UCMERCED UNIVERSITY OF CALIFORNIA School of Natural Sciences

CHEMISTRY SEMINAR 291

Investigating CH5+, "A Molecule that won't sit still"

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Date: **5/4/18**
Time: **1:30 PM**
Location: **COB1 267**

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ABSTRACT

Protonated methane (CH5+) has intrigued chemists for several decades. It was first detected by Tal'roze and Lyubimova in the early 1950's, and since then several groups have sought to obtain and assign an infrared spectrum of CH5+ as well as to understand it's structure. Bonding five hydrogen atoms to carbon results in a molecule with 120 (5!) equivalent structures. Unlike more typical organic molecules, the barriers that separate these structures are as low as 4 kJ mol-1 and the zero-point level has nearly equal probability amplitude at all 120 minima as well as 180 transition states that separate these minima!

In this talk I will discuss work in our group to understand the structure of CH5+ as well as possible spectral consequences of the very delocalized structure. I will also describe methods we use to explore questions of structure and spectra in a molecule that does not have a simple equilibrium structure. Finally, we will explore how deuteration may be the key to understanding and spectroscopy of CH5+.

BIO:

Anne B. McCoy received her B.S. degree in Chemistry from Haverford College in 1987, and taught chemistry for a year at The Hotchkiss School before receiving a Ph.D. at the University of Wisconsin, Madison with Professor Edwin L. Sibert in 1994. She was a Post Doctoral Fellow with Benny Gerber, traveling between the University of California, Irvine and Hebrew University in Jerusalem. She joined the faculty at the Ohio State University in 1994, where she rose through the ranks. In 2015 she moved to join the faculty at the University of Washington. She is a Fellow of the American Physical Society (2007), the American Chemical Society (2009) and the American Association for the Advancement of Science (2012). From 2005-2011 she was a Senior Editor for the Journal of Physical Chemistry, and has served as the Deputy Editor of the Journal of Physical Chemistry-A since 2011. In addition, she has been a member of the ACS Committee on Professional Training since 2008, and served as chair the committee from 2012-2014. She has also been active in the PHYS division of the ACS, serving as Secretary/Treasurer from 2006-2011 and will be program chair in 2019 and chair in 2020. Her research has been recognized through a CAREER Award from the NSF; Camille Dreyfus Teacher/Scholar Award and Crano Lectureship from the Akron Section of the ACS. While at Ohio State she received both the Distinguished Scholar Award and Harlan Hatcher Award Arts and Sciences Distinguished Faculty Award in 2013.