ROTATIONAL CONSTANTS FOR M-METHYLBENZALDEHYDE: A STUDY IN LOW BARRIER TORSIONAL SPLITTING

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We present the ground state spectrum for m-methylbenzaldehyde taken with a chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer. The presence of a methyl rotor on the molecule introduces a threefold internal rotation barrier. Tunneling through this barrier leads to splitting of the torsional energy level degeneracy into A and E states. Theory predicts a low torsional barrier for both the cis and trans conformers, which leads to large splitting in the frequency spectrum. The A states are simulated using the rigid rotor approximation and subsequent distortion terms. In order to predict the E states, a $V_3$ parameter must be determined that correlates to the torsional barrier. All four possible species have been fit and parameters will be presented, including rotational constants, distortion terms and $V_3$ values.