A COMBINED FREQUENCY ANALYSIS OF THE $\nu_3$, $\nu_9$, AND THE FAR INFRARED TORSIONAL SPECTRA OF ETHANE

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The lowest frequency nondegenerate fundamental band $\nu_3$ of ethane is Raman active and centered near $992 \text{ cm}^{-1}$. A stimulated Raman spectrum of the Q branch for this band (at a resolution of $0.0055 \text{ cm}^{-1}$) has been recorded by Bermejo et al.$^a$ The torsion-rotation branch with $\sigma = 3$ is perturbed by over $1 \text{ cm}^{-1}$.

The lowest frequency degenerate fundamental band $\nu_9$ is infrared active and occurs in the 12-$\mu$m region. A high resolution ($0.0014 \text{ cm}^{-1}$) Fourier transform spectrum of this band has been measured by Moazzen-Ahmadi et al.$^b$ The observed torsional splittings for this band are substantially larger than expected simply from the observed increase in the barrier height. Because of the proximity of the upper level $(i = -1; K = 17, \sigma = 0)$ in $\nu_9 = 1$ with its interacting partner $(\tau_9 = 0, \nu_4 = 3)$ a perturbation allowed band $3\nu_4$ has also been observed.

We have carried out a combined frequency analysis of $\nu_3$, $\nu_9$, and $3\nu_4$ bands together with the far infrared torsional spectra in the ground vibrational state (gs). A vibration-torsion-rotation Hamiltonian with 32 fitting parameters was used. Three interacting torsional stacks, one for each of the vibrational state, were considered. The large torsional splitting in the $\nu_9$ band is attributed to Coriolis-like interations between the torsional stacks of gs and $\nu_9 = 1$ whereas the large shift for the torsion-rotation branch with $\sigma = 3$ in the $\nu_9$ band is attributed to a Fermi-like interaction between the torsional stacks of gs and $\nu_9 = 1$.

The details of this analysis will be presented.
