ABSTRACTS

Laboratory Astrophysics: Enabling Scientific Discovery and Understanding

Kate Kirby*

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Abstract

NASA's Science Strategic Roadmap for Universe Exploration lays out a series of science objectives on a grand scale and discusses the various missions, over a wide range of wavelengths, which will enable discovery. Astronomical spectroscopy is arguably the most powerful tool we have for exploring the Universe. Experimental and theoretical studies in Laboratory Astrophysics convert "hard-won data into scientific understanding".[2] However, the development of instruments with increasingly high spectroscopic resolution demands atomic and molecular data of unprecedented accuracy and completeness. How to meet these needs, in a time of severe budgetary constraints, poses a significant challenge both to NASA, the astronomical observers and model-builders, and the laboratory astrophysics community. I will discuss these issues, together with some recent examples of productive astronomy/lab astro collaborations.

[2]NASA Science Strategic Roadmap, May 26, 2005, at http://www.spaceref.com/news/viewsr.html?pid=16753

Astrochemistry in sites of star formation

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Abstract

This talk will summarize recent observational and theoretical advances in understanding the chemistry of star formation. Chemical processes as- sociated with the formation and evolution of dense molecular clouds will be described. These clouds are sites of low-mass star formation, the ear- liest phases of which, from the prestellar core through to the Class I pro- tostar, exhibit remarkable chemical diversity and provide insight into the likely chemistry of the forming Solar System. Observational studies and theoretical astrochemistry modeling both rely heavily on the availability of specific laboratory datasets; several areas where such data are urgently needed will be highlighted.

Circumstellar Disks Around Young Stars

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Abstract

Disks represent a crucial stage in the formation of stars and planets. They are novel astrophysical systems, intermediate between the interstellar medium and stars. Their physical properties are very inhomogeneous and are affected by hard stellar radiation and by dynamical evolution, including instabilities. Observing disk structure is difficult because of their small sizes, ranging from 0.05 AU at the inner edge to 100-1000 AU at large radial distances. Nonetheless, substantial progress has been made by observing the radiation emitted by the dust from near infrared to mm wavelengths, the so-called spectral energy distribution of an unresolved disk. Many fewer results are available for the gas, which is the main mass component of disks over much of their lifetime. The inner disk gas of young stellar objects have been studied using the near infrared rovibrational transitions of CO and a few other molecules, while the outer regions have been explored with the mm and sub-mm lines of CO and other molecules. Further progress can be expected in understanding the physical properties of disks from observations with sub-mm arrays like SMA and ALMA, mid infrared measurements with SPITZER, and near infrared spectroscopy with large ground-based telescopes. Intense efforts have also been made to model such observations using complex thermal-chemical models. After a brief review of the existing observations and some preliminary modeling results, some of the weaknesses of the models will be discussed, including the absence of good laboratory and theoretical calculations of essential microscopic processes.

Astrochemistry

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Abstract

In this talk, I will emphasize some current needs of astrochemists for laboratory data. The data are urgently required both to detect molecules in assorted regions and to produce robust models of these regions. Three areas of laboratory-based research are particularly crucial and yet are not being studied in the United States: (i) reactions more complex than the formation of molecular hydrogen on interstellar grain analogs (or actual dust particles) at low temperatures, (ii) molecular spectroscopy in the THz (far-infrared) region of the electromagnetic spectrum, and (iii) gas-phase kinetics of reactions leading to simple and complex molecules. Reactions on cold granular surfaces are known to lead to species as large as methanol, yet the few that have been studied in any detail have been measured in Japanese laboratories. Molecular spectroscopy at THz frequencies will be needed to make sense out of the data to come from SOFIA and the Herschel telescope, yet currently only one laboratory is well-known for such measurements, and it is located in Germany. Finally, although ion-molecule reactions seem to explain, at least semi-quantitatively, much of the chemistry occurring in cold interstellar clouds, the far more complex gas-phase chemistry that occurs near star-forming regions in so-called hot cores and hot-corinos has not been studied with the completeness that is required. Moreover, there are even large gaps in our knowledge of low-temperature chemistry in the gas phase, some quite serious. Without solid knowledge of many unstudied but key reactions, both in the gas and on grains, astrochemists will not be in position to keep up with the large amount of new information expected to come from the next generation of telescopes.

NASA's Search for Habitable Environments and Life: The Role of Laboratory Astrophysics

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Abstract

Ongoing and future NASA astronomy missions need detailed information on the properties of a wide variety of molecular species and dust grains to convert observations into physical understanding. Examples include dust in protostellar disks around young stars and debris disks around mature disks; macro-molecules (PAHs) in nearby star forming regions and in distant galaxies; signatures of prebiotic chemistry in molecular clouds and comets; and biomarkers indicative of habitable environments and life itself in the atmospheres of nearby planets. NASA telescopes such as Spitzer, JWST, and the Terrestrial Planet Finder (TPF) will address these and many other scientific questions. A solid grounding in laboratory astrophysics is essential to addressing the goals of these scientific investigations.

Herschel

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Abstract

Herschel , short for the 'Herschel Space Observatory', is the fourth 'cornerstone' mission in the ESA science programme, with substantial NASA involvement. It will perform photometry and spectroscopy in approximately the $57-670\mu m$ range. It will have a radiatively cooled 3.5m diameter telescope, and a science payload complement of three instruments housed inside a superfluid helium cryostat.

Herschel is designed to observe the 'cool universe'; it has the potential of discovering the earliest epoch proto-galaxies, revealing cosmologically evolving AGN/starburst symbiosis, and unravelling the mechanisms governing the formation of stars and planetary systems, such as our own.

Herschel will be operated as an observatory facility offering three years of routine observations. It will be available for the entire scientific community, with roughly two thirds of the observing time being 'open time', which will be offered through a standard competetive proposal procedure.

Herschel will provide with a unique view of the IR and submillimeter universe. Its instruments are designed for very precise measurements. However, the accuracy of the molecular data - spectroscopy, excitation cross section, radiative transfer models, reaction cross sections - will be the limiting factor in the analysis and interpretation of this data. Europe has started an ambitious laboratory and theoretical program in the area of molecular astrophysics to provide the basic molecular physics data required for proper interpretation of the Herschel results. To this end, the Molecular Universe, a consortium of 21 institutes in 9 countries, has been funded by the European Commission under the Marie Curie FP6 program. The results of this program will be made available to the community through data bases and web-interfaces. In this talk I will review the status of Herschel, the molecular physics program required for the analysis and interpretation of its data, and the Molecular Universe program. Major areas of concern will be identified.

Lab Studies and the Pyramid of Science

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Abstract

Astrophysics, astrochemistry and astrobiology are the sciences we use to interpret observations of the universe beyond the Earth. They all deal with complex systems and complex interactions. Experience demonstrates that to understand a complex system, the necessary approach is modeling, and the fulcrum of modeling is the elimination of free parameters. With three parameters one could fit an elephant, and so to avoid the garbage-in-garbage-out situation, parameters must be defined so far as possible from laboratory studies, and these must be supplemented by copious empirical data and theoretical analyses. I will use the study of organic molecules in space as an example to demonstrate this. Despite the successes of quantum mechanics, precision determination of physical quantities must still come from the lab. The lab is the home of science, and science cannot make sense without it. And so, though occasionally and rarely, a simple observation made with a sensitive instrument will pin down the characteristics of a new phenomenon, the ultra sensitive instrument is just one tool in the toolkit of science, and it needs to be balanced by appropriate resources being spent on other tools - such as laboratory astrophysics. The current imbalance between national resources going towards extremely expensive sensitive telescopes and their auxiliary equipment and the lack of resources going to the bases of science, lab studies, education and theory, is turning the pyramid of science upside down and trying to balance it on a point! Such a use of resources sacrifices science for grandiosity.

Comets

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Abstract

High resolution spectroscopy of comets, both in the far ultraviolet, from space using the *Far Ultraviolet Spectroscopic Explorer* and the *Hubble Space Telescope*, and in the near infrared (2.9 – 5.0 μm), from the ground, have revealed a wealth of new information, particularly about the molecular consituents that make up the volatile fraction of the comet's nucleus. Interpretation of these data requires not only proper wavelengths for identification but also information about the photolytic processes at temperatures typical of the inner coma (70 – 100 K) that lead to the observed spectral signatures. Often, nearly simultaneous ultraviolet and infrared observations do not lead to consistent abundance determinations which may be the result of improper modeling of the excitation mechanisms in either or both regimes. Several examples, mainly from *FUSE* and *HST* spectra of comets observed during the last few years, will be given to illustrate some of the outstanding issues.

Laboratory Analysis for Planetary Science Research: Application for Cassini-Huygens

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Abstract

The Cassini-Huygens mission has been instrumental in extending our understanding of the Saturnian system, and in particular, the environment of Saturns largest moon Titan. In this investigation Titans composition, dynamics, and morphology have been examined and placed in the context of the origin and evolution of the solar system. However, the uniqueness of Titans environment that Cassini-Huygens has helped reveal requires particular attention in laboratory experiments. In particular, low temperature ultraviolet absorption cross sections and chemical kinetics data with an eye towards examining mechanisms for forming chemical complexes such as amino acids and macromolecular matter that is incorporated into Titan haze are needed. The current state of knowledge provided by Cassini-Huygens will be reviewed. Aspects of laboratory analysis that will facilitate the further interpretation of Cassini-Huygens data will also be addressed along with implications for planetary science research.

SOFIA: The Next Airborne Observatory

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Abstract

The Stratospheric Airborne Observatory will fly at altitudes of 12.5 – 13.7 km, above 99% of the atmosphere's water vapor. This will open nearly the entire spectrum for observations, from near-UV to beyond sub-millimeter wavelengths. SOFIA's spectrographs will see many atomic and molecular features which have been either poorly studied or undetected thus far; their interpretation will rely heavily on laboratory astrophysics data. The SOFIA observatory, instrumentation, and mission are described in this talk. Examples of observations of interest to laboratory astrophysicists will be given, and there will be some discussion of what laboratory astrophysics data are needed to ensure that SOFIA will achieve NASA's astrophysics goals.

Laboratory Simulations in Ices and Minerals

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Ujjwal Raut*

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Abstract

We will present the experimental capabilities of our laboratory at Virginia that have been applied over the years to address questions concerning airless bodies in the solar system and interstellar space. The processes investigated are thermal processes (gas-surface interactions, sublimation, phase changes) and interactions of energetic ions and ultraviolet photons with materials that lead to desorption / sputtering, chemical synthesis and alterations, amorphization, and electrostatic charging). The presentation will include data showing new aspects or considerations about conventional techniques, such as infrared reflectance and temperature programmed desorption, but it will include some innovative or unconventional techniques, such as piezoelectric microgravimetry, electron spectroscopies, nanosecond laser ablation, and UV-visible spectroscopic interferometry. Our goal will be to show the community what can be measured and what are the opportunities for collaborations. This will be illustrated with results that have been useful to solve some concrete problems: photodesorption of ice mantles, molecular synthesis by radiolysis, Na atmospheres around the Moon and Mercury, and the recently discovered "fountains" of Enceladus.

Spectroscopic Studies of PAHs in Supersonic Jets and Liquid Helium Droplets

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Abstract

Neutral and cationic polycyclic aromatic hydrocarbons (PAHs) are discussed as possible carriers of the diffuse interstellar bands (DIBs), still unassigned astrophysical absorption features observed in the spectra of reddened stars. Despite the importance of this class of molecules for astrophysics and nanophysics (PAHs can be regarded as nanoscale fragments of a sheet of graphite), the spectroscopic characterization of PAHs under well-defined conditions (low temperature and collision-free environment) has remained a challenge. Recently we have set up a cavity ring-down spectrometer combined with a pulsed supersonic jet expansion to study neutral and cationic PAHs under astrophysical conditions. PAHs studied so far include the neutral molecules anthracene and pyrene as well as the cationic species naphthalene$^+$ and anthracene$^+$. Employing another molecular beam apparatus, the same molecules (except of the cationic species) were also studied in ultracold liquid helium droplets. This novel technique combines several advantages of conventional matrix spectroscopy with those of gas phase spectroscopy. Notable advantages are the possibilities to study molecules with rather low vapor pressure, to achieve equilibrium between vibrational, rotational, and translational degrees of freedom, and to use a mass spectrometer facilitating spectral assignments. The most recent studies were devoted to phenanthrene and the more complicated (2,3)-benzofluorene. These molecules were investigated in the gas phase by cavity ring-down spectroscopy and in liquid helium droplets using depletion spectroscopy. For benzofluorene, the present studies constitute the first measurements carried out in the gas phase and in helium droplets. In contrast to previously studied PAHs, the shift induced by the helium droplets was very small (blue shift between 4.5 and 4.9 cm^{-1} for all vibronic bands). In addition to commercially available molecules, we have also studied PAHs which were produced by CO_2 laser pyrolysis of benzene/ethylene gas mixtures. Up to now, no coincidence between experimental and interstellar band positions was found.

Laboratory Studies on the Formation of Carbon-Bearing Molecules in Extraterrestrial Environments From the Gas Phase to the Solid State

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Abstract

A detailed knowledge of the formation of carbon-bearing molecules in interstellar ices and in the gas phase of the interstellar medium is of paramount interest to understand the astrochemical evolution of cold molecular clouds, circumstellar envelopes, and of star-forming regions. Since the present composition of each interstellar environment reflects the matter from which it was formed and the processes which have changed the chemical nature since the origin (cosmic ray exposure, photolysis, chemical reactions), a detailed investigation of the physico chemical mechanisms altering the pristine environment is of paramount importance to understand the contemporary composition. Once these underlying processes have been unraveled, we can identify those molecules, which belonged to the nascent setting, distinguish molecular species synthesized in a later stage, and predict the imminent chemical evolution of, for instance, molecular clouds. This talk overviews the experimental setups utilized in the current experiments (surface scattering machine, crossed beams machine) and portrays then typical results of each setup (formation of aminoacids, aldehydes, alcohols, epoxides; synthesis of hydrogen terminated carbon chains as precursors to complex PAHs and to carbonaceous dust grains in general). These laboratory results can predict then where in the interstellar medium complex, carbon bearing molecules can be formed on interstellar grains and in the gas phase.

Sticking and desorption of small physisorbed molecules: laboratory experiments and astrophysical applications

G.W. Fuchs

Abstract

Small molecules like O_2, N_2 and CO are key species in the chemical evolution of pre- and protostellar cores. Since O_2 and N_2 do not have an electric dipole moment, direct observations of these spieces in cold environments are difficult. Gaseous N_2 is known to be abundant in dense cores from indirect observations of the chemically related N_2H^+ ion, but gas-phase O_2 appears to be largely absent, with upper limits from space observations giving $N(O_2)/N(H_2) \leq 5{\cdot}10^{-8}$ [1]. At sufficiently high densities ($n(H_2) > 10^5$ cm^{-3}) and low temperatures (<20 K), even volatile molecules like CO, N_2 and O_2 freeze-out from the gas-phase onto grains, forming a water-poor icy mantle layer. This freeze-out significantly influences the gas-phase chemistry of many species including N_2H^+, since CO is one of its main destroyers. It also affects the abundance of H_3^+ and its level of deuterium fractionation [2]. Solid CO is readily observed through its stretching mode at 4.67 μm with an abundance comparable to, or larger than, that in the gas in the coldest regions [3]. Again, O_2 and N_2 cannot be detected directly in the ice but their presence may be inferred by their effect on the solid CO line profile. It is clear that in order to properly model the chemistry in cold dense cores, a good understanding of the freeze-out and desorption of these species is needed.

