## COLLEGE OF ARTS & SCIENCES Department of Chemistry

Brown and Williamson Series
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CBLL16



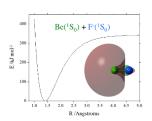
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Professor Emory University

# Beryllium bonding probed by electronic and anion photodetachment spectroscopy

#### **ABSTRACT:**

The chemistry of beryllium is known to be significantly different from the behavior exhibited by the heavier group IIA elements. Due to its high ionization energy and small size, the bonding of beryllium is significantly more covalent than the bonds of typical group IIA metals. As a consequence, beryllium and its compounds exhibit unique properties. However, the chemistry of beryllium is underexplored due to its toxicity. To circumvent this problem there have been many theoretical studies of beryllium and its compounds. Being a light element with just four electrons, beryllium appears to be well suited for investigation using non-relativistic quantum chemical methods. However, calculations for Be-compounds frequently prove to be difficult due to subtle (but dominant) electron correlation effects.



We are currently studying a series of Be<sub>n</sub> clusters and BeX diatomics by means of electronic spectroscopy and anion photodetachment spectroscopy to examine the bonding. Becontaining species are generated by pulsed laser ablation. For photodetachment measurements, anions are mass selected and then photodetached. Electron imaging and autodetachment techniques are used to recover spectroscopic data. Recent results for Be<sub>n</sub> clusters and the BeO-, BeS- and BeF- anions will be presented. BeO- and BeS- both exhibit dipole-bound excited states, permitting the observation of rotationally resolved spectra. BeF- shows an unusually strong bond between the closed-shell Be and F- moieties. Electronic structure calculations, validated by comparison with the spectroscopic observations, have been used to examine the bonding in the anionic and neutral species.

### BIO:

Editor in Chief, Journal of Molecular Spectroscopy, 2020 -

Vice-chair of the American Physical Society Division of Chemical Physics, 2021

ICLO 2018 Laser Optics Conference (St. Petersburg, Russia), June 2018. Member of the organizing committee for "High Power Lasers: Fiber, Solid State, Gas and Hybrid"

International Conference on Combustion Physics and Chemistry, Samara University (Samara, Russia). July 2018. Member of the organizing committee.

Advisory board member, Pacific Conference on Spectroscopy and Dynamics, 2017 -

Conference co-chair (with S. J. Davis, Physical Sciences Inc.) "Gas and Chemical Lasers and Intense Beam Applications", San Francisco, 2010, 2011, 2012, 2014, 2016

Conference co-chair (with Anne McCoy, OSU) "Dynamics on Multiple Potential Energy Surfaces", Telluride Workshop, July 2016, 2018, 2020

Conference co-chair (with Ken Brown, Georgia Institute of Technology), "Physical

Chemistry meets AMO Physics" ACS National Meeting, Philadelphia, Fall 2016.

Workshop chair, "Precision Chemical Dynamics and Quantum Control of Molecular Ion Reactions" Emory University, Oct. 2016.

Co-author of over 250 peer-reviewed papers that are published in the highest impact journals for the field of molecular spectroscopy. Supervised the PhD programs of 28 students and supervised 12 post-doctoral fellows. Presentation of approximately 10 invited talks per year at national and international meetings. Routinely involved in the organization of meetings and workshops (typically one or two per year). Research programs funded by the National Science Foundation, the Department of Energy, and the Department of Defense.