Broadband Microwave Spectroscopy of Highly Functionalized 5-Membered Ring Organic Molecules

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Chemistry Seminar on Microwave spectroscopy

Monday October 20 at 4 pm in 126 Schrenk

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Abstract: Succinimides and maleimides are highly polar cyclic organics that play important roles in biological chemistry, biotechnology, and organic synthesis. In this talk, I will describe our broadband rotational studies of Succinimide, N-methyl succinimide, N-methylmaleimide, N-ethyl succinimide, and N-ethyl maleimide. Microwave spectroscopy provides high-resolution rotational spectra of these molecules in the gas-phase and when combined with electronic structure calculations, the rotational fits can be used to extract the molecular structures. The broadband spectra of four succinimide derivatives has been investigated in the 26.5-40 GHz frequency range region using a chirped pulse Fourier transform microwave spectrometer coupled to a supersonic expansion. Details on the molecular structure of these five molecules, their molecular parameters, methyl internal rotations, the isotopologues of succinimide, and structural arrangements of the substituent group will be discussed.

About the speaker: Dr. Hernandez-Castillo is an Assistant Professor in the department of Chemistry at Harvey Mudd College in Claremont California. She attended the National and Autonomous University of Mexico (UNAM) for her undergraduate work. In the fall of 2014, she moved to the United States to do her graduate work at Purdue University under the supervision of Dr. Timothy S. Zwier. There she focused on detection and characterization of resonance stabilized radicals using broadband rotational spectroscopy. Her love for the development of new experimental techniques led her to a postdoc at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany. There she worked on establishing robust experimental schemes for preparing single enantiomers of chiral molecules in selected rotational states using an array of laser-based and broadband microwave methods. Since her arrival at Harvey Mudd College she has built a broadband microwave and a molecular beam time of flight mass spectrometer and has focused on the characterization of the structures of succinimide containing anticonvulsants. In her free time, she enjoys traveling, running, terrible puns, and chocolate.