Fourier Transform Microwave Spectroscopy of the Conformers of Perfluorobutane

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Nitrogen matrix IR spectroscopy and ab initio calculations of three distinct conformations of perfluoro-\(\eta\)-butane, \(\eta\)-C\(\text{F}_4\)\(\eta\), have recently been reported\(^{a}\). We have measured the Fourier Transform microwave spectrum of the gauche conformer of perfluoro-\(\eta\)-butane and determined the C-C-C-C dihedral angle to be \(\sim 51^\circ\). This is in good agreement with the ab initio calculations of Albinsson and Michl that predicted dihedral angles of 54\(^\circ\), 95\(^\circ\), and 165\(^\circ\), for the gauche, ortho, and anti conformations, respectively. The search for the other conformations continues. In addition, the spectrum of the symmetric top isomer, perfluoroisobutane, has been observed.

\(^{a}\)B. Albinsson and J. Michl, J. Phys. Chem. 100, 3418 (1996)