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-$n$-butane, $n$-$C_4F_{10}$, have recently been reported[a]. We have measured the Fourier Transform microwave spectrum of the $gauche$ conformer of perfluoro-$n$-butane and determined the C-C-C-C dihedral angle to be $\sim 51°$. This is in good agreement with the $ab\ initio$ calculations of Albinsson and Michl that predicted dihedral angles of 54°, 95°, and 165°, 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)