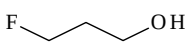
418 **C_3H_7FO** **3-Fluoro-1-propanol** **C_1** (aGG)

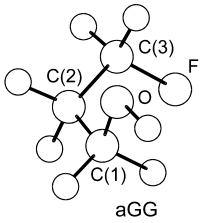
ED, DFT calculations



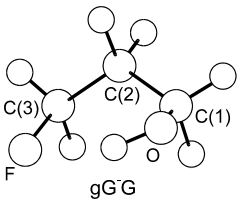
r_g	Å [a])	θ_α	deg [a])
O–H	1.026(4)	C–O–H	108.1 [b])
C–H (average)	1.113(4)	C–C–F	110.4(8)
C–O	1.380(8)	C–C–C, C–C–O (average)	111.1(6) [c])
C–F	1.448(7)	C–C–H (average)	110.0(7)
C(1)–C(2)	1.557(9)	H–O–C–C	191.2 [b])
C(2)–C(3)	1.492(5)	O–C–C–C	64.5 [b])
		C–C–C–F	61.7 [b])

The aGG conformer was found to be dominant, 47(19)%, among the 14 possible conformers. In the analysis of ED data, the differences between the corresponding parameters of these conformers and the relative abundances of 12 non-hydrogen-bonded conformers were assumed at the values from B3LYP/6-31G(d) calculations. The abundance of the hydrogen-bonded conformer, gG^-G and its enantiomer g^-GG^-, refined in the least-squares analysis separately from all the other conformers refined as a group, is found to be only 2(19)% of the sample. The sequence of a (*anti*) and g, G (*gauche*) indicates rotation around the C–O, C(1)–C(2) and C(2)–C(3) bonds, respectively, with the minus sign indicating clockwise rotation. The structural parameters are listed for the aGG conformer.
The nozzle temperature was 20 °C.

[a]) Twice the estimated standard errors.
[b]) Assumed at the value from B3LYP/6-31G(d) calculations.
[c]) Difference between the C–C–C and C–C–O bond angles was assumed at the value from B3LYP/6-31G(d) calculations.



aGG



gG^-G

Richardson, A.D., Hedberg, K.: J. Mol. Struct. **567-568** (2001) 187.

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