Project Title: RUI: Thermodynamics of Nucleation: From Water to Atmospheric Aerosols
Principle Investigator: Dr. George Shields, Professor of Chemistry, Dean College of Arts and Sciences
Funding Agency: National Science Foundation (NSF)
Award Amount: $106,433 for the first year. This award is expected to total $333,082
Award Period: 2015-2018

With this award, the Environmental Chemical Sciences Program of the Division of Chemistry is funding Professor George Shields of Bucknell University to determine structures and energies of molecular complexes relevant to atmospheric aerosols. These complexes are formed from water molecules, sulfuric acid molecules, and other trace molecules found in the atmosphere. These complexes are important because they are relate to the fundamental basis of how clouds form, and the mechanism for cloud formation is currently not known. The project is also having a broad impact through its model of a sustained and productive undergraduate research experience involving the same students, including minorities and women, throughout their undergraduate years.

Professor Shields and co-workers are perusing a joint computational/experimental study toward establishing the minimum energy structures and the thermodynamics for formation of hydrogen-bonded complexes. These studies allow for the assessment of the ability of state-of-the-art computational chemistry methods to model water clusters that can be directly compared, and help guide state-of-the-art microwave spectroscopy experiments. The Shields group is determining the structures and thermodynamics of molecular clusters containing sulfuric acid, bases, and water that are believed to serve as neutral and ionic cloud condensation nuclei. These methods are expected to allow for the prediction of the relative abundance of all potentially relevant complexes, providing insight on which ones are of atmospheric importance in the cloud nucleation process. In a much broader sense, the techniques being developed here may provide atmospheric scientists with new ways to relate air quality/composition to cloud nucleation/pattern development.

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