WE ARE FAMILY: THE CONFORMATIONS OF 1-FLUOROALKANES, $C_nH_{2n+1}F$ (n = 2,3,4,5,6,7,8)

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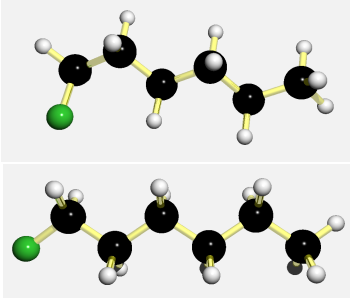
The pure rotational spectra of the n = 5, 6, 7, and 8 members of the 1-fluoroalkane family have been recorded between 7 GHz and 14 GHz using chirped pulse Fourier transform microwave spectroscopy. The spectra have been analyzed and results will be presented and compared with previous work on the n= 2, 3, and 4 members[b]. The lowest energy conformer for all family members has the common feature that the fluorine is in a gauche position relative to the alkyl tail for which all other heavy atom dihedral angles, where appropriate, are 180 degrees. For the n = 3 and higher family members the second lowest energy conformer has *all* heavy atom dihedral angles equal to 180 degrees. For each family member transitions carried by both low energy conformers were observed in the collected rotational spectra. Quantum chemical calculations were performed and trends in the energy separations between these two common conformers will be presented as a function of chain length. Furthermore, longer chain lengths have been examined using only quantum chemical calculations and results will be presented.



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[b]M. Hayashi, M. Fujitake, T. Inagusa, S. Miyazaki, J.Mol.Struct., 216, 9-26, 1990 ; W. Caminati, A. C. Fantoni, F. Manescalchi, F. Scappini, Mol.Phys., 64, 1089 ,1988 ; L. B. Favero, A. Maris, A. Degli Esposti, P. G. Favero, W. Caminati, G. Pawelke, Chem.Eur.J., 6(16), 3018-3025, 2000