COUPLED CLUSTER CHARACTERIZATION OF 1-, 2-, AND 3-PYRROLYL FOR VIBRATIONAL AND ROTATIONAL SPECTROSCOPY

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A wide variety of nitrogen-containing heterocycles have been detected on meteorites with non-terrestrial isotopic abundances, indicative of an interstellar origin. However, no N-heterocycles have been detected in space and their formation pathways are unclear. Experimental work has shown that N-heterocycles can likely form through barrierless radical-neutral gas-phase reactions, which are feasible in the low temperature environments of cold molecular clouds and the outer regions of protoplanetary disks. Astronomical searches and laboratory studies of potential precursors and depletion products are critical to determining if such mechanisms play a role in N-heterocycle formation. Pyrrolyl is both a photodissociation product of the N-heterocycle pyrrole (C_4H_5N) and a potential astrophysical precursor to larger N-heterocycles. Furthermore, pyrrolyl is a known intermediate in the combustion of biomass and was tentatively detected in Titan's atmosphere by the Cassini-Huygens mission. Here, the first treatment of 1-, 2-, and 3-pyrrolyl at the CCSD(T) level of theory and progress towards the first experimental detection in the cm-wave region will be discussed. Equilibrium geometries were optimized at CCSD(T)/cc-pwCVTZ and quadratic, cubic, and partial quartic force constants were evaluated at CCSD(T)/ANO0 in order to obtain harmonic and anharmonic vibrational frequencies. Additional parameters for vibrational and rotational spectroscopy were calculated at similar levels of theory. This work will enable astronomical searches, laboratory spectroscopy, and kinetics and dynamics studies.