

# Microwave Spectroscopy at Missouri S&T

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**Chemistry  
Seminar on  
Microwave  
spectroscopy**

**Monday  
Oct. 16 at 4  
pm in 303  
Schrenk**

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**Abstract:** Microwave spectroscopy, or rotational spectroscopy – which measures the distribution of nuclear masses in a molecule - has long been a very niche field with many people outside of the molecular spectroscopy community knowing little about it other than what is learned in a quantum mechanics/chemistry course. This all changed, however, with two major advances in the field in the past 20 years. Those were the chirped pulse, Fourier transform microwave (CP-FTMW) spectroscopy instrument of Pate and coworkers and the microwave three-wave mixing (M3WM) technique of Patterson, Schnell, and Doyle. These two advances immensely sped up the acquisition of spectra while also opening the door to use electric fields and, by extension, rotational principles to distinguish between enantiomers. This allowed for the greater physical and analytical communities to tap into the power of rotational spectroscopy which is its unparalleled bandwidth-to-resolution ratio (a single transition has a 1 in  $10^5$  probability of being anything but the molecule in question and can observe other phenomena like internal rotation dynamics). At Missouri S&T, we are both trying to improve on the CP-FTMW technique by using novel methods to increase the sensitivity while also using the power of the resolution to solve societal chemical problems such as the nature of  $f$ -electron contributions to bonding in actinide-containing molecules using laser ablation-equipped CP-FTMW and rapid detection of poly/perfluoroalkyl substances (PFAS) in mixtures. We have also constructed a M3WM instrument and are using the principles of pulse scheme construction and implementation to try and elicit enantioselectivity in chiral species using only microwave fields. In addition, more traditional microwave spectroscopy projects performed in our laboratory on silicon-containing molecules and biochemically relevant molecules will be discussed.

**About the speaker:** Bio: “Smitty” Grubbs, Associate Professor and Associate Chair of Chemistry, joined Missouri S&T in 2013. He received his BS from Texas A&M University in College Station, TX in 2006 and his PhD from the University of North Texas in Denton, TX in 2011. From 2011-2013 he was a postdoctoral fellow with Stew Novick at Wesleyan University in Middletown, CT. His research deals with the continuing improvement of molecular rotational spectra instrumentation and interpretation in order to unlock the potential uses of microwave rotational techniques, particularly as it applies to actinide-containing and chiral molecules. He has published over 50 peer-reviewed journal articles in this area. His group consists of postdoctoral fellows, graduate, undergraduate, and, occasionally, high school students. He is the editor of the Microwave Spectroscopy Information Letter, the premier source for up-to-date experimental happenings among the microwave rotational community. He is the organizer of the Midwest Microwave Spectroscopy Consortium which has nine investigators from eight different institutions. He is on the editorial board of the *Journal of Molecular Structure* and recently rotated off the editorial board of the *Journal of Molecular Spectroscopy*. He is the recipient of the 2019 Flygare Award in Molecular Spectroscopy which recognizes top Molecular Spectroscopist within 10 years of their PhD at the International Symposium on Molecular Spectroscopy.