INVESTIGATION OF THE TORSIONAL FAR-INFRARED OVERTONES AND HOT BANDS OF ACETALDEHYDE AND VIBRATIONAL-TORSIONAL-ROTATIONAL INTERACTIONS WITH THE $\nu_1 0$ FUNDAMENTAL BAND

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The torsional overtone spectrum of CH_3CHO has been recorded with a high resolution (0.003 cm^{-1}) Far-Infrared Fourier Transform spectrometer, between 40 and 90 cm^{-1} and between 180 and 230 cm^{-1}. This spectrum completes the far-infrared spectrum recorded a few years ago from 80 to 180 cm^{-1} to study the fundamental torsional band $v_t = 1$–0 and the two first overtones $v_t = 2$–1 and 3–2[a]. The spectral region between 40 and 90 cm^{-1} is very dense and allows us to assign many $v_t = 2$–1 lines and $v_t = 3$–2 lines. The region between 180 and 230 cm^{-1}, on the other hand, is less congested and allows us to search for weaker lines from the $v_t = 3$–1 and 4–2 overtone bands. Those overtone bands would correspond, in the free-rotor limit, to a change in the free-rotor quantum number m of ± 3 and are expected to arise when considering intensity contribution from the second terms in the Fourier expansion of the dipole moment $\mu_a^{(3)} \cos 3\alpha$ and $\mu_b^{(3)} \cos 3\alpha$ for the A and E species and also from the first non-zero term of $\mu_c^{(3)} \sin 3\alpha$ for the E species. The spectrum of the ν_{10} band was recorded last year at high resolution with a Fourier Transform spectrometer in the region of 450 to 550 cm^{-1} region and partly assigned. A number of strong perturbations arising likely from interactions with the $v_t = 4$ torsional levels of the ground state were observed. As a first step to investigate doorway states which facilitate passage of energy from the small amplitude manifold to the torsional manifold, the goal of this study is to consider a two-by-two theoretical model involving both ν_{10} and the ground vibrational state and to carry out a simultaneous fit of the perturbed lines from v_{10}=1 and from vt=4 of the vibrational ground state.

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