White paper submitted to the National Academies
Astro2010 Decadal Survey

Laboratory Astrochemistry Facility to underpin the next Decade of Astronomy and Astrophysics

Abstract

Among the most important foundations of our ability to interpret astrophysical observations and to create models of diverse cosmic phenomena are the laboratory-derived spectroscopic data, atomic, molecular, and chemical properties, and reaction rates that underpin them. The next decade of progress in astronomy and astrophysics will present great new opportunities for observations and for elaboration of simulations but these will be placed significantly at risk without commensurate advancement and range of new opportunities for laboratory astrophysics. To ameliorate this situation, we propose to develop a novel platform for the study of atoms, molecules, dust, and ices at the appropriate background temperatures relevant to planetary systems, star formation, and the interstellar medium, that is, a facility for laboratory astrochemistry. In particular, a molecular ion storage ring would allow development of accurate chemical networks and precision spectroscopy needed for a wide range of astrophysical studies. Consequently, we wish to underscore the need for prominent and fundamental consideration of laboratory astrophysics and for priority of support for the facilities needed for the next decade of discovery.

Prepared by:

David R. Schultz, (865) 576-9461
Physics Division
Oak Ridge National Laboratory
schultzd@ornl.gov

Initial Collaborators:

Daniel W. Savin, Columbia Astrophysics Laboratory
Phillip C. Stancil, University of Georgia
Gary Ferland, University of Kentucky
Robert Continetti, University of California, San Diego
Michael Fogle, Auburn University
C. Randy Vane, Oak Ridge National Laboratory
Mark E. Bannister, Oak Ridge National Laboratory
Charles C. Havener, Oak Ridge National Laboratory
Fred W. Meyer, Oak Ridge National Laboratory

Introduction

To a large extent, what we know about the cosmos and all that it contains comes from the observation and interpretation of photons. In addition to nuclear processes or emission from particles accelerated to very high energies, much of the rich mosaic of photons (or their absorption) across spectral bands are produced or affected by atomic, molecular, chemical, and surface processes. Therefore it is essential that appropriate capabilities exist to provide accurate and appropriately comprehensive laboratory astrophysics and astrochemistry data such as spectra of atoms, molecules, and larger complexes, and reaction rates for interaction among photons, electrons, atomic and molecular ions, atoms, molecules, dust and ices.

In particular, the opening up of new spectral sensitivity, resolution, and coverage within the next decade in the infrared, submillimeter, millimeter, radio, and optical wavebands, and commensurate improvements and elaborations in astrophysical models and computer simulations, will spur the need for new laboratory capabilities. At the same time, the greater focus on observing emission and absorption involving molecular systems, from the simplest species such as H_3^+, to carbon containing molecules, ices and dust, will necessitate construction of novel facilities to probe their interactions and further the work of deducing their spectra.

For example, dust grains, small clusters, and polycyclic aromatic hydrocarbons (PAHs) species are known to play important roles in the thermal balance of nearly all low-temperature astronomical objects and also provide key spectral signatures from the ultraviolet to the infrared. However, little quantitative information on the formation and destruction processes of PAHs is available. Novel laboratory astrochemistry capabilities would provide a unique opportunity to study PAH ion dynamics, currently not amendable to theoretical investigations, and to establish, for the first time, an accurate chemical network of these complicated astronomical species. PAHs are also suspected to emit in the far infrared and submillimeter and the coupling of far infrared photon sources with beams of PAH ions could provide precision spectroscopic data, which are currently lacking. Current matrix isolation techniques, which have provided comprehensive ultraviolet and optical spectroscopy, are not adequate for this spectral region.

One such required new facility is therefore a molecular ion storage ring facility to create and store a wide variety of molecular ions, allow interactions of them with electrons, photons, neutrals, and surfaces, and to observe the interactions through spectroscopy and reaction imaging. While Europe and Japan have made investments to develop molecular ion storage rings, the U.S. has not. Novel results from a complementary U.S. facility directed towards astrophysical research needs would underpin advances in understanding formation and evolution of stars and planetary systems, the interstellar and intergalactic media, and precursors to astrobiology, for example.

