THEORETICAL STUDY OF THE VIBRATIONAL SPECTROSCOPY OF THE ETHYL RADICAL

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The rich spectroscopy of the ethyl radical has attracted the attention of several experimental[ab] and theoretical investigations.[c] The purpose of these studies was to elucidate the signatures of hyperconjugation, torsion, inversion, and Fermi coupling in the molecular spectra. Due to the number of degrees of freedom in the system, previous theoretical studies have implemented reduced-dimensional models. Our ultimate goal is a full-dimensional theoretical treatment of the vibrations using both Van Vleck and variational approaches. The methods will be combined with the potential that we have calculated using the CCSD(T) method on the cc-pVTZ basis set. In this talk we will discuss our initial work, which builds up from these reduced-dimensional models. Our calculations use coordinates that exploit the system's G_{12} PI symmetry in a simple fashion. By systematically adding more degrees of freedom to our model, we can determine the effects of specific couplings on the spectroscopy.

[a] T. Häber, A. C. Blair, D. J. Nesbitt and M. D. Schuder *J. Chem. Phys.* **124**, 054316, (2006).
[b] G .E. Douberly, unpublished.
[c] R. S. Bhatta, A. Gao and D. S. Perry *J. Mol. Struct.: THEOCHEM* **941**, 22, (2010).