Mm and Sub-mm Wave Absorption in Low- and High-Density Amorphous Ice

N. I. Agladze and A. J. Sievers
Laboratory of Atomic and Solid State Physics and the Center for Radiophysics and Space Research, Cornell University, Ithaca, NY 14853-2501

Amorphous ice is believed to be one of the principal constituents of interstellar dust with about 10% of the total oxygen in dense molecular clouds contained in H_2O ice (Pollack 1994). Although single crystal ice has been measured over part of the mm-wave spectral region, surprisingly, no data are available on the mm-wave absorption of amorphous ice even though these optical constants will certainly play an important role in modeling calculations such as for the 'MRN' dust model (Mathis 1993). The discovery of the irreversible production of the high density amorphous (HDA) phase of ice by the compression of regular ice to 10 Kbar at 77 K (Mishima 1984) makes possible the spectroscopic measurement of bulk amorphous samples at atmospheric pressure. Upon then heating this substance to ≈ 120 K it transforms to the low density amorphous (LDA) form. At still higher temperatures ≈ 145 K it transforms to the cubic crystalline phase I_c and finally at 225 K it changes to I_h the hexagonal crystalline phase. Consequently, we are able to make mm and sub-mm wave measurements on a variety of phases at low temperature in a single sample by careful temperature cycling after the initial compression. We have measured the absorption spectra of these different phases in the spectral region from 5 to 0.33 mm wavelength at temperatures ranging from 1.5 to 70 K. Significant differences are found between the spectral properties of the HDA and the LDA ice forms. The absolute absorption of the HDA ice is 3 times larger than for either the LDA or the I_c ice phases. At 10 cm^{-1} (1 mm wavelength) its mass normalized single grain absorption coefficient for spherical particles small compared to the wavelength is 0.06 ± 0.008 cm^2g^{-1}. For temperatures up to 20 K the temperature dependent part of the absorption coefficient for the HDA ice is accurately described in the mm-wave region by a near uniform spectral distribution of two level systems, a characteristic feature of other disordered solids (Phillips 1987). Interestingly, over this same low temperature interval no corresponding temperature dependence of the absorption coefficient is found for the LDA ice. For temperatures above 20 K the absorption coefficient of all the different ice phases increases with temperature in a similar way indicating that a single temperature dependent absorption mechanism dominates in this higher temperature region.

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Electron collision properties and UV spectroscopy of H_2, HD, O, and H

J. Ajello, G. James, I. Kanik, C. Noren, L. Beegle, D. Dziczek, C. Jonin
Jet Propulsion Laboratory

D. Shemansky, X. Liu
University of Southern California

UV observations of diffuse molecular clouds and stellar atmospheres made by IUE, HST, Astro, FUSE and EUVE require accurate high resolution measurements of electron impact cross sections and oscillator strengths. The Laboratory Astrophysics program at the Jet Propulsion Laboratory concentrates on the measurement of the electron collision properties of atomic and molecular hydrogen, two species composing 90% of the ISM. The most recent developments for laboratory work are a 3m vacuum UV spectrometer ($\lambda/\Delta\lambda = 50000$), specialized discharge chambers for the production of atomic species, and installation of electrostatically focused electron guns.

Medium resolution ($\lambda/\Delta\lambda \sim 25000$) measurements of the H_2 Lyman and Werner systems have been obtained with the 3m facility in the 110 – 170 nm region (*Liu et al.*, 1995) allowing accurate comparison with the *Abgrall et al.*(1993a,b,c), and *Abgrall et al.*(1997) calculations of the rotational line strengths. Similar work on HD in the FUV and H_2 in the EUV to study the higher Rydberg states $^1\Sigma_u^+$ (B, B$'$, B$''$) and $^1\Pi_u$ (C, D, D$'$, D$''$) are underway. The electron impact cross sections of the H_2 Lyman and Werner systems have been reanalyzed in recent work (*Liu et al.*, in preparation), providing a much improved measure of the cross sections of the two systems. Our recent study of the Lyman continuum has revised by 15% the dissociation yield of this process, which represents the primary destruction path of H_2 in diffuse clouds.

Accurate ($< 10\%$) electron impact cross section measurement of the H(2p) resonance state of atomic hydrogen has been obtained over the range 0.020 – 1.8 keV (*James et al.*, 1997). This work is currently continuing to include the higher Rydberg states.

A new facility has been developed for producing an atomic oxygen beam, attached to a spectrometer with dual exit ports for simultaneous UV/Visible studies. The measurements are expected to provide definitive electron collision strength measurements of the atomic oxygen electronic direct and cascade cross sections of the important $^{3,5}S$ electronic states.

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Fifteen Years of Laboratory Astrophysics at Ames

L. J. Allamandola, S. A. Sandford, F. Salama, D. M. Hudgins, and M. Bernstein
NASA Ames Research Center, MS 245-6, Moffett Field, CA 94035-1000

Tremendous strides have been made in our understanding of interstellar material over the past fifteen years thanks to significant, parallel developments in two closely related areas: observational astronomy and laboratory astrophysics. Fifteen years ago the composition of interstellar dust was largely guessed at, the concept of ices in dense molecular clouds ignored, and the notion of large, abundant, gas phase, carbon-rich molecules widespread throughout the interstellar medium (ISM) considered impossible. Today the composition of dust in the diffuse ISM is reasonably well constrained to cold refractory materials comprised of amorphous and crystalline silicates mixed with an amorphous carbonaceous material containing aromatic structural units and short, branched aliphatic chains. In the dense ISM, these cold dust particles are coated with mixed-molecular ices whose compositions are very well known. Lastly, the signature of carbon-rich polycyclic aromatic hydrocarbons (PAHs), shockingly large molecules by early interstellar chemistry standards, is widespread throughout the ISM.

This great progress has only been made possible by the close collaboration of laboratory experimentalists with observers and theoreticians, all with the goal of applying their skills to astrophysical problems of direct interest to NASA programs. Such highly interdisciplinary collaborations ensure fundamental, in depth coverage of the wide-ranging challenges posed by astrophysics. These challenges include designing astrophysically focused experiments and data analysis, tightly coupled with astrophysical searches spanning 2 orders of magnitude in wavelength, and detailed theoretical modeling. The impact of our laboratory has been particularly effective as there is constant cross-talk and feedback between quantum theorists; theoretical astrophysicists and chemists; experimental physicists; organic, physical and petroleum chemists; and infrared and UV/Vis astronomers.

In this paper, two examples of the Ames Program will be given. We have been involved in identifying 9 out of the 14 interstellar pre-cometary ice species known, determined their abundances and the physical nature of the ice structure. Details on our ice work are given in the paper by Sandford et al.

Our group is among the pioneers of the PAH model. We built the theoretical framework, participated in the observations and developed the experimental techniques needed to test the model. We demonstrated that the ubiquitous infrared emission spectrum associated with many interstellar objects can be matched by laboratory spectra of neutral and positively charged PAHs and that PAHs were excellent candidates for the diffuse interstellar band (DIB) carriers. See Salama et al. and Hudgins et al.

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Low-Temperature Vapor Pressures of Some Light Hydrocarbons

John E. Allen, Jr. and Robert N. Nelson*
Astrochemistry Branch, NASA Goddard Space Flight Center

Interpretation of observations and proper modeling of planetary atmospheres are both critically dependent on accurate laboratory data for the properties and processes that give rise to the features and characteristics of those atmospheres. It is important, therefore, that these data be acquired over the appropriate ranges of parameters such as temperature, pressure, and composition. Thermodynamic data at low temperatures are particularly needed for the construction of first-order equilibrium and photochemical models of clouds and hazes in the atmospheres of the outer planets and their satellites. However, this information often does not exist or does not extend to the low temperatures prevalent in those environments. In the absence of the required low-temperature data, modelers must extrapolate high-temperature data to the temperature range of interest which can introduce significant errors.

To address the needs of the space sciences community for information of this nature, we have developed an apparatus specifically designed to provide low-temperature thermodynamic data. The system has been calibrated using propane (C_3H_8) over the temperature range from 84 to 241 K. Besides its role as a constituent in outer planet atmospheres, propane is a good calibration source since its vapor pressure is well determined over most of the temperature range of interest. The vapor pressure of ethylene (C_2H_4), for which there is little data below its triple point (104 K), was then determined from 97 to 147 K. And most recently the apparatus has been used to measure the vapor pressures of the critically important hydrocarbons methane (CH_4) and methane-d_1, i.e,, monodeuterated methane (CH_3D), from 62 to 90 K and 61 to 115 K, respectively. The results of these measurements are presented along with comparisons with existing data sets.

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* Also Department of Chemistry, Georgia Southern University.

High-resolution Absorption Cross Sections of Nitrogen in the 86.1-79.9 nm Region

L. M. Beaty, K. P. Huber
Steacie Institute for Molecular Sciences, NRC, Ottowa, ON, K1A 0R6, Canada

P. C. Hinnen
Laser Centre, Vrije Universiteit, De Boelelaan 1081-1083, 1081 HV Amsterdam, The Netherlands

K. Ito, T. Matsui
Photon Factory, KEK, 1-1 Oho, Tsukuba, Ibaraki, 305, Japan

G. Stark
Department of Physics, Wellesley College, Wellesley, MA 02181

An ongoing program at the Harvard-Smithsonian Center for Astrophysics and at the Steacie Institute for Molecular Sciences of the National Research Council in Ottawa aims at establishing reliable high-resolution cross sections for nitrogen in the 99.4-66.5 nm region of the dipole-allowed absorption spectrum (1). At the longest wavelengths, the data can contribute to a better understanding of the energetics of the Earth's upper atmosphere and to the interpretation of spacecraft-based observations of the atmospheres of the planetary satellites Titan and Triton (2). At intermediate wavelengths, the quantitative measurements in the near-threshold region complement the spectroscopic input data into multichannel quantum defect (MQD) calculations that seek to reproduce the observed spectrum by taking account of various channel interactions of the p and f Rydberg series with core-excited levels (3). Finally, the insight gained from the analyses of the discrete spectra can be used to extend the MQD calculations into the diffuse above-threshold region where quantitative absorption data become the principal source of information to guide the analysis. A preliminary analysis of room temperature and jet-cooled photoabsorption cross section measurements in the 79.9-86.2 nm region, carried out at the Photon Factory synchrotron radiation facility, will be presented.

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Spectral Catalogue of Multiply and Highly Charged Ions for Astrophysical Diagnostics in the Extreme Ultraviolet

P. Beiersdorfer[1], G. V. Brown[1], S. M. Kahn[2], D. L. Liedahl[1], S. B. Utter[1]
[1]*Lawrence Livermore National Laboratory*
[2]*Columbia University*

With the launch of the *Extreme Ultraviolet Explorer* (EUVE) in 1992, the extreme ultraviolet spectral region from 70 to 400 Å has been opened to stellar astrophysicists for high-resolution exploration. It was immediately apparent that EUVE could provide superb spectra of stellar coronae for deriving densities, abundances, and, very importantly, the coronal temperature structure not provided by any other means (Dupree et al. 1993, Brown 1994, Vedder et al. 1994, Mewe et al. 1995). The diagnostic opportunities are the result of the wealth of emission lines that mark the extreme ultraviolet spectral region. In particular, the region contains rich line emission from virtually all charge states of iron, i.e., transitions of the type 3ℓ-$n\ell'$ of the ionization states Fe IX–Fe XVII and transitions of the type $2s$-$2p$, of the ionization states Fe XVIII-Fe XXIV. These provide line diagnostics for the transition region ($T \leq 5 \times 10^5$ K), the "quiet" corona ($T \approx$ 1-2 $\times 10^6$K; e.g. Fe IX-Fe XII), active regions ($T \approx$ 2-5 $\times 10^6$ K; e.g. Fe XIV-Fe XX), and flares ($T \geq 10^7$ K; e.g. Fe XXI-Fe XXIV). The analysis of EUVE spectra is, however, not without problems. In fact, the spectra, especially those in the short wavelength band 70-180 Å, cannot be properly fitted without making controversial assumptions about the completeness of the available line lists covering the intermediate charge state iron ions. We are addressing this controversy by establishing a definitive spectral catalogue of the intermeditate ionization states of iron in the extreme ultraviolet based on measurements carried out under precisely controlled laboratory conditions using the LLNL Electron Beam Ion Trap facility. The measurements are providing a complete line list, wavelength assignments, line intensities, and branching ratios, including the contributions from weak, unresolved lines to the overall flux level. These measurements support the development of reliable modeling codes for the analysis of data from present and future space astrophysics missions sensitive to extreme ultraviolet radiation.

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Application of Laboratory UV Measurements of CO and C_2H_2 Absorption Coefficients to Hubble Space Telescope Observations of Neptune

Naomi Black, John Caldwell and Xin-Min Hua
York University, Toronto, Canada

C. Y. Robert Wu, D. L. Judge,
University of Southern California, Los Angeles, California

The Faint Object Spectrograph aboard the HST has observed both Uranus and Neptune from 1700 to 3300Å. The data have previously been analyzed by Courtin *et al.* (1996). Their goal was to determine the CO abundance on Neptune, using the Cameron (0,0) band at 2060Å. CO is known to be present there from millimeter wavelength observations, but it is not in chemical equilibrium in that environment. It therefore requires that there be a source of CO to maintain its presence as observed. Courtin *et al.* were motivated by the potential of the UV observations to clarify the vertical distribution of CO in the upper atmosphere. If one could determine the abundance gradient, with vertical resolution made possible by the multi-spectral data set from submicro- to millimeters, it would then be possible to distinguish between an internal and an external source for the CO. There would be significant implications for the origin and internal structure of the entire planet. Here, we re-analyze the data, with a number of differences from the procedures used by them, the most important being:

1) our inclusion of the effects of C_2H_2 (Chen *et al.* (1991), which are significant,

2) our use of *ab initio* calculations and supporting low-temperature laboratory observations of UV absorption coefficients CO (White *et al.* (1993) , and

3) a more rigorous analysis of errors, which shows that the true errors are significantly less than claimed by Courtin *et al.*.

We do, however, retain one important feature that was developed by Courtin *et al.*. Because the albedos of Uranus and Neptune are very similar, and because CO has not been found at millimeter wavelengths on Uranus, they ratioed Neptune to Uranus, instead of to the Sun, to form a UV quasi-albedo spectrum with reduced spectrographic signatures.

We report a UV non-detection of CO on Neptune, with an upper limit of 5×10^{-6} in the pressure range 0.4-200 mbar, as opposed to the marginal detection $2.7 \pm 1.8 \times 10^{-6}$ found by Courtin *et al.*. A major factor in this contradiction is the different abundances of C_2H_2 on Neptune and Uranus, which mask the true abundance of CO on Neptune.

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Application of Laboratory UV Measurements of NH_3 and C_2H_2 Absorption Coefficients to Hubble Space Telescope Observations of Jupiter

John Caldwell, Ilana Dashevsky
York University, Toronto, Canada

C. Y. Robert Wu, D. L. Judge,
University of Southern California, Los Angeles, California

Spectrographs aboard the HST have observed Jupiter at the center of the disk and at the limb. Local air masses at the two equatorial positions are 1.0 and 2.5 respectively. The central spectrum includes GHRS G200M and FOS G190H and G270H data, from 1700 to 3300Å. The limb spectrum includes only FOS G190H data, up to 2300Å. The spectra were obtained during consecutive HST Earth-orbits, such that the G190H data at each location measure the same parcel of Jovian air, that planet having rotated in the interim between HST observations. The respective G190H observations contain essentially all of the information on Jovian NH_3 and C_2H_2 in the current data set.

