A COMBINED FREQUENCY ANALYSIS OF THE ν_3, ν_9, AND THE FAR INFRARED TORSIONAL SPECTRA OF ETHANE

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The lowest frequency nondegenerate fundamental band ν_3 of ethane is Raman active and centered near 992 cm^{-1}. A stimulated Raman spectrum of the Q branch for this band (at a resolution of 0.0055 cm^{-1}) has been recorded by Bermejo et al.[a] The torsion-rotation branch with $\sigma = 3$ is perturbed by over 1 cm^{-1}.

The lowest frequency degenerate fundamental band ν_9 is infrared active and occurs in the 12-μm region. A high resolution (0.0014 cm^{-1}) Fourier transform spectrum of this band has been measured by Moazzen-Ahmadi el 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 ($l = -1; K = 17, \sigma = 0$) in $v_9 = 1$ with its interacting partner ($v_9 = 0, v_4 = 3$) a perturbation allowed band $3\nu_4$ has also been observed.

We have carried out a combined frequency analysis of ν_3, ν_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 ν_9 band is attributed to Coriolis-like interations between the torsional stacks of gs and $v_9 = 1$ whereas the large shift for the torsion-rotation branch with $\sigma = 3$ in the ν_3 band is attributed to a Fermi-like interaction between the torsional stacks of gs and $v_3 = 1$.

The details of this analysis will be presented.

[a]D. Bermejo, J. Santos, P. Cancio, J.M. Fernandez-Sanchez, and S. Montero, J. Chem. Phys. **97**, 7055 (1992).

[b]N. Moazzen-Ahmadi, J. Schroderus, and A.R.W. McKellar, J. Chem. Phys. **111**, 9609 (1999).