THE ROLE OF TORSIONAL HOT BANDS IN MODELING ATMOSPHERIC ETHANE

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The strong and sharp ${}^{p}Q_3$ subbranch of the ν_7 band of ethane near 2976.8 cm^{-1} is relatively free of interfering lines of methane, water and ozone and has been utilized as the signature of ethane for atmospheric monitoring [a]. This subbranch is unresolvable at the Doppler limit, even at low T (119 K) [b]. However, the rotational structure and torsional splittings have been obtained by subDoppler molecular-beam spectroscopy [c], along with the air-broadening coefficients and their temperature dependence, so that the fundamental band can be well characterized, apart from a minor perturbation evident at high J. This still leaves a significant fraction of the observed structure and intensity in this region unassigned. The strong temperature dependence of this extraneous structure enables us to attribute it to torsional hot bands, which improves the quantitative estimates of atmospheric ethane. We also discuss various approximations to the ethane partition function, accounting for the highly anharmonic torsional mode, needed for the accurate scaling of the intensities over the wide range of atmospheric temperatures.

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[b] A. Pine and W. Lafferty, J. Res. NBS. 87, 237 (1982).
[c] A. Pine and S. Stone, J. Mol. Spectrosc. 175, 21 (1996).