ROTATIONAL SPECTRA AND STRUCTURES OF $(CF_3)_3CH$ AND $(CF_3)_3CF$

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1,1,1,3,3,3-Hexafluoro-2-(trifluoromethyl)-propane $(CF_3)_3CH$ and perfluoroisobutane $(CF_3)_3CF$ are hydrofluorocarbon(HFC) and perfluorocarbon(PFC), respectively, and environmental concerned. Both are vapor at room temperature and symmetric-top molecules with the $(CF_3)_3C$ group. The comparison of these structures seemed interesting. We have, therefore, investigated the structures of these molecule by microwave spectroscopy and ab initio MO calculation. The rotational spectra have been observed using a Stark modulation and a supersonic free jet Fourier transform microwave spectrometers. The samples of 1% in Ar/Ne were used to form the supersonic expansion. The Stark modulation microwave spectrum have been assigned for the normal $(CF_3)_3CH$ and deuterated $(CF_3)_3CD$ species. Ab initio MO calculations of MP2/6-311+G(d,p) level have been made.
The C-C bond length and the C-C-C bond angle are found higher in $(CF_3)_3CF$ than those in $(CF_3)_3CH$. For both molecules, the two fluorine atoms in the CF_3 groups do not align in a plane, but are rotated ca. 18 degree. All these facts are considered due to the repulsion between the fluorine atoms in the molecules.