In this contribution laboratory experiments will be presented using our new ultra-high vacuum experiment CRYOPAD to determine fundamental properties of ices, in particular sticking probabilities at low temperatures and molecular desorption energies. CO, N_2 and O_2 have been deposited on a poly-crystalline gold surface at 14 K in pure, mixed and layered structures [4,5,6]. For astrophysical relevance, ices with different thicknesses between 10 and 160 mono-layers have been investigated using Temperature Programmed Desorption (TPD) and Reflection Absorption InfraRed Spectra (RAIRS) techniques. The TPD spectra are used to determine the binding energies and desorption kinetics of these species under various conditions. It is concluded that N_2 and CO molecules interact significantly with each other whereas O_2 and CO molecules do not. The sticking coefficients of CO, N_2 and O_2 are all close to unity at low temperatures. The RAIR spectra of mixed and layered N_2 -CO and O_2 -CO ices are discussed and conclusions are drawn for the underlying intermolecular interactions. The astrophysical consequences will be discussed and kinetic models for use in astrochemical calculations are presented.

[1] Liseau, R. & Odin Team, 2005, astro-ph/050989
[2] Roberts et al., 2002, Astron& Astrophys., 381, 1026
[3] Pontoppidan et al. 2003, Astron.&Astrophys., 408, 981.
[4] Öberg et al. 2005, Astrophys.J.Lett. 621, L33.
[5] Bisschop et al., 2006, Astron.& Astrophys., in press, astro-ph/0601082
[6] Fuchs et al. 2006, Faraday Discuss., DOI:10.1039/B517262B

Use of Laboratory Data to Model Interstellar Chemistry

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Abstract

We show that experiments conducted in the laboratory under simulated astrophysical conditions have yielded quantitative information on molecule formation on and ejection from dust grain analogues. Data on processes leading to the formation of molecular hydrogen on different surfaces of dust grain analogues will be presented. We then illustrate how, in close collaboration with theoretical groups, these results are used in models of the chemical evolution of ISM environments. As the result of these studies, a new picture of the formation of molecular hydrogen on dust grains is emerging.

This work was supported by NASA through grants NAG5-9093, NAG5-11438, and NNG05 GF 07G (G.V) and by the Italian Ministry for University and Scientific Research through grant 21043088 (V.P).

Nucleosynthesis

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Abstract

Abundance observations indicate the presence of neutron capture (*i.e.*, *s*- and *r*-process) elements in old Galactic halo and globular cluster stars. These observations provide insight into the nature of the earliest generations of stars in the Galaxy – the progenitors of the halo stars – responsible for neutron-capture synthesis. Comparisons of abundance trends can be used to understand the chemical evolution of the Galaxy and the nature of heavy element nucleosynthesis. In addition age determinations, based upon long-lived radioactive nuclei abundances, can now be obtained. These stellar abundance determinations depend critically upon atomic data. Improved laboratory transition probabilities have been recently obtained for a number of elements. These new gf values have been used to greatly refine the solar photospheric abundances of, especially, rare-earth elements, and has allowed for more reliable determinations of the abundances in metal-poor Galactic halo stars. These newly determined stellar abundances are consistent with a (relative) Solar System *r*-process pattern, and are also consistent with abundance predictions expected from such neutron-capture nucleosynthesis.

This work has been supported in part by NSF and by STScI.

Laboratory Astrophysics for High Resolution Astrophysical X-ray Spectroscopy

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Abstract

The most obvious need for laboratory experiments in X-ray astronomy is in basic data for high resolution spectroscopy. Astrophysical X-ray spectroscopy of highly ionized gas has taken off with the launch of the *Chandra* and *XMM-Newton* observatories, and the success of this work can be attributed partially to the availability of reliable spectroscopic atomic data derived from, or benchmarked against, laboratory experiments. I'll briefly review some of the issues in this area. Astrophysical X-ray spectroscopy of near-neutral material is new, and has been found to lack some of the most basic spectroscopically reliable information required to exploit the potential of these data. I will review the astrophysical data, and the areas in which laboratory experiments could make a decisive difference.

X-ray Plasma Models: Current Achievements and Future Needs

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Abstract

Before the launch of the Chandra X-ray Observatory and the XMM/Newton satellite, there was great concern about the available X-ray spectroscopic data, including not only the rates needed to calculate line strengths but even fundamentals such as wavelengths for iron L-shell lines. This inspired a substantial and successful effort to improve the situation. This included many laboratory measurements along with more detailed atomic modeling and better communication between the atomic physics and astrophysics communities.

We now have over 5 years of experience with high-resolution X-ray spectra, and have begun serious plans for Constellation-X which will achieve even higher resolutions. I will discuss what we have learned from this experience, including what our atomic data needs are now and what they will be in the near future.

Ultraviolet and X-ray Spectroscopy of Multiphase Hot Gas in the Interstellar Medium and the IGM

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Abstract

The Space Telescope Imaging Spectrograph and the *Far Ultraviolet Spectroscopic Explorer* have observed a large number of hot stars and low-redshift QSOs and AGNs for the purpose of studying interstellar and intergalactic gases and their roles in galaxy evolution and cosmology. The spectra of these objects show an array of remarkable absorption lines ranging from cold, molecular gas (e.g., traced by C I and H_2) to highly ionized and hot gas (e.g., traced by O VI and Ne VIII transitions). Many of the gas clouds detected in UV absorption cannot be studied by any other technique, especially in intergalactic regions where the densities are likely to be quite low. The O VI absorption lines detected in intervening gas clouds have particularly important implications regarding the chemical enrichment, physical conditions, and baryonic content of intergalactic gas in the nearby universe. For example, these absorbers can be used to search for the "warm-hot intergalactic medium", a shock-heated phase of the IGM that is theoretically predicted to be a major baryon reservoir at the present epoch. In parallel, X-ray telescopes with grating spectrographs have detected absorption lines of even more highly ionized species (e.g., O VII and Ne IX) that complement the UV studies. This talk will briefly review studies of the low-z IGM based on UV and X-ray observations of O VI and related absorption lines, including findings on the metallicity, ionization, and cosmological mass of these systems as well as their relationships with galaxies. Comments will be interspersed about how these science programs require and motivate supporting work from laboratory astrophysics.

NASA's Ultraviolet Spectrographs: Science and Atomic Data Needs

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Abstract

I will summarize some of the exciting science capabilities of NASA's ultraviolet spectrographs, including the Far Ultraviolet Spectroscopic Explorer mission and Hubble's Space Telescope Imaging Spectrograph and planned Cosmic Origins Spectrograph. These instruments have provided a vast archive of data for a broad range of studies, from the interstellar medium of the Milky Way and other nearby galaxies to the study of the intergalactic medium, from the atmospheres of stars to stellar remnants and black hole accretion disks. This talk will focus on the capabilities of these instruments and some of the important atomic data needs for the optimization of their scientific legacy.

Laboratory astrophysics in Europe and the ties to various missions

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Abstract

The forthcoming NASA missions are expected to provide spectral energy distributions and a multitude of molecular line data in a variety of astrophysical environments. Identification, analysis and interpretation of these data in terms of the physical and chemical characteristics of the astronomical sources require a concerted effort by physicists, chemists and astronomers.

Related projects are presently in progress and supported by the European community within the frame of a FP6 network labelled "The Molecular Universe". I will report on such recent achievements and tasks undertaken in different european groups. The areas of molecular spectroscopy, collisional excitation processes and chemical reactions will be addressed specifically.

Laboratory Rotational Spectroscopy of Astrochemically Interesting Metal Cyanides and Isocyanides

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Radio Astronomy Observatory, University of Arizona

Abstract

The most common metal-bearing molecules in the interstellar medium are metal cyanides and isocyanides. For example, NaCN, MgCN, MgNC, KCN, and AlNC all have been observed in the circumstellar gas of asymptotic giant branch stars. These findings suggest that other metal cyanides might be present in circumstellar gas. Their detection would have implications for nucleosynthetic processes in stars, as well as for the chemistry in the interstellar medium. Studies are being conducted in the laboratory to measure the rest frequencies of these potential interstellar molecules. The current focus is on transition metal cyanides and isocyanides. We have previously recorded the spectra of CoCN, NiCN, CuCN, and ZnCN. Most recently, we have identified the spectrum of CrCN/CrNC ($X^6\Sigma^+$) in the laboratory, and preliminary work is underway on MnNC ($X^7\Sigma^+$) and FeNC ($X^6\Delta_i$). The most recent results will be presented.

Laboratory Spectroscopy of CH+ and isotopic CH

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Abstract

The A singlet Pi to X singlet Sigma electronic band of the CH+ ion has been used as a probe of the physical and dynamical conditions of the ISM for 65 years. In spite of being one of the first molecular species observed in the ISM and the very large number of subsequent observations with large derived column densities, the pure rotational spectra of CH+ has remained elusive in both the laboratory and in the ISM as well. We report the first laboratory measurement of the pure rotation of the CH+ ion and discuss the detection of 13CH+ in the ISM. Also reported are the somewhat unexpected chemical conditions that resulted in laboratory production.

Recent Selected Ion Flow Tube (SIFT) Studies Concerning the Formation of Amino Acids in the Gas Phase

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Abstract

Recently the simplest amino acid, glycine, has been detected in interstellar clouds, ISC, although this has since been contested. In order to substantiate either of these possibilities, plausible routes to amino acids need to be investigated. For gas phase synthesis, the SIFT technique has been employed to study simple amino acids via ion-molecule reactions of several ions of interstellar interest with methylamine, ethylamine, formic acid, acetic acid, and methyl formate. Carboxylic acid type ions were considered in the reactions involving the amines. In reactions where the carboxylic acid and methyl formate neutrals were studied, the reactant ions were primarily amine ion fragments. It was observed that the amines and acids preferentially fragment or accept a proton whenever energetically possible. NH3+, however, uniquely reacted with the neutrals via atom abstraction to form NH4+. These studies yielded a body of data relevant to astrochemistry supplementing the available literature. However, the search for gas phase routes to amino acids using conventional molecules has been frustrated. Our most recent research investigates the possibility that ion-molecule reactions of acrolein and ethylene oxide may lead to amino acid precursors.

Calculation of Ro-vibrational Spectra: State-of-the Art

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Abstract

The state-of-the art in the calculation of ro-vibrational spectra of small molecules of interest in astronomy and astrophysics is demonstrated through several examples. The highly accurate quantum chemistry method, singles and doubles coupled-cluster theory with a perturbational correction for triple excitations, denoted CCSD(T), is used to compute a purely ab initio potential energy surface (PES). Corrections for correlation of core electrons, higher-order correlation effects, and scaler relativistic effects, among others, are incorporated into the final purely ab initio PES. Ro-vibrational calculations show that such potentials are highly accurate and, for example, can produce fundamental vibrational frequencies to within 1 cm-1. It is shown that further refinement of the potential using high resolution experimental data, can decrease errors for ro-vibrational energy levels by several orders of magnitude. In fact, potentials constructed in this way lead to the most reliable opacity data for small molecules available. Examples of this work will be shown for several small molecules.

Laboratory Study of Magnetorotational Instability and Hydrodynamic Stability at Larger Reynolds Numbers

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Abstract

Rapid angular momentum transport in accretion disks has been a longstanding astrophysical puzzle. Molecular viscosity is inadequate to explain observationally inferred accretion rates. Since Keplerian flow profiles are linearly stable in hydrodynamics, there exist only two viable mechanisms for the required turbulence: nonlinear hydrodynamic instability or magnetohydrodynamic instability. The latter, also know as magnetorotational instability (MRI), is regarded as a dominant mechanism for rapid angular momentum transport in hot accretion disks ranging from quasars and X-ray binaries to cataclysmic variables. The former has been proposed mainly for colder protoplanetary disks, whose Reynolds numbers are typically large. Despite their popularity, however, both candidate mechanisms have been rarely demonstrated and studied in the laboratory. In this talk, I will describe a laboratory experiment in a short Taylor-Couette flow geometry ongoing at Princeton intended for such purposes. Based on the knowledge leant through prototype experiments and simulations, the apparatus contains novel features for better controls of the boundary-driven secondary flows (Ekman circulation). Initial results on hydrodynamic stability have shown, somewhat surprisingly, robust quiescence of the Keplerian-like flows with million Reynolds numbers, casting questions on viability of the nonlinear hydrodynamic instability.

This project is supported by NASA, DoE, and NSF.

Targeting inaccurate atomic data in the η Car ejecta absorption

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Abstract

The input from the laboratory spectroscopist community has at many occasions improved the analysis of the η Car spectrum. The η Car ejecta have different characteristics ranging from a 760 K environment consisting of molecules and neutral elements to a 6400 K inner ejecta observed in predominantly singly-ionized iron-group elements. We have analyzed the ejecta spectrum using medium to high resolution HST/STIS and VLT/UVES spectra. Our analysis, based on classical curve-of-growths in combination with cloudy modeling, has targeted spectra such as V II, Ti II and Cr II where improved wavelengths and oscillator strengths were needed. We will show how new and improved set of atomic data have enhanced the accuracy of our spectral analysis and illuminate where more work still is necessary. This work has been supported through STIS GTO/HST GO programs and is a collaboration between NASA/GSFC, London Imperial College, Lund Observatory and Lund Laser Center.

A Spatial Heterodyne Spectrometer for Laboratory Astrophysics; First Interferogram

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Abstract

Spatial Heterodyne Spectrometer (SHS) designs have the potential to revolutionize interferometric spectroscopy in the VUV. The advantages of interferometric spectrometers such as the Kitt Peak 1m Fourier Transform Spectrometer (FTS) in the near UV, visible, and IR for laboratory measurements of spectroscopic data including emission branching fractions, improved level energies, and hyperfine/isotopic parameters are well documented. These advantages include: (1) very high spectral resolving powers, (2) excellent absolute wavenumber accuracy, (3) extremely broad spectral coverage, (4) high data collection rates, and (5) insensitivity to source drift during branching fraction measurements. We are designing and building a very broadband, high resolution VUV compatible SHS. In order to address certain design issues including scattered light, order separation, and phase stability in a broadband SHS, we have built a Phase 1 SHS with a transmitting beamsplitter. We are planning to start construction of an all reflection Phase 2 SHS in the near future. Our Phase 1 SHS has a CaF2 beamsplitter and a matched pair of very coarse (23.2 groove/mm) echelle gratings blazed for 63.5 degrees. Key mechanical components have temperature compensated designs and many parts, including the entire optical bread board, are made of Invar for long term phase stability. The 96 mm wide gratings blazed at 63.5 degrees are compatible with a limit-of-resolution of 0.125 cm-1 using a symmetric interferogram, and a smaller limit-of-resolution using an asymmetric interferogram. The localized fringes of equal thickness from a SHS should be straight and equally spaced. The fringes are imaged onto a CCD camera in an SHS. We are purchasing a 4 Mega-pixel VUV compatible CCD camera. The first interferograms from our Phase 1 SHS were recorded with an older 0.25 Mega-pixel VUV compatible CCD camera. These interferograms are quite satisfactory. The equally spaced straight fringes in our first interferograms are indication that the beamsplitter and grating surfaces are flat to a fraction of a wave. Optical imperfections are much more serious in a traditional Michelson FTS than in a SHS. We are anticipating some slight fringe deviations as our Phase 1 instrument is pushed to shorter (VUV) wavelengths, but small deviations can be corrected with software after transferring the interferogram from the CCD. Similar optical imperfections from either figure or index of refraction variations in a Michelson FTS lower fringe contrast and degrade the instrument sensitivity. The use of a CCD camera to record the spatially distributed interferogram means that the SHS is quite compatible with transient, low duty cycle sources which are common in the VUV.