HST UV imaging shows significant UV limb-brightening at the location of the limb spectrum. It is necessary to invoke a thin, high-altitude, strongly back-scattering haze layer to reconcile the central and limb continuum albedos near 2300Åwavelength. With that constraint satisfied, it is then possible to explain both spectra of Jupiter well with a simple model consisting of 15 km-am of clear H_2, which exhibits both Rayleigh and Raman scattering, and minor amounts of NH_3 and C_2H_2. These minor gases are distributed nonuniformly with altitude, with the C_2H_2 being concentrated toward the top and NH_3 toward the bottom. NH_3 and C_2H_2 absorption coefficients used in this work have been described further by Wu *et al.* (this volume). Additional trace amounts of other molecules, including polyacetylenes, are compatible with, but not compelled by, these data.

While the reality of NH3 absorption on Jupiter is beyond doubt, a comparison of laboratory observations (Wu *et al.*) and HST spectra reveals detailed differences for some individual subband structures. In particular, the (0,0) and (1,0) bands on Jupiter, at 2157 and 2166Å respectively, are much narrower than those in the laboratory data of Wu *et al.*, obtained at 175K. The Jovian bandwidths are more consistent with the data of Ziegler (JCP 82(1985)664) obtained at 25K. The (2,0) and (3,0) NH3 bands are expected to resemble the (0,0) and (1,0) bands, as opposed to the (4,0) and higher bands, because the (0,0) to (3,0) bands are not subject to pre-dissociation but (4,0) and higher bands are. However, the HST data indicate that the (2,0) and (3,0) bands are as wide as the (4,0) and higher bands.

Future modelling will investigate the influence of PH_3 on the continuum albedo of Jupiter near 2000Å. Future laboratory studies of very low temperature NH_3 spectra will require open cell techniques, as described by Wu *et al.*.

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Measurement of Absolute Electron Excitation Cross Sections in Multiply-Charged Ions Using Electron Energy-Loss Methods

Ara Chutjian, Steven J. Smith and Jason D. Greenwood
Atomic and Molecular Collisions Team, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109

Electron-collision excitation rates and cross sections in multiply-charged positive ions are one of the more important quantities required to analyze optical-emission spectra from astrophysical objects. These data are needed to both test theoretical methods (such as close-coupling and distorted-wave methods), and to provide benchmark laboratory data for the infrared to x-ray transitions observed in stellar, pulsar, nebular, etc. emission spectra. Within the appropriate models, the data provide estimates of electron and ion densities and temperatures in these high electron temperature objects. Past, present and future NASA flight missions include HUT, EUVE, ORFEUS, STIS/HST, FUSE, and AXAF.

The experimental program at JPL addresses two important phenomena involving multiply-charged ion collisions in astrophysics: collisional excitation and emission lifetimes (for obtaining f-values). JPL pioneered the use of the electron energy-loss method in collisional excitation of ions. This technique has several major advantages over more conventional optical-emission measurements. First, optically-forbidden transitions (forbidden by spin or g,u/+,- symmetry) as well as optically-allowed transitions are routinely detected. Second, there is no "wavelength barrier" to the measurements: a transition in the infrared, at 1μ, corresponds to an electron energy loss of 1.2 eV; while a transition in the X-ray region, at 10 nm, corresponds to an energy loss of 124 eV. Both extremes are accessible by the energy-loss technique in one experimental apparatus!

We have recently placed on line a new, state-of-the-art electron-cyclotron resonance ion source ("Caprice"). The source operates in the Ku band, and has produced ample currents of, for example, O III-V, Mg III-VIII, and Fe III-XIII, all in low-power ($\leq$ 100 watts microwave power) operation. Higher charge states are obtained at 500- and 1000-watt operation. Two beam lines have been constructed, with allowance for a third. Using the old source and beam line, absolute collision cross sections have been most recently reported for O II [1], C II [2], S II [3]; and cross sections in S III have been measured using the new Caprice source [4]. Near-term measurements are planned for the ions C III, N V, Si III and Fe X.

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Laboratory Formation and Properties of Carbonaceous Particles for Astrophysical and Cometary Comparisons

Regina J. Cody
NASA Goddard Space Flight Center

Spacecraft and ground instruments have observed infrared absorption features in interstellar and circumstellar phenomena for many years. The sources of a number of these features has been attributed to grains of various organic compositions. Thus far, no one molecule or class of compounds has provided a definitive fit to the observational spectra. Interstellar grains were incorporated into the solar nebula and may have survived to now in comets. Particles in the coma of Comet Halley were analyzed by the Giotto spacecraft to be composed of carbon, hydrogen, oxygen, and nitrogen and have been labeled as the "CHON" particles. A recently developed laboratory technique can generate small carbonaceous particles from gas mixtures of varying organic compositions either in the presence or the absence of water. FTIR spectra of these particles can provide comparison with observational spectra.

Small carbonaceous particles are formed in the laboratory by photolysis of a gas mixture of parts per million of small organic molecules in a carrier gas at atmospheric pressure. The photolysis source is an excimer laser at 193 nm. Since the flow area of the gas is larger than that of the laser beam, a mixture of irradiated and unirradiated gases are producing the particles. A visible laser (He-Ne at 633 nm) is used to monitor the particles by scattering. Nitrogen, Argon, or Helium are the carrier gases in slowly flowing gas streams. Initially, the laser beam penetrates 10 - 40 cm of the 150 cm long flow tube where the gas is flowing counter to the laser beam propagation direction; therefore, a particle formation front is established. The particles are collected on ZnS substrates, and their IR spectra from 2.5-14 microns is measured with an FTIR instrument.

The most extensive set of experiments has consisted of photolyzing a gas mixture of several parts per million of small aromatic molecules (benzene, toluene, ethylbenzene, xylenes) and water with each of the carrier gases. Small spectral differences were noted depending upon the carrier gas. Low temperature heating (40°C) of the samples produced some spectral changes. Aromatic gas mixtures without water were photolyzed to be more representative of interstellar and circumstellar conditions. Gas mixtures containing either alkynes or alkenes were photolyzed to determine the effect of the type of carbon bond upon the particle generation process. Aromatic molecules have what is loosely called a "bond and a half" C-C bond. The alkynes, of which acetylene is a member, have a triple bond structure, which is a strong molecular bond. A mixture of C_2 - C_4 alkynes were photolyzed. The alkene or olefin family of organic molecules have a weaker double C=C bond. A mixture of C_2 - C_6 organics were photolyzed. In previous experiments the alkanes which contain a single C-C bond or simple alcohols did not produce particles.

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Laboratory Investigations into the Temperature Dependence of the Collisional Removal of Oxygen in the Herzberg States

R. A. Copeland, E. S. Hwang, C. G. Bressler, and A. Bergman
Aeronomy Program, Molecular Physics Laboratory, SRI International
Menlo Park, California 94025

Emission from the O_2 Herzberg states ($A^3\Sigma_u^+$, $A'^3\Delta_u$, $c^1\Sigma_u^-$) is an important component of the ultraviolet nightglow on earth and Venus. Collisional processes involving these excited electronic states affect the altitude distribution, intensity, and temporal evolution of the nightglow. The oxygen emission comes from an atmospheric layer near 95 km where the temperature varies between 150 and 250 K. Unfortunately, most laboratory collisional energy transfer studies are performed at room temperature.[1,2] At SRI, we are in the midst of a laboratory program to measure collisional removal rate constants for the important atmospheric colliders at the temperature of the emitting O_2 layer.

We use a two-laser state-specific multiphoton ionization method to study these states. The first laser pulse excites O_2 to a specific level in one of the states and the second time-delayed laser pulse ionizes from either the excited level or a neighboring level. Thus far, we have measured the temperature dependence of the collisional removal of O_2 in the $v = 9$ level of the $A^3\Sigma_u^+$ state[3] and in the $v = 9$ and 10 levels of the $c^1\Sigma_u^-$ state. For the $A^3\Sigma_u^+$ state, the removal rate constant with O_2 collider is independent of temperature between room temperature and 200 K and increases by 50% going from 200 K to 150 K.[3] For the colliders N_2 and CO_2 the rate constant is independent of temperature between room temperature and 150 and 225 K, respectively. Unlike the trend for $O_2(A^3\Sigma_u^+, v = 9)$, the rate constants for the $v = 9$ level of the $c^1\Sigma_u^-$ state decrease as temperature decreases by a factor of five and three at 125 K when compared to the values at room temperature for the colliders O_2 and N_2, respectively. Preliminary results for the $v = 10$ level indicate that the removal rate constant with O_2 is five times faster than that for the $v = 9$ level and that about 80% of the removal collisions result in vibrational cascade to the $v = 9$ level of the $c^1\Sigma_u^-$ state. This significant difference in the temperature dependence of the collisional removal between the $A^3\Sigma_u^+$ state and $c^1\Sigma_u^-$ results shows the importance of examining each state for all atmospherically relevant colliders.

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Laboratory Measurements for Supernovae Expansion Opacities

Eastman, R.G., Springer, P.T., Goldstein, W.H., Hammer, J.H., Iglesias, C.A.
Lawrence Livermore National Laboratory
Pinto, P.A.
Steward Observatory, University of Arizona
Deeney, C.
Sandia National Laboratory

Experiments using 0.5 - 2 MJ pulsed power plasma sources are being used to generate high velocity shear, low density plasmas characteristic of gas in the exploded remnants of Type Ia supernovae (SNe Ia), and which can be used to benchmark SNe Ia radiation transport models and opacity calculations.

Supernovae are one of the most violent events in the modern Universe. They play a central role in the origin and evolution of the elements. Their optical brilliance rivals that of a large galaxy, making them visible at great distances. For this reason supernova, and SNe Ia in particular, have become one of the most important cosmological tools available for determining the geometry of space-time. An improved understanding of these standard candles is therefore of considerable importance.

The use of SNe Ia as cosmological distance indicators hinges upon an empirically derived correlation (the so-called Philip's Relation) between the absolute luminosity at maximum light and the distance- and reddening- independent decline rate. This relationship is calibrated from observations of nearby (i.e. recent supernovae),and then applied to more distant ones which exploded when the Universe was younger. However, there is not now any general consensus on what accounts for the Philip's Relation. Nor is there yet a good understanding of how evolutionary effects such as pre-explosion metallicity might affect the light curve. This is because explosion calculations are very sensitive to the opacity. Useful results are dependent on an accurate knowledge of the complex line spectra of the iron peak elements Fe, Co and Ni.

Experiments are currently being planned that will address the physics of radiative transfer in a scaled analog of the supernovae plasma. Understanding the supernovae light curves depends not only upon accurate atomic models, but also on accurate models for radiative transport in the presence of large velocity gradients. Laboratory analogs of this situation are available in the low density, expanding plasmas created in the pulsed power experiments. In these experiments, high velocity gradient plasmas, in the Sobolev regime, will be created and the absorption properties measured as a function of velocity field. Approximations for the atomic physics used in the OPAL opacity code, as well as others, will be applied with various approximations for the radiative transport, and tested directly by comparing with the experiment. Techniques will then be extended to modeling of supernovae light curves.

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Oscillator Strengths for Ultraviolet Lines of Interstellar Atoms and Molecules

S.R. Federman, R.M. Schectman, J. Zsargó, W. Lee, H. S. Polvony, and L.J. Curtis
University of Toledo
J.A. Cardelli
Villanova University
K.L. Menningen and J.B. Stoll
University of Wisconsin - Whitewater

In order to obtain precise oscillator strengths for ultraviolet transitions in atoms and molecules of interest to interstellar studies, several techniques are employed at the University of Toledo. Radiative lifetimes and branching fractions for transitions in S I and Si II were measured using the Toledo Heavy Ion Accelerator [1,2]. The laboratory results for S I [1] were used as the basis for a self-consistent set of f-values for the suite of lines seen in spectra acquired with the Goddard High Resolution Spectrograph on the *Hubble Space Telescope* [3,4]. Our measurements on the Si II multiplet at 1531 Å [2] resolve the discrepancies among earlier f-value determinations. In another set of experiments at the Synchrotron Radiation Center of the University of Wisconsin-Madison, band oscillator strengths for transitions involving the $A\ ^1\Pi$ and $X\ ^1\Sigma^+$ states for CO clarified the situation regarding the appropriate values to use in interstellar work [5].

Our determination of a self-consistent set of f-values for S I lines was based on curves of growth. Accurate laboratory f-values yielded the column density and broadening parameter for S I, and the f-values for other lines were made self consistent by insuring that the results for all lines fell on the curve of growth. This technique was also applied to UV lines in C I [6] and Ni II [7]. For Ni II, because no laboratory data exist for the lines of interest, only relative f-values were obtained. Experiments are now being carried out to rectify this situation. Branching fractions are measured at the University of Toledo and Denison University and lifetimes are obtained at the University of Wisconsin-Madison (see poster of Lawler, Mullman, and Fedchak). In a similar vein, laboratory measurements at the University of Wisconsin were used to provide an absolute calibration of interstellar Co II observations obtained with the *HST* by the University of Toledo [8].

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New Developments In Small-Angle Electron Scattering: Aid To Measurements

Zineb Felfli, Daniel Bessis and Alfred Z. Msezane
Department of Physics and Center for Theoretical Studies of Physical Systems
Clark Atlanta University, Atlanta, Georgia 30314

The understanding of the interactions of electrons with atoms/ions/molecules is fundamental to the development of innovative propulsion technologies of a spacecraft and its environment and communication systems. In particular, in ion propulsion technology, NASA's selected primary propulsion system for the New Millennium, spacecraft contaminations and interactions result from participating neutral and ionized atomic species in their ground and excited states. Small-angle electron differential cross sections (DCSs), which are generally poorly known, are important to spacecraft propulsion technologies and planetary atmospheres. The difficulties of obtaining reliable measurements of the electron DCSs for atomic, ionic and molecular transitions at and near zero scattering angles are well documented [1,2]. Hence, the need for reliable theoretical calculations.

Recently, three theoretical developments have been used to investigate and guide the measurement of small-angle, including zero, electron DCSs in atoms, ions and molecules. The first method, the momentum dispersion method (mdm) [3], based upon Regge pole theory, uses the analytical continuation of the generalized oscillator strength (GOS) function to obtain the smaller angle, including zero, data from the more reliably measured larger angular data. The second method, the forward scattering function (fsf) [4], uses the OOS as the only input. It represents a unique path of the GOS function to the OOS without traversing the non-physical region, which is always present for finite impact energies, E^2 as E varies from near threshold to the Born approximation limit. The fsf is, therefore useful for normalizing the measured relative electron DCSs through the GOSs [5]. In an appropriate representation, consistent with the mdm, the GOS for both dipole allowed and forbidden transitions varies linearly with K^2 for small scattering angles. This linear variation is more dramatic for values of E close to threshold, where it can involve scattering angles as large as 40 or more. We have exploited this linear variation in our international collaborations to investigate the electron DCSs at small scattering angles for transitions in $He, Cd, Xe, Hg, N_2, SF_6, N_20$, etc., including the normalization of the measured relative DCSs, and found that many measurements experience difficulties obtaining reliable data at and near zero scattering angles.

Very recently [6], we have found singular behavior in the electron-atom scattering at small momentum transfer K coming from second-order terms. This result, combined with a Regge pole representation, yields a new generalized two-term Lassettre expansion to evaluate OOSs from GOSs at $K^2 = 0$; the results for $H1s - 2p$ are outstanding even at low impact energies. Representative results will be presented.

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Photoluminescence Measurements of the EURECA organic residue : Does it match the ERE?

