Invited Lectures I

September 6, Thursday, 9:00 – 10:30

Reactive and Highly Reactive Species: Characterizing Key Intermediates in Combustion, Atmospheric, and Interstellar Chemistries by Rotational Spectroscopy

Michael C. McCarthy

Atomic & Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA, mccarthy@cfa.harvard.edu

Fourier transform microwave spectroscopy of supersonic molecular beams has developed into a remarkably sensitive technique for studying unstable molecules. It has proven particularly effective for the detection and characterization of transient species such as radicals and carbenes, and both positively- and negatively-charged molecular ions, which are even more reactive once formed, often reacting at the gas-kinetic or Langevin rate. Although laboratory detection remains challenging, the rotational spectra of several hundred entirely new carbon, silicon, and sulfur molecules have been detected. Precise molecular geometries have been determined by means of isotopic substitution for nearly one-half of the newly found molecules. Many of these species are of astronomical interest, and on the basis of the laboratory data, slightly less than 10% have been detected in space with large radio telescopes, including anions for the first time. A total of six carbon-chain anions have now been detected in rich interstellar or circumstellar sources in the span of five years, and C_6H^-, the most readily observed anion, has now been detected in at least eight astronomical sources, suggesting that negatively-charged molecules may be widely distributed in the interstellar gas.

This talk will provide a broad overview of our recent work, illustrating with a few specific examples the power of our laboratory techniques, and how these techniques can be applied to detect and characterize key reactive intermediates that are believed to play important roles in combustion, atmospheric, and interstellar chemistries. Many of the results are of general interest to the chemical physics community; they contribute to comparative studies of bonding between different elements in the Periodic Table, providing further evidence of the rich architecture of the chemical bond; and establish important benchmarks for theoretical chemistry. Recent isotopic work on the HOXO (X=C, O, S, N) radicals and the detection of positively-charged species such as nitrogen-protonated nitrous oxide and vinyl cyanide will likely be highlighted.

New Telescopes, New Expectations, Puzzling Results

Eric Herbst[1]

[1]University of Virginia, United States, eh2ef@virginia.edu

The exciting new spectral results from the Herschel Space Observatory, SOFIA (Stratospheric Observatory for Infrared Astronomy), and ALMA (Atacama Large Millimeter/Submillimeter Array) among other telescopes are leading astrochemists into a new era, in which our level of understanding of the molecular universe will be challenged as never before. New observations of both reasonably well-known and novel environments with exquisite spatial detail plus vastly increased spectral intensity will quickly yield a huge amount of data, much of which will require new and more detailed chemical simulations to understand. Successful simulations, which contain both gas-phase chemistry and chemistry on the surfaces of dust particles, will probably require the coupling of chemistry with both dynamics and heterogeneity.[1] In addition, the role of surface chemistry will have to be better understood, and incorporated into models via more exact methods, while exotic gas-phase processes such as radiative attachment will have to be calculated or measured in the laboratory. In my talk I will emphasize some new results about the interstellar medium that are puzzling to astrochemists, because they are not fully understandable in terms of the environments we thought we knew well. These results include a polyatomic chemistry in diffuse (low-density) clouds, the detection of intense spectra from species that should be destroyed on every collision with H_2, the dominant interstellar molecule, (e.g. OH^+, H_2O^+) and strong spectra from species in similar environments that require H_2 for their formation (e.g. HF), as well as unusual ortho-to-para ratios, such as the value of 4.8 ± 0.5 for H_2O^+ in the direction of the galactic centre. I will also discuss our current views of how the most complex interstellar molecules are formed, and what role chemistry plays in new observations that show different complex molecules in the same star-forming region to often occupy different regions of space.[2]

References

[1] Y. Aikawa, V. Wakelam, R. T. Garrod, E. Herbst, Astrophys. J. **674,** 984, 2008
[2] E. Herbst, E. F. van Dishoeck, Ann. Rev. Astron. Astrophys. **47,** 427, 2009