A PROPOSAL FOR A GENERAL METHOD FOR DETERMINING SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURES OF CARBON ATOM BACKBONES

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Semi-experimental equilibrium structures are determined from ground state rotational constants derived from the analysis of rotational transitions in high-resolution spectra and from the quantum chemical calculation of spectroscopic alphas. In the full application of this method, spectra of numerous isotopic species must be investigated. Most of these isotopic species require specialized synthesis. We now propose focusing on the carbon atoms, for which microwave spectroscopy routinely yields spectra for polar molecules with ^{13}C substitution in natural abundance. Needed spectroscopic alphas can be computed with Gaussian software. Application of the Kraitchman substitution relationships gives Cartesian coordinates for the carbon atoms and thence bond parameters for the carbon backbone. This method will be evaluated with ethylene, 1,1-difluoroethylene, 1,1-difluorocyclopropane, propene, and butadiene. The method will then be applied to *cis*-hexatriene[a] and the two conformers of glycidol.[b]

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[a]R. D. Suenram, B. H. Pate, A. Lessari, J. L. Neill, S. Shipman, R. A. Holmes, M. C. Leyden, and N. C. Craig, J. Phys. Chem. A 113, 1864-1868 (2009).

[b]A. R. Conrad, N. H. Teumelsan, P. E. Wang, and M. J. Tubergen, J. Phys. Chem. A 114, 336-342 (2010).