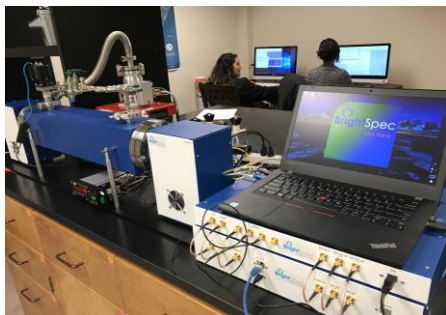


M.S. Assistantship- Molecular spectroscopy and quantum chemical study of micro-solvation process

We are seeking a motivated student for a graduate position (MS) in molecular spectroscopy of micro-solvation process. The research will consist of spectroscopic studies in the microwave regions. The student will work to (1) carry out measurement of rotational spectra of the interested species using our newly acquired BrightSpec K-band Fourier transform microwave spectrometer, (2) analyze the spectra, (3) carry out quantum chemical calculations using the cluster computer from Texas Advanced Computational Center (TACC) on the related molecules. (4) write up papers and present research results in national conferences. This appointment is to begin in Fall 2025 in the Chemistry Department at the University of Texas Rio Grande Valley. Student support is offered through a departmental teaching assistantship.

Applicant must have a Bachelor's degree in chemistry or a related field and have research interest in gas phase molecular spectroscopy. Successful candidates must demonstrate an aptitude for research and ability to work independently. As a TA, the student will be expected to work 19 hours/week as assistant instructor in undergraduate chemistry laboratory classes, assist his/her faculty teaching mentor with laboratory preparation and grading, and participate in departmental outreach events. The successful applicant will be expected to enroll full time in the UTRGV Chemistry Master of Science program pursuing the thesis option. The teaching assistantship will be provided in the form of a stipend, and is benefits eligible.

A minimum undergraduate GPA of 3.0 and GRE scores are required. Interested applicants should send to Dr. Wei Lin (wei.lin@utrgv.edu) a copy of their CV or resume, GPA and GRE scores, a written statement of graduate research interests, and letters from two references. Review of applications will begin immediately and will continue until the position is filled.



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Microwave measurements of the tropolone–formic acid doubly hydrogen bonded dimer

Aaron M. Pejlavas,¹ Agapito Serrato III,² Wei Lin,² and Stephen G. Kukolich¹

¹Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721, USA

²Department of Chemistry, University of Texas Rio Grande Valley, Brownsville, Texas 78520, USA

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The microwave spectrum was measured for the doubly hydrogen bonded dimer formed between tropolone and formic acid. The predicted symmetry of this dimer was $C_{2v}(M)$, and it was expected that the concerted proton tunneling motion would be observed. After measuring 25 a- and b-type rotational transitions, no splittings which could be associated with a concerted double proton tunneling motion were observed. The calculated barrier to the proton tunneling motion is near $15\,000\text{ cm}^{-1}$, which would likely make the tunneling frequencies too small to observe in the microwave spectra. The rotational and centrifugal distortion constants determined from the measured transitions were $A = 2180.7186(98)\text{ MHz}$, $B = 470.87390(25)\text{ MHz}$, $C = 387.68984(22)\text{ MHz}$, $D_J = 0.0100(14)\text{ kHz}$, $D_{JK} = 0.102(28)\text{ kHz}$, and $D_K = 13.2(81)\text{ kHz}$. The B3LYP/aug-cc-pVTZ calculated rotational constants were within 1% of the experimentally determined values. © 2016 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4940775>]