MICROWAVE SPECTROSCOPY AND STRUCTURES OF PERFLUOROHEXANE AND 1H-HEPTAFLUOROPROPANE

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The lowest energy conformer of perfluorohexane is helical and its microwave rotational spectrum has been observed and assigned. The molecular parameters were characterized by scaling computed models by the square root of the ratio of the observed second moments to those computed. The scaled structures exactly reproduce the observed second moments. From this scaling approach, the exterior $C_1C_2C_3C_4$ dihedral angle is 16.7° and the interior $C_2C_3C_4C_5$ dihedral angle is 18.0° away from trans. In addition, two conformers of 1H-heptafluoropropane have been observed and characterized by its microwave spectrum. The HCCC dihedral angle is analogous to the CCCC dihedral angle in butane and exhibits both trans and gauche conformations. The trans conformer shows no evidence of a helical twist. It appears that the steric and dipole interactions which cause a twist in longer perfluoroalkane oligomers are not sufficient in a three carbon chain. Computations at the PBE0/cc-pVTZ level are in excellent agreement with the experimental results for both compounds.