

HIGH RESOLUTION SPECTROSCOPY OF THE TWO LOWEST VIBRATIONAL STATES OF QUINOLINE C₉H₇N

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PAHs molecules and derivatives have long been suspected to be present in different objects of the universe but no unambiguous detection (based on rotationally resolved spectroscopy) has been reported yet. Pure rotation transitions in the ground state (GS) of quinoline (which belongs to the C_s point group) have been analyzed in a previous work of Kisiel et al.^c using micro-wave and sub-mm techniques. We will present in this talk a collective effort to record and assign the rotational structure of the two lowest vibrational states of quinoline (namely ν_{45} and ν_{44} centered at about 168.5 cm⁻¹ and 177.6 cm⁻¹ respectively). In this study, high resolution synchrotron based FT-FIR together with pure rotation spectroscopy in the sub-mm range permitted to obtain very complementary data. The spectral analysis permitted to identify relatively large perturbation patterns across a K_a difference of 2 between the two excited states (both states are A' symmetry). Successful treatment of the perturbations allowed for the accurate determination of i) the rotational constants in the excited states ii) the Fermi and Coriolis perturbation terms and iii) the relative energies of ν_{45} and ν_{44} to the GS. Since most of the PAHs molecules possess low frequency out of plane vibrations which are relatively close in energy, this study emphasizes the difficulties encountered to simulate accurately the rotational structures of such large molecules in excited vibrational states.

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