LABORATORY ASTROPHYSICS WHITE PAPER
(BASED ON THE 2002 NASA LABORATORY ASTROPHYSICS WORKSHOP AT NASA ARC, Moffett Field, 1-3 MAY, 2002)

EXECUTIVE SUMMARY OF THE NASA LABORATORY ASTROPHYSICS WORKSHOP

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The NASA Laboratory Astrophysics Workshop (NASA LAW) met at NASA Ames Research Center from 1-3 May 2002 to assess the unique role that laboratory astrophysics plays in the optimization of NASA missions, both at the science conception level and at the science return level. Space missions provide understanding of fundamental questions regarding the origin and evolution of galaxies, stars, and planetary systems by deciphering the nature of their gaseous and solid components, including some that may be the precursors of life.

In the following we express a general consensus of the workshop as to the guiding principle of the Laboratory Astrophysics program, a list of general programmatic findings, and finally a list of more specific scientific areas that need attention.

I. General findings:

- The number of NASA missions requiring spectroscopic laboratory data has risen dramatically, but the funding for Laboratory Astrophysics has remained flat. The current funding profile cannot meet the needs of existing missions or prepare for future missions.

- Critical compilation of databases was identified as a high priority need. For example, NIST has been maintaining the highest quality atomic database in the world, a resource relied upon for basic data in several communities. But the overstrained NASA budget has not been able to provide the level of support required to maintain this database, and resources from other agencies have also diminished.

• Laboratory equipment is aging, and major funding is required to replace it with modern, state-of-the-art apparatus. Unless new facilities can be built, it will become increasingly difficult for laboratory astrophysics to keep up with the demand for atomic and molecular data to support space-based and ground-based observatories.

• Lack of funding is making it harder and harder to attract students and train the scientists of tomorrow to provide the required laboratory data.

• Until the 1990s, sensitivities in most spectral ranges were too low to permit high resolution spectroscopy, and missions like IRAS and ROSAT concentrated on mapping and photometry. The situation is drastically different today; with ISO, HST, FUSE, Chandra, and XMM-Newton we can look at detailed chemical and physical processes on solar system, stellar, galactic, and extragalactic scales.

• Within the next decade, four major infrared astronomical observatories will be launched, while major needs exist for the interpretation of data from current and planned UV and X-ray missions. Furthermore, high redshift observations from IR missions will require UV laboratory data for interpretation. All of these missions have spectroscopic capabilities with exquisite sensitivity, and most will have extremely high resolving power, with instrumental resolutions as high as $R = \lambda/\Delta\lambda = 10^6 - 10^7$. A host of new spectral features numbering in the millions will need to be identified and interpreted. This will not be possible without the support of:

(a) Laboratory wavelength measurements;
(b) Experimental and theoretical line strength work;
(c) Data on interaction cross sections;
(d) Accessible archives of these data.

To meet the objectives of these planned missions and to make their findings accessible to the public in clear, understandable terms, we will need the support of a coherent and vigorous Laboratory Astrophysics program that integrates theory, modeling, and experiment.

II. Needs for laboratory data supporting specific missions and spectral bands.

We now consider the scientific returns of laboratory astrophysics to various current and planned NASA missions. These differ significantly among wavelength ranges, and the lab astro program should support work across all spectral bands. The various spectral regions are considered here in order of increasing wavelength.

The X-Ray Spectral Region

Missions: Chandra, XMM-Newton, Astro-E2, and Constellation-X

X-ray observations can be used to address a number of fundamental questions in astrophysics. Relativistically broadened metal lines in AGN and quasars can be used to study black holes. High resolution spectra of AGN, quasars, XRBs, and CVs help us learn about accretion in the vicinity of compact objects. X-ray emission from infrared bright galaxies tell us about the relationship between the AGN and starburst components of galaxies. Stellar winds, supernova remnants, and the ISM can be used to study nucleosynthesis and the evolution of our Galaxy and the universe. Observations of galaxy clusters and the IGM provide information on the formation of large scale structure in the universe, the formation of galaxies, and provide constraints on the dark matter component of the universe. Stellar coronal observations can be used to study the connection between the stellar photosphere and corona and the physical processes involved in heating and mass supply to stellar coronae.

X-rays provide a quantitative understanding of highly ionized plasmas, both electron-ionized and photoionized. Electron-ionized plasmas are formed in stellar coronae, supernova remnants, the ISM, galaxies, and clusters of galaxies. Photoionized plasmas are found in planetary nebulae, H II regions, the IGM, AGN, XRBs, and CVs. Interpreting X-ray spectra from all these sources depends critically upon input from laboratory astrophysics. Priorities for measurements include atomic rate coefficients for low and high temperature dielectronic recombination, state-specific and total charge transfer for multiply charged ions on H and H_2, collisional excitation, inner shell photoabsorption, and photoexcitation and photoionization cross sections as well as fluorescence and Auger yields. Measurements of fundamental spectroscopic quantities are also needed, including M- and L-shell emission and satellite line identifications and wavelengths (accurate to one part in 10^5) for Ne, Mg, Si, S, Ar, Ca, Fe, and Ni.

