

Announcing the Final Examination of Mr. Conner Penson for the degree of Doctor of Philosophy

Date: November 6th, 2025

Time: 9:30 a.m.

Room: CSB 221

Attendance Link: <https://ucf.zoom.us/j/95758203798>

Dissertation Title: A Theoretical Study Investigation of Molecular Photoionization: Applications to Molecules of Astrophysical and Atmospheric Interest

This thesis is devoted to the development of the model for total molecular photoionization spectra which is general to diatomic molecules and the application of this model to two benchmark systems, CH and N₂, for verification. This model combines multi-channel quantum defect theory, first-principles ab initio molecular calculations, and vibrational frame transformation to accurately model molecular photoionization and electron impact including vibrational dynamics. The scattering data and transition dipole moments for the molecular systems were calculated using R-matrix method through the UKRMol+ suite of codes. A vibrational frame transformation is then performed and multi-channel quantum defect theory is used to calculate closed channel resonances. The matrix of closed-channel coefficients is then analyzed to characterize all of the resonant structures present in the spectra. The electron impact (de-)excitation cross sections were also calculated for the first 9 vibrational levels of the X²Σ_g, A²Π_u and B²Σ_u of N₂⁺. The photoionization spectra were compared with current experimental data for their associated molecule in order to verify the model. The experimental studies are the ion yield measurement by Gans et al. for CH and the measurement by Randazzo et al. for N₂. To verify the electron impact calculations, the results were compared with the recent theoretical study by Abdoulanziz et al. Both calculated photoionization spectra successfully represented and characterized most resonant structures present in the experimental data. An identification of double-cathedral resonance in the N₂ photoionization spectrum shows agreement for the first peak but an argument is made for the missing second peak. The comparison between this calculation of the electron impact rate coefficients and the previous group's model reveals differences in temperature thresholds, but an argument is made for the rates found within this work. Potential future improvements and additions to the investigation are proposed and discussed.

Outline of Studies:

Major: Physics

Educational Career: B.A., 2021, Embry-Riddle Aeronautical University

Committee in Charge (UCF):

Dr. Viatcheslav Kokoouline

Dr. Robert Peale

Dr. Nicolas Douguet

Dr. Mehdi Ayouz

Committee in Charge (UP-S):

Dr. Ioan Schneider

Dr. Guillaume Lombardi

Dr. Thierry Stoecklin

Dr. Arnaud Bultel

Dr. Olivier Dulieu

Dr. Nadia Bouloufa

Approved for distribution by Viatcheslav Kokoouline, Committee Chair, on October 16, 2025.

The public is welcome to attend.