Supported by NASA.

Magnetic Field Sensitive Line Ratios in EUV and X-ray Spectra

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Abstract

While performing detailed laboratory measurements aimed at cataloguing the L-shell line emission of astrophysically abundant ions in the extreme ultraviolet and X-ray bands we discovered a class of lines that are sensitive to the strength of the ambient magnetic field. We have identified one such line in S VII and one in Ar IX. Currently we are performing measurements to identify the corresponding line in Fe XVII. The intensity of the line increases as the magnetic field strength increases. As a result, the ratio of the intensity of this line to those of neighboring lines that are not sensitive to the magnetic field represents a diagnostic of the magnetic field strength. Calculations show that the magnitude of field strengths that can be measured with this line ratio ranges from a few hundred gauss to several tens of kilogauss depending on the particular ion emitting the line.

This work was supported by NASA Astronomy and Physics Research and Analysis program work order NNH04AA751, and was performed under the auspices of the Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.

Sensitivity Analysis Applied to Atomic Data Used for X-ray Spectrum Synthesis

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Abstract

A great deal of work has been devoted to the accumulation of accurate quantities describing atomic processes for use in analysis of astrophysical spectra. But in many situations of interest the interpretation of a quantity which is observed, such as a line flux, depends on the results of a modeling- or spectrum synthesis code. The results of such a code depends in turn on many atomic rates or cross sections, and the sensitivity of the observable quantity on the various rates and cross sections may be non-linear and if so cannot easily be derived analytically. In such cases the most practical approach to understanding the sensitivity of observables to atomic cross sections is to perform numerical experiments, by calculating models with various rates perturbed by random (but known) factors. In addition, it is useful to compare the results of such experiments with some sample observations, in order to focus attention on the rates which are of the greatest relevance to real observations. In this paper I will present some attempts to carry out this program, focussing on two sample datasets taken with the Chandra HETG. I will discuss the sensitivity of synthetic spectra to atomic data affecting ionization balance, temperature, and line opacity or emissivity, and discuss the implications for the ultimate goal of inferring astrophysical parameters.

The Southeast Laboratory Astrophysics Community: Our experience and outlook

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Abstract

The Southeast Laboratory Astrophysics Community (SELAC) was formed in 2002 through a collaboration of researchers from eight institutions and its activities have had broad participation from many others within the region and nationwide. SELAC's primary goal is to stimulate communication and deep interaction between the laboratory astrophysics and the modeling and observer communities by providing various forums. In these forums, the needs for new, improved, more comprehensive, and recommended data can be made known as well as the recent accomplishments and capabilities of experimental and theoretical laboratory astrophysicists.

Towards these ends, SELAC has organized two major workshops thus far: the first was held in 2003 at the University of Georgia ("Frontiers in Laboratory Astrophysics") and the second at the University of Kentucky in 2005 ("Understanding the Universe through IR and Submillimeter Astrophysics"). Each brought together speakers and participants from a national and international scope who surveyed topics of recent astrophysical interest along with the associated status and needs for laboratory astrophysics.

In addition to providing such forums, SELAC seeks to promote laboratory astrophysics broadly to help raise the level of recognition of the importance of the field and to encourage the development of the next generation of laboratory astrophysicists. SELAC has also served as a vehicle by which new collaborations and joint proposals for new work have been spurred and facilitated.

The members of the SELAC plan to continue activities such as these in the future, but also have recognized the need to do more. In particular, profound funding and demographic changes threaten the future of the laboratory astrophysics field motivating action. Specifically, funding agencies outside of NASA (i.e. NSF, DOE, DOC, ...) have greatly shifted or curtailed their support of research providing collisional and spectroscopic data, as well as the collection and organization of such data, decreasing dramatically the number and capabilities of reserach groups, facilities, and even individual PIs that are the foundation on which rests all of the laboratory astrophysics legacy and future production for space- and ground-based observations and models.

The SELAC Executive Committee believes that this situation must be addressed by a firming of NASA's committment to its existing programs that support laboratory astrophysics and, moreover, that new action must be proposed on the roadmap for the future. For example, SELAC believes that a network of new laboratory astrophysics facilities, centered around a synergistic ensemble of new apparatus, theoretical science, data collection and evaluation, and a strong interface with modeling and observations, should be created.

Recent Excitation, Charge Exchange, and Lifetime Results in Highly Charged Ions Relevant to Stellar, Interstellar, Solar, and Comet Collision Phenomena

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Abstract

Recent results from the JPL Atomic and Molecular Physics Group will be presented in the following areas relevant to a range of stellar, interstellar, solar, and cometary phenomena: (a) measurement of absolute collisional excitation cross sections in highly-charged ions (HCIs) for stellar, solar, and interstellar plasma modeling, (b) measurement of absolute HCI-neutral charge exchange cross sections with neutral species that are present in cometary atmospheres, (c) measurements of lifetimes of metastable levels in highly- charged Fe ions, and (d) measurement of X-ray emission phenomena following HCI-neutral collisions, and HCI-mineral (olivine, augite, quartz) collisions.

This work was carried out at JPL/Caltech, and was supported through NASA.

Laboratory Studies of the Stabilities of Heterocyclic Aromatic Molecules and Suggested Gas Phase Ion-Molecule Routes to their Production in Interstellar Gas Clouds, ISC

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Abstract

Over the years, several small ring compounds have been detected in ISC, including the aromatic, benzene. Polycyclic aromatic hydrocarbons, PAHs, have been implicated as carriers of diffuse interstellar bands, DIBs, and unidentified infrared (UIR) bands. Heterocyclic aromatic rings of intermediate size containing nitrogen, possibly PreLife molecules, were included in early searches (1973-81) but were not detected and a recent search for Pyrimidine was unsuccessful, although there have been tentative detections of the less biochemically important 2H-azirine and Aziridine. Also, the recent disputed detection of the simple amino-acid, glycine, has emphasised the difficulty of such searches. Our laboratory investigations of routes to such molecules could establish their existence in ISC and suggest conditions under which their concentrations would be maximized in ISC thus aiding the searches. The stability of such compounds (Pyridine, C_5H_5N; Pyrimidine, $C_4H_4N_2$; Piperidine, $C_5H_{11}N$ and also Dioxane, $C_4H_8O_2$) has been tested in the laboratory using charge transfer excitation in ion-molecule reactions. Some of these reactions, notably those with N^+ and N_2^+, may also be important in the Titan atmosphere. The stabilities of the compounds are also being tested in less energetic proton transfer reactions some of which are directly relevant to ISC. The fragmentation paths, including production of $C_4H_4^+$, $C_3H_3N^+$ and HCN, suggest reverse routes to the parent molecules, which are presently under investigation as production sources.

Visible to near infrared emission spectra of electron-excited H_2

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Abstract

H_2 is the most abundant molecule in the universe and is an active component of star formation. Inside dense molecular clouds, heating and ionization occur by cosmic rays, X-rays and shock waves, generating energetic electrons. Collisional excitation by electrons is the source of both UV and Visible-optical-IR (VOIR) H_2 fluorescence in the ISM, circumstellar disks and certain classes of stars [1]. The importance of collisional excitation processes has been verified with analysis of HST and IUE observations of Herbig-Haro (HH) Objects, T Tauri stars and reflection nebulae [2,3]. In particular, intense H_2 transitions in the VOIR from various vibrational levels have been observed in highly-collimated jets of matter from young stellar objects [4]. These observed lines trace the colder molecular part of the post-shocked gas [5].

In recent work, we have demonstrated [6] that the gerade series ($\mathrm{EF}^1\Sigma_g^+$, $\mathrm{GK}^1\Sigma_g^+$, $\mathrm{H}^1\Sigma_g^+$, $\mathrm{I}^1\Pi_g$, $\mathrm{J}^1\Delta_g$...) makes a significant contribution to the UV spectrum of H_2 via its cascade spectrum in the visible/near IR to the $n = 2p\sigma\mathrm{B}$ and $2p\pi\mathrm{C}$ states, the upper states of the Lyman and Werner bands, respectively. Here, we have measured the electron-impact-induced emission spectrum of H_2 in the VOIR wavelength region 700 nm to 950 nm at a spectral resolution of 2 nm (FWHM). A model spectrum of H_2, based on newly calculated transition probabilities and line positions including rovibrational coupling for the strongest band systems is in excellent agreement with observed intensities.

The VOIR emission spectra of H_2 and HD have never been studied before in optically-thin single-scattering conditions. This work will complete analytic models for use in electron transport codes of the two most fundamental sets of electronic cross sections in UV astronomy: the Lyman and Werner band systems ($\mathrm{B}^1\Sigma_u^+ 1s\sigma 2p\sigma - \mathrm{X}^1\Sigma_u^+$ and $\mathrm{C}^1\Pi_u^+ 1s\sigma 2p\pi - \mathrm{X}^1\Sigma_u^+$) of H2 and HD [7].

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Formation of Silicate Grains in Circumstellar Environments: Experiment, Theory and Observations

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Abstract

SiO is one of the most abundant reacting oxygen bearing condensable gas-phase species in molecular astronomical regions. Based on laboratory smoke condensation experiments and analysis of end products, it was conjectured that silicate formation in the circumstellar envelopes surrounding M-type giants begins with the formation of pure SiOx clusters. There are no direct and almost no experimental studies on the role of molecular processes on formation of silicates in high temperature clouds.

In contrast to previous identification of amorphous disordered nature of silicates, the most recent infrared space observatory (ISO) observation shows the widespread presence of crystalline silicates throughout the galaxy. The "nominal" molecules of observed crystalline silicates such as forsterite (MgO)2(SiO2) do not exist in the gas-phase. The growth of crystalline silicates occurs by heterogeneous chemistry in unique catalytically active pathways through gas-surface interactions at high temperatures. Thus one of the most fundamental questions in grain formation studies is which one among the high-temperature condensable gas-phase species is going to nucleate first at a significant condensation rate to provide a molecular surface(cluster) enabling condensed phase growth of minerals.

In an attempt to resolve this critical question on condensation processes and the formation of cosmic silicates, samples of silicon and its oxides have been laser ablated under a series of different ambient environments. During the course of laboratory experiments an unexpected chemically anomalous composition of (SiO)x(SiO2)y was observed in both neutral and ionic clusters. The beams of molecular clusters are detected by ultrafast multiphoton ionization process in a time-of-flight reflectron mass spectrometry using femtosecond pulsed lasers. The observed anomalous compositions in SiOx clusters and their formation kinetics must be taken into account, prior to a mechanism is invoked for or an argument is presented against the role of SiO molecules in chemical models of formation of circumstellar silicates.

The gradient corrected density-functional theoretical studies have been carried out on the geometry, electronic structure and stability of SixOy clusters. It is found that the structures of the ground states of small SixOx clusters containing upto 4 units are single rings. The Si-Si bond appears first at Si5O5, and starting at this size, the elementary rings begin to assemble into multiple rings that eventually lead to cages. It is shown that the ground state structures at larger sizes have a central core of pure Si atoms decorated by outer shell of SiO2 units. The results of our investigations on the stability of SixOx-1 and SixOx+1 species will also be presented. In particular, we will examine the specific chemical processes in which the properties of SiOx clusters are involved, and could lead to the formation of SiO2 from the abundant SiO molecules in circumstellar space.

The present findings offer an expectation that a quantitative understanding of the chemistry of formation of silicate grains and nanoparticles in interstellar dust models may be reached through coordinated efforts of infrared observational astronomy, and the union of large-scale quantum theoretical calculations and laboratory spectroscopy and dynamics experiments of the type reported here.

Low-Temperature Thermodynamic Properties of Some Light Hydrocarbons

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Abstract

Light hydrocarbons are important constituents in a variety of astrophysical systems and their components, including ices and icy mantles on grains. The first-order equilibrium models developed to describe these systems require accurate laboratory data as inputs. It is important that these data be acquired over the appropriate range of parameters, e.g., temperature, and in this regard there is a particular need for thermodynamic properties of molecular constituents at low temperatures. We have developed an apparatus capable of measuring low-temperature vapor pressures, experimentally determined values for which are extremely limited, and have undertaken a program to systematically provide this information for molecules and mixtures of importance to the astrophysical and planetary communities. Here we describe our apparatus and present results for the low-temperature vapor pressures and heats of sublimation for a group of light hydrocarbons.

Difficulties in Laboratory Studies and Astronomical Observations of Organic Molecules: Hydroxyacetone and Lactic Acid

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Abstract

Organic molecules in interstellar space likely play a role in prebiotic chemistry. Hence, it is very important to properly identify the organic species present and to accurately evaluate their abundance. Owing to the rich molecular spectra found in many interstellar sources, accurate laboratory rest frequency measurements are crucial to accomplish these goals.

Two key molecules are hydroxyacetone and lactic acid. A previous study on hydroxyacetone by Kattija-Ari and Harmony (1980) was not extensive enough to accurately predict even the A-state of this molecule, which has a methyl internal rotor. The E-state proved even more difficult as they found the molecule to possess a very low barrier to internal rotation. A more recent study by Braakman et al. (2005) provided rest frequencies for the A-state by measuring its spectrum at 3 mm and 1 mm, but they too reported that a definitive assignment of the E-state was proving difficult. Just prior to that time, we started measuring the microwave spectrum of hydroxyacetone, which was critical for the assignment of the E-state. We have now extended those measurements to cover the entire spectrum at 3 and 2 mm, where the strongest low-K interstellar transitions are predicted. Using the methods described for fitting low-barrier molecules by Hougan and co-workers and a modified computer code provided by Kliener et al., we now have fitted rotational constants that reproduce the data to experimental accuracy in both the A- and E-states simultaneously. The application of these methods will be described.

An extensive interstellar search has been conducted for hydroxyacetone based on these new laboratory results, as well as for lactic acid. Upper limits to the abundance of these species will be reported along with a discussion of problems in identifying these and other organic species owing to a high degree of spectral confusion.

