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

WILLIAM STYERS, BRIAN J. ESSELMAN, MARIA ZDANOVSKAIA, ANDREW N. OWEN, SAMUEL M. KOUGIAS, Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA; BRANT E. BILLINGHURST, JIANBAO ZHAO, Materials and Chemical Sciences Division, Canadian Light Source Inc., Saskatoon, Saskatchewan, Canada; R. CLAUDE WOODS, ROBERT J. McMAHON, Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA.

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 (\(\mu_a = 4.3\) D, \(\mu_b = 0.7\) D and \(\mu_a = 4.0\) D, \(\mu_b = 0.4\) 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 (\(\nu_{17}\) and \(\nu_{24}\)). 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 \(\nu_{23}\) 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.