

In general our research interest involves computational/theoretical chemistry, as it applies to materials and atmospheric chemistry. Currently our group is working in aerosol chemistry and metal silicate clusters.

**Aerosol Chemistry** – The fundamental knowledge derived from studies of molecular complex formation is of great importance in understanding atmospheric chemical process and aerosol formation. This project centers its attention on molecular complexes formation that serves as nucleus for fine aerosol particle formation.

**Condense Phase** – We look at the molecular and electronic structure of small molecules adsorbed on metal silicate clusters and semiconductor or metal surfaces. Our goal is to look at biomolecules synthesis catalyzed by these surfaces. A motivation for this project is the recent discovery of aminoacetonitrile<sup>1</sup> (Figure 1.a) in the dense molecular cloud Sagittarius B2. A publication in the Journal of Physical Chemistry<sup>2</sup> looked at the mechanism in which this particular molecule can be transform into glycine (Figure 1.b), which is the smallest amino acid commonly found in proteins.

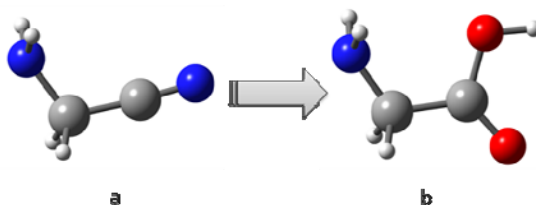


Figure 1: Optimized structure at the B3LYP/6-31+G(d) level of theory of a) aminoacetonitrile and b) glycine. Color code: Grey=carbon, blue=nitrogen, red=oxygen and white=hydrogen.

To accomplish these studies we will perform electronic structure calculations using density functional theory and post Hartree-Fock methods employing the Gaussian software package.

Students will learn without difficulty how to do molecular and electronic structure calculations.

#### References:

1. Belloche, A.; Menten, k.M. et al; Astronomy and Astrophysics 2008, 482, 179
2. Koch, D.M.; Toubin, C. et al; Journal of Physical Chemistry C 2008, 112, 2972-2980