ROTATIONAL SPECTROSCOPY AS A TOOL TO INVESTIGATE INTERACTIONS BETWEEN VIBRATIONAL POLYADS IN SYMMETRIC TOP MOLECULES: LOW-LYING STATES OF METHYL CYANIDE

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Recently, interactions between vibrational polyads were studied for propyne, $H_3C{-}C{\equiv}CH$; in particular those between $v_{10} = 1$ at 30 μm with the 15 μm dyad ($v_9 = 1$, $v_{10} = 2$),[ab] as well as between that dyad and the 10 μm tetrad ($v_5 = 1$, $v_9 = v_{10} = 1$, $v_{10} = 3$, $v_8 = 1$)[b]. Pronounced effects were caused by $\Delta v_{10} = \pm 1$, $\Delta K = 0$, $\Delta l = \pm 3$ Fermi-type resonances at $K \approx 12$. Such resonances had not been found thus far for the isoelectronic methyl cyanide, $H_3C{-}C{\equiv}N$, molecule despite extensive previous spectroscopic work. As methyl cyanide is also an important interstellar molecule, in particular in hot and dense molecular cores, and as it may play a role in the atmospheres of planets or of Titan, we have recorded extensive rotational and rovibrational spectra up to ~ 1.6 THz and $\sim 1500\,\mathrm{cm}^{-1}$, respectively. The present investigations focus on the $v_8 = 0$, 1, and 2 states. The ν_8 mode in methyl cyanide corresponds to the ν_{10} mode in propyne, and it is at a rather similar energy. While the infrared data pertaining to these states help to constrain their K level structures they do not reach $K \approx 14$ which are perturbed most; the $l = 0$ component of $2\,\nu_8$ may be an exception. The pure rotational data on the other hand access K levels well beyond these perturbations which can be easily recognized in the spectra. Since the $\nu_9 = \delta$(CCH) mode in propyne is missing in methyl cyanide one would expect easier assignments and analyses. However, besides $\Delta v_8 = \pm 1$, $\Delta K = 0$, $\Delta l = \pm 3$ Fermi-type resonances around K of 14, additional fairly strong resonances occur at similar K values which are described by $\Delta v_8 = \pm 1$, $\Delta K = \mp 2$, $\Delta l = \pm 1$. The latter type of resonance takes even place weakly between $v = 0$ and $v_8 = 1$; an indication for this was seen previously.[c] The analyses of interactions between states with $v_8 \leq 2$ have been largely completed. The results will be compared with those in propyne.

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[a] H. S. P. Müller, P. Pracna, and V.-M. Horneman, *J. Mol. Spectrosc.* **216** (2002) 397−407.

[b] P. Pracna, H. S. P. Müller, S. Klee, and V.-M. Horneman, *Mol. Phys.* **102** (2004) 1555−1568.

[c] M. Šimečková *et al.*, *J. Mol. Spectrosc.* (2004) 123−126.