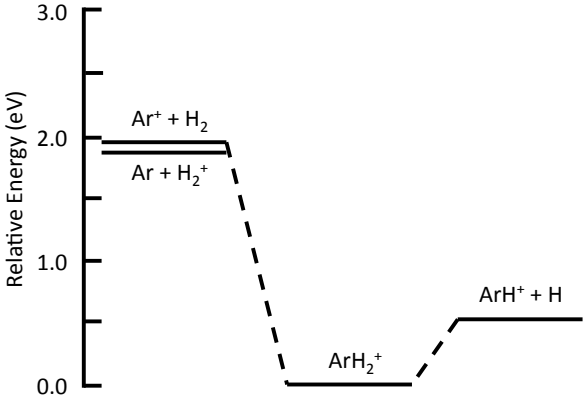
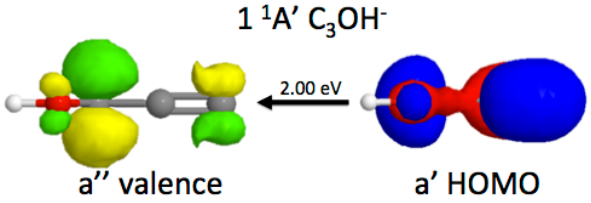
NOBLE GAS CHEMISTRY, ROVIBRONIC SPECTRA, AND MULTIPLE EXCITED STATES OF ANIONS FROM QUANTUM CHEMICAL COMPUTATIONS. R. C. Fortenberry, Georgia Southern University (P.O. Box 8064 Statesboro, GA 30460, rfortenberry@georgiasouthern.edu).

Introduction: The environments of the interstellar medium, photodissociation regions, and exoplanetary atmospheres, among other astronomical environments, are often populated by molecular species that are often transient, at best, on Earth. Quantum chemical computation is an excellent tool for the study of these species since it not hindered in the analysis of molecules the same way in which laboratory experiments can be. Granted, quantum chemistry has it own set of drawbacks, but this tool has shown significant promise and use in the analysis of astronomically-relevant molecules for some time.



Presentation: First, this presentation will include new computational insights into the formation and spectra of emerging noble gas compounds [1] ($ArH^+/ArH_2^+/ArH_3^+$) now known to exist in the Crab nebula. Next, discussion of computed rovibrational and even new rovibronic spectra will include novel insights into the HOC and C_2H radicals, as well as the *c*-C_3H^- anion [2-4]. Finally, new insights into both valence and dipole-bound excited states of anions and how these states affect the creation and spectra of astrochemicals will be provided for CH_2CN^-, CH_2SiN^-, C_3N^-, C_3P^-, C_5N^-, C_3H^-, C_3OH^-, $HBCN^-$, and polycyclic aromatic hydrocarbon anion derivatives both with and without the inclusion of nitrogen heteroatoms (PANHs and PAHs, respectively), among others [5-9]. The growth of understanding for these species will provide deeper insights regarding the chemistry of astronomical environments and, ultimately, the creation pathways for the molecular building blocks of life.



References: [1] Theis, R. A.; Morgan, W. J.; Fortenberry, R. C. *Mon. Not. R. Astron. Soc*. (2014), 446, 195. [2] Morgan, W. J.; Fortenberry, R. C. *Spectrochim. Acta A*. (2015), 135, 965. [3] Morgan, W. J.; Fortenberry, R. C. *J. Chem. Phys.* (2015), *submitted*. [4] Fortenberry, R. C.; Huang, X.; Crawford, T. D.; Lee, T. J. *Astrophys. J.* (2014), 796, 139. [5] Fortenberry, R. C.; Crawford, T. D. *J. Chem. Phys.* (2011), 134, 154304. [6] Fortenberry, R. C. *Mol. Phys*. (2013), 111, 3265. [7] Fortenberry, R. C.; Morgan, W. J.; Enyard, J. D. *J. Phys. Chem. A*. (2014), 118, 10763. [8] Theis, M. A.; Candian, A.; Tielens, X. G. G. M.; Lee, T. J.; Fortenberry, R. C.; *Phys. Chem. Chem. Phys.* (2015), *submitted.* [9] Fortenberry, R. C. *J. Phys. Chem. A*. (2015), *submitted.*

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