Brian C. Friedmann Adolf N. Witt
University of Toledo

J. Mayo Greenberg
University of Leiden

Organic residues are thought to be a candidate for grain mantle materials and they have been shown to produce a close match to the observed interstellar 3.4μm absorption feature. The dust grains that produce the 3.4μm absorption feature are also thought to produce the Extended Red Emission (ERE). ERE is a broad emission band with a peak wavelength between 610 nm and 850 nm depending on the astrophysical environment, such as reflection nebulae, planetary nebulae, and the interstellar medium (ISM). If there is a connection between the 3.4μm absorption feature and ERE, then this organic residue should also photoluminesce with a peak wavelength in the range 610 nm $\leq \lambda \leq$ 850 nm.

Photoluminescence (PL) measurements have been obtained for a laboratory organic residue that has been exposed to long-term solar ultraviolet radiation aboard the EURECA satellite. Excited by a 488 nm Ar laser, the photoluminescence of the organic residue peaked around 560 nm at room temperature. Upon annealing the sample at successively higher temperatures, from 100° C to 350° C, we did not find a measureable shift in the peak wavelength, but we did observe a marked decrease in the relative PL efficiency of the sample. The relative intensity of the PL peak after annealing at 350° C for 30 min was down by a factor of 1500 from the peak intensity prior to annealing. This organic residue, therefore, cannot be the source of the ERE based on its PL peak wavelength, the stability of the peak as a function of temperature, and the decrease in the relative PL efficiency.

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IR Spectroscopy of Solids Containing Si-H Bonds: Source of the Interstellar 4.62 micron Absorption Feature?

D.G. Furton, Todd Scungio
Rhode Island College

A.N. Witt
University of Toledo

Recent mid-IR observations of a number of embedded protostars by Pendleton et al. (1998) clearly reveal the general presence in dense molecular clouds of a broad absorption feature at 2165 cm^{-1} (4.62 μm). While this feature is often referred to as the "XCN band", its source has not yet been conclusively identified. Two broad catagories of astrophysically relevent materials—nitrogen-bearing species such as nitriles, and compounds containing Si-H bonds—are known to absorb in the 2200–2100 cm^{-1} spectral region on the basis of laboratory spectroscopy of individual molecules (both free and isolated in polar and nonpolar ices), and of energetically processed ice mixtures. In this work, thin films of *a*-Si:H and *a*-Si(x)C(1-x):H were produced by plasma enhanced chemical vapor deposition from silane, silane/methane mixtures and from tetramethylsilane, oxidized by exposure to the atmosphere and UV radiation, and characterized by IR absorbance spectroscopy. It is shown, consistent with other published reports (i.e., Moore, Tanabe & Nuth 1991, Strazzulla et al. 1998), that the Si-H stretching frequency is variable in the range $2200-2100$ cm^{-1}, depending on the electronegativity of the other heavy atoms bonded to Si in the solid. The Si-H band in freshly deposited *a*-Si:H and *a*-Si(x)C(1-x):H is observed at 2100 cm^{-1}, and found to shift through 2165 cm^{-1} to 2200 cm^{-1} and broaden as the materials oxidize. *a*-Si(x)C(1-x):H appears to oxidize more rapidly and thoroughly than pure *a*-Si:H, producing an absorption feature at 2165 cm^{-1}, but this feature is much broader than that observed in dense molecular clouds.

While these experiments do not completely rule out the possibility that the 2165 cm^{-1} interstellar absorption feature observed in dense molecular clouds is due to oxidized *a*-Si(x)C(1-x):H, they do highlight a problem with this and other identifications: the feature appears to be remarkably constant in frequency in astrophysical environments and remarkably variable in the lab.

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ISO–SWS Observations of Interstellar CO_2 Ice

P. A. Gerakines & D. C. B. Whittet
Department of Physics, Applied Physics, & Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180

A. C. A. Boogert & A. G. G. M. Tielens
Kapteyn Astronomical Institute, P.O. Box 800, 9700 AV Groningen, the Netherlands

P. Ehrenfreund
Leiden Observatory, P.O. Box 9513, 2300 RA Leiden, the Netherlands

Infrared absorption features near 4.3 & 15.2 μm associated with the fundamental vibrational modes of the carbon dioxide molecule (CO_2) have been observed toward 13 sources (which include 3 toward the Galactic Center and 10 embedded protostars) using the Short-Wavelength Spectrometer (SWS) aboard the Infrared Space Observatory (ISO). CO_2 has long been predicted to exist in the interstellar medium in the results of computational models and laboratory experiments involving solid H_2O and CO, but is unobservable from the ground (or even high-altitude observatories) due to the strength of its atmospheric absorptions. The column densities derived from the observed spectra indicate that CO_2 makes up 10 - 20 % of the H_2O abundance and from 0.8 - 5 times the CO abundance in each of these lines of sight. The shapes and positions of the bending mode at 15.2 μm and the stretching mode of $^{13}CO_2$ at 4.38 μm are quite sensitive to the ice environment, and their profiles are compared to laboratory data in order to determine the nature of the CO_2 ice and the molecules with which it resides.

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Accurate Measurements of Atomic Branching Fractions Using Fourier Transform Spectrometry and Progress on the NIST VUV– Fourier Transform Spectrometer

Ulf Griesmann, Gillian Nave, Krzysztof Dzierzega and Wolfgang L. Wiese
National Institute of Standards and Technology, Gaithersburg, MD 20899, U.S.A

Radiative transition probabilities in atoms are important quantities for a very wide range of applications of plasma physics, from astrophysics to semiconductor processing. Until very recently the uncertainty for the resulting transition probabilities was often limited by the uncertainty of the lifetime data [1]. Advances in beam–gas–laser spectroscopy (BGLS) have achieved sub–percent accuracy for lifetimes of levels in neutral alkali– and noble gas atoms [2]. Based on these new lifetime measurements, transition probabilities with relative accuracies better than 5% can now be determined once branching fractions for all transitions from an upper level have been measured.

Fourier transform (FT) spectrometry provides a reliable and very efficient method for the measurement of branching fractions with good accuracy. This is illustrated by the results of our recent measurements of branching fractions for transitions from 5p levels in neutral Kr with the NIST high–resolution IR–vis–UV Fourier transform spectrometer [3]. A high–current hollow cathode lamp was used to excite the 5p levels in Kr. To overcome the problem of self–absorption, Ar or Ne was used as a carrier gas for the hollow cathode discharge with an admixture of only a few % of Kr gas. A tungsten strip standard lamp served to determine the spectral response of spectrometer and detectors. Results for the transition probabilities of 5p–5s transitions in Kr I, and an analysis of their uncertainties will be presented.

NIST has recently acquired a UV–Fourier transform spectrometer manufactured by Chelsea Instruments Lt. (London) [4]. The FT spectrometer is currently being refurbished. A new CaF_2 beam splitter will be installed to extend the wavelength range of the instrument into the VUV down to ≈140 nm. The new spectrometer will enable us to efficiently carry out very accurate wavelength– and intensity measurements in VUV spectra. We will report on the status of the VUV Fourier transform spectrometer.

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The Capture of Electrons by Molecular Ions in Planetary Ionospheres and the Interstellar Medium

Steven L. Guberman
Institute for Scientific Research

Dissociative recombination (DR) reactions often have high rate constants allowing them to play important roles in the interstellar medium, comet atmospheres and planetary ionospheres. In these reactions, a diatomic or polyatomic ion, e.g. AB^+, captures an electron, e^-, and breaks up into neutral fragments,

$$AB^+ + e^- \rightarrow A + B \tag{1}$$

where A or B can be in the ground or an excited state. If AB^+ is a polyatomic molecule, the products can be atoms and/or molecules. The identity of the products can be sensitive to the electronic and vibrational state of the ion undergoing DR.

We describe an ab initio theoretical approach for the calculation of DR cross sections and rate coefficients. Potential curves for both molecular ions and neutral dissociative states have been determined using large scale configuration interaction wave functions. Cross sections and rate coefficients have been calculated using Multichannel Quantum Defect Theory.

In recent work [Guberman, 1997], we have identified the mechanism by which DR of O_2^+ generates the $O(^1S)$ excited state. Electron capture takes place mostly into a state which does not dissociate to $O(^1S)$ but which has a high capture probability. Vibrationally excited mixed symmetry neutral Rydberg states couple the capture state to another state which dissociates to $O(^1S)$. The calculated DR rate constant for generating $O(^1S)$ from the lowest vibrational level is $3.9x10^{-9} cm^3/sec$ at an electron temperature of 300K. Recent results for the DR of HeH^+, CO^+ and H_3^+ will also be reported.

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Cosmic Dust Exploration using Broadband Microwave Analogues

B. Å. S. Gustafson, L. Kolokolova, J. Loesel, J. Thomas-Osip, T. Waldemarsson, Y.-l. Xu
Department of Astronomy, University of Florida, Gainesville

Cosmic grains are often expected to be irregularly shaped complex structures of inhomogeneous composition that are hard or nearly impossible to reliably model using common numerical techniques. As a consequence, the interpretation of observational data is similarly difficult. We use microwave analog experiments to study almost any combination of particle composition, size and shape. Notable advantages with the microwave method are: I) the controlled environment where all particle properties are precisely known and can be systematically varied and II) the ability to model exotic volatile materials using their stable microwave analogues.

There are two directions to our approach I) theory development and validity testing [1,2] and II) a systematic exploration of scattering by complex particles using our microwave analogue laboratory. While the diversity of particles of interest to astronomy and astrophysics is more diverse, it is convenient to identify two broad classes: I) relatively primitive particles such as circumstellar, interstellar, and cometary dust, respectively II) fragments of evolved and possibly differentiated bodies such as asteroids, planetary satellites, and ejectae from planetary surfaces. Sample results from both categories of particles will be discussed.

The "primitive" targets include low packing factor aggregates of a few hundred to approximately 6,000 cylindrical or spherical particles ranging from 0.07 wavelengths to 0.4 wavelengths in radius. Their refractive index, ranging from 1.6-0.003i to 1.74-0.005i, is selected to represent silicates and organic refractory materials. These structures have scattering properties reminiscent of zodiacal dust and some cometary dust [3] as well as aerosols in the atmosphere of Saturn's satellite Titan.

Dust from evolved bodies may be irregular compact aggregates or angular fragments produced in collisions. We have obtained results for silicate cubes ranging from 3.25 to 14 wavelengths to the side and from ~ 14 to ~ 20 wavelengths to the side tetrahedrae. We also have results for irregularly shaped particles of homogeneous materials and mixtures.

While the scattering by these structures are very different from that by a Mie-sphere, they have several similarities to the scattering by the "primitive" class of particles. We point out differences between the optical properties of the various models as well as similarities.

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Thermal Evolution of Amorphous Magnesium Silicate Smokes: Comparison to Circumstellar and Cometary Spectra

Susan L. Hallenbeck and Joseph A. Nuth III
NASA Goddard Space Flight Center, Astrochemistry Branch, Code 691, Greenbelt, MD 20771 USA

Highly amorphous silicate grains which form in the outflows of mass losing stars or in the ISM must undergo some degree of thermal processing to form more ordered materials. Amorphous magnesium silicate smokes were prepared in the laboratory by vapor phase condensation and annealed in vacuum. The samples were monitored by IR spectroscopy as a function of annealing time and temperature (1000 - 1200 K), focusing on the development of the 10 micron silicate feature. The IR spectrum of the initial condensate displayed a broad band at 9.3 microns. As annealing proceeded, the maximum shifted to longer wavelengths and was eventually observed at 9.7 microns, the value typically reported for silicates in the interstellar medium and in circumstellar outflows of oxygen-rich stars.

Further thermal evolution of the amorphous magnesium silicate smokes led to the appearance of a dual maximum at 9.8 and 11 microns, indicative of "crystalline" olivine. The dual maxima 10 micron feature is a natural consequence of the thermal evolution of the amorphous condensate, rather than a mixture of amorphous and "crystalline" materials. There appears to be a natural pause in the spectral evolution of these samples, midway between the initially chaotic condensate and the more ordered glass. Thereafter, individual features sharpened as the sample became more ordered. The "olivine-rich" comets Halley, Bradfield, Levy, Mueller, and Hale-Bopp all display emission features with dual maxima at 9.8 and 11.2 microns which closely resemble the magnesium silicate smoke stall spectra.

Since grain temperatures range from 500 - 1000 K in typical stellar outflows, any magnesium silicate grain sufficiently annealed to exhibit the stall spectrum should remain at this stage of evolution for the remainder of its lifetime. The stall spectrum is therefore a practical endpoint in the spectral evolution of magnesium silicate condensates in natural systems. Currently, we are investigating how the appearance and duration of the dual maxima stall is effected by the magnesium concentration of the anhydrous silicate smokes.

The C_2N_2 C^1B_u - $X^1\Sigma_g^+$ Transition: Assignment of the Excited Electronic State, Its Origin and Vibrational Frequencies

Joshua B. Halpern and Yuhui Huang
Department of Chemistry, Howard University, Washington, DC 20059

C_2N_2 has been detected in Titan's atmosphere and may also be present in comets. A new analysis is presented for the VUV C_2N_2 C^1B_u - $X^1\Sigma_g^+$ transition. Contrary to previous studies this is shown to be a linear to bent transition with a trans-bent C^1B_u excited electronic state. The electronic origin is at 59,848 cm^1, about 550 cm^1 lower than previously thought [1]. Vibrational bands between 170 and 145 nm are assigned. The C^1B_u symmetric CN stretching frequency, ν_1, is as previously noted 2050 $\pm$ 20 cm^1 [1]. It has been possible to assign four of the five other vibrational frequencies. The symmetric CC stretching frequency, ν_2, is 926 $\pm$ 20 cm^1. The trans-bending vibrational frequency, ν_3, is 532 $\pm$ 10 cm^1, the torsional bending frequency, ν_4, is 110 $\pm$ 10 cm-1^1 and the cis bending frequency, ν_6, is 140 $\pm$ 10 cm^1. Anharmonicities have also been determined for the various vibrational modes.

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Nanotechnology Fabrication of Polysilicon Film/Metal Grid Infrared Filters

Brian Hicks, Milt Rebbert, Pete Isaacson, Christie Marrian, Jackie Fischer
Naval Research Laboratory

Howard Smith
Smithsonian Astrophysical Observatory

Peter Ade, Rashme Sudiwala
Queen Mary and Westfield College

Matt Greenhouse, Harvey Moseley, and Ken Stewart
NASA Goddard Space Flight Center

We have studied the possibility of making high transmission, precisely controlled FIR filters from stacks of precisely formed metal grids separated by thin polysilicon films. The grids are photolithographically deposited using techniques[1] we have patented for metal mesh Fabry-Perot etalons. The polysilicon films are evaporatively deposited using new silicon technology. With the current fabrication techniques we could make filters usable from about 20 microns and longward.

It is observed that commercial crystalline silicon has small absorptions in the FIR which, when "amplified" by the presence on its surface of a resonant metal grid, limit the transmission of any filter of which it is a part. We have prepared a set of samples using our preferred polysilicon films, and present their transmission properties. We discuss the potential and/or limitations of polysilicon devices.

