Millimeter-wave Rotational Spectroscopy of Pyridine (C_5H_5N), Pyridazine ($C_4H_4N_2$), and Their Discharge Products with efforts toward Phenyl Radical (C_6H_5), *ortho*-Benzyne (*o*-C_6H_4), Protonated Benzene ($C_6H_7^+$)

Brian J. Esselman, Brent K. Amberger, Mitchell A. Daane
R. Claude Woods,* and Robert J. McMahon*

Department of Chemistry, University of Wisconsin, 1101 University Avenue, Madison, WI 53706

esselman@wisc.edu

In order to gain insight into the behavior of small aromatic species in a DC discharge, we have been studying pyridine and pyridazine. These molecules are advantageous due to their dipole moment which allows us to determine the relative abundance of the parent molecule with relative ease as well as any discharge products. Thus far, we have observed several previously identified species in a pyridine discharge including previously reported vibrationally exicted states of pyridine. We have also measured the unpublished millimeter lines of pyridazine and compared them with predictions based upon published rotational constants and centrifugal distortion constants. This work should provide insight on the conditions necessary to produce large ions and radicals using our spectrometer.

A detection of benzene has been reported in proto-planetary nebula CRL 618 via infrared spectroscopy by the Infrared Space Observatory. Due to its symmetry and resulting lack of a dipole moment, however, benzene does not exhibit rotational transitions that allow detection by radioastronomy. Fortunately several closely-related reactive aromatic species, such as phenyl radical (C_6H_5), *ortho*-benzyne (*o*-C_6H_4), and protonated benzene ($C_6H_7^+$) have dipole moments and should be detectable in the interstellar medium via their rotational spectra. At this point, the rotational spectra of phenyl radical and *ortho*-benzyne have been reported in the microwave region of the spectrum, but experimental values are not available in the millimeter region. We are attempting to generate all three of these molecules in a gas discharge tube and measure their absorptions over a region of 240 to 450 GHz, thus expanding their known rotational spectra. We aim to explore the conditions necessary to produce each species and their discharge coproducts. The measured laboratory frequencies may provide the basis for future radioastronomical searches for these molecules.

The millimeter-wave absorption spectrometer being used in this research project has been used previously for the investigation of numerous small inorganic molecules and ions. The apparatus consists of a three-meter Pyrex discharge chamber with cylindrical electrodes at each end. The discharge operates at mTorr pressures and at temperatures as low as 77 K. The microwave signal is generated by a Gunn-diode microwave source, which is then further amplified and multiplied to reach the desired frequencies. The signal is focused onto a liquid-helium-cooled indium antimonide detector. Recent modifications include the addition of an internal glass tube designed to distribute our parent molecules evenly throughout the chamber and the introduction of a chiller to provide fine-tuned control of the experimental temperature. These improvements should allow for a more uniform discharge and greater control of conditions.