ANHARMONIC RESONANCES AMONG LOW-LYING VIBRATIONAL LEVELS OF METHYL ISO-CYANIDE (H_3CNC)

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Vibrational levels up to 1000 $\mathrm{cm}^{-1}$of H_3C-N≡C are currently studied in FTIR spectra together with rotational transitions within these levels. This investigation comprises the low-lying excited vibrational levels of the CNC doubly degenerate bending vibration $v_8 = 1^{\pm 1}$ (267.3 cm^{-1}), $v_8 = 2^{0,\pm 2}$ (524.6 cm^{-1}(A), 545.3 cm^{-1}(E)), and $v_8 = 3^{\pm 1,\pm 3}$ (792.5 cm^{-1}(A1+A2), 833.9 cm^{-1}(E)), respectively, and the next higher fundamental level of the C-N valence vibration $v_4 = 1$ (945 cm^{-1}). All these vibrational levels exhibit cubic and quartic anharmonic resonances localized to moderate values of the rotational quantum number $K \leq 10$. Therefore the system of rovibrational levels has to be treated as a global polyad in order to describe all the available data quantitatively. The ground state constants have been improved considerably by extending the assignments to higher J/K rotational states both in the purely rotational spectra recorded in the ground vibrational level and in the ground state combination differences generated from the wavenumbers assigned in the fundamental ν_4 band. Similarities and differences with respect to isoelectronic molecules CH_3CN and CH_3CCH are discussed.