Reference:

Kattija-Ari and Harmony, Inter. J. Quant. Chem., 14, 443 (1980) Braakman et al., 60th International Symposium on Molecular Spectroscopy, Columbus, Ohio, Talk RA07

Experimental and Theoretical Studies of Pressure Broadened Alkali-Metal Atom Resonance Lines

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Abstract

The pressure-broadened absorption lines of the alkali-metal atoms are prominent in the spectra of L-dwarfs and T-dwarfs. In particular, the resonance lines of sodium and potassium are each observed to be broadened by many tens of nm on either side of line center due to collisions with helium and molecular hydrogen in the atmospheres. Accurate broadening parameters are necessary for modeling atmospheric opacities. Validated models can be used to characterize properties such as metallicity and effective temperature of dwarfs or predict spectra of irradiated extrasolar giant planets, in advance of missions such as TPF-C. We are undertaking a program of experimental and theoretical studies of the pressure broadening of Na and K by He and H_2. The experiment utilizes a hot cell and spectrometer to yield absorption spectra over the visible spectrum at temperatures of around 900 K and perturber gas pressures of up to several hundred torr. The atomic densities are known precisely using the anomalous dispersion (or "hook") method. The theoretical calculations utilize accurate molecular potential energies and transition dipole moments and fully quantum-mechanical methods. We will present our results and comparisons to available data, where available. Supported by NASA under award NAG5-12751.

Accurate VUV laboratory measurements of Fe III transitions for astrophysical applications.

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Abstract

We report preliminary measurements of Fe III branching fractions covering the wavelength range 1150 to 2500Å. Spectra of iron-neon Penning discharge lamps between 1600 and 2500Å were recorded at Imperial College (IC) using Fourier transform spectroscopy (FTS). Deuterium standard lamps provided a radiometric calibration of the spectra. These spectra are the first radiometrically calibrated measurements of a doubly-ionized element using vacuum ultraviolet FTS. The FTS measurements were extended down to 1150Å using high-resolution grating spectroscopy at the National Institute of Standards and Technology (NIST). Phosphor image plates were used as detectors, and the spectra were radiometrically calibrated with a deuterium lamp. These detectors have a linear intensity response with a dynamic range of at least 10000, enabling us to measure branching fractions of doubly-ionized spectra down to 1150Å or below.

Accurate branching fractions have been determined for all transitions from the upper level $^7\mathrm{P}_j$, including the intercombination branches. These will be combined with lifetimes to yield oscillator strengths. The spectral range of the new laboratory measurements corresponds to recent HST/STIS observations of sharp-lined B stars and of Eta Carinae. The new improved atomic data can be applied to abundance studies and diagnostics of astrophysical plasmas.

This work was partially supported by NASA under the inter-agency agreement W–10,255.

Assessing the Requirements for Completeness and Accuracy of Atomic Data for X-ray Spectroscopy

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Abstract

We present several examples which illustrate the application of complete and/or accurate atomic data to problems in X-ray astrophysics. Large efforts in both theory and experiment since the launches of Chandra and XXM-Newton are beginning to pay off. For example, we can now determine the opacity of the solar corona, study episodic heating in active stars, measure the mass of the white dwarf in a cataclysmic variable, and find the distance from the central source to the outflowing winds of Active Galactic Nuclei. These case studies allow us to assess the needs for both completeness and accuracy of future laboratory astrophysics work.

Processing of Interstellar Silicate Grains by Cosmic Rays

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Abstract

Observations have shown that an appreciable fraction of silicates formed in the outflows from red giants and supergiants have a crystalline structure. Yet, the fraction of crystalline silicates in the interstellar medium is very small, pointing towards an efficient crystalline-to-amorphous conversion process. Here we report experimental and modeling results that show that low energy (0.1 5 GeV) heavy ion cosmic rays can rapidly amorphize crystalline silicate grains ejected by stars into the ISM. We have also examined the effects of cosmic ray processing of silicates in the solar system and in stellar debris disks. In the latter systems, cosmic ray processing may play a role for grains trapped in resonance with planetary companions. Similar effects on the evolution of interstellar dust grains are likely to be even more important in the early universe and in forming (starburst) galaxies, which have higher cosmic ray fluxes due to much larger star formation rates and emerging active black holes.

Laboratory measurements of the electron impact excitation cross section of Fe XVII x-ray transitions

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Abstract

We have used a large-area, gain-stabilized microcalorimeter array built by the NASA-Goddard Space Flight Center and operated at Lawrence Livermore National Laboratory's electron beam ion trap to measure the electron-impact excitation cross sections for the dominant x-ray lines in the Fe XVII spectrum as a function of electron impact energy. The results reveal a consistent overestimation by recent calculations of the excitation cross section of the resonance transition, which is shown to be at the root of several long-standing problems associated with modeling solar and astrophysical Fe XVII spectra. These results establish a benchmark for atomic calculations frequently used to analyze high-resolution celestial spectra measured using the Chandra, XMM-Newton, or Suzaku X-ray observatories. Work by the U.C. LLNL was performed under the auspices of the D.o.E. under contract No. W-7405-Eng-48 and supported by NASA APRA grants to LLNL, GSFC, and Stanford University.

Collisional Ionization Equilibrium for Optically Thin Plasmas

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Abstract

Reliably interpreting spectra from electron-ionized cosmic plasmas requires accurate ionization balance calculations for the plasma in question. However, much of the atomic data needed for these calculations have not been generated using modern theoretical methods and their reliability are often highly suspect. We have carried out state-of-the-art calculations of dielectronic recombination (DR) rate coefficients for the hydrogenic through Na-like ions of all elements from He to Zn. We have also carried out state-of-the-art radiative recombination (RR) rate coefficient calculations for the bare through Na-like ions of all elements from H to Zn. Using our data and the recommended electron impact ionization data of Mazzotta et al. (1998), we present improved collisional ionization equilibrium calculations. We compare our calculated fractional ionic abundances using these data with those presented by Mazzotta et al. (1998) for all elements from H to Ni, and with the fractional abundances derived from the modern DR and RR calculations of Gu (2003a,b, 2004) for Mg, Si, S, Ar, Ca, Fe, and Ni.

This work is supported in part by the NASA APRA program.

Excitation Cross Section Measurement for n=3 to n=2 Line Emission in Fe^{17+} to Fe^{23+}

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Abstract

We report the measurement of electron impact excitation cross sections for the strong iron L-shell $3 \rightarrow 2$ lines of Fe XVIII to Fe XXIV at the EBIT-I electron beam ion trap using a crystal spectrometer and NASA-Goddard Space Flight Centers 6×6 pixel array microcalorimeter. The cross sections were determined by direct normalization to the well established cross section of radiative electron capture through a sophisticated model analysis which results in the excitation cross section for 48 lines at multible electron energies. This measurement is part of a laboratory X-ray astrophysics program utilizing the Livermore electron beam ion traps EBIT-I and EBIT-II. This work was performed under the auspices of the U.S. DOE by LLNL under contract No. W-7405-Eng-48 and supported by NASA APRA grants to LLNL, GSFC, and Stanford University.

Measurements of Polyatomic Molecule Formation on an Icy Grain Analog Using Fast Atoms

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Abstract

Measurements are reported for production of CO2 resulting from the impact of a monoenergetic O(3P) beam upon a surface cooled to 4.8 K and covered with a CO ice. Using temperature-programmed desorption and mass spectrometer detection, one clearly detects increasing amounts of CO2 formation with O(3P) energies of 2, 5, 10, and 14 eV. This is the first measurement of polyatomic molecule formation on a surface with superthermal atoms. The chosen surface coverage, surface temperature, and superthermal atom energy simulate conditions in shock-heated circumstellar and interstellar regions.

This work was carried out at JPL/Caltech, and was supported through NASA.

Laboratory Measurements of Dissociative Recombination

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Abstract

Dissociative recombination (DR) reactions serve as a primary loss mechanism of electrons, both within the interstellar medium and in planetary atmospheres. A quantitative knowledge of DR reaction rates is crucial to an accurate modeling of these environments. Ab initio calculation of quantitative DR rates is exceedingly difficult; hence laboratory measurements have provided the main source of information on these processes. It has only been within the last decade that reliable laboratory measurements have become available through advances in ion source technology to control the internal energy in the molecular ion reactants and in the use of heavy ion storage rings to control the electron-ion interaction. This paper will report on the progress that has been made in characterizing the internal energy distributions of the O_2^+ and H_3^+ molecular ions and measuring the DR reaction rates and products for these species.[1,2] This work is in collaboration with W. van der Zande (Nijmegen), M. Larsson (MSL), A. Petrignani (FOM) and their colleagues and is partially funded by NASA grants NAG5-12666 and NNG05GP60G.

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Lifetimes and Oscillator Strengths for Ultraviolet Transitions in P II, Cl II, and Cl III

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Abstract

Oscillator strengths for transitions in P II, Cl II, and Cl III are derived from lifetimes and branching fractions measured with beam-foil techniques. The focus is on the multiplets with a prominent interstellar line at 1154 Å in P II which is seen in spectra of hot stars, and the lines at 1071 Å in Cl II and 1011 Å in Cl III whose lines are seen in spectra of diffuse interstellar clouds and the Io torus acquired with the *Far Ultraviolet Spectroscopic Explorer*. These data represent the first complete set of experimental f-values for the lines in the multiplets. Our results for P II $\lambda1154$ agree well with Curtis' semi-empirical predictions, as well as the large-scale computations by Hibbert and by Tayal. The data for Cl II $\lambda1071$ also agree very well with the most recent theoretical effort and with Morton's newest recommendations. For Cl III, however, our f-values are significantly larger than those given by Morton; instead, they are more consistent with recent large-scale theoretical calculations. Extensive tests provide confirmation that LS coupling rules apply to the transitions for the multiplets in Cl II and Cl III.

This work was supported by NASA grant NAG5-11440 to the University of Toledo.

Oscillator Strengths and Predissociation Widths for Rydberg Transitions in Carbon Monoxide

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Abstract

CO is used as a probe of astronomical environments ranging from planetary atmospheres and comets to interstellar clouds and the envelopes surrounding stars near the end of their lives. One of the processes controlling the CO abundance and the ratio of its isotopomers is photodissociation. Accurate oscillator strengths for Rydberg transitions are needed for modeling this process. We present results of recent analyses on absorption from the $E-X$ (1-0), $B-X$ (6-0), $K-X$ (0-0), $L'-X$ (1-0), $L-X$ (0-0), and $W-X$ (ν'-0, $\nu'=0$ to 3) bands acquired at the high resolution (R $\approx$ 30,000) SU5 beam line at the SuperACO Synchrotron (Orsay, France). Spectra were obtained for the $^{12}C^{16}O$, $^{13}C^{16}O$, and $^{13}C^{18}O$ isotopomers. Absorption bands were analyzed by synthesizing the profiles with codes developed independently in Meudon and Toledo. Each synthetic spectrum was adjusted to match the experimental one in a non-linear least-squares fitting procedure with the band oscillator strength, the line width (instrumental and predissociation), and the wavelength offset as free parameters. In order to perform the synthesis, the CO column density was required. Because a differentially pumped cell was used, the measured CO pressure had to be corrected to determine the CO column density. This was accomplished by fitting absorption obtained at the same pressure from the $E-X$ (0-0) band, whose oscillator strength is well known. For the $K-X$, $L'-X$, and $L-X$ bands, the substantial amount of mixing among the upper states was considered in detail. Predissociation widths determined for the $B-X$ band varied widely among isotopomers. For the $W-X$ bands, when possible, J-dependent widths and widths for both e and f parities were extracted from the data. Our results will be compared with earlier determinations.

This work was funded in part by NASA through grant NAG5-11440 and the CNRS-PCMI program.

Electron-Impact Ionization of Be-like C, N, and O

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Abstract

Previous experimental studies of the electron-impact ionization of Be-like C, N, and O have not explicitly accounted for the contribution of metastable 2s2p ^{3}P ions in ion beam preparation, which has suggested some uncertainty in previously published cross sections and rate coefficients. In an effort to ascertain the accuracy of previously suggested cross sections and rate coefficients,the total electron-impact ionization cross sections of Be-like C, N, and O ions have been studied using the crossed beams apparatus at Oak Ridge National Laboratory with ions prepared by an electron cyclotron resonance ion source. The metastable fractions of the ion beams were measured using a He gas attenuation technique. Recommended cross sections and temperature dependent rate coefficients will be presented along with a comparison to various theoretical results.

Dielectronic Recombination of C, N, and O Ions

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Abstract

Electron temperature and elemental abundance determinations are of paramount importance to models used in spectral analysis. There have been recent indications in planetary nebulae observations that collisionally excited lines and optical recombination lines result in elemental abundances that are up to 20 times different. In an effort to clarify the available recombination data, electron-ion recombination has been investigated for Be-like C^{2+}, N^{3+}, and O^{4+} and B-like N^{2+} and O^{3+} using the heavy ion storage ring CRYRING. A detailed comparison of calculations made with the AUTOSTRUCTURE code and various literature recombination rates is made for each ion and recommended Maxwellian temperature dependent rate coefficients are produced. Special attention is given to dielectronic recombination at low temperatures where theoretical models have historically encountered discrepancies with experiment. The formation of triply excites states, via double excitation of core electrons in a process analogous to dielectronic recombination, in some Be-like ions has been observed; termed "trielectronic recombination". In the case of O^{4+}, a large trielectronic recombination resonance at low energy has a drastic effect on the low temperature recombination rate.

Measurements of Electron Impact Excitation Cross Sections at the Harvard-Smithsonian Center for Astrophysics

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Abstract

The analysis of absolute spectral line intensities and intensity ratios with spectroscopic diagnostic techniques provides empirical determinations of chemical abundances, electron densities and temperatures in astrophysical objects. Since spectral line intensities and their ratios are controlled by the excitation rate coefficients for the electron temperature of the observed astrophysical structure, it is imperative that one have accurate values for the relevant rate coefficients. Here at the Harvard-Smithsonian Center for Astrophysics, we have been carrying out measurements of electron impact excitation (EIE) for more than 25 years. We will illustrate our experimental approach and apparatus by discussing a measurement of EIE in C^{2+} (2s2p $^3P^o$ $\rightarrow$ $2p^2$ ^3P). The technique employed utilizes a modulated beam of a single ion species which is crossed at 45 degrees with a similarly modulated electron beam. Photons from the decay of ions excited by collisions with the electrons are collected synchronously with the beams' modulation pattern by an absolutely calibrated optical system comprised of a mirror with an appropriate reflective coating, suitable filters, and a microchannel plate based photon counting detector. The experiment is being modified to enable measurements where the decay photon has a wavelength shortward of the cutoff wavelength of commonly available transmitting materials (e.g., MgF_2), which we have traditionally used as windows to limit the optical bandpass and isolate the photon detector system.

This work has been supported by NASA Supporting Research and Technology grants NAG5-9516 and NAG5-12863 in Solar and Heliospheric Physics and by the Smithsonian Astrophysical Observatory.