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10 μm Ethylene: Spectroscopy, Intensities and a Planetary Modeler's Atlas

J. J. Hillman, D. C. Reuter, J. M. Sirota
NASA/Goddard Space Flight Center

W. E. Blass, S. J. Daunt, L. R. Senesac, A. C. Ewing, L. W. Jennings, M. C. Weber, J. S. Hager, S. L. Mahan
University of Tennessee, Knoxville

A. Fayt
U. Louvain, Louvain-la-Neuve, Belgium

FTS and TDL spectra of ethylene in the 10 μm region have been observed, measured, calibrated, assigned and intensities measured working toward the goal of a planetary modeler's atlas. A spectrum taken in double pass configuration at the 1-m McMath FTS instrument at Kitt Peak National Observatory has been measured and calibrated against CO_2 laser bands with a calibration standard deviation of 0.0002 cm^{-1}. Using the results of a previous analysis (Cauuet et al., 1990) we have assigned the FTS spectrum and have measured over 500 intensites of ethylene lines in the 900-1000 cm^{-1} region. Using measurements of 15 isolated transitions in this region made independently at the University of Tennessee and Goddard Space Flight Center using TDL spectrometers, the FTS intensities have been calibrated and transformed to 296 K. A benefit of this calibration approach is the improvement of the accuracy of intensity determination as well as compensation for the pressure and temperature determinations of an FTS spectrum taken for line position determination. Using a calculated spectrum, including mixing coefficients for ν_4, ν_7, ν_{10}, and ν_{12} interactions and calculated relative intensities (A. Fayt, 1996), we have used the calibrated FTS intensities as the independent variable in a non-linear regression to determine the vibrational band intensities of ν_7, ν_{10}, and ν_{12} (ν_4 is not determined by the data). These vibrational band intensities (scaled dipole moment derivatives) make it possible for us to generate an ethylene atlas at temperatures of our choice, which will be useful to the planetary atmosphere modeling community.

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ELECTROSTATIC CHARGING OF LUNAR DUST

Mihály Horányi
LASP, U.of Colorado, Boulder, CO 80309-0392

Bob Walch
Physics Department, U.of Northern Colorado, Greely, CO 80639

Scott Robertson
Physics Department, U.of Colorado, Boulder, CO 80309-0391

The chemical and mineralogical composition of lunar dust is well matched by two widely used lunar simulants: MLS-1 (Minnesota Lunar Simulant)[1] and JSC-1 (Johnson Space Center)[2]. However, their electrostatic charging properties were not compared to that of the lunar soil[3]. We have constructed an experiment, where individual dust grains can be exposed to a thermal plasma background and a flux of fast electrons. We have conducted experiments using glass, copper, graphite and silicon particles[4] and also grains from MLS-1 and JSC-1 lunar substitute materials[5]. We report our new set of measurements comparing Apollo-17, MLS-1 and JSC-1 samples. The secondary electron production from these materials, in the energy range of $20 \leq E \leq 90$ eV of the bombarding electrons, are similar. The measured secondary electron yield for the Apollo-17 sample was intermediate between MLS-1 and JSC-1 simulants, closer to that of MLS-1. On the day side of the Moon, photoelectron production becomes dominant. We are now modifying our plasma chamber to accommodate a solar UV simulant light source to examine charging due to photoelectron production.

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The Unidentified Infrared Emission Bands: Identified

Douglas M. Hudgins, Louis J. Allamandola, and Scott A. Sandford
NASA Ames Research Center, Moffett Field, CA

The so-called Unidentified Infrared or simply UIR bands, the infrared emission band spectrum associated with a wide variety of interstellar objects, can be modeled *in detail* by laboratory spectra of neutral and positively charged polycyclic aromatic hydrocarbon (PAH) mixtures. Fits are presented for the UIR emission from the protoplanetary nebula IRAS 22272+5435, the diffuse galactic medium, and the Orion HII/photodissociation front - a selection of objects which span the evolutionary range of interstellar material. These data directly address the spectroscopic criticisms previously leveled at the PAH hypothesis and demonstrate that PAH-related molecular species are indeed responsible for this widespread emission. Furthermore, these fits reflect the structure, abundance, and ionization state of the interstellar PAHs and, in turn, provide direct insight into the processes of carbon nucleation, growth and evolution in circumstellar shells and the interstellar medium. To date, no other candidate material which has been proposed to account for the UIR emission can as readily and specifically reproduce these spectral variations. Given the ubiquity of these species, this work demonstrates the tremendous potential of these species as probes of a new and heretofore largely unexplored facet of astrochemistry - potential which should make PAHs the probe of the next millennium much as CO has been for the last quarter century.

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$O_2(^5\Pi_g)$ and Atmospheric Oxygen Atom Recombination

D. L. Huestis, C. G. Bressler, and R. A. Copeland
Molecular Physics Laboratory, SRI International, Menlo Park, CA 94025

Understanding oxygen atom three body recombination is crucial for modeling and interpreting the spectral distributions and intensities of the oxygen nightglows of the Earth and the planets [1]. Recent laboratory studies at SRI [2] have provided an unexpected new means of improving this understanding.

Collisions of oxygen or nitrogen molecules with laser-excitated high vibrational levels of $O_2(A^3\Sigma_u^+)$ produce a longer lived excited state, whose resonant multiphoton ionization (REMPI) spectrum cannot be assigned to any known singlet or triplet system. We attribute the lower state of this new transition to the often-invoked but previously unobserved $^5\Pi_g$ state of O_2. Although quite weakly bound, at large internuclear distances this state is predicted [3,4] to be the lowest of the states dissociating to ground state atoms, and because of its high degeneracy could be a key intermediate state in O + O recombination, contributing more than 70% according to early estimates [5].

Recent calculations [4] of the potential energy curves gave a shallow well depth (0.16 eV) which Bates [6] concluded made $O_2(^5\Pi_g)$ a relatively insignificant participant, under the assumption that the rate of collisional relaxation is orders of magnitude slower than the rate of collision-induced dissociation. The recent SRI measurements [2] show that the rates of collisional removal (presumably by electronic relaxation to the more strongly bound states) for both oxygen and nitrogen are actually about a factor of 6 *faster* than the dissociation rate estimated by Bates [6]. Thus the first experimental information on $O_2(^5\Pi_g)$ reestablishes its significance in oxygen atom recombination.

The new observations motivate efforts to develop a more detailed and quantitative theoretical model of O + O + M collisions. In addition to the experimental results, we will also present preliminary work on spin-orbit resolved long-range potential curves for O_2 and implications for atmospheric recombination and the role of $O_2(^5\Pi_g)$ in predicting nightglow emissions.

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High Resolution UV Emission Spectroscopy of CO and N_2 Excited by Electron Impact

G. James, J. Ajello, I. Kanik, C. Noren, L. Beegle, D. Dziczek, C. Jonin
Jet Propulsion Laboratory

D. Shemansky, X. Liu
University of Southern California

Photodissociation via discrete line absorption into predissociating Rydberg states is the dominant destruction mechanism of CO and other molecules in the interstellar medium and molecular clouds. Accurate values for the oscillator strengths and predissociation yields of these transitions are required for input into the photochemical models which attempt to reproduce observed abundances.

We present our latest experimental results of the electron collisional properties of CO and N_2 obtained using the 3 meter high resolution spectroscopic facility at JPL.

Medium resolution (0.031 nm FWHM) measurements of the CO (A-X) 4th Positive band system produced by electron impact excitation at 20 eV and 100 eV have been obtained in the 130 to 205 nm region (*Beegle et al.*, 1998). These spectral data were used in combination with those of *DeLeon et al.* (1988) to determine the dependence of the electric dipole transition moment (R_e) on the r-centroid. High resolution measurements (0.0034 nm FWHM) of the CO (A-X) (5,1) and (3,0) bands show excellent agreement between the observed spectra and a synthetic model developed at JPL. In addition, the excitation function of the CO (A-X) (0,1) band at 159.7 nm has been measured from threshold to 500 eV and compared to previous measurements.

A high resolution (0.0036 nm FWHM), optically thin emission study of the N_2 ($c_4' - X$)(4,3) and (3,2) Rydberg bands excited by electron impact at 100 eV has been completed in the extreme ultraviolet (*Ajello et al.*, 1998). A model of the perturbed rotational line intensity distribution of the bands shows the effects of electronic state mixing between the c' Rydberg state and the b' valence state. By normalizing the model to the predissociation yield for $J' = 9$ measured by *Walter et al.* (1994) the laboratory spectrum has been used to determine the c' predissociation yields for each rotational level of $v' = 3$ and 4.

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Laboratory X-ray Spectroscopy Experiments in Support of NASA's X-ray Satellite Missions

S. M. Kahn[1], P. Beiersdorfer[2], G. V. Brown[2], M. F. Gu[1], D. L. Liedahl[2]
D. W. Savin[1], S. B. Utter[2], K. Widmann[2]
[1]*Columbia University*
[2]*Lawrence Livermore National Laboratory*

The power of moderate-to-high resolution x-ray spectroscopy to probe physical processes and conditions occurring in cosmic high temperature plasmas has become widely recognized by the astrophysical community following the launch of the *ASCA* Observatory. Moreover, it was realized that simple spectral models, which had been invoked in the past to analyze low-resolution, low-statistics data, do no longer fit the data. The new observations require more sophisticated astrophysical models that include a correct treatment of the atomic processes underlying the X-ray spectra. Not only simple atomic parameters such as oscillator and collision strenghts must be known correctly but the balance of all excitation and deexcitation processes that feed and deplete relevant quantum levels. The problems encountered in modelling of *ASCA* data will increase considerably when we begin to analyze the spectra acquired by the next series of X-ray observatories: *AXAF, XMM*, and *ASTRO E*.

In order to gain a quantitative understanding of which processes are important, we have established a state-of-the-art laboratory spectroscopy research program devoted to the measurement of key atomic processes central to the interpretation of high resolution X-ray spectroscopic observations of cosmic sources. Using an integrated set of spectroscopic equipment at the LLNL Electron Beam Ion Trap facility we have studied a broad range of processes peculiar to equilibrium and non-equilibrium plasmas, including electron-impact excitation, dielectronic recombination, resonance excitation, and innershell ionization. Measurements were carried out, for example, for the diagnostically relevant K-shell ions Ne VIII through Fe XXIV. Presently, we are focussing on definitve measurements of line emissivities for iron L-shell ions in optically thin, thermal plasmas in equilibrium to address systematic discrepancies between *ASCA* spectra and spectral synthesis codes in the vicinity of the iron L-shell complexes and to aid the development of spectral modeling codes for the upcoming high-resolution x-ray missions.

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Analysis of Ammonia Line Parameters in the 3-μm Region

I. Kleiner
Laboratoire de Photophysique Moleculaire, Universite Paris Sud, Unite propre du C.N.R.S., Batiment 213, 91405 Orsay Cedex, France.

L. R. Brown
Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA, 91109 USA.

G. Tarrago, Q. L. Kou, N. Picque,
Laboratoire de Physique Moleculaire et Applications, Universite Paris Sud, Batiment 350, 91405 Orsay Cedex, France.

V. Dana and J. Y. Mandin
Laboratoire de Physique Moleculaire et Applications, Universite Paris VI, Tour 13, boite 76, 4 Place Jussieu, 75252 Paris, Cedex 05, France.

Improved spectroscopic line parameters of ammonia in the 3-μm region are now available. These have been obtained from extensive new measurements using two Fourier transform spectrometers. For line positions, spectra were recorded in France at 0.0054 cm^{-1} resolution, and for line intensities, 16 spectra from the Kitt Peak FTS in Arizona were used. Some 1800 transition positions and nearly 1000 line strengths (of the ν_1 and ν_3 fundamentals at 3323.7 and 3443.8 cm^{-1} and the $2\nu_4$ overtone at 3229.8 cm^{-1}) were modelled using an effective rotation-inversion Hamiltonian to obtain a new ammonia linelist in HITRAN format between 3000 and 3700 cm^{-1}.

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Evidence for Comet Dust Evolution based on Microwave Analogue Experiments and Polarimetric Observations

L. Kolokolova, B. Å. S. Gustafson, J. Loesel, and J. Thomas-Osip
Department of Astronomy, University of Florida, Gainesville

Cometary dust particles, most likely, can be represented as aggregates of grains with dimensions close to the wavelength of visible light or smaller. At the same time, the dimensions of each aggregate may span a broad range of size and sometimes be large compared to the wavelength. These circumstances make a theoretical study of light scattering by cometary dust and many other cosmic grains exceedingly difficult and, at least in part, beyond the capability of common numerical techniques. As a consequence, the interpretation of observational data is similarly difficult.

A basis for such an interpretation can be the laboratory simulation of light scattering by dust particles. Microwave analog experiments, which allow us to study particles of almost any combination of composition, size and shape, may be the most suitable. We have taken advantage of this ability and the broadband nature of the University of Florida microwave facility to obtain the intensity, polarization, color and polarimetric color for a range of particle types [1].

We selected aggregates made of acrylic and nylon for comparison to polarimetric CCD images for comets Hyakutake and Hale-Bopp [2,3]. These materials are, with their refractive indices near 1.605-0.003i and 1.74-0.005i, microwave analogues to silicates and organic materials expected in comet dust. Thus, the aggregates are among the most complicated for theoretical study, namely aggregates larger than the wavelength (circumference to wavelength ratio $X = 30$ to 100) with the constituent particles comparable to the wavelength $X \sim 1$. For each aggregate, we obtained the dependencies of intensity and polarization on the wavelength and on the scattering angle in the [0,165] degree range.

Based on these microwave data and on the polarimetric imaging by Jockers *et al.*, we present evidence for a change in scattering regime as particles transit the inner coma.

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Electron Capture by Silicon Ions from Helium at eV Energies

Victor H. S. Kwong and Z. Fang
Department of Physics, University of Nevada, Las Vegas

Silicon is commonly found in a variety of astrophysical plasmas. Several charge-transfer recombination reactions by multiply charged silicon ions have been suggested and their effects on the ionization equilibrium of the plasmas have been discussed. We measured the charge transfer rate coefficients of Si^{3+} and Si^{4+} with helium at electronvolt energies by using the technique of laser-induced-plasma ion source and ion storage. The Si^{3+} and Si^{4+} ions are produced by laser ablation of solid silicon or tungsten disilicide targets and stored in an rf ion trap. The decay rates of the stored silicon ions are measured while the vacuum chamber of the ion trap is filled with helium gas with known pressures. The charge transfer rate coefficients are obtained from the decay rates and the helium densities. The equivalent reaction temperatures are estimated to be 3.9×10^3 K for $Si^{3+} + He \rightarrow$ products and 4.6×10^3 K for $Si^{4+} + He \rightarrow$ products. The comparison of the measured values with the calculated ones are given. A summary of our previous electron capture measurements (O^{2+}+ He, H_2, N_2 and CO; N^{2+}+ He, H_2, N_2 and CO; Fe^{2+}+ H_2) will also be given.

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ISM abundances from accurate *f*-values for the VUV resonance lines of FeII, CoII, and NiII

J. E. Lawler, K. L. Mullman and J. A. Fedchak
Department of Physics, University of Wisconsin, 1150 University Ave., Madison, WI 53706

A High Sensitivity Absorption Experiment which measures absolute UV and VUV oscillator strengths has been developed at the University of Wisconsin-Madison. This experiment uses a hollow cathode discharge as an absorbing sample, the Aladdin storage ring at the Synchrotron Radiation Center as a continuum source, and a 3m focal length vacuum echelle spectrometer equipped with a CCD detector array. The experiment achieves spectral resolving powers of 350,000 and sensitivities to fractional absorptions much smaller than 1% at deep UV and VUV wavelengths. Column densities of sputtered metal atoms and ions as small as 3.0×10^8 cm^{-2} can be detected. The absorption experiment measures relative oscillator strengths for lines from a common lower level, usually a VUV transition relative to a well known UV transition. An accurate absolute scale for all of these measurements is established using radiative lifetimes from laser induced fluorescence measurements on atomic/ionic beams. This experiment is applicable to essentially every element in the periodic table, both neutral atoms and atomic ions. The experiment is used to measure oscillator strengths for the most important UV and VUV resonance lines of Fe^+, Co^+, and Ni^+ [1-3]. These resonance lines are prominent in absorption spectra on the Interstellar Medium (ISM) recorded using the Hubble Space Telescope. The Fe measurements include a number lines with widely varying *f*-values. Cardelli and Savage [4] used these *f*-values to establish accurate absolute column densities along a variety of sight lines through the ISM. They were then able to perform "self-consistent analysis of ISM FeII over a large dynamic range (e.g. between different sight lines sampling a large range of column densities and in single sight lines with multiple and widely varying component structure)." Recent work with Zsargo and Federman [3] established that gas phase cobalt is significantly less depleted onto dust grains in the ISM than determined previously. The depletion of nickel may be one of the best probes for grain evolution in galaxies [5]. Our work in progress will establish an accurate absolute scale for the relative NiII *f*-values reported by Zargo and Federman from ISM observations [5].

