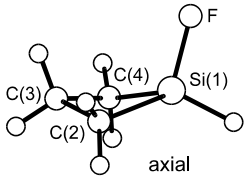
θ_a	deg [a])	
H–Si–F	106.8(6)	
C–Si–C	80.8(6)	
C–C–Si	85.3 [b])	
C–C–C	98.6(19)	
H–C–H	110.0 [b])	
	equatorial	axial
φ [c])	37.4(20)	23.5(70)
γ_1 [d]) [e])	5.2 [b])	14.0 [b])
γ_2 [e]) [f])	14.6 [b])	15.0 [b])
γ_3 [e]) [g])	6.6 [b])	7.0 [b])

The equatorial conformer was found to be lower in energy than the axial conformer by 4.30(21) kJ mol^{-1} corresponding to the ratio of the conformers eq : ax = 85(5) : 15(5).
The nozzle was at room temperature.
According to MP2/6-31G** calculations, the energy difference is equal to 6.04 kJ mol^{-1}.

[a]) Three times the estimated standard errors.
[b]) Assumed.
[c]) Ring puckering angle.
[d]) Rocking angle of the H–Si–F group.
[e]) Rocking angles are positive when the two axial bonds attached to the diagonal atoms are brought closer to each other by rocking.
[f]) Rocking angle of the H–C(2)–H group.
[g]) Rocking angle of the H–C(3)–H group.



equatorial



axial

Dakkouri, M., Grosser, M.: J. Mol. Struct. **559** (2001) 7.