Calculation of Atomic Data for NASA Missions

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Abstract

The interpretation of cosmic spectra relies on a vast sea of atomic data which are not readily obtainable from analytic expressions or simple calculations. Rather, their evaluation typically requires state-of-the-art atomic physics calculations, with the inclusion of weaker effects (spin-orbit and configuration interactions, relaxation, Auger broadening, etc.), to achieve the level of accuracy needed for use by astrophysicists. Our NASA-supported research program is focused on calculating data for three important atomic processes, 1) dielectronic recombination (DR), 2) inner-shell photoabsorption, and 3) fluorescence and Auger decay of inner-shell vacancy states. Our DR work has produced rate coefficients for all H-like through Na-like ions up to nuclear charge $Z = 30$. We compare some of these to existing experimental measurements. Present work is focused on the more challenging third-row isoelectronic sequences, some of which will be presented. K-shell photoabsorption cross sections for all oxygen and neon ions will be presented and compared to existing experimental measurements (i.e., neutral species only). These newly computed data have already been used to infer elemental abundances in the ISM by Juett, Schulz, and Chakrabarty. We also present new fluorescence yields for all second-row K-shell-vacancy isoelectronic sequences, where the inclusion of higher-order effects frequently give results that differ considerably from the currently recommended data.

This work was supported in part by a NASA APRA grant.

Laboratory Measurement and Theoretical Modeling of K-shell X-ray Lines from Inner-shell Excited and Ionized Ions of Oxygen

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Abstract

We present high resolution laboratory spectra of K-shell X-ray lines from inner-shell excited and ionized ions of oxygen, obtained with a reflection grating spectrometer on the electron beam ion trap (EBIT-I) at the Lawrence Livermore National Laboratory. Only with a multi-ion model including all major atomic collisional and radiative processes, are we able to identify the observed K-shell transitions of oxygen ions from O III to O VI. The wavelengths and associated errors for some of the strongest transitions are given, taking into account both the experimental and modeling uncertainties. The present data should be useful in identifying the absorption features present in astrophysical sources, such as active galactic nuclei and X-ray binaries. They are also useful in providing benchmarks for the testing of theoretical atomic structure calculations.

The work at Lawrence Livermore National Laboratory was performed under the auspices of the Department of Energy under Contract No. W-7405-Eng-48 and was supported by the National Aeronautics and Space Administration under work order W19,878 issued by the Space Astrophysics Research and Analysis Program. M.F.G and S.M.K acknowledge the support by the NASA grant NAG5-5419. E.T. acknowledges travel support from the German Research Association (DFG). E.B. was supported by grant No. 2002111 from the United States Israel Binational Foundation.

Laboratory Survey of Fe L-shell X-ray Emission Lines between 7 and 11 Å

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Abstract

We present a comprehensive survey of Fe L-shell X-ray lines between 7 and 11 Å using the electron beam ion trap at the Lawrence Livermore National Laboratory. A set of flat crystal spectrometers are used to measure the wavelengths of all significant Fe emission lines in the 7–11 Å range, most of them being transitions from high n (up to $n = 10$) configurations to the $n = 2$ shell. The identification and assignment of transitions are made with the help of detailed theoretical modeling using the Flexible Atomic Code. The present work is an extension of Brown et al. (2002, ApJ 140, 589) where Fe lines above 10.6 Å are measured and identified. The combination of the previous and the present work provides the most extensive and accurate laboratory X-ray line list for Fe L-shell ions to date.

The work at Lawrence Livermore National Laboratory was performed under the auspices of the Department of Energy under Contract No. W-7405-Eng-48 and was supported by the National Aeronautics and Space Administration under work order W19,878 issued by the Space Astrophysics Research and Analysis Program. M.F.G and S.M.K acknowledge the support by the NASA grant NAG5-5419.

The Homunculus: a Unique Astrophysical Laboratory

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Abstract

In the 1840s, Eta Carinae underwent a massive ejection, repeated to a lesser extent in the 1890s. Today we see the Homunculus, an expanding bipolar neutral structure expanding outward at 500 km/s with a more slowly moving, internal bipolar ionized structure, the Little Homunculus. The central source is found to be a massive binary stellar system with a 15000 K primary star with a hot, O or WN companion in a highly elliptical 5.54 year orbit. The system is ideal as an astrophysical laboratory for absorption and emission line spectroscopy. In the line-of-sight, multiple narrow line absorption components are observed with densities around 10^7 cm^{-3} and temperatures ranging from 760 to 6400 K at 10,000 and 1300AU distance from Eta Carinae, respectively. Thousands of metal lines are identified, plus molecular hydrogen, CH, OH, NH and likely other molecules. The Strontium Filament, a truely unique emission nebula located in the skirt region between the bipolar lobes, is found to be a neutral emission gas excited by photons with energies below 7.9 eV (Fe II ionization potential), No hydrogen, helium or nitrogen emission is associated with this structure thought to be excited by Balmer continuum from the central source. For most of the spectroscopic cycle, bright emission blobs and the Little Homunculus are highly excited, but relax for a few months during the periastron passage. During this short period of time, spectral lines in [Ar III].[Ne III], [Fe III], [Fe IV] and Lyman alpha continuum-pumped Fe II and Cr II emission lines disappear due to a cut-off in UV-radiation. Given the changes in spectra, we are learning not only about the binary system and its ejecta, but in turn can use this system to test atomic spectroscopy. Examples that can be presented include the greatly improved Cr II curve-of-growth, based upon new experimental atomic data sets, improved V II wavelengths due to inconsistencies in the velocity measures that correlated with energy levels. Problems we continue to face include transition probabilities for Fe I, lifetimes of metastable states of many iron peak singly ionized species, limited atomic data on Ca II and Sr II, and indeed understanding the effects in a nitrogen-rich, carbon poor gas. Finally we note that the recent GRB high dispersion spectra demonstrate local ejecta of GRB progenitors are relatively hot, photoexcited gases (which include detectible oxygen and carbon). The studies of the Eta Carinae ejecta are proving to be invaluable for interpreting these new and exciting results.

Observations leading to these studies were obtained with the Hubble Space Telescope with the Space Telescope Imaging Spectrograph and the Very Large Telescope with the UltraViolet Echelle Spectrograph.
Funding was through STIS GTO and HST GO resources.

Laboratory astrophysics on the ASDEX-Upgrade tokamak: Measurements and analysis of O, F, and Ne spectra in the 8 - 20 Å region

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Abstract

High-resolution measurements of K-shell emission from O, F, and Ne have been performed under various plasma conditions at the ASDEX Upgrade tokamak in Garching, Germany. The tokamak plasma is well characterized, with temperature and density profiles obtained independently of the spectroscopic data, providing an excellent test bed for spectroscopic modeling. The measured spectra show intriguing deviations from the typical thermal emission patterns of coronal plasmas, including anomalously intense high-Rydberg emission, high ratios of forbidden to resonance lines, and intense satellites. The possibility that these features are due to the presence of fast electrons is investigated by comparing the measured spectra with calculations from a multi-charge collisional-radiative model.

Fully-First-Principles Quantum Calculations of Helium-Broadened Metal Resonance Lines

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Abstract

Alkali and alkaline earth atomic resonance lines, broadened by collisions between the metal atoms and ambient H_2 and He, make substantial contributions to the atmospheric opacity of several brown dwarfs and other low mass astronomical objects. Analysis of these collisionally-broadened absorption features can in principle provide information about the composition and physical conditions of the atmospheres of these objects. This has stimulated both a variety of studies of the absorption features' line shapes and several attempts to use model line shapes to fit the observed dwarf spectra.

Here we present fully first-principles quantum calculations of the He-broadened Na I resonance line, calculations based on high-quality quantum chemical studies of the Na–He potential energy and transition dipole moment curves. We also investigate the sensitivity of the collisionally-broadened Na I line shape to the underlying potential and transition moment functions. This makes it possible to assess the reliability of commonly-used simplifications, such as the assumption that the transition moment is independent of the Na–He distance. If time permits, we will also present some preliminary work on the He-broadened K I and Ca I resonance lines.

Investigations into the Astrochemistry of H_2O_2, O_2, and O_3 in Ion-Irradiated Ices

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Abstract

Features due to solid-phase H_2O_2, O_2, and O_3 have been found in the reflectance spectra of some of the icy satellites of Jupiter and Saturn (Spencer and Calvin, 2002; Noll *et al.*, 1997; Carlson *et al.*, 1999). These molecules can form by high-energy jovian magnetospheric and cosmic radiations bombarding the H_2O-ice on the surfaces of these worlds. This radiation breaks chemical bonds in the ice, forming species that can react to produce new molecules. Gravitational loss of H_2 then leaves an oxygen-richer ice containing H_2O_2, O_2, and O_3. The radiation chemistries of these three molecules are linked since H_2O_2 is a proposed precursor for O_2 formation, and O_2 is itself a precursor for O_3.

In the Cosmic Ice Laboratory at NASA-Goddard we have studied these processes by using a 0.8 MeV protons to bombard H_2O-ices (Moore and Hudson, 2000) containing H_2O_2, O_2, and O_3. We are able to measure rates of molecular formation and destruction, and IR spectra as a function of temperature, sample concentration, and radiation dose. In this presentation we show some of our most-recent results on the radiation chemistries of H_2O, H_2O_2, O_2, and O_3, such as the formation of the HO_3 radical in irradiated H_2O + O_3 ices. Since O_2 is now known to be an interstellar molecule (Liseau *et al.*, 2006), our results may also apply to the chemistry of icy interstellar grain mantles.

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Critical Evaluation of Chemical Reaction Rates and Collision Cross Sections of Importance in the Earth's Upper Atmosphere and the Atmospheres of other Planets, Moons, and Comets

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Abstract

We recommend establishment of a long-term program of critical evaluation by domain experts of the rates and cross sections of atomic and molecular processes that are needed for understanding and modeling the atmospheres in the solar system. We envision products resembling those from the ongoing JPL/NASA Panel for Data Evaluation and the efforts of the international combustion modeling community funded by US DOE and its European counterpart. Both of these endeavors already provide some important inputs for modeling the atmospheres of the Earth, planets, moons, and comets. However, their applications restrict the choice of which processes to evaluate and the temperature and pressure ranges to cover, thus leaving large gaps that need to be filled. Interestingly, an older evaluation program once filled some of these gaps. Funded by the US DoD in the 1960s-1980s, the DNA Reaction Rate Handbook provided a thorough treatment of numerous types of collisions and reactions that are important in the Earth's lower ionosphere, and the program even provided funding for new laboratory measurements. Other examples could be given, with the on-line resources at NIST being among the best, but most provide a narrower scope or less critical evaluation. What is needed is not a just a list of processes and numbers (i.e., a "database"), but rather serious comparison of the available information and specific statements from independent expert laboratory/theory data providers about what should be believed, what uncertainty to assign, and what is most in need of redetermination. The major topic areas would include the following: 1. Chemical reactions of neutral atoms and molecules in their ground electronic states 2. Ion-molecule reactions 3. Chemistry, relaxation, and radiation of electronically excited atoms and molecules 4. Vibrational and rotational relaxation and radiation 5. Photoabsorption, photodissociation, and photoionization 6. Electron-impact excitation, dissociation, ionization, and recombination 7. Energetic heavy particle excitation and charge exchange

Metastable State Populations in Laser Induced Plasmas

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Abstract

Laser ablation plasma has been used as a source of neutrals and ions. The purity of state of this source is critical to the measurement of collisional parameters such as the charge transfer rate coefficients between ions and neutrals used in the modeling of astrophysical plasmas. However, there appears to be some uncertainty on the presence of metastable state population in this source. We address this issue in this paper by reviewing theoretical and experimental evidences to show that the temperature of the laser-induced plasma is a rapidly decreasing function of time and that the temperature of the plasma is initially high but cools off rapidly by collision with the expanding plasma electrons as the neutrals and ions streams into to the vacuum. Similar to a supersonic jet, this rapid expansion of the plasma drastically lowers the internal energy of the neutrals and ions. Measurements on the time evolution of the population ratio of metastable state to ground state indicate that the population ratio freezes out at 3.5μs after the plasma is produced. The freeze-out population ratio suggests Te$\sim$1000 K. This measurement is consistent with the observations (1,2) that the charge transfer rate coefficient is independent of the power of the laser used in the production of the ions. We conclude that the metastable fraction in both the neutral and ion source must be negligibly small if the metastable state is more than 0.4 eV above the ground state.

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Astrochemistry in the Early Universe

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Abstract

Chemistry plays a critical role in controlling the formation of the first objects through cooling the clouds as they collapse. The radiation emitted in this cooling will also be the most precise diagnostics of the physical conditions of these clouds. In the first objects the cooling was likely dominated by molecular hydrogen, H_2. We have computed state to state cross sections for H on H_2 collisions. This will improve the our understanding of cooling in the early universe, and line emission in the formation of the first objects. I will present an overview of that chemistry including these new calculations of H on H_2 collision rates.

Laboratory measurements of the line emission from mid-Z L-shell ions in the EUV

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Abstract

We are continuing measurements of line lists in the extreme ultraviolet spectral region for use in astrophysical diagnostics. We recently completed line lists of sulfur S VII - S XIV, and are close to completing the analysis of laboratory spectra of silicon Si V - Si XII. These measurements were done at the Lawrence LIvermore National Laboratory's electron beam ion traps, in which a monoenergetic electron beam excites the transitions of interest, and were used to determine wavelengths and intensities of these transitions. We have also obtained data for the same transitions in collisional plasmas produced in the Princeton NSTX tokamak. We present here L-shell EUV transitions of argon in the 20 – 50 Å band and show density-sensitive line ratios for the 2p-3d lines of Ar XIV and the 2p-3s lines of Ar IX, comparing them to calculations from the Flexible Atomic Code. The tokamak plasmas are at 100 times higher density than the EBIT plasmas, allowing us to calibrate these diagnostic ratios at the high density limits. This work was supported by NASA Astronomy and Physics Research and Analysis program work order NNH04AA751, and was performed under the auspices of the Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.

Quenching of excited Na due to He collisions

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Abstract

The quenching and elastic scattering of excited Sodium by collisions with Helium have been investigated for energies between 0.01 meV and 10 eV. With the *ab initio* adiabatic potentials and nonadiabatic radial and rotational couplings obtained from multireference single- and double-excitation configuration interaction approach, we carried out scattering calculations by the quantum-mechanical molecular-orbital close-coupling method. Cross sections for quenching reactions and elastic collisions are presented and compared with other available theoretical predictions and experimental data. Quenching and elastic collisional rate coefficients as a function of temperature between 1 K and 10,000 K are also obtained. The results are relevant to modeling non-LTE effects on Na D absorption lines in extrasolar planets and brown dwarfs.

This work is funded by NASA grant NNG04GM59G.

Dielectronic Recombination In Active Galactic Nuclei

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Abstract

XMM-Newton and Chandra observations of active galactic nuclei show a rich spectrum of X-ray absorption lines. These observations have detected a broad unresolved transition array (UTA) between $\approx$ 15-17 Å. This is attributed to inner-shell photoexcitation of M-shell iron ions. Modelling these UTA features is currently limited by uncertainties in the low temperature dielectronic recombination (DR) data for M-shell iron. In order to resolve this issue and to provide reliable iron M-shell DR data for plasma modeling, we are carrying out a series of laboratory measurements using the heavy-ion Test Storage Ring at the Max-Planck-Institute for Nuclear Physics in Heidelberg, Germany. Storage rings are currently the only laboratory method capable of studying low temperature DR. We use our results to produce experimentally-derived DR rate coefficients. We are also providing our data to atomic theorist to benchmark their DR calculations. Here we will report our recent DR results for selected Fe M-shell ions. At temperatures where these ions are predicted to form in photoionized gas, we find a significant discrepancy between our experimental results and previously recommended DR rate coefficients.

