MICROWAVE STUDIES OF PERFLUOROPENTANE AND ITS HELICITY

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Unlike hydrocarbons, fluorocarbons are helical in their all-trans most stable conformations. A definitive experimental determination of the helical angle has not been accomplished because single crystal X-ray studies are not available due to the lack of suitable crystallization solvents, but a value of 17° from exactly trans is generally accepted from X-ray fiber studies. Using a pulsed-jet Fourier Transform microwave spectrometer, we have observed and assigned the rotational spectra of the lowest energy all-anti C_2 symmetry form of perfluoro-n-pentane and all three of its ^{13}C isotopomers. A, B, and C values of the parent species are 990.6394(4) MHz, 314.00020(14) MHz, and 304.37034(14) MHz, respectively. A range of effective r_0 structures incorporating various model constraints are consistent with about 16° torsion and a Kraitchman analysis of the parent and ^{13}C species gives 13.3°. Ab initio calculations are consistent with the experimental results.