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A Synergistic Approach to Modeling Astrophysical X-Ray Spectra

D.A. Liedahl, P. Beiersdorfer, G.V. Brown, and S. Utter
Lawrence Livermore National Laboratory

S.M. Kahn, M.F. Gu, and D.W. Savin
Coulmbia Astrophysics Laboratory

Plasma emission models used in X-ray astronomy need to simulate X-ray spectra from at least 15 elements. Development of comprehensive models involve large-scale calculations; for example, Fe M-shell spectra, K-shell fluorescence from near-neutral ions, and dielectronic recombination satellite spectra from L-shell ions. Current and recent missions (*EUVE*, *ASCA*, *DXS*, etc.) have already demonstrated the need for major, rapid improvements in spectral models. The deployment in the near future of three major X-ray observatories – *AXAF*, *XMM*, and *Astro-E* – with instruments of high spectral resolving power, promises to push X-ray spectral models to their limits.

Atomic modeling problems derive from limitations in our abilities to achieve adequate levels of accuracy and completeness simultaneously. Problems related to completeness have gained attention as the result of confrontations with astrophysical data. Problems related to accuracy (wavelengths, line ratios, etc.), those that compromise our ability to extract precise physical information from high-resolution data, are best studied in the laboratory. The controllable, well-characterized conditions available in EBIT experiments at LLNL allow us to isolate specific line-formation processes in ions chosen for their astrophysical interest. The overlap of astrophysical data, laboratory data, and the results of atomic modeling works to maximize the utility of plasma emission models in interpreting high-resolution spectra from more complex (uncontrolled) environments encountered in high-energy astrophysics. Some specific examples of this interplay are presented.

Photoionization Cross Sections of Atoms and Ions Related to Astrophysical Problems

Steven T. Manson
Department of Physics and Astronomy, Georgia State University

A project of calculation for the photoionization cross sections of atoms and ions of astrophysical interest has been initiated. The project envisions three principle goals: To provide cross sections as input for modelling of various astrophysical problems; To develop methodologies to calculate such photoionization cross sections which provide results of known accuracy; To offer a check on the accuracy of the extensive (but unassessed) Opacity Project data base[1]. The most difficult systems to deal with are those with a high degree of correlation (many- body interactions) among the target electrons. To test methodologies on such systems, we concentrate, to begin with, upon transition metal atoms and ions, where the open 3d shell opens a Pandora's Box of many-body correlations, and negative ion photoabsorption, where many-body interactions are required even for binding the ground state. Among the theoretical methodologies which are being brought to bear on these problems, often with in tandem and with modifications to enhance accuracy, are many-body perturbation theory (MBPT), multiconfiguration Hartree-Fock (MCHF), relativistic random phase approximation (RRPA), R-matrix with pseudostates (RMP), eigenchannel R-matrix (ERM), multichannel quantum defect theory (MQDT), and Fano continuum configration interaction (FCCI), among others.

Prelimimary results of this research program have been most encouraging. We have studied photoionization of the ground states of Sc and Sc^{++} among the transition metal atoms and ions [2,3] using a modified MBPT in conjunction with MCHF and a coupled channel matrix diagonalization technique. Investigation of the excited metastable 1s2s2p ^4P state of He^- employing MCHF in a FCCI formalism has also taken place [4,5]. The Ne isoelectronic sequence has also been scrutinized using a combination of RRPA and MQDT, along with some new enhancements we have introduced [6]. A selection of these and other results will be presented for a number of cases to give a flavor of the success of this program to date.

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Laboratory Observations of Wave-Induced Radial Transport within an "Artifcial Radiation Belt"

Michael E. Mauel
Columbia University

Energetic electrons trapped within a strong dipole magnetic field have been produced by applying microwave electron cyclotron resonance heating to a low-pressure hydrogen discharge. The microwaves are absorbed at the fundemental cyclotron resonance, and the energetic electrons (1 keV $< E_h <$ 50 keV) are localized to a small region where the cyclotron absorption layer intersects the dipole's equator. We refer to these energetic particles as an "artificial radiation belt.". In the experiment, the collision time, τ_{col}, of the energetic electrons is long, and thousands of gradient-$|B|$ drift orbits are possible between collisions, $\omega_{dh}\tau_{col} \geq 10^3$. As the intensity of the radiation belt increases, large-amplitude drift-resonant instabilities, $\omega \simeq \omega_{dh}$, are excited. The frequency spectrum of these instabilities are time-varying and complex, and chaotic radial transport is induced whenever the frequency spectrum is both intense and compact. Since the energetic electrons are strongly magnetized, the first and second adiabatic invariants, μ and J, are preserved during the nonlinear drift-resonant, wave-particle interactions. The energetic electrons act as a one-dimensional Vlasov fluid, and this allows a relatively simple self-consistent model of the growth and saturation of the drift-resonant instability. The model agrees with the temporal characteristics of the measured radial transport and the observed frequency sweeping of the instability.

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Critical Compilation of Atomic Wavelength and Energy Level Data

W. C. Martin, J. Sugar, A. Musgrove, C. J. Sansonetti, J. E. Sansonetti, E. B. Saloman
National Institute of Standards and Technology

V. I. Azarov, A. E. Kramida, A. N. Ryabtsev
Institute for Spectroscopy, Troitsk, Russia

T. Shirai
JAERI, Tokai-mura, Japan

Our past work on spectra of astrophysical interest has produced new critical energy-level compilations for some 350 spectra of the first 30 elements, including all spectra of Na through S (Z=11−16), the iron-group elements and Cu and Zn (Z=19−30). We have also published very complete new wavelength lists with energy-level classifications for all spectra of Mg, Al, S, and Sc [1]. In addition, the NIST Atomic Spectra Database [1] has fairly complete data for the C, N, and O spectra, including the extensive transition probability data compiled by Wiese, Fuhr, and Deters [1].

Our main goal is to carry out the additional compilations needed to have more complete energy-level and wavelength data for the first 30 elements. In our most recent and current work we are compiling complete new energy level and wavelength data, together, for each spectrum. Such tables have been published for Be I and O II [1] and will be submitted for all the Ar spectra this year. We have prepared at least preliminary tables for most spectra of Be, B, F, Ne, and Cl. Completion of these tables and of updated compilations for several other elements in the range up to P (Z=15) are an important part of our program.

Large extensions of energy level and wavelength data for important iron-group spectra have been produced in several laboratories during the past 10 years or so. We plan to edit, format, and incorporate these new results in our Atomic Spectroscopic Database to supplement the extensive Fe-group data already accesible there [1].

We are also making good progress on a special “handbook” compilation covering the neutral and singly-ionized atoms of all elements. In addition to wavelengths and relative intensities for some 10,000 lines, this compilation has separate tables of the persistent lines with their energy-level classifications and (where available) transition probabilities. Tables of selected energy levels, ionization energies, and basic nuclear data are being included.

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[1] The list of references for this abstract is too long for inclusion here. These references and others are accessible through the Website http://physics.nist.gov.

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Atomic Spectra Database

W. C. Martin, W. L. Wiese, A. Musgrove, J. R. Fuhr, J. Sugar, J. Reader,
D. E. Kelleher, K. J. Olsen, P. J. Mohr, G. R. Dalton
National Institute of Standards and Technology

C. Stern Grant, G. Eichhorn
Center for Astrophysics

Version 1 of this database is accessible at the NIST Physics Laboratory Web site (physics.nist.gov, select Physical Reference Data). It has data on atomic energy levels for some 500 spectra, transition probability data for spectra of the iron-group elements, and wavelength data for spectra of a few elements. This current version includes no data for one or more of these three types of data for many important spectra, however.

Pending new critical compilations of the most needed data, we have extended the database by editing and adding data from earlier NIST compilations, selected non-NIST compilations, and selected recent publications or unpublished material. The new Version 2.0 ("ASD"), which will be put on-line this year, includes data for observed transitions of 99 elements and energy levels of 52 elements. It contains data on 950 spectra, with 70,000 energy levels and 90,000 lines from 1 Å to 200 μm, about 40,000 of which have transition probabilities.

The two principal categories of queries handled by ASD are for data on energy levels and for data on spectral lines. All current NIST-evaluated data associated with each transition are combined under a single listing. The presentation of the data is much improved and many options, search criteria, and a "Help" file are provided.

ASD has additional energy level data for 12 elements in the range Z=1 to 36 taken largely from material compiled by R. L. Kelly. Additional transition probability data include new NIST compilations for the C, N, and O spectra and data from other, mostly earlier, NIST compilations. ASD thus has energy level data for most spectra of H through Kr (Z=1−36), Mo (Z=42), and for 65 spectra of the rare-earth elements La through Lu (Z=57−71). Wavelengths of observed transitions are included for 99 elements. Energy-level classifications and transition probabilities are included for the lines of most spectra of H through Ni (Z=1−28). Comprehensive lists of observed wavelengths with classifications based on critically compiled level data are available for some elements, including all spectra of Mg, Al, S, and Sc. At a minimum, wavelengths with relative intensities are included for prominent lines of up to the first five spectra of Cu through Es (Z=29−99), with selected transition probabilities for the first two spectra. Several extensive data sets from recent NIST compilations are being prepared for inclusion in a later version of ASD.

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Spectroscopy and Dynamics of H_3^+ in the Laboratory and in Space

B. J. McCall and T. Oka
Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, IL 60637

The recent detections of interstellar H_3^+ in dense[1] and diffuse[2] clouds and towards the Galactic Center[3] have revealed the remarkable abundance and ubiquity of this fundamental molecular ion which has been proposed as the cornerstone of the ion-neutral reaction scheme of interstellar chemistry. Because of the low temperature of interstellar space, only two rotational levels, (J,K)=(1,0) for ortho-H_3^+ and (1,1) for para-H_3^+ are significantly populated. While thermalization between two states with different spin modifications is extremely slow for neutral molecules such as NH_3, it is rapid for ions because of efficient ion-neutral reactions. We will discuss thermalization of ortho- and para-H_3^+ based on a recent laboratory experiment[4] and its significance in the conversion between ortho- and para-H_2 in interstellar space.

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Large Organic Molecules in the Laboratory and in Space

Michael C. McCarthy, Carl A. Gottlieb, and Patrick Thaddeus
Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138

Discoveries of large new organic molecules in space help provide a foundation for understanding the role of the chemical bond and organic chemistry on a cosmic scale, and by extension, an opportunity to begin to address the interesting questions of biological and chemical origins and the issues that relate to them.

Most of the large organic molecules so far detected in the interstellar gas and circumstellar shells are carbon chains, a configuration of linear carbon which is unstable at high density, and therefore unfamiliar on Earth. Laboratory detection of long carbon chains was until recently extremely difficult or impossible, but more than 25 have now been detected over the past two years in this laboratory with a very sensitive Fourier transform microwave spectrometer. The largest molecule so far discovered is a chain ($HC_{17}N$) with 19 atoms and a molecular weight of 219 amu — more than three times that of glycine, the simplest amino acid. All are good candidates for astronomical detection with radio telescopes, and four have already been found in space, including the largest interstellar molecule $HC_{11}N$; with large telescopes under construction or the discovery of better astronomical sources, it is possible that nearly all can be found. Laboratory detection of other known and postulated astrophysical carbon chains and rings should be possible if we exploit the nearly two orders of magnitude between the detection sensitivity of our present microwave spectrometer and the fundamental limit set by modern technology — the same technology routinely exploited by radio astronomers.

Synthesis of ethane in ion-irradiated water ice mixtures with organics relevant to comets

M. H. Moore
NASA's Goddard Space Flight Center, Greenbelt, MD

R. L. Hudson
Eckerd College, Department of Chemistry, St. Petersburg, FL

During the recent apparitions of Comets C/1996 B2 Hyakutake and C/1995 O1 Hale-Bopp, abundant ethane, methane, and acetylene were detected. To investigate the possibility of condensed-phase synthesi s of C_2H_6 in interstellar ices due to radiation processing, we have examined the role of CH_4 and C_2H_2 in the synthesis of C_2H_6 in laboratory-formed low-temperature ices (Hudson and Moore, 1997; Moore and Hudson, 1998). Water dominated icy mixtures containing CH_4 and/or C_2H_2 were bombarded with MeV protons. Results showed that yields of C_2H_6 from CH_4 du e to dimerization reactions were similar to yields of C_2H_6 from H atom addition reactions with C_2H_2. In water dominated mixtures, CH_4 was not a source of C_2H_2, suggesting that C_2H_2 is part of the natal chemistry of these comets. Other new products were CH_3OH, C_2H_5OH, CO, CO_2, HCO, H_2CO, and CH_3CHO.

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NH_3 reactions in ion-irradiated $H_2O + CO_2$ ices–in search of the identification of the 6.8 micron interstellar absorption band

M. H. Moore
NASA's Goddard Space Flight Center

R. K. Khanna
University of Maryland, Department of Chemistry, College Park, MD

Attempts to fit the 6.8 micron feature observed in ISO SWS spectra such as NGC 7548 IRS9 and RAFGL 7009S using laboratory data have included a variety of species. Schutte et al. (1996) discusses candidates such as ices containing CH_3OH or NH_4+ ions but these alone can not explain the observed intensity. We have begun examining reactions between carbonic acid, H_2CO_3, and the base, NH_3, in search of new species which may contribute to the 6.8 micron feature. A layer of NH_3 ice is first formed under a layer of $H_2O + CO_2$. H_2CO_3 is formed in the H_2O +CO_2 ice layer during irradiation (Moore and Khanna, 1991). During slow warming the NH_3 diffuses through the upper layer containing the carbonic acid. Our first major result was the formation of a new residual ice above 250 K which is tentatively identified as carbamic acid (NH_2COOH) (Khanna and Moore, 1998). This compound has not been isolated or characterized by any other experimental technique. The spectrum of carbamic acid is a good match with the 6.8 micron band, but because it also contains a strong 7.7 micron band, it will not be a good candidate for the interstellar features. However, the acid is important because of the existence of its CN bond; structurally it has similarities with glycine, the simplest amino acid.