Background

By the 1990's, molecular ions were introduced into existing magnetic storage rings that were built for nuclear physics research motivated by applications requiring knowledge of electron – molecular ion interactions such as astrophysics and low-temperature plasma science. For example, pioneering studies of dissociative recombination of H_3^+ were made, resolving long-standing uncertainties in the magnitude of this process at low electron energies, both of fundamental interest and of great importance in astrophysics. To date dozens of molecular ions up to a few tens of Daltons have been studied in this way at magnetic storage rings. Also during this time, the first ideas and the first deployment of electrostatic storage rings came about, with the goal of studying molecular ions of greater mass owing to the essentially mass independent character of electrostatic deflection compared to magnetic deflection. To date several "first" generation electrostatic, molecular ion storage rings have been built, with a "second" or "advanced" generation of devices under construction or planned. Again, none of these facilities have been built in the U.S., Europe and Japan taking the lead (e.g., ELISA in Aarhus, DESIREE in Stockholm, and CSR in Heidelberg).

Storing and circulating ions

All the proposed studies are enabled by one or more of the unique characteristics of storage rings. Specifically, storage rings are a particularly advantageous geometry for a particle trap in which ions are circulated in a beam without any significant changes in particle velocity. That is, trapping in a ring avoids slowing the particles (for example, in the electrostatic mirrors of a reflecting beam ion trap) where undesired, deleterious reactions with background gas in the vacuum system are greatest because the cross sections are largest for low velocities. Another advantage of the ring geometry is that the stored particles can be synchronously "re-used" on each orbit. As we have mentioned, such rings are essentially not mass limited and so can store particles up to very large masses (e.g., large biomolecules, clusters, dust) albeit at relative low circulation velocities. Thus, ion beams generated from a wide variety of sources can be accumulated, stored, and repeatedly used in a ring.

State-preparation

By confining molecular ions (with permanent electric moments) in the ring for storage periods longer than radiative lifetimes, they reach thermal equilibrium with the blackbody temperature of the surrounding vacuum vessel. Storage in the ring therefore acts to cool them to a low internal (rotation and vibration) state, enabling experiments on a controlled initial state rather than the broader distribution of internal states populated in the process of creating the ions. This process is practically limited by two factors, storage time and vessel temperature. Various rings are designed for room temperature, liquid nitrogen, or liquid helium temperatures to address the latter constraint. Storage time is principally limited by the vacuum maintained in the ring – greater background pressure leads to more collisions of the stored beam with residual gas and thus greater loss from the phase space for confinement.

Interactions with other species

Another significant advantage of storage rings is the ability to cause controlled interactions with other species in the so-called merged beams geometry. We envision deploying merged electron, neutral (atoms, molecules), and photon beams. In the first two of these, the advantage stems from two factors: (1) the merged geometry allows very low relative velocities between the merging beam (e.g., electrons) and the stored beam of molecular ions, where the most interesting physics and chemistry occurs and where the needs from astrochemistry arise, and (2) this geometry also allows for a significant overlap of the beams for greater efficiency. Merged laser beams will similarly be afforded large overlaps with the stored ions for laser induced fluorescence or other spectroscopies.

Ring-intrinsic reaction detection schemes

The ring geometry also lends itself intrinsically to particular schemes of detecting the products of reactions. Since ions are only confined if their charge and velocity vectors stay within a particular range, any interaction that changes these significantly causes the ion (or its fragments) to become unconfined. For example, if while merged with the electron beam an ion recombines with an electron and dissociates, the neutral fragments will continue along trajectories undeflected by the electrostatic elements and can thus be detected as they leave the nominal ion orbit. Therefore one of the principal detectors envisioned will be patterned after the neutral particle imaging detectors pioneered at existing magnetic storage ring facilities. Another primary kind of detector will be photodetectors to probe absorption or emission of light following illumination of the stored beam by lasers and from exoergic reaction processes.

Proposed Astrochemistry Facility, Budget

To taking advantage of the capabilities of molecular ion storage rings, we propose that a facility be constructed containing the appropriate sources of atomic, molecular, cluster, ice, and dust ions, a storage ring for cooling and preparing them, interaction targets using electrons, neutral atoms, molecules, photons, and surfaces, and means of analysis of the reactions through a variety of spectroscopic and particle detection apparatus. A preliminary design for this facility has been carried out and it is estimated that it could be built for approximately $15M and operated at a cost of about $2M/year.

Summary and Prospective

The next decade of astronomy and astrophysics will require advances in laboratory astrophysics and astrochemistry commensurate with the advances made observationally and through modeling and simulation. In particular, knowledge of the spectra and reactions of systems involving photons, electrons, atoms, molecules, clusters, ice, and dust underpin interpretation of observation and the creation of accurate physical and chemical models spanning wavebands ranging from radio to visible.

New facilities are required to reach these goals and a molecular ion storage ring facility is a key one. Moreover, these facilities will require significant increases in funding available from NASA and NSF for laboratory astrophysics and astrochemistry. We urge the community to prominently and fundamentally consider support for such laboratory facilities and their complementary theoretical efforts.