This work has been supported in part by NASA, the German Federal Ministry for Education and Research, and the German Research Council.

The Atomic and Ionic Data for Astrophysics (AIDA) Project at Georgia State University

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Abstract

Data on atoms and ions that are present in astrophysical objects are crucial to interpreting astronomical data and, thereby, crucial to the understanding of these objects and the ultimate success of NASA missions. Among the most important data are photoionization rates (cross sections) of atoms and ions and the relaxation of the photoionized ion to the ejection of one or more photoelectrons. This relaxation is of critical importance for inner-shell ionization after which the photoion decays *via* either radiation (typically in the far UV or x-ray range), or radiationless Auger decay accompanied by the emission of an Auger electron (usually a quite energetic electron.

At Georgia State University, there is a long history of calculations of atomic and ionic photoionization cross sections, along with the resulting relaxation processes, spanning five decades. Many of these calculations have been performed with an eye towards astrophysical applications. In the course of this work, an array of state-of-the-art methodologies have been developed to perform the photoionization calculations, e.g., R-Matrix (in a number of different forms including the Breit-Pauli and Eigenchannel versions), Relativistic Random Phase Approximation (RRPA) and the associated Relativistic Multichannel Quntum Defect Theory (RMQDT), Randon Phase Approximation with Exchange (RPAE), and Augmented Many-Body Perturbation Theory (AMBPT). This arsenal of methodologies has allowed us to fit the methodology to the problem, not the other way around. In addition, the variety of methodologies allows us to provide "quality control" for our results. Furthermore, we work in close collaboration with experimenters for the ultimate "quality control".

This work has morphed into the AIDA project at present. Here we are concerned with providing accurate photoionization data to the astrophysical community on both inner shells and outer shells of ground and metastable states of atoms and ions of astrophysical interest, eventually posting the data on an AIDA web site. Some examples of our recent results will be presented along with a prospectus of future calculations.

The work reported is supported by NASA.

The effect of non-equilibrium kinetics on oxygen chemistry in the interstellar medium

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Abstract

The $O+H_2 \rightarrow OH+H$ reaction is considered to be the key step in initiating oxygen chemistry in shocked interstellar molecular clouds. We present extensive quantum scattering calculations of rate coefficients of the $O+H_2 \rightarrow OH+H$ reaction involving both ortho and para hydrogen in the temperature range 100–4000 K. The reaction is slow at low temperatures with ground state reactants due to an energy barrier in the entrance channel of the reaction. The role of non-equilibrium vibrational populations of H_2 is examined and it is shown that vibrational excitation of the molecule has a significant effect on reactivity, especially at low temperatures. At 100 K, the rate coefficient increases by about 11 orders of magnitude when the H_2 vibrational quantum number is increased from $v = 0$ to $v = 3$. Initial vibrational state selected cross sections, rate coefficients as well as product OH vibrational level distributions are presented for $v = 0 - 3$ of the H_2 molecule.

Atomic Oscillator Strengths in the Vacuum Ultraviolet

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Abstract

Transitions in singly-ionized and doubly-ionized iron-group elements give rise to prominent emission lines from a wide variety of astrophysical objects. Some of the most important lines are formed when the upper energy level is excited by radiation from hydrogen at 1216 Å(Ly-α), giving strong fluorescence lines from the vacuum ultraviolet to the infrared. These emission lines are important diagnostics of astrophysical plasmas, but laboratory oscillator strengths are unavailable.

The established way to measure accurate oscillator strengths for atomic lines combines the measurement of a lifetime of an upper energy level with a separate measurement of the branching fractions of all the lines emitted from that level. This technique relies on being able to observe *all* the spectral lines emitted by the upper level, which range down to Ly-α or below for many fluorescence lines. Methods of measuring branching fractions using Fourier transform spectroscopy are limited to wavelengths above about 1400 Å and cannot observe all the spectral lines required.

We have developed techniques to measure branching fractions in the vacuum ultraviolet using our 10.7 m normal incidence grating spectrograph. For this we use phosphor image plates as replacements for the photographic plates previously used on this instrument. Image plates are sensitive to wavelengths from the X-ray region to 2200 Å, and have a linear intensity response with a dynamic range of at least 10^{4}. We have recorded spectra of iron-neon hollow cathode and Penning discharges, using a deuterium standard lamp for radiometric calibration. Our measurements of Fe II branching ratios around 1600 Å agree with previously-published measurements to within 8 %. The reproducibility of our D_2 standard lamp spectra at shorter wavelengths is 4 % , enabling us to measure branching ratios down to 1150 Å. We are also investigating methods of radiometric calibration below 1150 Å using hollow cathode standard lamps. This will enable us to measure branching ratios down to 800 Å or below – a region with many resonance lines of doubly-ionized spectra and critical for the analysis of data from the Far Ultraviolet Spectroscopic Explorer.

This work is partially funded by NASA under the inter-agency agreement W-10,255.

Circumstellar Silicates Do Nucleate: New Vapor Pressure Data for SiO

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Abstract

We have measured the vapor pressure of solid SiO as a function of temperature over the range from 1200K up to 1950K in vacuo using a modified Thermo-Cahn Thermogravimetric system. Although the vapor pressure measured near 2000K is close to that predicted from the work of Schick[1] under reducing conditions, the vapor pressures measured at lower temperatures diverge significantly from such predictions and are several orders of magnitude lower than predicted at 1200K. This new vapor pressure data has been inserted into a simple model for the gas expanding from a late stage star. Using the new vapor pressure curve makes a significant difference in the temperature and stellar radius at which SiO gas becomes supersaturated, although SiO still becomes supersaturated at temperatures that are too low to be consistent with observations. We have therefore explored including the effects of vibrational disequilibrium2 of SiO in the expanding shell on the conditions under which nucleation occurs. These calculations are much more interesting in that supersaturation now occurs at much higher temperatures. We note however, that both vibrational disequilibrium and the new vapor pressure are required to induce SiO supersaturation in stellar outflows at temperatures above 1000K.

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THz Spectroscopy and Spectroscopic Database for Astrophysics

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Abstract

Molecule specific astronomical observations rely on precisely determined laboratory molecular data for interpretation. The Herschel Heterodyne Instrument for Far Infrared, a suite of SOFIA instruments and ALMA are each well placed to expose the limitations of available molecular physics data and spectral line catalogs. Herschel and SOFIA will observe in high spectral resolution over the entire far infrared range. Accurate data to previously unimagined frequencies including infrared ro-vibrational and ro-torsional bands will be required for interpretation of the observations. Planned ALMA observations with a very small beam will reveal weaker emission features requiring accurate knowledge of higher quantum numbers and additional vibrational states. Historically, laboratory spectroscopy has been at the front of submillimeter technology development, but now astronomical receivers have an enormous capability advantage. Additionally, rotational spectroscopy is a relatively mature field attracting little interest from students and funding agencies. Molecular data base maintenance is tedious and difficult to justify as research. This severely limits funding opportunities even though data bases require a similar level of expertise. We report the application of some relatively new receiver technology into a simple solid state THz spectrometer that has the performance required to collect the laboratory data required by astronomical observations. Further detail on the lack of preparation for upcoming missions by the JPL spectral line catalog is given.

Challenging the Identification of Silicon Nitride Dust in Extreme Carbon Stars

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Abstract

It has been well established that SiC is a dominant mineral in the condensation sequence of carbon-rich stars (or C-stars). The presence of other mineral species in interstellar dust surrounding C-stars may be indicative of exotic formation conditions for these objects. Observers have long held out hope for detecting the compound silicon nitride (Si_3N_4) in stellar spectra; however, previous attempts to identify Si_3N_4 in dust material around novae, planetary nebulae, and late-type binary and C-stars have proved to be unsuccessful (Clément et al. 2005, ApJ, 821, 985 and references therein). Clément et al. (2005) suggested that a broad, double-peaked 9-11 μm absorption feature in the ISO SWS spectra of two extreme C-stars (AFGL 2477 and AFGL 5625) is due to Si_3N_4. This assignment was based on the correlation of several weak observational spectral features with laboratory spectral features of α-Si_3N_4 in the 15-30 μm range. The broad 9-11 μm feature had been previously attributed to a mixture of SiC and interstellar silicate (Speck et al. 1997, MNRAS, 20, 431), and more recently to amorphous SiC (Speck et al. 2005, ApJ, 634, 426). We dispute the Si_3N_4 assignment on the basis of expected interstellar abundances, Si_3N_4 meteoritic isotope studies, blackbody correction methods, and spectral peak assignment as compared to noise. Speck et al. (2005) discovered another extreme carbon star (IRAS 00210+6221) that exhibits a 9-11 μm absorption feature identical to those found in AFGL 2477 and AFGL 5625. A preliminary re-analysis of the spectra of these three extreme carbon star spectra has revealed that neither AFGL 2477 nor IRAS 00210+6221 display any of the 15-30 μm features. For AFGL 5625, any features present in this range are at $> 2\sigma$ level, and therefore may just be noise. We compare the observational spectra to independently acquired laboratory spectra for Si_3N_4, as well as other nitride minerals consistent with recently published condensation sequences (e.g., AlN, TiN), carbides, and silicides. Our thin film laboratory absorbance spectra of α- and β-Si_3N_4 appear to give good agreement with the KBr pellet method transmission spectra of Clément et al. (2005). Based on these analyses, we conclude that a unique identification of Si_3N_4 has not yet been made and calculate an upper limit to the abundance based on a non-detection.

This work is supported through NASA APRA04-000-0041.

Diagnostics of laboratory plasmas with the high resolution XRS instrument at the EBIT-I facility: a critical tool for understanding spectral signatures of x-ray emitting astrophysical sources

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Abstract

The X-ray Spectrometer (XRS) instrument is a revolutionary non-dispersive spectrometer that was developed for the Suzake (Astro-E2) observatory. We have installed a flight spare XRS detector array in a laboratory cryostat and deployed it as a unique diagnostic spectrometer at the Electron Beam Ion Trap facility (EBIT I) at Lawrence Livermore National Laboratory. The XRS microcalorimeter is an x-ray detector that senses the heat deposited by the incident photon in a high Z absorber. It achieves a high energy resolution by operating below 0.1K and by carefully controlling the heat capacity and thermal conductance of each detector. The XRS/EBIT instrument has 32 pixels in a square geometry and achieves an energy resolution of 6 eV at 6 keV, with a bandpass from 0.1 to over 60keV. The instrument allows detailed studies of the x-ray line emission of laboratory plasmas. This provides critical diagnostics for x-ray emission models including absolute cross sections for L shell transitions, verification of thermal emission models of, for example, K shell Fe, and charge exchange interactions between a hot plasma and a cold target. These measurements are critical for guiding and verifying plasma codes used to interpret the high resolution spectra from the Chandra, XMM, and Suzaku observatories and will form the basis for the scientific interpretation of data from the Constellation-X observatory. We will discuss the current state of the instrument, near term significant upgrades, and some of our recent measurements. The authors wish to thank NASA's APRA program for funding this work.

Atomic Spectroscopic Databases at NIST

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Abstract

The NIST Physics Laboratory provides a number of atomic spectroscopic databases on the World-Wide-Web that are widely used in astrophysics. The data consist mainly of wavelengths, energy levels, and oscillator strengths that have been critically evaluated in the NIST Atomic Spectroscopy Data Center. These data play an important role in line identification, spectra modeling, and other astrophysical research. All databases can be accessed from the NIST Physics Laboratory home page: www.physics.nist.gov; select Physical Reference Data.

Since the last Workshop, some of the existing databases were significantly expanded, and a number of new databases became available on the Web. The NIST "Atomic Spectra Database" (ASD) has been upgraded from version 2.0 to 3.0. It now contains detailed information on more than 75,000 energy levels and almost 130,000 spectral lines for ions of 99 elements. New large sets of data were recently added for the spectrum lines and energy levels of Ne I, Hg I and II, Be II, Xe and Rb in all ionization stages, highly-charged ions of the iron period of elements, Cu, Mo, and Kr (taken from Mon. 8 of J. Phys. Chem. Ref. Data), Zr III and IV, Ba I and II, and W I and II. Data for the transition probabilities of Ba I and II were also added.

A new relational database management system allows a high level of data integration and consistency, while the innovative user interface provides convenient access to various parameters. Several new additions to the ASD interface should be of special value to astrophysicists. Among those is the online Saha-LTE spectrum generation tool, which allows calculation of plasma emission spectra under Saha-LTE equilibrium for user-defined values of electron density and temperature. The calculated spectrum can also be Doppler-broadened for arbitrary values of ion temperature. This also may be used for simulation of instrumental broadening. Another example of a new graphical interface is the availability of Grotrian diagrams. This provides an intuitive visualization of the atomic energy level structure and transitions as well as direct access to the fundamental atomic data (energy levels, wavelengths, transition probabilities).

In recent years, two new databases became available. The "Handbook of Basic Atomic Spectroscopic Data," now upgraded to v.1.1, provides the most frequently used atomic spectroscopic data in an easily accessible format. It includes data for the neutral and singly-ionized atoms of all elements hydrogen through einsteinium (Z = 1-99). Wavelengths, intensities, line classifications, and transition probabilities are given in a separate table for each element. The data for 12,000 lines of all elements are also collected into a finding list sorted by wavelength. "Spectral Data for the Chandra X-ray Observatory" contains critically compiled wavelengths, energy levels, line classifications, and transition probabilities for ionized spectra of neon (Ne V to Ne VIII), magnesium (Mg V to Mg X), silicon (Si VI to Si XII), and sulfur (S VIII to S XIV) in the 20 to 170 region. These tables provide data of interest for the Emission Line Project in support of analyses of astronomical data from the Chandra X-Ray Observatory. The transition probabilities were obtained mainly from recent sophisticated calculations carried out with complex computer codes.

Work continues on the bibliographic databases for atomic transition probabilities and spectral line broadening, as well as the database on electron impact ionization cross sections. We expect our bibliographic database on energy levels and spectral lines to be available in the near future.

Work on these databases is supported in part by the National Aeronautics and Space Administration and by the Office of Fusion Energy Sciences of the U. S. Department of Energy.

Quantum chemical characterization of dimeric polyaromatic hydrocarbons

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Abstract

Polyaromatic hydrocarbon (PAH) has been considered to be an important interstellar species for a relatively long time because of its possible linkage to lifeforms. Despite its importance, however, interactions of individual PAH molecules have not been well understood. In this study, characteristics of dimers of various PAHs are investigated using ab initio quantum chemical approach. It is found that various homo- and heterodimers can be formed with significant stability especially from cationic monomers, which may exist in abundance in the interstellar space. Such dimeric species are also found to have strong absorption features in a wide range of wavelengths. It is hypothesized that the combination of the stability and the large absorptivity can lead to chemical reactions between monomers, opening a possible route to the growth of PAH and other organic substances in space.

