THE CONFORMATIONS AND STRUCTURES OF 1H-NONAFLUOROBUTANE

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The all trans conformers of perfluorocarbons, unlike hydrocarbons, are helical with C-C-C-C dihedral angles about 164^0. Fluorocarbons with H substitution can replace chlorofluorocarbons as propellants and compressor fluids without the disadvantage of causing ozone depletion in the upper atmosphere. 1H-perfluorobutane, $CHF_2CF_2CF_2CF_3$, has been studied by pulsed-jet Fourier transform microwave spectroscopy. The spectrum is very rich. Quantum chemical calculations identify five stable conformers with relative energies up to 1.1 kcal/mol. Thus far three conformers have been characterized and many lines remain unassigned. The assigned species have CCCCanti/CCCH gauche as well as the anti/anti and gauche/anti forms. Rotational constant values are 1428.9501(2) MHz, 593.323877(6) MHz, and 546.43578(6) MHz for the anti/gauche species, 1323.664(3) MHz, 617.6051(5) MHz for the ant/anti species, and 1066.9384(4) MHz, 768.4736(4) MHz, and 671.3145(4) MHz for the gauche/anti form.