

FOURIER TRANSFORM SPECTRA AND INVERTED TORSIONAL STRUCTURE FOR A CH₃-BENDING FUNDAMENTAL OF CH₃OH

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The high-resolution Fourier transform spectrum of CH₃OH has been investigated in the 1400-1650 cm⁻¹ region, containing the CH₃-bending fundamental bands. Twenty-two perpendicular $\Delta K = +1$ subbands have been identified so far, with origins ranging from 1490 to 1570 cm⁻¹ for transitions $K = 2 \leftarrow 1$ up to $11 \leftarrow 10$ for various torsional symmetries. Assignment of the subbands to the ν_4 in-plane (A') or ν_{10} out-of-plane (A'') asymmetric methyl-bending modes is not yet clear, but the one subband so far observed with resolved K -doublet structure suggests *c*-type selection rules consistent with a ν_{10} vibrational assignment. The pattern of the K -reduced torsion-vibration energy τ -curves is inverted compared to the normal 1-dimensional picture for $n = 0$ torsional levels, in agreement with prediction based on fitting torsional variation of *ab initio* CH₃-bending frequencies to a local mode model. However, the periodicity of the curves is unusual and significantly different from the ground state. The vibrational energy for the bending mode is 1481 cm⁻¹, and the mean B -value is 0.008 cm⁻¹ higher than that of the vibrational ground state.