

A COMPLETE STRUCTURE FOR THE GAUCHE ROTAMER OF 1,1,2,2-TETRAFLUOROETHANE FROM MICROWAVE SPECTROSCOPY

NORMAN C. CRAIG, *Department of Chemistry, Oberlin College, Oberlin, OH 44074*; BELÉN MATÉ, ANGELA HIGHT WALKER, and RICHARD D. SUENRAM, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899*.

The complete molecular structure of the high-energy, gauche rotamer of 1,1,2,2-tetrafluoroethane, Freon F134, has been determined using Fourier transform microwave spectroscopy. A total of five different ^{13}C - and ^2H -substituted isotopomers and the normal species have been studied. Unlike the nonpolar anti rotamer, the gauche form has a permanent electric dipole moment, which permits a direct rotational analysis. The electric dipole moment was also determined using the Stark effect of two low-J transitions. The resulting dipole moment is $\mu_e = 8.186(7) \times 10^{-30}$ C.m [2.454(2) Debye]. Two recent ab initio calculations, one using the hybrid Hartree-Fock, density functional method (ACM)^a and the other an MP2/6-31G** model^b, are in reasonable agreement with experimental findings.

^a M. Muir and J. Baker, *J. Mol. Phys.* **89**, 211 (1996).

^b S. Papasavva, K.H. Illinger, and J.E. Kenny, *J. Phys. Chem.* **100**, 10100, (1996).