While most atomic data used to interpret X-ray plasmas are compiled from theoretical calculations, laboratory measurements are needed to determine the accuracy of rates for critical diagnostics. As an example, the strong set of Fe XVII X-ray emission lines provides information on temperatures, densities, and opacities, but, despite recent laboratory studies, their astrophysical interpretations remain unclear. Laboratory surveys of the X-ray spectral content are also needed to provide critical tests of the completeness of spectral models. For moderate resolution X-ray data, complete models are required for global spectral fitting; at higher resolution, completeness studies are necessary in order to assess blending around diagnostic lines.

The atomic data for collisionally ionized plasmas, relevant to stellar coronae, galaxies, and clusters of galaxies, have received the best critical evaluations and laboratory tests. Non-equilibrium effects of X-ray spectra, such as those expected in supernova remnants, require further studies, as the atomic rate coefficients are often less accurate away from equilibrium temperatures. Priorities for future work need to include critical tests of the atomic data used for X-ray photoionized plasmas, such as found in accretion disks and black hole environments. Since spectral models for photoionized sources need to make assumptions about the astrophysics (e.g. energy balance and geometry) to incorporate atomic physics, it is critical that laboratory studies benchmark the essential atomic data, therefore studies of low temperature dielectronic recombination should receive high priority.

New results from Chandra and XMM-Newton suggest additional areas in need of laboratory astrophysics. Recent astrophysical observations have tentatively identified X-ray absorption by molecules, a new area for laboratory measurements of edge physics, which can lead to differentiation between gas and dust in diffuse media. Closer to home, objects in the solar system, such as comets, the Jovian aurora, the Io plasma torus, and the Jovian Galilean satellites (Io, Europa, Ganymede), emit X-rays. Cometary X-ray emission is tentatively attributed to charge transfer between the solar wind ions and the comet. If charge transfer is the correct mechanism, these observations provide a sample of the comet coma material as well as information on the solar wind velocity and elemental charge states. Accurate cross sections for charge transfer are needed, to compute both state-specific partial rates and total rates, for multiply charged ions on H and H_2. Laboratory measurements of charge exchange cross sections will help to validate the models for solar system X-ray emission, and may be of importance in X-ray photoionized plasmas as well.

The UV Spectral Region

Missions: HST(STIS), HST(COS), and FUSE, for low redshift; SOFIA, Herschel, and NGST for higher redshifts

This spectral region will provide ages and metallicities of old galaxies, the sequence of galaxy formation, tests of cosmological models, and an understanding of the relative importance of r- versus s-process nucleosynthesis of neutron capture elements as a function of time since the Big Bang. The UV region also provides insights on chemically/isotopically peculiar stars, on segregation of elements in stellar photospheres, and on mass transfer in binary systems. These problems need comprehensive classified spectral line lists in the UV, including wavelengths accurate to 1 part in 10^7, transition probabilities accurate to 5 to 10%, and hyperfine/isotopic parameters for high abundance Fe group elements in the first three stages of ionization, and similar spectral line lists in the UV for strong lines of lower abundance elements including the neutron capture elements.

The UV region is key to interpreting visible and UV spectra of important interstellar molecules, such as large organic species that carry the ubiquitous IR emission bands (UIBs) and diffuse interstellar bands (DIBs) and that may be related to the origin of life. Identification of UV spectra of large aromatics is especially important to address the key science goal of the HST(COS). UV spectra are uniquely capable of identifying specific molecules, in contrast with the less specific transitions observed in the IR. Lab studies provide spectroscopy of large organic molecules (such as PAHs) and their ions in the solid and in the gas phases, measurements of chemical reaction rate coefficients, and recombination cross sections. This work must be complemented by quantum theory calculations so that the lab data are properly interpreted.

The molecule CO is a key component of dense interstellar clouds and a probe of local interstellar conditions. Measurements are needed of oscillator strengths for UV intersystem bands for CO and its isotopomers, improved wavelength measurements in the UV, and photodissociation cross sections including their J-dependence at appropriate interstellar temperatures.

Astronomers also require an improved understanding of the energetics of interstellar dust in a variety of environments (photon-pumping mechanisms, etc.). Such insight arises from spectroscopic signatures that provide direct information on the composition and evolution of dust. Previous studies in the UV have focused on the only identified spectral feature (at 2200 Å), but all materials should show UV spectral signatures, as indicated by the recent detection by higher-resolution HST observations of a weaker absorption band on the UV extinction curve. Laboratory measurements of the optical properties of bulk materials such as carbonaceous solids, metallic carbides, sulfides, oxides, as well as weak features of other common materials, are needed, as well as studies of the properties of very small (nano-sized) particles of the same substances, which differ from the bulk properties.

