

SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURES; RESULTS FROM DIFFERENT CALCULATIONS OF ALPHAS AND COMPARISON WITH THEORY

NORMAN C. CRAIG, *Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074*;  
DAVID FELLER, *Department of Chemistry, Washington State University, Pullman, WA 99164-4630*; PE-  
TER GRONER, *Department of Chemistry, University of Missouri-Kansas City, Kansas City, KS 64110-2499*;  
DONALD C. MCKEAN, *School of Chemistry, University of Edinburgh, EH9 3JJ, U.K.*

Semi-experimental equilibrium structures for ethylene, butadiene, and 1,1-difluorocyclopropane have been determined from ground state rotational constants and alphas (vibration-rotation constants) computed with scaled harmonic force constants. These results are compared with optimized structures from high-level ab initio calculations and with structures obtained with alphas computed by Gaussian 03 without force constant scaling. A similar, comparative analysis is reported for the equilibrium structures for cyclopropene and 3,3-difluorocyclopropene. Caution is advised in using alphas from Gaussian. Also reported is the length of a pure  $sp^2$ - $sp^2$  single bond in twisted ( $90^\circ$ ) butadiene as computed with high-level ab initio calculations.