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Laboratory Investigations of C_2H_4 by Infrared Heterodyne Spectroscopy

V. Morozhenko
National Research Council at NASA/Goddard Space Flight Center

T. Kostiuk, D. Buhl
NASA/Goddard Space Flight Center

Heterodyne Spectroscopy can make a significant contribution to remote studies of planetary atmospheres and other gaseous astronomical objects. Infrared heterodyne investigations of planetary atmospheres permits the determination of their composition, distribution of pressure and temperature with altitude, and investigation of local physics and chemistry[1]. But this method is especially important for investigations of atmosphere dynamics. It has a high spectral resolution ($\lambda/\Delta\lambda \approx 10^7$), which makes it possible to remotely determine the direction and speed of winds with an accuracy 2 m/s [2]. However, in order to retrieve atmospheric parameters from atmospheric line measurements, it is important to know the molecular parameters of the lines being measured. Ethylene is an important hydrocarbon present in atmospheres of Jupiter, Saturn, and Titan (*e.g.*, 3). It is a product of methane chemistry in the stratospheres of these planets and has a complicated spectrum in middle IR region. This makes it a very interesting and usable probe of physical-dynamical properties of these atmospheres. In this report we present initial results of laboratory investigations of absorption lines of ethylene (C_2H_4) in the ν_7 band near 10.5 μm. The measurements were made using a laboratory infrared heterodyne spectrometer with the ethylene gas at temperatures 293–297K and pressures 0.05–0.5 Torr.

Positions of more then 150 lines were measured relative to lines in the P and R branches of the $^{12}C^{16}O_2$ laser. Absolute frequencies of the stronger lines were determined to $\pm 5 \times 10^{-5}$ cm^{-1}. Their intensities were determined to $\approx 10\%$. Comparison of our results with other experimental and theoretical results (J. Hillman *et al.*, this meeting) will be discussed. A number of unknown absorption lines were discovered. The possible source of these lines will be discussed, including foreign gas admixture (although 99.99% ethylene was used), isotopic $^{13}C^{12}CH_4$ or weak $^{12}C_2H_4$ lines

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The Electronic Rydberg and Valence Structures of Molecular Oxygen

J. S. Morrill
E.O. Hulburt Center for Space Research, Naval Research Laboratory, Washington, DC 20375-5352

M. L. Ginter
IPST, Univ. of Maryland, College Park, MD 20742-2431

B.R. Lewis and S.T. Gibson
The Australian National Univ., Canberra, ACT 0200, Australia

The spectra and electronic structures of molecular oxygen play dominant roles in many terrestrial and astrophysical processes. This includes the absorption of solar radiation, the observed emission spectrum of the airglow and aurora, as well as processes involving reactions and recombination of atomic oxygen. The details of these processes are governed, in turn, by the details of the molecular potentials of the electronic states involved in these phenomena. As part of a comprehensive review of the electronic structure of molecular oxygen currently nearing completion, data on all known valence and Rydberg states is being compiled and corrected. This presentation emphasizes both a summary of our current understanding of the valence electronic states as well as the complex electronic potentials which arise from the interaction between the Rydberg-Rydberg and Rydberg-valence states. We will present a discussion of the application of these electronic structures to typical problems of atmospheric interest.

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Laboratory Studies of Strengths and Pressure-broadened Widths of Lines in the 10 μm Band of Ammonia Molecule.

V. Nemtchinov and P. Varanasi
Institute for Terrestrial and Planetary Atmospheres,
The University at Stony Brook,
Stony Brook, NY 11794-5000

The proper identification and interpretation of the infrared signatures in the spectroscopic observations of the outer planets by orbiting probes and ground-based astronomers creates a sustained need for laboratory data on individual spectral lines obtained at temperatures and pressures relevant to the respective atmospheres. The analysis of the infrared spectra of Jovian atmosphere in the 10 μm region is influenced by the accuracy of laboratory data on spectral lines of $^{14}NH_3$ and $^{15}NH_3$. We present here recent high-resolution studies of the absolute intensities and collision-broadened widths of lines in the ν_2 bands of ammonia performed in our laboratory. These data were obtained with our coolable cells and a Fourier transform spectrometer. The effects of pressure-broadening by H_2, N_2 and O_2 were investigated at 200, 255 and 296 K. The coefficients of temperature dependence of linewidths were derived for individual transitions in the 10 μm spectral region from these data.

Absorption Spectra and Absorption Coefficients for the 790 nm and 889 nm bands of Methane obtained using Intracavity Laser Spectroscopy

James J. O'Brien, Elizabeth A. Amin and Balazs L. Kalmar
Department of Chemistry and Center for Molecular Electronics, University of Missouri-St. Louis, St. Louis, MO 63121-4499.

Methane spectral features are prominent in the reflected sunlight spectra from the outer planets and some of their major satellites (e.g., Titan) and can provide detailed information on the atmospheres of those bodies. Methane bands in the visible to near-IR are particularly important because for many of these planetary bodies, the methane bands occurring in the IR are found to be saturated. Laboratory data acquired at appropriate low temperature conditions are required to interpret the observational data. Because methane bands in the visible to near-IR region consists of high overtone and/or combination transitions, the spectra are intrinsically weak. Consequently, sensitive techniques such as intracavity laser spectroscopy (ILS) are required to perform the laboratory measurements. In this paper, the ILS technique with an argon-ion laser pumped Ti:sapphire laser is used to record spectra in the 790 nm band (from 12,125 cm^{-1} to 13,235 cm^{-1}) and the central portion of the 889 nm band (from 10,975 cm^{-1} to 11,345 cm^{-1}), for room (298 K) and liquid nitrogen temperature (77 K) methane. Spectra for the more strongly absorbing sections of these bands will be presented. These spectra are acquired at a resolution of approximately 500,000. From the spectra, absorption coefficients are determined and these are presented as averages over 1 Å and 1 cm^{-1} intervals. The results are compared with low resolution measurements on methane at room temperature and with absorption coefficients derived from methane features observed in spectra of the outer planets and Titan. To obtain our results, spectra are deconvolved for the instrument function using a Fourier transform technique. The validity of the approach is verified from studies of isolated water absorption lines occurring in the same spectral region. Good agreement is observed between the intensity values determined from the FT deconvolution and integration method and those derived by fitting the observed line profiles to Voigt lineshapes convoluted with the instrument function.

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Ammonia-Water Low Temperature Vapor-Liquid Equilibrium: Applications to the Atmospheres of Outer Planets

Dr. Nimmi C. Parikh
Richard Stockton College of New Jersey

Dr. John Zollweg
Cornell University

Knowledge of atmospheres of other planets is important not only for its intrinsic value but also for the insights which this knowledge can provide to us about the atmosphere of our own planet, the origins of our solar system, and perhaps even the origins of life on earth. Accurate interpretation of remote sensing data and high quality atmospheric models require thermodynamic data on the condensible trace constituents which are expected to form clouds in these planetary atmospheres. Specifically, for studies of Jupiter's atmosphere, a good thermodynamic model of Vapor-Liquid Equilibrium (VLE) in the ammonia-water system under conditions relevant to Jupiter (below 20C) is of vital importance for understanding the composition of condensing ammonia-water clouds, constraining ammonia gas phase abundances, and reducing extrapolation uncertainties in atmospheric models. While there is substantial VLE data on the ammonia-water system at high temperatures, low temperature VLE data in general use are old, sparse, and inconsistent between different investigators. We have obtained experimental data on temperature, pressure, and liquid composition of ammonia-water mixtures from 20C to 0C. We have combined these data with select, carefully evaluated, literature data to create an updated maximum-likelihood model of the ammonia-water system which takes into account experimental uncertainties in all measured data. From the temperature-dependent model parameters we have calculated new cloud profiles (mole fraction of ammonia in condensing droplet versus altitude) for potential condensing ammonia-water clouds on Jupiter.

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Laboratory Fourier transform spectroscopy for astronomers' special requests

J.C.Pickering, A.P.Thorne, R.C.M.Learner & G.Cox
Blackett Laboratory, Imperial College, London SW7 2BZ

We have exploited the high resolving power and excellent wavenumber accuracy of our visible/ultraviolet Fourier transform (FT) spectrometers not only for systematic studies to update the old, inaccurate and incomplete database for the astrophysically important transition element spectra (see [1] for the most recent summary of this work) but also to provide answers to specific questions posed by astronomers on a 'one-off' basis. This activity started a decade ago with a refutation of suspicions that measurements of the solar boron abundance were affected by a weak iron line [2] . It continued with two separate sets of measurements on weak Fe, Ni, Co and V lines blended with the Th II line used in the thorium-neodymium stellar chronometer. In the second set the hyperfine structure of the Co line was evaluated, and the gf-value of the weak intercombination V line was measured and shown to be significantly higher than predicted [3]. In recent years our laboratory spectra have been used in conjunction with GHRS spectra from Hubble Space Telescope to determine isotopic abundances in chemically peculiar stars for Pt [4] and Pb. FT spectra of Au, Tl and Hg from our colleagues in Lund have been used for the same purpose. Our most recent specifically requested measurements, on the resonance lines of Mg I and II, have had the entirely different purpose of establishing very accurate rest wavelengths for comparison with high quality ground-based recordings of quasar spectra with high red shifts; the object of this comparison is to establish whether there are significant space-time variations of the fine-structure constant.

Although not all of our efforts to provide data for specific problems have been successful, we are open to requests of limited scope that do not diverge too far from our main programme and that match the capabilities of our FT spectrometers. These may be summarised as follows: resolving power of up to 1.5 million from the visible region into the VUV (present limit about 1400 Å), wavenumber accuracy 0.001 to 0.005 cm^{-1} (10-50 $\mathrm{m\,s}^{-1}$), depending on line strengths, and relative intensities with uncertainties from 5%, again depending on line strengths and spectral region.

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Outer atmosphere and wake of space objects, kinetic simulation

Ponomarjov Maxim
State Academy of Aviation Technology, Promyshlennaya str.1 (Box 22), 152300 Tutaev, Yaroslavl region, Russia

Problems of the kinetic simulation of charged and neutral particle flows due to interactions of bodies with space magnetoplasma are dealt with. The image method (see [1], [2]) is considered in application to modeling disturbances of space plasma near a space station taking into account interactions with boundaries and pollution clouds. Different special cases of the objects wake are considered in detail. The correlations of boundary material properties and space plasma disturbances are discussed on the basis of the simulation results.

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Ion-Electron Behaviour near Plasma Sheet Boundary Layer During Substorm

Manju Prakash

Department of Physics and Astronomy, SUNY at Stony Brook, New York 11794- 3800

Recently Parks et al. (1997) have reported correlated observations based on WIND spacecraft data on the characteristics of ions and electrons near the plasma sheet boundary layer (PSBL). The ion distribution is anisotropic with multiple beams and, therefore departs from Maxwellian. The ion distribution often includes several different populations. The electron distribution is usually composed of a single component which is nearly isotropic. Correlated observations with POLAR UVI show that during substorm times the ion distribution is dynamic and undergoes large changes. For example, each component can vary independent of the other components. The electron distribution remains relatively stable. The counter streaming ion beams are predominantly observed in a layer between the PSBL and the lobe. The present work examines theoretically the origin of the complex features of the plasma.

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Absolute Cross Section for Electron Impact Excitation of Ground State Si^{2+}

D. B. Reisenfeld[1], P. H. Janzen[1], L. D. Gardner[1], D. W. Savin[2], and J. L. Kohl[1]
[1]*Harvard-Smithsonian Center for Astrophysics*
[2]*Columbia University*

Electron-impact excitation (EIE) is the dominant mechanism for the formation of emission lines in many astrophysical plasmas. Absolute line intensities and their ratios to one another can provide diagnostics of the temperature and density of the emitting plasma, and of the abundances of the elements within the plasma. Modern space observatories such as the Hubble Space Telescope, the SOHO solar mission, and the upcoming AXAF mission measure UV and X-ray line intensities with detectors calibrated to a high degree of accuracy, placing more demand than ever on the atomic physics community to provide accurate atomic data. Theoretical calculations can provide the vast numbers of atomic rates used for the interpretation of emission line measurements, but experimental benchmark measurements are required to test the accuracy of the calculation methods.

At the CfA Ion Beam Facility we are continuing an ongoing program to measure absolute cross sections for EIE and dielectronic recombination. We have recently completed a measurement of the absolute cross section for EIE of $\mathrm{Si}^{2+}(3s^2\ ^1S - 3s3p\ ^1P)$ for energies below threshold to 11 eV above. A beams modulation technique with inclined electron and ion beams was used, where the radiation from the excited ions at $\lambda 120.6$ nm was detected using an absolutely calibrated optical system. The population of the $\mathrm{Si}^{2+}(3s3p\ ^3P^o)$ metastable state in the incident ion beam was determined to be $22.4 \pm 2.5\%$. The data have been corrected for contributions to the signal from excitation of the metastable state, and for higher energies, from excitation of the ground state to levels above the $3s3p\ ^1P$ level. The experimental 0.5 ± 0.05 eV energy spread allowed us to resolve complex resonance structure throughout the studied energy range. At the reported 15% uncertainty level (90% confidence limit), the measured structure and absolute scale of the cross section are in good agreement with 12-state close-coupling R-matrix calculations[1][2].

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Hydrodynamics experiments for astrophysics using intense lasers

Bruce A. Remington[†], S. Gail Glendinning, Kimberly S. Budil, Jave Kane, Dave Gold, Dimitri Ryutov, Gilbert Collins, and Robert Cauble
Lawrence Livermore National Laboratory

In a broad-based collaboration with universities, we are developing astrophysically relevant hydrodynamics experiments on the Nova and PetaWatt lasers at Lawrence Livermore National Laboratory (LLNL), and in the future on the Omega laser at the University of Rochester, and the National Ignition Facility, currently under construction at LLNL. Issues that we are or planning to investigate are deep nonlinear, compressible hydrodynamic mixing in 2D and 3D, relevant to supernovae [1]; strong-shock hydrodynamics relevant to supernova remnant formation [2]; radiative shocks and blast waves, of potential interest to gamma-ray burst models [3]; cratering experiments, of possible interest to hypervelocity meteoroid impacts [4], and equation-of-state measurements of hydrogen at multi-Mbar pressures, relevant to the interiors of giant planets and brown dwarfs [5]. An overview of this work will be given, and the issue of scaling will be addressed [6].

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[†]remington2@llnl.gov

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LABORATORY EXPERIMENTS RELATING TO POLAR MESOSPHERIC CLOUDS

Scott Robertson
Department of Physics, University of Colorado Boulder, CO 80309-0390

Mihály Horányi
Laboratory for Atmospheric and Space Physics, University of Colorado, Boulder, CO 80309-0392

Laboratory experiments are in progress to create nanometer-size ice crystals in plasma to investigate the role of charging processes in noctilucent clouds (NLC) and polar mesospheric summer echoes (PMSE). Rocket-borne probes have observed localized "bite-outs" in the density of free electrons caused by small ice particles in the lower ionosphere. Charge collectors have recently found evidence for both positive and negative aerosols near NLC and PMSE layers[1]. The mass distribution of these particles and the reaction rates for electron attachment, photoionization, photodetachment, etc. which are necessary for modeling are not known. Two new experiments are underway to answer these questions[2].

First, a rocket-borne charge-collecting probe with a magnetic field for mass discrimination has been constructed and tested in the laboratory. The magnetic field prevents collection of singly-charged species with mass below a threshold determined by the rocket velocity and the magnetic field strength. Several of these probes with differing mass thresholds will be used to provide a low-resolution mass spectrum of NLC particles. Laboratory tests of a prototype probe show that the magnetic field is effective in preventing collection of low energy electrons.

Second, a large plasma chamber (0.9 m diameter x 1.2 m) is being fitted with a supersonic nozzle which generates ice clusters. Clusters which become charged will be detected by Faraday cups and their mass distribution will be determined by mass spectrographs. Electron attachment rates will be inferred from the dependence of the charged fraction on the electron density. An arc lamp source with a cutoff wavelength similar to that of the solar spectrum at 80 km will be used to determine the role of photodetachment and possibly photoionization. Sodium or other impurities may be added to the flow creating the ice particles to determine whether or not their presence results in a lower work function.

