# A HAMILTONIAN TO OBTAIN A GLOBAL FREQUENCY ANALYSIS OF ALL THE VIBRATIONAL BANDS OF ETHANE

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The interest in laboratory spectroscopy of ethane stems from the desire to understand the methane cycle in the atmospheres of planets and their moons and from the importance of ethane as a trace species in the terrestrial atmosphere. Solar decomposition of methane in the upper part of these atmospheres followed by a series of reactions leads to a variety of hydrocarbon compounds among which ethane is often the second most abundant species. Because of its high abundance, ethane spectra have been measured by Voyager and Cassini in the regions around 30, 12, 7, and 3 $\mu$m. Therefore, a complete knowledge of line parameters of ethane is crucial for spectroscopic remote sensing of planetary atmospheres. Experimental characterization of torsion-vibration states of ethane lying below 1400 cm$^{-1}$ have been made previously [a], but extension of the Hamiltonian model for treatment of the strongly perturbed $\nu_8$ fundamental and the complex band system of ethane in the 3 micron region requires careful examination of the operators for many new torsionally mediated vibration-rotation interactions. Following the procedures outlined by Hougen [b, c], we have re-examined the transformation properties of the total angular momentum, the translational and vibrational coordinates and momenta of ethane, and for vibration-torsion-rotation interaction terms constructed by taking products of these basic operators. It is found that for certain choices of phase, the doubly degenerate vibrational coordinates with and symmetry can be made to transform under the group elements in such a way as to yield real matrix elements for the torsion-vibration-rotation couplings whereas other choices of phase may require complex algebra. In this talk, I will discuss the construction of a very general torsion-vibration-rotation Hamiltonian for ethane, as well as the prospect for using such a Hamiltonian to obtain a global frequency analysis (based in large part on an extension of earlier programs and ethane fits[a] from our laboratory) of all the vibrational bands of ethane at or below the 3-micron region.

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[a]N. Moazzen-Ahmadi and J. Norooz Oliaee, J. Quant. Spectrosc. Radiat. Transfer, submitted.

[b]J.T. Hougen, Can. J. Phys., 42, 1920 (1964)

[c]J. T. Hougen, Can. J. Phys., 43, 935 (1965)