AB INITIO SPECTROSCOPIC PARAMETERS OF PYRIDYL RADICALS

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Nitrogen-substituted polycyclic aromatic hydrocarbons (PANHs) are fundamental species important in biological molecules, astrochemistry, and combustion. They have been detected on meteorites with non-terrestrial isotopic abundances, potentially play a role in prebiotic chemistry, and have been observed in the atmosphere of Titan. They are suggested to be responsible for some of the unidentified infrared (UIR) emission bands in the interstellar medium and have been identified as intermediates in the combustion of biomass. Pyridine is a prototypical nitrogen-containing aromatic molecule, and recent studies suggest that the pyridyl radicals are key intermediates to the formation of PANHs. However, no high-resolution spectra or coupled-cluster calculations of the pyridyl radicals are available. To complement our search for the pyridyl radicals with rotational spectroscopy, we calculated the equilibrium geometries, relative energies, and spectroscopic parameters for the three pyridyl radicals at the CCSD(T) level of theory. In addition, anharmonic vibrational frequencies were evaluated using second-order vibrational perturbation theory. We will discuss the results of our calculations and our progress to measure the rotational spectra of the pyridyl radicals using Fourier transform microwave spectroscopy.