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Searching For the Interstellar Signatures of Large Carbon Molecules and Ions from the Ultraviolet to the Near IR.

F. Salama, L. Allamandola and T. Halasinski
NASA-Ames Research Center, Space Science Division, Moffett Field, CA 94035-1000.

Multiwavelength observations from space (HST, ISO, IRTS) indicate that interstellar molecules range from simple diatomic molecules and ions to very large molecules and clusters containing up to hundreds of atoms. This large molecular distribution which links the gas phase to solid phase of IS dust is dominated by carbon-containing materials among which polycyclic aromatic hydrocarbons (PAHs) are an important component. Although the study of atoms, small molecules and ions in space based on laboratory measurements is now well established, almost no information has been available on large molecular systems until recently. The importance of this issue and its impact on our understanding of the evolution of the ISM is one of the cited priorities in the NASA/UVGA Laboratory Astrophysics list of recommendations.

In response, we have developed, a laboratory program to: (i) simulate realistic IS environments and (ii) measure the spectroscopy of large, refractory, molecular systems. Since IR observations show that PAHs are widespread throughout the ISM, absorption spectra of neutral and ionized PAHs isolated in a cryogenic (5 K) neon matrix were measured together with the oscillator strengths of the bands. This laboratory program has resulted in a *unique* data base on the spectroscopy of neutral and ionized PAHs from the UV to the NIR spectral range (1800-10,000 Å). The data base consists of the electronic spectra of about 30 species containing up to 25 carbon atoms and includes regular PAHs in their neutral and cationic forms as well as hydrogenated PAHs and PAHs with side groups. The experimental results will be compared with theoretical calculations and astronomical observations and important astrophysical implications discussed. These include possible diffuse interstellar band carriers, UV absorptions, molecular budget of the diffuse ISM, UV-to-IR energy conversion in the ISM, etc.... The UV, visible and NIR IS spectral features which should be searched for using space platforms and in existing archival data will be discussed. It will be argued that the next phase in the study of carbon- containing materials should also include parallel studies of the gas phase spectroscopy of isolated molecules and ions. This next step is technically very challenging. We propose to measure the UV-to-NIR vibronic spectra of neutral and ionized PAHs and derivatives (fullerenes) using supersonic jet techniques and to build a data base (wavelengths and oscillator strengths) of the characteristic UV and visible bands of these molecules and their ions. This data base will be used to predict structures that can be searched for with the HST (new diffuse UV and visible bands) and to test for the presence of specific PAHs or derivatives in the ISM and derive their IS abundances. Providing such data is fundamental and represents an experimental challenge which needs to be addressed.

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Laboratory Studies of Interstellar/Cometary Ice Analogs

S. A. Sandford, M. P. Bernstein, and L. J. Allamandola
NASA-Ames Research Center, Mail Stop 245-6, Moffett Field, CA 94035-1000 USA

Interstellar molecules condense on cold grains in dense clouds and spend most of their time in icy mantles. New species form when reactive species combine on the grain surfaces or within ices subjected to radiative and thermal processing. Ices are also a significant part of comets, possibly some asteroids, and the surface materials of many outer Solar System bodies. Spectral analysis of lab ice analogs, especially in the IR, has proven to be necessary to identify these materials and understand their formation and evolution. Several examples of recent progress made at the Astrochemistry Laboratory at NASA-Ames will be presented.

Interstellar ices undergo both UV and cosmic ray processing. This breaks bonds and generates new ions, radicals, and molecules. For example, photolysis and warm up of ices containing H_2O, CH_3OH, CO, and NH_3, all known to exist in ices in space, produces organic residues with new molecules of interest to interstellar astrochemistry. Since the ISM contains polycyclic aromatic hydrocarbons (PAHs) and related materials, they too should be in interstellar ices. We have found that PAHs in ices are somewhat susceptible to attack by H, O, and OH liberated from photolyzed H_2O. The result is loss of some aromaticity and production of PAHs with peripheral ketone (C=O) groups and excess H atoms (H_n-PAHs). The IR signatures of these variants explain some enigmatic spectral features seen towards low excitation objects, and having dipole moments, allow for submillimeter search and detection.

The organic residues have other important properties relevant to extraterrestrial samples. Some of the complex organics in meteorites and IDPs are highly D-enriched. We have demonstrated that D in interstellar/cometary ice analogs concentrate into certain complex photoproducts. The C-rich fractions of meteorites also contain large concentrations of noble gases trapped by an unknown mechanism. However, using isotopically-spiked noble gases, we have shown that ice photolysis produces residues that trap noble gases at concentrations up to 100+ times above anything previously attained (Xe = 10^{-6} CC-STP per gram, values comparable to those seen in meteorites). These noble gas trapping and D results suggest that a significant fraction of the organics in meteorites have an interstellar connection.

Another use of spectral data from our ice analogs is to identify the molecular components of interstellar ices, determine their column densities, grain sizes, etc. Most recently, we have shown that the strength of the N=N fundamental at 2328 cm^{-1} produced by N_2-rich ices can vary by up to *three orders of magnitude* depending on what other molecules are in the ice. This effect can profoundly alter current estimates of the abundance of N_2 in interstellar ices and certain outer Solar System bodies.

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Wavelengths and Oscillator Strengths for Space Astronomy

Craig J. Sansonetti and Joseph Reader
National Institute of Standards and Technology, Gaithersburg, MD 20899

Over a period of more than a decade the Atomic Spectroscopy Group at NIST has carried out laboratory research to support the observing program of the Hubble Space Telescope. Our measurements of the spectral lines emitted by a Pt/Ne hollow cathode lamp have been used for wavelength calibration of the Goddard High Resolution Spectrograph and will continue in use for calibration of the Space Telescope Imaging Spectrograph. Our comprehensive atlas [1] covering the spectrum from 1100 to 4000 Å, which contains accurate wavelengths and photometric scans, is now accessible at http://physics.nist.gov.

Recently we have studied species needed for interpretation of HST spectra of chemically peculiar stars. Our spectral analyses provide wavelengths and oscillator strengths for modelling stellar atmospheres, and our detailed studies of particular spectral lines are used to determine elemental and isotopic abundances.

We are currently completing extensive new analyses of Hg II and III, which are of special interest because of the high abundance of Hg in chi Lupi. Results of this work are used in a current analysis of Hg in chi Lupi and HR7775 [2]. Our wavelengths for Zr II and III support the identification of Zr in chi Lupi [3]. We have also presented a full analysis for Zr III [4]. Members of our Group have calculated oscillator strengths for Gd III and Eu III and made the first analysis of Dy III [5].

For determination of isotopic abundances in chi Lupi we have made observations of selected lines of Hg III with separated isotopes [6]. These measurements helped to prove that all Hg on chi Lupi is the heaviest isotope: ^{204}Hg [3]. In connection with the recent identification of Bi in HR7775 [7] we made new measurements of Bi I, II, and III in the far UV. Our measurement of the 1553-Å line of Pb III established the identification of Pb in chi Lupi, and separated isotope measurements with ^{204}Pb and ^{207}Pb showed that the Pb on chi Lupi is predominantly isotope 207 [8].

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Ion Storage Ring Measurements for Understanding Line Emission and Ionization and Thermal Structures of Photoionized Gas

D. W. Savin[1], S. M. Kahn[1], A. Müller[2], and A. Wolf[3]

[1]*Columbia Astrophysics Laboratory and Department of Physics, Columbia University*

[2]*Institut für Kernphysik, Strahlenzentrum der Justus-Liebig-Universität*

[3]*Max-Planck Institut für Kernphysik und Physikalisches Institut der Universität Heidelberg*

In photoionized gas ions are formed at electron temperatures far below those where they would be formed in collisional ionization equilibrium. As a result of the low electron temperature, radiative recombination (RR) and dielectronic recombination (DR) are often the dominant line formation mechanisms. RR and DR also play an extremely important role in determining the ionization and thermal structure of the photoionized gas. Storage ring measurements can aid in understanding photoionized plasmas such as planetary nebulae, H II regions, cold novae shells, AGNs, XRBs, and CVs. Ion storage rings are unique for their ability to study electron-ion recombination at low energies. DR and RR measurements are carried out by merging the stored ions with a co-linear electron beam. The merged beams arrangement allows for a low center-of-mass collision energy.

Using the heavy ion Test Storage Ring (TSR) at the Max-Planck-Institute for Nuclear Physics in Heidelberg, Germany, we have undertaken to measure the DR rates for the Fe L ions (Fe XVII to Fe XXIV). These rates play an important role in determining the thermal stability of X-ray photoionized gas. Our recent measurement of Fe XVIII to Fe XVII DR (Savin et al. 1997) has shown that at low electron temperatures, DR can proceed primarily via $2p_{1/2} \rightarrow 2p_{3/2}$ excitation of core electrons. This channel is not accounted for by LS-coupling calculations or the Burgess formula and our measured DR rate is a factor of ~ 2 times larger than predicted by previously existing theoretical calculations. Our results indicate that a reevaluation of low temperature DR rates is needed.

Our Fe XVIII results suggest that there may be a factor of ~ 2 error in the low temperature Fe L DR rates. We have used XSTAR (Kallman & Krolik 1997) to investigate the affect of such an uncertainty on the thermal instability of photoionized gas. We find that increasing the low temperature Fe L DR rates by a factor of two significantly increases the range in parameter space over which the instability exists. Correspondingly, a factor of two decrease significantly decreases the range. These results demonstrate that our understanding of the importance of thermal instabilities is limited by uncertainties in the atomic data.

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Theoretical Atomic and Molecular Physics and Data Activities for Astrophysics

D.R. Schultz, P.C. Stancil, P.S. Krstić, W. Liu, and D.J. Jeffery
Physics Division, Oak Ridge National Laboratory

The atomic astrophysics group at ORNL produces, collects, evaluates, and disseminates atomic and molecular data relevant to astrophysics, and actively models various astrophysical environments utilizing this information. With the advent of the widespread use of the World Wide Web, these data are also being placed on-line to facilitate their use by end-users in various applications communities. The group's recent activities in data production and modeling will be highlighted in this presentation. For example, recent calculations and applications of elastic scattering and derived transport cross sections for ionospheric studies, charge transfer between metal ions and metal atoms for supernova nebular spectral modeling, ion-atom collision data relevant to planetary atmospheres and comets, and data for early universe modeling will be described.

Low Temperature Mm-wave Properties of Model Celestial Grains

A. J. Sievers and N. I. Agladze
Laboratory of Atomic and Solid State Physics and the Center for Radiophysics and Space Research, Cornell University, Ithaca, NY 14853-2501

Interstellar and interplanetary dust consists mainly of silicates, organics, iron compounds and ices, the exact mix depending on the local environment. The observations of thermal radiation from these particles are often converted to total particle mass by using the theoretical absorptivity of these constituents. This method has been particularly important in the mm-wave region where it is used for mass estimates of particles orbiting stars, of molecular cloud complexes and of distant galaxies. The best estimates for silicates generally predict values for isolated grain mass opacity coefficient of interstellar particles: $\kappa_\nu \approx A\left(\tilde{\nu}/10cm^{-1}\right)^{\beta}$ cm^{2}g^{-1} where $\tilde{\nu} = 1/\lambda$, $A = 0.3$ and $\beta = 2$ (Draine & Lee 1984). Although current theories of interstellar dust agree that the grains are probably porous and amorphous (Mathis 1993), the effect of porosity and structure on the strength and temperature dependent mm-wave optical constants of model interstellar dust still needs to be explored experimentally. The first low temperature measurements on realistic analogs of silicate grain materials (Agladze 1996) showed that the millimeter-wave mass opacity coefficient at 1 mm wavelength ranged up to $A = 1.6$ at a temperature of 1.2 K and decreased with increas ing temperature to $A = 1.0$ at 20 K. The decrease in the opacity coefficient with increasing temperature has been identified with resonant absorption by a continuous distribution of two level systems (TLS) associated with amorphous solids (Agladze 1996). To examine the influence of porosity we compare our findings for amorphous silicate grains synthesized by sol-gel reaction with those measured for SiO_2 aerogel which has an extremely open structure. For samples of aerogel with a volume fill fraction of 5% SiO_2 at 1.5 K we find in the region between 0.7 and 2.9 mm wavelength (3.5 - 15 cm^{-1}) that $A = 1.3$ and $\beta = 1.2$. Temperature dependences are found for both coefficients: by 16 K the coefficient A decreased to 0.8 and β increased to 1.6. The large change in the coefficients with increasing temperature, which corresponds to a 50% bleaching effect in absorption, occurs because the TLSs have large dipole moments and extend to much larger frequencies, consequently, for open grain structures the mm and sub-mm wave absorption produced by TLS represents a more significant contribution than for bulk amorphous solids.

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The $O_2(b^1\Sigma_g^+)$ State - Nightglow Observations and Laboratory Kinetics

T. G. Slanger, P. C. Cosby, D. L. Huestis, E. S. Hwang, H. I. Bloemink, A. Bergman, and R. A. Copeland
Aeronomy Program, Molecular Physics Laboratory
SRI International, Menlo Park, CA 94025

D. E. Osterbrock and J. P. Fulbright
University of California Observatories/Lick Observatory, UC Santa Cruz
Santa Cruz, CA 95064

Ground-based observations of the $O_2(b^1\Sigma_g^+)$ state in the terrestrial nightglow have been limited to the 0-1 band of the Atmospheric Band system, at 864 nm. Countless observations of this feature have been made, in order to monitor temperature and gravity waves, and to determine the variability of oxygen atom densities in the 95 km region. Although other O_2 emission systems (cf. the Herzberg transitions) exhibit a range of emitting vibrational levels, vibrational excitation has not been reported in either the $b^1\Sigma_g^+$ or the $a^1\Delta_g$ states. It is generally understood that this is a consequence of the long radiative lifetimes of the two states and the large difference in collisional quenching rates for v = 0 and v > 0 levels. Recent spectra obtained with the Keck telescope and the HIRES echelle spectrometer on Mauna Kea demonstrate that with adequate sensitivity and resolution, vibrational excitation can in fact be observed in the $b^1\Sigma_g^+$ state.[1] We have shown that levels up to at least v = 15 are generated in the nightglow, and that the v = 0,1 levels exhibit high rotational-temperature components. At the same time, we are pursuing a program of laboratory investigations[2] of the temperature-dependent collisional removal of vibrational excitation in the $b^1\Sigma_g^+$ and $a^1\Delta_g$ states of O_2 which will ultimately lead to an understanding of relationships between the observed nightglow band intensities, the production rates of the vibrationally-excited levels, and the ultimate source function - atom recombination in most cases. These measurements will also impact auroral observations, and observations of the Venus and Mars atmospheres.

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Improved VUV Spectroscopy of Doubly-Ionized Atoms

Peter L. Smith
Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138

Juliet C. Pickering
Blackett Laboratory, Imperial College, London SW7-2BZ, U.K.

State-of-the-art UV and VUV astronomy with the GHRS, and now the STIS, on HST requires wavelengths accurate to a few parts in 10^7 (Morton 1992; Carpenter 1993; Leckrone *et al.* 1997). Smith *et al.* (1998) give a quantitative justification for this value. Fourier transform (FT) spectrometry in the laboratory has provided wavelengths of this accuracy for singly-charged ions, but application of this method to doubly-charged ions (*i.e.*, to so called "third spectra") has been hindered by the lack of a suitable light source. Third spectra, particularly of the iron group, are of great interest to observers of chemically peculiar and other hot stars.

