AB INITIO DETERMINATION OF MOLECULAR PARAMETERS FOR ETHANE-LIKE MOLECULES

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A new method has been developed for the ab initio determination of several vibration-torsion-rotational spectroscopic parameters for a symmetric top molecule with an internal rotor. In contrast to existing methodologies [a,b] which employ vibrational contact transformations either numerically or algebraically, the present model treats the molecule as vibrationally static but with a density distribution characteristic of the vibrational wavefunction. The second-order rotational constants A and B and torsional constant F, distortion parameters D_J, D_K, and D_{JK}, and torsional distortion parameters D_m, D_{Jm}, and D_{Km} have been determined for a series of ethane-like molecules from the results of ab initio calculations done at the CCSD(T) level. The technique has been applied to the molecules CH_3CH_3, CH_3CD_3, CD_3CD_3, and CH_3SiH_3 with very promising results. Preliminary results for the potential constants F_{3J} and F_{3K} are also in excellent agreement with global fit values.

[a] Y.-B. Duan, L. Wang, X.T. Wu, I. Mukhopadhyay, and K. Takagi, *J. Chem. Phys.* **111**, 2385 (1999).
[b] T.J. Lukka and E. Kauppi, *J. Chem. Phys.* **103**, 6586 (1995).