ROTATIONAL SPECTROSCOPY AS A TOOL TO INVESTIGATE INTERACTIONS BETWEEN VIBRATIONAL POLYADS IN SYMMETRIC TOP MOLECULES: LOW-LEYING STATES $v_8 \leq 2$ OF METHYL CYANIDE

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Rotational and rovibrational spectra of methyl cyanide were recorded to analyze interactions in low-lying vibrational states and to construct line lists for radio astronomical observations as well as for infrared spectroscopic investigations of planetary atmospheres. The rotational spectra cover large portions of the 36–1627 GHz region. In the infrared (IR), a spectrum was recorded for this study in the region of $2v_8$ around 717 cm$^{-1}$ with assignments covering 684–765 cm$^{-1}$. Additional spectra in the $v_8$ region were used to validate the analysis.

Using $v_8$ data$^b$ as well as spectroscopic parameters for $v_4 = 1$, $v_7 = 1$, and $v_8 = 3$ from previous studies,$^c$ we analyzed rotational data involving $v = 0$, $v_8 = 1$, and $v_8 = 2$ up to high $J$ and $K$ quantum numbers. We analyzed a strong $\Delta v_8 = \pm 1, \Delta K = 0, \Delta l = \pm 3$ Fermi resonance between $v_8 = 1 \pm 1$ and $v_8 = 2 + 2$ at $K = 14$ and obtained preliminary results for two further Fermi resonances between $v_8 = 2$ and 3. We also found resonant $\Delta v_8 = \pm 1, \Delta K = \mp 2, \Delta l = \pm 1$ interactions between $v_8 = 1$ and 2 and present the first detailed analysis of such a resonance between $v_8 = 0$ and 1.

We discuss the impact of this analysis on the $v_8 = 1$ and 2 as well as on the axial $v = 0$ parameters and compare selected CH$_3$CN parameters with those of CH$_3$CCH and CH$_3$NC.

We evaluated transition dipole moments of $v_8$, $2v_8 - v_8$, and $2v_8$ for remote sensing in the IR.

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