ROTATIONAL SPECTROSCOPY AND STRUCTURE DETERMINATION OF FURONITRILE AND ITS COMPLEX WITH WATER

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Recent astronomical observations reported on the first interstellar detection of various pure and substituted aromatic rings via emission of their rotational transitions[1]. However, searches for nitrogen-, oxygen-, and sulfur-bearing heterocycles have been unsuccessfully so far[2]. Since oxygen is the most abundant element among heteroatoms and the presence of a cyano group typically results in a large value of the molecular electric dipole moment, furonitrile represents one of the best candidates for the first detection of an interstellar heterocycle via its rotational emission.

In this context, an accurate spectroscopic characterization of the rotational spectra of both regioisomer of furonitrile, namely 2-furonitrile and 3-furonitrile, has been carried out with the aim of obtaining accurate spectral predictions to be used for astronomical observations. Moreover, we have investigated the rotational spectra of several of their isotopologues, namely all their singly-substituted ^{13}C species, the ^{15}N, and the ^{18}O isotopic species. The rotational constants obtained have been used in combination with computed vibration-rotation interaction constants (within the so-called semi-experimental approach) to derive a precise geometry of both 2- and 3-furonitrile.

Lastly, in order to provide insights on how water interacts with aromatic rings when an heteroatom is introduced, the rotational spectra of some molecular complex formed by 2- or 3-furonitrile with one water molecule (including various water isotopologues) have been recorded and analyzed. The interaction occurring in the furonitrile-water cluster is then compared with those reported for similar species, such as benzonitrile[3] and acrylonitrile[4].

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