TOWARD A GLOBAL MODEL OF LOW-LYING VIBRATIONAL STATES OF CH$_3$CN: THE $v_4 = 1$ STATE AT 920 cm$^{-1}$ AND ITS INTERACTIONS WITH NEARBY STATES

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Methyl cyanide, CH$_3$CN, 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 $\approx 1.6$ THz and $\approx 1500$ cm$^{-1}$, respectively. The present investigation extends our analysis of states with $v_8 \leq 2$ at vibrational energies below 740 cm$^{-1}$ and takes into consideration findings from an analysis of the $v_4$ band and the higher-lying $v_7$ (at $\approx 1042$ cm$^{-1}$) and $3v_6$ (at $\approx 1078$ cm$^{-1}$) bands. 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 $\Delta k = 0, \Delta I = 3$ 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 $v_8 = 3$.

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