ANALYSIS OF COMBINED MILLIMETER-WAVE AND HIGH-RESOLUTION INFRARED SPECTRA OF 2- AND 3-FURONITRILE

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2-Furonitrile and 3-furonitrile are highly polar CN-substituted derivatives of furan. These molecules are attractive targets for interstellar search due to their strong dipole moments (μ_a = 4.3 D, μ_b = 0.7 D and μ_a = 4.0 D, μ_b = 0.4 D, respectively) and their ability to serve as tracer molecules for furan. In our recent work, we analyzed and assigned the millimeter-wave and high-resolution infrared (IR) spectra of 2- and 3-furonitrile for the first time. From 140-750 GHz and 140-500 GHz, respectively, the vibrational ground-state transitions of each molecule have been least-squares fit to partial octic, distorted-rotor Hamiltonians with each data set containing several thousand independent transitions. The two lowest-energy fundamental modes of both furonitriles are the Coriolis-coupled bending modes of the nitrile (ν_{17} and ν_{24}). High-resolution infrared spectra were obtained from the Canadian Light Source and provided the precise band origins of these modes for both furonitriles, as well as of ν_{23} for 2-furonitrile. We recently reported our work on 2-furonitrile [1] and will discuss our progress in the analysis of the ground state and first two fundamental modes of 3-furonitrile.

[1] Millimeter-Wave and High-Resolution Infrared Spectroscopy of 2-Furonitrile - A Highly Polar Substituted Furan. *J. Phys. Chem. A*, ASAP (2023)