Laboratory Spectroscopy of Large Carbon Molecules and Ions in support of Space Missions. A New Generation of Laboratory & Space Studies

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Abstract

Polycyclic Aromatic Hydrocarbons (PAHs) are an important and ubiquitous component of carbon-bearing materials in space. A long-standing and major challenge for laboratory astrophysics has been to measure the spectra of large carbon molecules in laboratory environments that mimic (in a realistic way) the physical conditions that are associated with the interstellar emission and absorption regions [1]. This objective has been identified as one of the critical Laboratory Astrophysics objectives to optimize the data return from space missions [2]. An extensive laboratory program has been developed to assess the properties of PAHs in such environments and to describe how they influence the radiation and energy balance in space. We present and discuss the gas-phase electronic absorption spectra of neutral and ionized PAHs measured in the UV-Visible-NIR range in astrophysically relevant environments and discuss the implications for astrophysics [1]. The harsh physical conditions of the interstellar medium - characterized by a low temperature, an absence of collisions and strong VUV radiation fields - have been simulated in the laboratory by associating a pulsed cavity ringdown spectrometer (CRDS) with a supersonic slit jet seeded with PAHs and an ionizing, penning-type, electronic discharge. We have measured for the *first time* the spectra of a series of neutral [3, 4] and ionized [5, 6] interstellar PAHs analogs in the laboratory. An effort has also been attempted to quantify the mechanisms of ion and carbon nanoparticles production in the free jet expansion and to model our simulation of the diffuse interstellar medium in the laboratory [7]. These experiments provide *unique* information on the spectra of free, large carbon-containing molecules and ions in the gas phase. We are now, for the first time, in the position to directly compare laboratory spectral data on free, cold, PAH ions and carbon nano-sized carbon particles with astronomical observations in the UV-NIR range (interstellar UV extinction, DIBs in the NUV-NIR range). This new phase offers tremendous opportunities for the data analysis of current and upcoming space missions geared toward the detection of large aromatic systems i.e., the "new frontier space missions" (Spitzer, HST, COS, JWST, SOFIA,...).

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Acknowledgments:

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Computational Spectroscopy of Polycyclic Aromatic Hydrocarbons In Support of Laboratory Astrophysics

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) are strong candidates for the molecular carriers of the unidentified infrared bands (UIR) and the diffuse interstellar bands (DIBs). In order to test the PAH hypothesis, we have systematically measured the vibronic spectra of a number of jet-cooled neutral and ionized PAHs in the near ultraviolet (UV) to visible spectral ranges using the cavity ring-down spectroscopy. To support this experimental effort, we have carried out theoretical studies of the spectra obtained in our measurements. *Ab initio* and (time-dependent) density functional theory calculations are performed to obtain the geometries, energetics, vibrational frequencies, transition dipole moments, and normal coordinates of these PAH molecules. Franck(Condon (FC) calculations and/or vibronic calculations are then performed using the calculated normal coordinates and vibrational frequencies to simulate the vibronic spectra. It is found that vibronic interactions in these conjugated (electron systems are often strong enough to cause significant deviations from the Born(Oppenheimer (BO) approximation. For vibronic transitions that are well described by the BO approximation, the vibronic band profiles are simulated by calculating the rotational structure of the vibronic transitions. Vibronic oscillator strength factors are calculated in the frame of the FC approximation from the electronic transition dipole moments and the FC factors. This computational effort together with our experimental measurements provides, *for the first time*, powerful tools for comparison with space-based data and, hence, a powerful approach to understand the spectroscopy of interstellar PAH analogs and their contribution to the interstellar extinction, the UIR and the DIBs.

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Cosmological Implications of the Uncertainty in Astrochemical Rate Coefficients

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Abstract

The cooling of neutral gas of primordial composition, or with very low levels of metal enrichment, depends crucially on the formation of molecular coolants, such as H_2 and HD within the gas. Although the chemical reactions involved in the formation and destruction of these molecules are well known, the same cannot be said for the rate coefficients of these reactions, some of which are uncertain by an order of magnitude. In this presentation, we discuss two reactions for which large uncertainties exist – the formation of H_2 by associative detachment of H^- with H and the destruction of H^- by mutual neutralization with protons. We show that these uncertainties can have a dramatic impact on the effectiveness of cooling during protogalactic collapse.

This work was supported in part by a NASA SARA/APRA grant.

Studying Atomic Physics Using the Nighttime Atmosphere as a Laboratory

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Abstract

Many of the atomic transitions observed in low-ionization plasma astrophysical environments, such as planetary nebulae and H II regions, are also manifest in the terrestrial night airglow or nightglow. Ground-based observations of astrophysical objects inevitably capture the spectrum of the nightglow. The combination of the high resolution of these spectra, their associated high-sensitivity detectors, and the ability to calibrate these spectra to high precision in terms of wavelength and absolute intensity, have allowed the observation and measurement of weak permitted and optically-forbidden atomic transitions that are difficult to observe in the laboratory. We present here a summary of our recent work in this area, including a new determination of the wavelengths of the [O I] $^2D^o$–$^2P^o$ $\lambda\lambda$7320,7330 doublets that are used to characterize the velocity field of the Orion Nebula outflow. Also presented are experimental tests of the theoretical intensity ratios of [N I] $^4S^o$–$^2D^o$ $\lambda5198/\lambda5200$ and [O I] ^3P–^1D $\lambda6300/\lambda6364$, used as electron density and temperature diagnostics, and our observations of high-energy triplet and quintet Rydberg series neutral oxygen permitted lines, arising from electron radiative recombination, that allow calculations of effective recombination coefficients used for elemental abundance determination to be verified. Finally, we present our re-confirmation in these spectra of a discrepancy between the observed intensity ratio of [O I] $^1D_2$–$^1S_0$ $\lambda5577$ to [O I] $^3P_1$–$^1S_0$ $\lambda2972$, and the ratios predicted by *ab initio* theory calculations and laboratory experiment, in some cases differing by more than a factor of two.

Physical data needs for select problems in stellar atmospheres

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Abstract

Over the past ten years there has been a renewal of interest in stellar atmospheric and spectrum modeling and the information it can provide. This has been driven by several observational developments: 1) the discovery and characterization of Brown Dwarfs, 2) the discovery of extremely metal poor (XMP) stars, 3) the discovery of extra-solar planetary systems, and 4) the surprising revision in the abundances of important elements in the solar atmosphere. Various of these fields are dependent upon, and plagued by uncertainty in, physical data for atomic and molecular radiative and collisional processes. Particular areas of concern include data for Iron group elements and collisional cross-sections for molecules. At stake is our ability to use stars as accurate tracers of the chemical evolution of galaxies, and the interaction of planetary systems with their host stars.

New Measurements of Doubly Ionized Iron Group Spectra by Fourier Transform and Grating Spectroscopy

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Abstract

We use the unique high resolution vacuum–UV Imperial College Fourier transform spectrometer (FTS) to measure spectra of astrophysically important ions. The IC FTS combines high wavelength resolution (1:10^8) with a broad spectral range from the visible to 135 nm. The new high resolution laboratory spectra are required to fully interpret new astrophysical spectra obtained by the latest generation of spectrographs such as HST/STIS and FUSE. Astronomers urgently require accurate wavelengths, energy levels, line broadening effects and oscillator strengths.

Our measurement program has included many neutral and singly ionized iron group elements (e.g. Cr I, V I & II, Co I & II and Mn I). Difficulties in measuring doubly ionized spectra using an FTS have recently been overcome by a Penning discharge lamp. These ions are particularly important in the analysis of B-type (hot) stars whose spectra they dominate, however existing measurements are in many cases incomplete or inaccurate.

We report new measurements of Co III and Cr III taken with the Imperial College VUV FTS and measurements of Co III taken with the normal incidence vacuum (grating) spectrograph at the National Institute of Standards and Technology, below 135 nm. We report the completion of measurements of Fe III, with new grating spectra to complement our FT spectra. Work towards transition wavelengths, energy levels and branching ratios (which, combined with lifetimes, produce oscillator strengths) for these and other doubly ionized iron group elements is presented.

This work is supported in part by NASA Grant NAG5-12668, NASA inter-agency agreement W-10,255, PPARC, the Royal Society of the UK and by the Leverhulme Trust.

Collisional De-excitation of Molecular Hydrogen in the Interstellar Medium

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Abstract

With the new development of NASA ground- and space-based missions, peering into the universe with higher spatial and spectral resolution at infrared and sub-millimeter wavelengths has become possible and will be further enhanced in the near future. Molecular hydrogen is the most abundant chemical species in the universe and therefore plays a significant role in astrophysical environments such as starburst galaxies, interstellar molecular clouds, and star-forming regions. However, the scarcity of both accurate and complete data sets for rovibrational inelastic cross sections involving collisions with H_2 has set a serious limitation on the development of reliable astrophysical models. In particular, the investigation of cooling processes, molecular emission, and non-equilibrium effects in molecular gaseous nebulae and other molecular environments requires collisional de-excitation data for H-, He-, and H_2-impact on H_2. Recently, a number of observations, performed using the NASA Spitzer Space Telescope's infrared spectrograph, have identified emissions arising from pure rotational transitions in H_2. In order to identify, analyze and interpret these spectral lines, an accurate set of data for thousands of cross sections is needed, thus requiring large scale molecular physics computer codes to make extensive theoretical predictions. A sample of rate coefficients for quenching of rotationally- and vibrationally-excited H_2 will be presented. This work was partially supported by NASA APRA grant NNG05GD81G and the Spitzer Cycle 2 Theoretical Research Program.

Molecular nitrogen photoabsorption cross sections and line widths in support of analyses of planetary atmospheres.

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Abstract

The analyses of VUV occultation measurements of the N2-rich atmosphere of Titan require reliable photoabsorption cross sections and line widths for the approximately 100 vibronic bands of N2 in the 80 to 100 nm wavelength region. We report measurements of these fundamental parameters of the absorption spectrum of 14N2 in the 93.5 100 nm spectral region. The room temperature absorption measurements were performed with the 6.65-meter vuv spectrometer at the Photon Factory synchrotron facility with a resolving power of approximately 125,000. A line-shape fitting routine is used to extract individual rotational line f-values and predissociation-broadened line widths within the fifteen bands reported in this study. Within individual bands, we find significant departures from the predicted line strength distributions based on isolated band models. Line width analyses within each band indicate that predissociation-broadening is often highly dependent on the rotational quantum number. We illustrate the importance of N2 line widths in the analysis of Cassini occultation measurements with sample N2 transmission models over selected wavelength regions. We gratefully acknowledge funding support from NASA grant NAG5-9059.

X-ray Spectroscopy of Neon-like Ions at the NIST EBIT Facility

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Abstract

X-ray spectra of highly charged ions (HCIs) can be useful diagnostics for hot plasmas found in astrophysical objects. To provide benchmark data for the development of models and computational codes, HCIs are produced and confined within the controlled conditions of an electron beam ion trap (EBIT). Experiments at the NIST EBIT facility include the investigation of HCI excitations from closed-shell configurations, such as neon-like Fe XVII, Ni XIX, Cu XX, and Kr XXVII. Advances in X-ray quantum calorimetry have made it feasible to measure spectral features over the broad energy range of interest. We will present results obtained using the recently commissioned SAO microcalorimeter with a 1x4-array of NTD-Ge detectors.

Cross Sections for Electron Impact Excitation of Astrophysically Abundant Atoms and Ions

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Abstract

Electron collisional excitation rates and transition probabilities are important for computing electron temperatures and densities, ionization equilibria, and for deriving elemental abundances from emission lines formed in the collisional and photoionized astrophysical plasmas. The electron excitation rates including cascades are needed. Oscillator strengths for the UV and FUV lines of abundant and trace elements are needed to study absorption by gases in the interstellar medium. Accurate representation of target wave functions that properly account for the important correlation and relaxation effects and inclusion of coupling effects including coupling to the continuum are essential components of a reliable collision calculation. Non-orthogonal orbitals technique in multiconfiguration Hartree-Fock approach is used to calculate oscillator strengths and transition probabilities. Comparison of the computed excitation energies and oscillator strengths with experiment can provide a check on the accuracy of target wave functions. The effect of coupling to the continuum is included through the use of pseudostates which are chosen to account for most of the dipole polarizabilities of target states. The B-spline basis is used in the R-matrix approach to calculate electron excitation collision strengths and rates. Recent results for oscillator strengths and electron excitation collision strengths for transitions in N I, O I, O II, O IV, S X, and Fe XIV will be presented.
This research work is supported by NASA.

Fluorescence Spectroscopy of Gas-phase Polycyclic Aromatic Hydrocarbons

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Abstract

The purpose of this investigation was to produce fluorescence spectra of polycyclic aromatic hydrocarbon (PAH) molecules in the gas-phase for comparison with blue luminescence (BL) emission observed in astrophysical sources (Vijh et al. 2004, 2005a,b). The BL occurs roughly from 350 to 450 nm, with a sharp peak near 380 nm. PAHs with three to four rings, e.g. anthracene and pyrene, were found to produce luminescence in the appropriate spectral region, based on existing studies. Relatively few studies of the gas-phase fluorescence of PAHs exist; those that do exist have dealt primarily with the same samples commonly available for purchase such as pyrene and anthracene. In an attempt to understand the chemistry of the nebular environment we also obtained several nitrogen substituted PAHs from our colleagues at NASA Ames. In order to simulate the astrophysical environment we also took spectra by heating the PAHs in a flame. The flame environment counteracts the formation of dimmers and permits the spectroscopy of free-flying neutral molecules. Experiments with coal tar and coal tar extracts demonstrate that fluorescence spectroscopy reveals primarily the presence of the smallest molecules, which are most abundant and which possess the highest fluorescence efficiencies. One gas-phase PAH that seems to fit the BL spectrum most closely is phenanthridine, a 3-ring PAH with a single nitrogen substitution. In view of the results from the spectroscopy of coal tar, a compound containing PAH structures ranging from small, simple PAHs to very large PAH molecules, this fit in no way precludes the presence of larger PAHs in interstellar sources exhibiting BL.

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Intra-molecular interactions during the fragmentation of small systems.

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Abstract

Recent dissociative recombination (DR) experiments have investigated the role of the parent ion's structure, bonding and charge centre on the DR process. For examples, in the DR of the H_5^+ and $D_5O_2^+$[1] cluster ions, the dominant product channels greatly reflect the structure of the parent ion, $H_3^+{\cdot}H_2$, and $D_2O{\cdot}D^+{\cdot}D_2O$[1] respectively, and the question arises on the role played by the "neutral" constituent in the cluster, i.e. as spectator or participant. To investigate this question we have studied the DR of one of the simplest such systems, $Li^+{\cdot}H_2$, which is a weakly bound cluster with the charge centre located on the lithium atom. All these systems represent excellent models for providing insight into the dynamics occurring in the fragmentation of small systems.

