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

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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°) butadiene as computed with high-level ab initio calculations.