EXPERIMENTAL AND THEORETICAL STUDIES OF ETHYL

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First detected in 1988, the $-CH_2$ wagging fundamental of C_2H_5 recorded at high resolution by diode laser absorption extends from approximately 470 to more than 600 cm^{-1}. The mode corresponds to the out-of-plane motion at the radical center and this is strongly coupled to the torsion or internal rotation in this species. We published[a] a preliminary analysis of the spectrum in 1996, but at the time recognized many questions remained. Aided by extensive ab initio calculations and the detection[b] of part of the spectrum at $3\mu m$ in a jet-cooled sample, we have recently made much progress understanding the details of the $20\mu m$ spectrum and the internal dynamics in the radical. In total, close to 500 transitions have been assigned in 18 rotation-torsion branches. The observation of branches involving levels with $m_{torsion}$ = 3 and low k_a, in particular, has allowed much more precise estimates of the barrier to internal rotation and its change on vibrational excitation. Calculations of the torsion/wag potential surface have allowed a physical interpretation of these experimental results.

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[a] T. J. Sears, P. M. Johnson, P. Jin and S. Oatis, J. Chem. Phys., 104, 781 (1996)

[b] S. Davis, D. Uy, and D. J. Nesbitt, Paper FE03, 52nd Ohio State University International Symposium on Molecular Spectroscopy, 1997.