

TOWARD A GLOBAL MODEL OF LOW-LYING VIBRATIONAL STATES OF CH₃CN: THE $v_4 = 1$ STATE AT 920 cm⁻¹ AND ITS INTERACTIONS WITH NEARBY STATES

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Methyl cyanide, CH₃CN, is an important interstellar molecule, in particular in hot and dense molecular cores, and it may play a role in the atmospheres of planets or of Titan. Therefore, we have recorded extensive rotational and rovibrational spectra up to ~ 1.6 THz and ~ 1500 cm⁻¹, respectively. The present investigation extends our analysis of states with $v_8 \leq 2$ at vibrational energies below 740 cm⁻¹^a and takes into consideration findings from an analysis of the ν_4 band and the higher-lying ν_7 (at ~ 1042 cm⁻¹) and $3\nu_8^1$ (at ~ 1078 cm⁻¹) bands.^b The rotational data extend to $J = 87$ and $K = 15$, infrared assignments currently extend to 55 and 12, respectively. Parameters affecting only $v_7 = 1$ or $v_8 = 3$ as well as some additional interaction parameters were kept fixed to values from (b). The largest perturbations of $v_4 = 1$ are caused by a $\Delta k = 0, \Delta l = 3$ interaction with $v_8 = 3$ at $K = 8$. Despite the inclusion of the interaction parameter and a centrifugal distortion correction, residuals amount to more than 200 MHz very close to the resonance. Removal of these residuals probably requires explicit inclusion of $v_8 = 3$ data. Several additional perturbations exist at lower as well as higher K with $v_8 = 2, v_7 = 1$ and $v_8 = 3$. Higher values of K are difficult to reproduce in spite of an extensive set of distortion parameters which, at highest orders, have rather large magnitudes, possibly indicating unaccounted interactions which would probably occur with states even higher than $v_8 = 3$.

^aH. S. P. Müller et al., contribution WG03, presented at the 62nd International Symposium on Molecular Spectroscopy, June 18–22, 2007, Columbus, Ohio, USA.

^bA.-M. Tolonen et al., *J. Mol. Spectrosc.* **160** (1993) 554–565.