The UV wavelength region, often used in conjunction with other wavelengths, provides an understanding of the fundamental processes (and especially the energy balance) associated with emissions from planetary atmospheres and magnetospheres, including planetary aurora and dayglow emissions (relevant for all planets and satellites with atmospheres and magnetospheres), as well as comets. Laboratory studies must provide reaction rates and electron impact excitation rate coefficients.

Light reflected from atmospheres of planets, in which absorption from the planetary atmosphere is superposed upon the solar spectrum, leads to a determination of the composition and structure of planetary atmospheres and interiors. Different wavelengths probe various depths in the atmosphere. Laboratory studies must provide line lists for the parent species (primarily those arising from methane, water, and carbon monoxide), extensive sets of rate coefficients for all classes of reactions used in the photochemical models, and an understanding of the radiative transfer and temperature effects on line shapes. Low temperature rate constants are needed in many cases. It is not known how the products of many photodissociation rates are distributed in energy states. Equations of state, solubility, and molecular diffusion in H_2/He mixtures at low temperature and high density are needed for studies of giant planets that can also be used as a basis for understanding brown dwarfs.

The Infrared and Sub-mm Spectral Region

Missions: HST(NICMOS), SIRTF, SOFIA, Herschel, and NGST

Accurate wavelengths and transition probabilities of far-IR/sub-mm fine structure transitions of atoms and atomic ions are needed to diagnose low density astrophysical plasmas.

IR/sub-mm transitions of interstellar dust grains must be used to determine their specific mineral composition, leading to grain opacities in various environments. These opacities, uncertain now by an order of magnitude, determine inferred grain temperatures and the masses of the ISM within entire galaxies. Emission bands from warm astronomical environments such as circumstellar regions, planetary nebulae, and star-forming clouds lead to the determination of the molecular composition and physical conditions in regions where stars and planets form. The compositions of cool stars provide the nucleosynthetic history of our galaxy and of others.

The laboratory data essential for these investigations are measurements of emission and absorption spectra (opacities at various wavelengths, especially in the FIR) of candidate grain materials (both carbonaceous and silicaceous). Metallic carbides, sulfides, oxides, as well as weak features of common materials, are important. For abundant materials (e.g., forms of carbon such as PAHs), the measurements should range from molecules to nano- particles to bulk materials. Also vital are measurements of molecular wavelengths and transition probabilities in the near-IR, where cool stars emit most of their flux. There are many as-yet unexploited transitions of important species. Frequency measurements and band analyses for molecular species whose transitions lie between 500 GHz and 2 THz are needed.

Non-Wavelength-Specific Needs involve fundamental physical and chemical processes that affect the scientific output of all NASA missions

Understanding of celestial objects requires knowledge of the rates of relevant physical and chemical processes. Only laboratory data can provide reaction rates, sticking coefficients, and desorption rates for processes in the gas phase, on the surfaces of small (nano-sized) and larger (micro-sized) grains, within interstellar ices, and on solar system objects such as icy satellites and Kuiper Belt objects. For instance, a quantitative understanding of the formation of the most important interstellar molecule, H_2, is very important and still incomplete. The quantitative understanding of the energy balance of the ISM (from the diffuse component to dense clouds) and the resulting phase structure requires studies of photoelectric yields and the effects of particle bombardment, X-rays, and FUV radiation on laboratory materials such as interstellar molecules, dust grain and ice analogs. Studies of porous regoliths are needed where sticking to neighboring grains is relevant.

Lack of reflectance spectra (UV-visible-NIR) of low temperature frosts/volatile ices has inhibited interpretation of the Galileo data. Unless something is done in the near future, the situation will be similar for Saturn Cassini data. Water is reasonably well covered, and the mid- and far-IR has been done for astrophysical ices, although not at the 50-150K temperatures relevant for solar system objects. Optical constants/properties of organic solids (important for most "red" solid bodies in the outer solar system) and of solid sulfur are needed. Low velocity collisions of icy dirt balls and mechanical properties of cryogenic porous ice/rock aggregates have direct relevance to the Kuiper Belt. The limitations on the available lab data will also hamper interpretations of thermal IR spectra to be obtained from the surface in 2004 by the Mars Exploration Rovers. The situation is similar in the visible to NIR, which will be studied extensively at the tens of meters scale by a NIR spectrometer on the 2005 Mars Reconnaissance Orbiter mission.

Web-accessible, critically evaluated data bases should become available. The efficiency gains obtained by eliminating the need for individual scientists to search original literature for data are significant. Critical evaluation and the establishment of reliable error bars on the data are important. Reliable error bars add much confidence to scientific conclusions based on the interpretation of astrophysical observations with the data and modeling with the data.