[1] Någård et al. J. Chem. Phys. 117, 5264 (2002)

Charge Exchange Spectra of H-like and He-like Iron

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Abstract

In our experiments, bare iron (Fe^{26+}) and hydrogen-like iron (Fe^{25+}) ions are produced in the Livermore electron beam ion trap, and a neutral target gas (either N_2, He, or H_2) is injected into the trap. The ions then undergo charge exchange reactions at a collision energy of ~10 eV/amu and produce Fe XXV and Fe XXVI emission. These spectra are recorded with a solid-state Ge detector and/or the X-Ray Spectrometer (XRS) microcalorimeter provided by the Goddard Space Flight Center, which has an energy resolution of better than 10 eV. As expected, strong enhancement of emission from the Fe XXV forbidden and intercombination lines is observed, compared with the dominance of the resonance line in electron-impact-excitation spectra. Surprisingly, however, the Fe XXVI high-n Lyman lines have a summed intensity that in most instances is greater than that of Lyα; this is substantially stronger than predicted from theoretical calculations of charge exchange with atomic H. We conclude that the angular momentum distribution resulting from electron capture using a multi-electron target gas is significantly different from that obtained with H, resulting in the observed high-n enhancement.

Metal Hydride and Alkali Halide Opacities in Extrasolar Giant Planets and Cool Stellar Atmospheres

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Abstract

The lack of accurate and complete molecular opacity data for a large number of metal hydrides and alkali halides has been a serious limitation to developing atmospheric models of cool stars and extrasolar giant planets. In fact, sophisticated modeling programs require high quality opacity data in order to produce synthetic spectra and predict important physical parameters (surface chemical composition, effective temperature, etc). Typically, atmosphere models include molecular bands with hundreds of millions of spectral lines, mostly derived from molecular band models.

In this work, we report our progress on the calculations of line opacities resulting from the presence of CaH and LiCl. Fully quantum-mechanical techniques have been applied to compute comprehensive and complete transition energies and absorption line oscillator strengths for all possible allowed transitions from the electronic ground state. *Ab initio* potential energies and dipole transition moment functions have been used, with the former adjusted to account for experimental data.

For calcium monohydride, line lists for the electronic transitions from the $X\ ^2\Sigma^+$ ground state to the $A\ ^2\Pi$, $B/B'\ ^2\Sigma^+$, $C\ ^2\Sigma^+$, $D\ ^2\Sigma^+$ and $E\ ^2\Pi$ bound excited states have been calculated using electronic structure calculations from the literature. The spectrum of CaH is characterized by strong perturbations of various types, from local shifts to large interactions between electronic states [1]. For lithium chloride, we have obtained the potential curves and dipole transition moment functions between the $X\ ^1\Sigma^+$ ground state and the purely dissociative $B\ ^1\Sigma^+$ and $A\ ^1\Pi$ excited states [2]. Using these data for LiCl and CaH, we have calculated synthetic spectra for cool dwarf test models with the `PHOENIX` stellar atmosphere code [3, 4, 5].

This work was supported in part by NSF grants AST-9720704 and AST-0086246, NASA grants NAG5-8425, NAG5-9222, and NAG5-10551 as well as NASA/JPL grant 961582. Some of the calculations were performed on the IBM SP2 of the UGA EITS, on the SP *Blue Horizon* of the San Diego Supercomputer Center, with support from the NFS, and on the IBM SP of the NERSC with support from the DoE.

1. P. F. Weck, P. C. Stancil and K. Kirby, J. Chem. Phys. **118**, 9997 (2003).
2. P. F. Weck, P. C. Stancil and K. Kirby, J. Chem. Phys. **120**, 4216 (2004).
3. P. H. Hauschildt and E. Baron, Journal of Computational and Applied Mathematics **102**, 41 (1999).
4. P. F. Weck *et al.*, Astrophys. J. **613**, 567 (2004).
5. D. Homeier *et al.*, ASP Conf. Series **334**, 209 (2005).

Photoelectric Emission from Dust Grains Exposed to Extreme Ultraviolet and X-ray Radiation

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Abstract

Photoelectric emission from dust plays an important role in grain charging and gas heating. To date, detailed models of these processes have focused primarily on grains exposed to soft radiation fields. We provide new estimates of the photoelectric yield for neutral and charged carbonaceous and silicate grains, for photon energies exceeding 20 eV. We include the ejection of electrons from both the band structure of the material and the inner shells of the constituent atoms, as well as Auger and secondary electron emission. We apply the model to estimate gas heating rates in planetary nebulae and grain charges in the outflows of broad absorption line quasars. For these applications, secondary emission can be neglected; the combined effect of inner shell and Auger emission is small, though not always negligible. Finally, we investigate the survivability of dust entrained in quasar outflows.

New Critical Compilations of Atomic Transition Probabilities for Neutral and Singly Ionized Carbon, Nitrogen and Iron[1]

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Abstract

Because of the strong astrophysical interest in the above cited spectra and because of new literature data of significantly improved quality, we have undertaken new critical assessments and tabulations of the transition probabilities of important lines of these spectra. For Fe I and Fe II, we have carried out a complete re-assessment and update, and we have relied almost exclusively on the literature of the last 15 years, so that this new compilation supersedes our 1988 data volume. Our new tables are about 25% larger for Fe I and almost 50% larger for Fe II, and the estimated accuracies are now for the majority of lines in the 3 - 10% range for Fe I and in the 10 - 25% band for Fe II.Our updates for C I, C II and N I, N II address primarily the persistent lower transitions involving principal quantum numbers 2 and 3, as well as a now greatly expanded number of forbidden lines (M1, M2, and E2). For these transitions, sophisticated multiconfiguration Hartree-Fock (MCHF) calculations have been recently carried out, which have yielded data considerably improved from our 1996 NIST compilation and have also yielded many additional forbid-den transitions. We plan to enter all this new material into our comprehensive NIST Atomic Spectra Database (ASD).

EUV-VUV Photolysis of Molecular Ice Systems of Astronomical Interest

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Abstract

We wish to report laboratory simulation results obtained from extreme ultraviolet (EUV) and vacuum ultraviolet (VUV) photolysis of molecular ices relevant to the cometary-type ices and icy satellites of planetary systems. Specifically, we identify the type of molecules that form in the ices and/or those that come off the ice surfaces, quantify their production yields and destruction yields, understand their production mechanisms, and ascertain their significance in astronomical environments.

A FTIR spectrometer was employed to identify IR absorption features of the *in-situ* ice samples. We have recently installed a Quadrupole Mass Spectrometer in the experimental apparatus which will allow us to carry out simultaneous measurements of fragments ejected by EUV photon sputtering. A tunable intense synchrotron radiation light source available at the National Synchrotron Radiation Research Center, Hsinchu, Taiwan, was employed to provide the required photons from the soft x-ray region on through the VUV. However, we have mainly selected the photon wavelengths to center at the prominent solar lines, namely, the 121.6 nm, 58.4 nm, 30.4 nm, and other photon wavelengths of interest.

So far, we have studied the following ice systems using the FTIR spectrometer: (1) pure ices such as pure CH_4, CO, N_2, and NH_3 ices. (2) Mixtures of two molecules such as H_2O+CH_4, H_2O+C_2H_2, H_2O+CO, H_2O+CO_2, CH_4+NH_3, CO+NH_3, H_2O+NH_3. (3) Mixtures of three or more molecules such as H_2O+CO+NH_3, CO+CH_4+NH_3, H_2O+CO+CH_4+NH_3.

New molecular species were produced in the ice samples at 10 K as a result of EUV photon irradiation. The photon-induced chemical products that have been observed in the above studies include radicals, such as CH_2, CH_3, C_2H_3, C_2H_5, light hydrocarbons, such as, C_2H_2, C_2H_4, C_2H_6, C_3H_8, carbon-containing compounds, such as C_3O_2, C_2O, CO, CO_2, CO_3, alcohols, such as CH_3OH, C_2H_5OH, and others such as HCO, H_2CO, HCOOH, HCN, XCN, CN^-, CH_2N_2. While new molecular species were formed, the original parent molecules were depleted due to their conversion to other species. The production yields of the products and the destruction yields (or lifetime) of the parent molecules in the ices, and the typical reaction mechanisms will be presented.

The Temperature-Dependent Photoabsorption Cross Section Measurements Program at the Space Sciences Center, USC

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Abstract

One of our recent laboratory efforts is concerned with the interaction of ultraviolet (UV) and extreme ultraviolet (EUV) photons with the atmosphere of the Earth, other planets, and cometary gases under various temperature and spectral resolution conditions. The cross section measurements in the temperature range from 140 K to 650 K with a spectral resolution from ultrahigh (0.0003 nm and 0.0008 nm), and high (0.008 nm), to medium (0.01 nm). A closed absorption cell was used to carry out measurements between 140 K and 400 K while a windowless high-temperature absorption cell was used for temperatures up to 650 K. The 6VOPE spectrometer available at the synchrotron radiation facility of the Photon Factory, KEK, Tsukuba, Japan, is used in the ultrahigh resolution studies, whereas the 4-m NIM spectrometer available at the Synchrotron Radiation Center, Madison, Wisconsin, is utilized in the high and medium resolution measurements.

Typical ultrahigh-resolution, high-temperature results on: (1) N_2 with a resolution of 0.0003 nm and 0.0008 nm in the 91.6 nm and the 83.4 nm regions at temperatures of 650, 555, 445, and 295 K and, (2) O_2 with a resolution of 0.0008 nm in the 83.4 nm, 91.6 nm, 108.5 nm regions at temperatures of 535 and 295 K will be presented. The data will contribute to a correct interpretation of the NII 91.6 nm, the OII 83.4 nm, and the NII 108.5 nm extreme ultraviolet airglow emissions of the Earth, by elucidating the effect of temperature on the atmospheric extinction due to absorption by N_2 and O_2.

We have also obtained temperature-dependent absolute absorption cross sections of molecules at temperatures between 140 K and 400 K for CO, C_2H_2, NH_3, PH_3, H_2S, OCS, CS_2, and SO_2. The data have been applied in modeling optical albedos of Venus, Mars, Saturn, Jupiter, Titan, Io, and Jupiter. We have also carried out low temperature cross section measurements on CH_4, C_2H_4, and C_2H_6 and have studied pressure-induced broadening effects on C_2H_2 in the presence of high pressure H_2 and N_2. Most recently the Cassini UVIS experiment detected CH_4, C_2H_2, C_2H_4, C_2H_6, C_4H_2, and HCN in the atmosphere of Titan using data from a stellar occultation by Titan [Shemansky et al., Science 308, 978 (2005)]. Our low- temperature CH_4, C_2H_2, C_2H_4, and C_2H_6 data have been applied to a model using Cassini UVIS observations. The observations cover an unprecedented range of altitudes from 450 km to 1600 km, allowing the first determination of the mesopause. However, there exists no previous high resolution and low temperature cross section data of HCN and C_4H_2. Therefore, we plan to carry out such measurements in our laboratory in the very near future. Typical low temperature data for a variety of atmospheric gases will be presented.

Vibrational and rotational quenching of CO by collisions with H, He, and H_2

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Abstract

Collisional quenching of molecular species by atoms and molecules is an important process in a variety of astrophysical environments. Advanced atmospheric modeling and spectral synthesis of extrasolar giant planets (EGPs), brown dwarfs (BDs), photodissociation regions (PDRs), and other cool astrophysical environments requires an extensive array of accurate molecular data, i.e. state-to-state cross sections and rate coefficients. A large portion of the data is either currently unavailable (as the requisite experiments or calculations have not been carried out) or the available data are insufficient to meet the demands required by the modeling applications. Comprehensive experimental and theoretical studies of such processes are now becoming feasible.

Due to their astrophysical importance as these species are the most common ones in a wide range of astronomical sources, collisions of CO with H, He, and H_2 have been the subject of numerous experimental and theoretical studies. Accurate data for state-to-state cross sections and rate coefficients for these systems are crucial to quantitative models of astrophysical environments. In this work, quantum mechanical scattering calculations have been performed for the rovibrational and rotational relaxation of CO in collisions with H, He and both para-H_2 and ortho-H_2 in their rovibrational ground states using the close-coupling approach and coupled-states approximation.

Cross sections and rate coefficients for the quenching of the v=0-2, j=0-10 levels of CO will be presented and comparisons with previous calculations and measurements, where available, be provided. This work was partially supported by NASA grant NNG04GM59G from the Origins of Solar Systems Program.

Charge transfer between S^{2+} and He: A comparative study of quantal and semiclassical approaches

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Abstract

A comparative study on charge transfer in collisions of ground-state S^{2+} ions with He has been performed within fully quantal and semiclassical molecular-orbit close-coupling approaches. The processes for capture into $S^+(^4S^o, {}^2D^o, {}^2P^o)$ + He^+ are taken into account. Quantal and semiclassical cross sections were evaluated, respectively, in the diabatic and adiabatic representations and found to be in good agreement. The calculations show that at collision energies below about 40 eV/u, the charge-transfer processes are dominated by $S^{2+}(^3P) + He \rightarrow S^+(^2D^o) + He^+$, and capture into the $^2P^o$ and $^4S^o$ states become comparable with that into the $^2D^o$ state above 40 eV/u and 600 eV/u, respectively. The multireference single- and double-excitation configuration-interaction method was utilized to obtain adiabatic potentials and nonadiabatic coupling matrix elements. A detailed comparison of quantal and semiclassical transition probabilities is discussed. State-selective and total rate coefficients are presented with temperatures between 10, 000 K and 5.0×10^6 K.

Sub-millimeter Spectroscopy of Astrophysically Important Molecules

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Abstract

With the advent of SOFIA, Herschel, and SAFIR, new wavelength regions will become routinely accessible for astronomical spectroscopy, particularly at sub-mm frequencies (0.5-1.1 THz). Molecular emission dominates the spectra of dense interstellar gas at these wavelengths. Because heterodyne detectors are major instruments of these missions, accurate knowledge of molecular transition frequencies is crucial for their success. The Ziurys spectroscopy laboratory has been focusing on the measurement of the pure rotational transitions of astrophysically important molecules in the sub-mm regime. Direct absorption methods and ion-selective velocity modulation techniques have been employed. Of particular interest have been metal hydride species and their ions, including CrH, CrH^+, VH, and MnH. Also of interest have been metal halides such as ZnF and metal cyanides, including CrCN. A new avenue of study has included metal bearing molecular ions such as $FeCO^+$. Large organi c species with internal rotation have also been investigated, such as hydroxyacetone. Results of these various molecules will be discussed.

Hydrogen Atom Collisions and Tomography of the Dark Age Universe

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Abstract

We present collision data for hyperfine level changing transitions in atomic hydrogen. Recent proposals[1] have suggested that observation of the red-shifted hydrogen 21 cm line could provide unprecedented information on matter density fluctuations in the early universe. If the spin temperature of atomic hydrogen falls below the temperature of the background radiation field (CBR), regions of dense primordial hydrogen absorb radiation at 21 cm. The resulting features could be detected with proposed next generation radio telescopes. However, the decoupling of matter and radiation temperature depends crucially on the collision properties of the hydrogen system[2]. Our calculated collision data, which significantly improves upon previous results, confirms that for $30 < z < 200$, 21 cm absorption is efficient and enables proposed tomography of the dark age universe. We also discuss the role of spin-exchange vs. long range dipolar spin changing transitions in determining the level populations of atomic hydrogen in the dark age epoch.

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[2] B. Zygelman, ApJ 622 1356 (2005).

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