HIGH-RESOLUTION STUDY OF THE ROTATIONAL SPECTRUM OF 2-AMINOPROP-2-ENENITRILE

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The high-resolution rotational spectrum of 2-aminopropen-2-enitrile (APN) was recorded in two frequency ranges: 204–240 and 292–328 GHz employing the Prague semiconductor millimetre-wave spectrometer[1]. Several hundreds of *a*- and *b*-type transitions corresponding to the 0^+ and 0^- inversion states arising from the inversion motion of the amino group were identified and assigned. Bauder et al.[2] estimated the energy difference between the energy levels to be 54 ± 22 cm^{-1} based on the relative intensity measurements. Since no *c*-type transitions connecting the inversion states were assigned in the present spectrum, the value of ΔE separating the levels could not be derived with a better accuracy. Hence, the rotational transitions from both vibrational states were analysed separately by means of the A-reduced Hamiltonian using the SPCAT/SPFIT program package[3]. The experimentally determined molecular parameters of APN are presented in comparison with their quantum chemical counterparts.

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