Rotational Spectroscopy Investigation of Interactions between Carbon Dioxide and N-containing Cyclic Compounds

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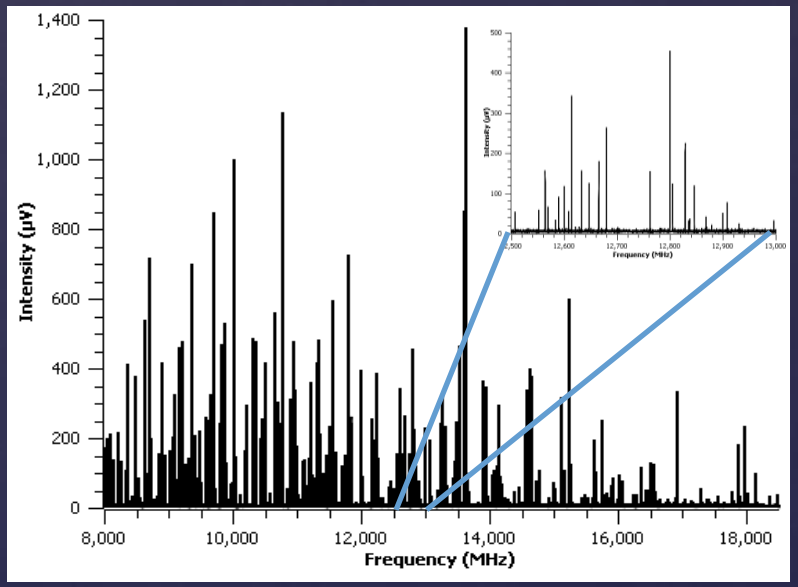
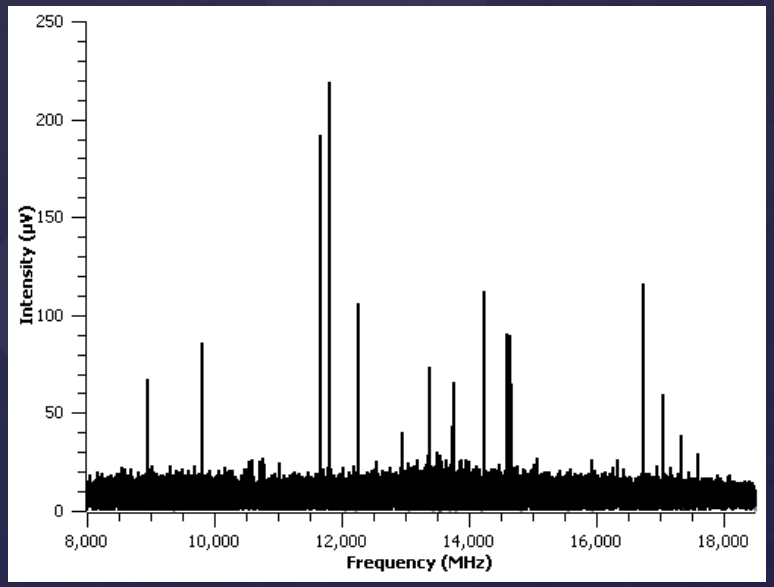
In this project, our main goal is to measure, assign, and analyze the rotational spectra of van der Waals complexes of carbon dioxide with four nitrogen-containing cyclic molecules: pyrimidine, pyridazine, pyrazine, and imidazole. The purpose of this study is twofold. First, we hope to better guide the next generation of materials developed for carbon capture and storage (CCS). Second, this study will provide an important test of previously published theoretical data.



The above figure shows the spectrum of 3-vinylbenzaldehyde (3VBA). After significant upgrades to the Coker microwave spectrometer, made possible by the PRF grant, we successfully measured, assigned, and analyzed the above spectrum. This successful experiment highlights the utility of the upgraded spectrometer.



The above figure shows the spectrum of the pyrrole-CO_2 complex. For this experiment, the pyrrole monomer was measured separately, and all lines from the monomer were removed from the above spectrum. Therefore, all of the lines shown on the spectrum above are due to the pyrrole-CO_2 complex.