The goal of this project was to apply a new light source (Heise *et al.* 1994) to FT spectrometry of multiply charged ions, in particular, Fe III (Fe^{2+}). The previous recent measurements of Fe III wavelengths were those of Ekberg (1993), who used a photographic grating spectrometer. The resulting wavelengths had an accuracy of, at best, between 5 mÅ and 10 mÅ, *i.e.*, only several parts in 10^6. Literature wavelengths for most other third spectra are less accurate.

The quality of the new Fe III spectra we obtained is unprecedented; the new wavelengths that we have derived are at least an order of magnitude more accurate that those currently used by astronomers. Thus, this project has shown that the urgently needed improvements in accuracy of the laboratory atomic data for doubly ionized species are now possible. An extensive study of Fe III is in progress; branching ratio measurements and studies of other doubly charged ions will follow.

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Oscillator Strengths for VUV lines of CO, H_2, and HCl

Peter L. Smith, K. Yoshino, J. R. Esmond & W. H. Parkinson
Harvard-Smithsonian Center for Astrophysics, Cambridge, MA

K. P. Huber
Steacie Institute for Molecular Sciences, NRC, Ottowa, ON, K1A 0R6, Canada

K. Ito & T. Matsui
Photon Factory, KEK, Tsukuba, Japan

Incomplete or inconsistent molecular parameters contribute to many of the difficulties and anomalies that arise in interpreting observations of molecules in diffuse and translucent interstellar clouds and planetary atmospheres and in modelling those environments. As a consequence, the acquisition of improved photoabsorption cross section and spectroscopic data for molecules (*e.g.*, CO, N_2, H_2O, SO_2, HCl) at UV and VUV wavelengths has been a major focus of our research program in the past few years.

We have studied the photoabsorption cross sections of the $d(15)$, $a'(20)$, $d(14)$, $a'(19)$, $a'(17)$, $d(12)$, $a'(16)$, $d(11)$, $e(8)$, $d(10)$, $a'(14)$, $e(5)$, $d(7)$, $e(4)$, and $a'(11) - X(0)$ intersystem (*i.e.*, spin-changing) bands of CO at 77 K using the 6VOPE spectrometer at the Photon Factory (Ito *et al.* 1985) and synchrotron radiation as a background continuum source. Cooling significantly reduces the number of rotational levels populated and thus overlapping with the lines of the much stronger $A - X$ bands. Federman *et al.* (1994) detected some of these intersystem bands in observations with the GHRS on HST along the line of sight to ζ Oph. The intersystem bands are relatively weak and, therefore, more likely than 'allowed' bands to be on the linear portions of curves-of-growth. The f-values are the most likely cause of the discrepancies between observed and modelled spectra.

We have also studied two absorption bands of H_2O, $C - X$ at $\sim$124 nm and $F - X$ at 116 nm. The analysis of the measurements is almost complete. In addition, we have remeasured the absorption cross sections of the $C(0)-X(0)$ and $C(1)-X(0)$ bands of HCl. Our peak cross sections are significantly larger than in previous work, demonstrating that high spectral resolving power is required for accurate cross section measurements of narrow spectral features. Measurements on N_2 and SO_2 are discussed elsewhere at this workshop; measurements on some $E - X$, $B - X$, and $C - X$ bands of CO are planned.

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Measurement of Lifetimes and f-Values in Multiply-Charged Positive Ions

Steven J. Smith, Ara Chutjian, Jason Greenwood
Atomic & Molecular Collisions Team
Jet Propulsion Laboratory/Caltech

Measurements will continue to be made of lifetimes of metastable levels in singly- and multiply charged ions (MCI) which have significant density and can contribute to the optical absorptions, emissions and energy balance in the ISM, stellar atmospheres, etc. These ion charge states are important for interpretation of data obtained from GHRS/HST, EUVE, STIS/HST, and the planned FUSE missions. Accurate column densities of abundant species found in the ISM are limited by the presence of strong electric dipole transitions with equivalent widths (EW) that lie on the saturated part of the curve of growth. Hence reliable column densities require metastable state measurements with small f-values, where EW's are on the linear part of the curve. Intensity ratios between forbidden and allowed transitions are density and temperature sensitive, and critically depend on the lifetimes of the metastable or intersystem line. However, calculated and measured lifetimes in some cases can differ by a factor of three. The vast majority of transition rates required are presently being calculated by theory alone,which if unchecked by benchmark experiments can lead to orders of magnitude error in the estimation of electron densities and temperatures from diagnostic line ratios. MCI metastable lifetime measurements reported here use the JPL CAPRICE electron-cyclotron resonance ion source (ECRIS) which provides microampere currents of charge states such as C II-VII, S II-VII, Ne II-VI, and Mg II-VI. Metastable ions are injected into a Kingdon ion trap and stored for times longer than the metastable lifetimes (.001 to 1 second). Decay channels include intercombination, electric quadrupole E2, magnetic dipole M1 and double photon decay 2E transitions. The UV photon emission are detected by (a) interference filter and phototube using a UV grade quartz optical system and (b) for transitions shorter than 180 nm, a cesium-iodide coated microchannel plate enhanced for UV performance. The JPL ion trap, constructed in collaboration with Texas A & M University[1] is on a dedicated beam line. The measured lifetimes for C II at 232.5 nm, N II at 215.5 nm and Ar III at 519 nm will be presented. Results are in good agreement with other experiments and theoretical calculations. Additional series of measurements will be made of the astrophysically relevant species N III at 174 nm, Ne V at 113.4 nm, and S III at 171.3 nm. The accuracy is at the 5-10% level.

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Photoluminesence of Carbonaceous Grain Mantle Materials with Silicon Impurities

T. Smith, B. Friedmann, A.N. Witt, R. Wang, X. Deng
The University of Toledo

D. Furton
Rhode Island College

The high abundance of carbon in the local universe and its ability to form refractory solids makes carbon a likely interstellar grain candidate. The abundance of carbon and the association of the 3.4 micron C-H stretch band with dust grains has lead to the adoption of hydrogentated amorphous carbon (HAC) as a major component of IS dust. HAC could therefore be responsible for the IS photoluminesence (PL) process known as Extended Red Emission (ERE). Astronomical ERE spectra exhibit peak positions in the 610 - 850 nm range, and the observed ERE intensities suggest a quantum yield of at least 10% in the diffuse ISM. HAC analogs produce efficient photoluminesence near 570 nm but become inefficient in the observed ERE wavelength range.

The technique of bandgap engineering was employed in an attempt to lower the lab HAC bandgap from ≈ 2.85 eV to ≈ 2.1 eV through the incorporation of silicon impurities (bandgap $\approx$ 1.1 eV). The goal is to shift the photoluminesence peak toward longer wavelengths. Fourteen a-Si(x)C(1-x):H thin films were made using chemical vapor deposition (CVD) in an RF glow discharge reactor with silane, a hydrocarbon gas and argon as feed gases. The films were then illuminated by a blue laser and then separately by UV laser light. The resulting PL peaks were compared for central wavelength and efficiency and to see if the "bluer" UV illumination caused a shift to the blue of the resultant PL peaks. Infrared absorption spectra of the films show the presence of the Si-H stretch band near 4.6 microns and confirm the incorporation of Si into the films.

We present spectral evidence showing that the CVD-produced a-Si(x)C(1-x):H films do not solve the band gap issue and that the resultant film PL is therefore still too blue to match interstellar ERE. Furthermore, the inclusion of Si into HAC leads to a strong absorption band (Si-H stretch) near 4.6 microns which is not observed in the diffuse ISM.

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Laboratory Studies of PAH Cations of Interest for Studies of the Diffuse Interstellar Medium

Theodore P. Snow, Valery LePage, and Veronica Bierbaum
University of Colorado

We describe laboratory studies of the chemical properties of small PAH cations which have been suggested as possible carriers of the unidentified diffuse interstellar bands. Our measurements, carried out through the use of a tandem-flowing afterglow-selected ion flow tube (FA-SIFT), show that PAH cations and dehydrogenated PAH cations will quickly migrate to their protonated forms in the diffuse ISM, through the addition of atomic or molecular hydrogen. To date we have made these measurements for ionized benzene ($C_6H_6{}^+$), napthalene ($C_{10}H_8{}^+$), and pyrene ($C_{16}H_{10}{}^+$), as well as their dehydrogenated forms, with similar results in each case. The reaction rates with hydrogen are greater than those for other neutral collision partners (including small molecules); this, combined with the overwhelming abundance superiority of hydrogen, means that protonation is the dominant chemical process. Physical processes such as electron attachment and dehydrogenation via UV absorption may be competitive, so full models are needed in order to determine the ultimate fate of small PAH cations in the diffuse ISM. For now we can say that small PAH cations are probably not good candidates as diffuse band carriers, but large PAHs, large PAH ions, and various forms of radical PAH fragments are not ruled out. In addition to summarizing results already obtained, we describe plans for future laboratory work on this problem.

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Laboratory Data Needed in Support of the FUSE (Far Ultraviolet Spectroscopic Explorer) Mission

Theodore P. Snow and J. Michael Shull
University of Colorado

Donald C. Morton
National Research Council of Canada

The *Far Ultraviolet Spectroscopic Explorer* (*FUSE*) will be launched within a few months. *FUSE* will obtain spectroscopic data in the wavelength interval from 912 to 1175Å with a nominal resolving power of $\lambda/\Delta\lambda = 30{,}000$ on a wide variety of astronomical sources with far-UV flux levels in the range from 10^{-15} to 10^{-10} erg cm^{-2} s^{-1}Å^{-1}. *FUSE* spectra will be applied to a wide variety of astrophysical problems including measurements of the D/H ratio, studies of hot ionized gas in the interstellar and intergalactic media, observations of AGNs and quasars, observations of molecular hydrogen and other molecular species, studies of stellar winds and extended atmospheres, analyses of nebulae and supernova remnants, and general ISM abundances and depletions in our galaxy and in the Magellanic Clouds. The *FUSE* wavelength region has not been well-studied spectroscopically since the *Copernicus* mission of the 1970s. As a result, fundamental data are lacking for a number of transitions of atoms, ions, and molecules. We provide a list of species known to be of interest, in the hope that we can stimulate laboratory measurements of transition probabilities. We also invite input, suggestions, and data on species and transitions not in our list which may be relevent to the *FUSE* mission.

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This paper represents the collective contributions of the entire *FUSE* science team, which is headed by H. Warren Moos of Johns Hopkins University and funded by NASA.

Laboratory Measurment of Opacity for Stellar Envelopes

Springer, P.T, Eastman, R.G., Goldstein, W.H., Hammer, J.H.,Iglesias, C.A.
Lawrence Livermore National Laboratory

Pinto, P.A.
Steward Observatory, Univerisity of Arizona

Deeney, C.
Sandia National Laboratory)

Using the world's most energetic pulsed power accelerators, we create stellar plasma conditions in the laboratory and perform measurements of importance for stellar modeling and astrophysics. We have recently completed a series of experiments to critically test the accuracy of opacity models used in calculations of the structure and pulsation properties of Cepheid Variable stars. Understanding of these stars is important since they serve as a standard candle for extragalactic distances up to 60 million light-years. Astronomical observations of double-mode Cepheid's indicated a lack of understanding for these stars, attributed to inaccuracies in earlier opacity models. The measurements provide the first direct validation of the OPAL opacity models in regimes of interest for stellar envelopes, and resolve long-standing puzzles in stellar pulsation and evolution.

Cepheid pulsation depends critically on the absorption properties of mid-Z elements, mostly iron, at temperatures of order 20 eV, and densities of order 10^{-4} g/cc, where the contribution of the M-shell $\Delta n = 0$ transitions to the Rosseland mean opacity is maximal. Calculations of the opacity at this low density are particularly difficult because they depend sensitively on the treatment of millions of individual lines, and the merging of these lines into quasi-continua. Using the 500 kJ Saturn pulsed power facility at Sandia National Laboratory, we created and measured the opacity of Fe and Ni plasmas at stellar envelope conditions. In particular, the absorption properties of the M-shell $\Delta n = 0$ transition arrays were studied at high spectral resolution and compared to predictions used in Cepheid Variable modeling. Experimental requirements include: high spectral resolution, large homogenous plasma sources, and Planckian radiation fields lasting tens of nanoseconds.

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High-resolution oscillator strength measurements for high-v′ bands of the A(v′)-X(0) system of carbon monoxide

Glenn Stark
Physics Department, Wellesley College, Wellesley, MA

Brenton R. Lewis, Stephen T. Gibson, Julian P. England
Research School of Physical Sciences and Engineering, Australian National University, Canberra, ACT, Australia

Band oscillator strengths for six bands of the CO A(v′) - X(v″=0) system with 12 < v′ < 22 have been determined from high-resolution (resolving power = 750,000) absorption spectra recorded with a tunable VUV laser system. The instrumental bandwidth of the system, 0.11 cm^{-1} FWHM, was significantly less than the widths of the Doppler-broadened CO lines (0.20 cm^{-1} FWHM). Integrated cross sections of individual rotational lines were determined by a least-squares fitting routine, taking into account the effects of the finite instrumental resolution on the measured absorption features. Our derived f-values for the A(13)-X(0), A(14)-X(0), and A(16)-X(0) bands are consistent with other recent measurements, with the ab initio electronic transition moment calculations of Kirby and Cooper (1989), and with f-values derived from the ab initio electronic transition moment calculations of Spielfiedel and Feautrier (1997) in Jolly et al. (1997). Our f-values for the A(18)-X(0), A(20)-X(0), and A(21)-X(0) bands, the first directly measured values for these bands, progressively deviate from band oscillator strengths derived from the electronic transition moment function of Kirby and Cooper (1989). In addition, a pressure-broadening coefficient of (3.1 ± 0.6) × 10^{-4} cm^{-1}/Torr was determined for room temperature CO-CO collisions.

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N_2 and SO_2 VUV Oscillator Strengths for Planetary Atmosphere Studies

Glenn Stark
Physics Department, Wellesley College, Wellesley, MA 02181

Peter L. Smith
Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138

Juliet C. Pickering, Geoff Cox & James Rufus
Blackett Laboratory, Imperial College, London, U.K.

Analyses of Voyager EUV occultation measurements of the N_2-rich atmospheres of Titan and Triton have been hampered by the lack of fundamental spectroscopic data for N_2 — in particular, by the lack of reliable *f*-values and linewidths for electronic bands of N_2 in the 800 to 1000 Å wavelength region. In order to address this shortfall, we have studied the photoabsorption spectrum of N_2 with a resolving power ($\lambda/\delta\lambda$) of 90,000 to 170,000. New band-integrated photoabsorption cross sections (*i.e., f*-values) for the region 900 to 950 Å will be presented. Data for linewidths — which, in the case of the EUV bands of N_2, are often determined by predissociation lifetimes rather than by Doppler effects — are as essential as *f*-values in calculations of the transmission of radiation through the high column densities of N_2 ($nl \simeq 10^{19}$ cm^{-2}) observed by the Voyager spacecraft at Titan and Triton. We will present preliminary linewidth results for some $b(v')$-X(0) bands of N_2. We will also demonstrate that, for some bands and for high column densities, isotopically rare $^{15}N^{14}N$ may contribute disproportionately to N_2 absorption.

Determination of the chemical composition of the atmosphere of Io from Hubble Space Telescope observations in the 190-220 nm wavelength region requires knowledge of the photoabsorption cross sections of SO_2 at temperatures ranging from 110 to 300 K. We have initiated a laboratory program to measure SO_2 absorption cross sections with very high resolving power ($\lambda/\delta\lambda \simeq 500,000$) and at temperatures appropriate to the Io atmosphere. Previous photoabsorption measurements, with $\lambda/\delta\lambda \leq 100,000$, have been unable to fully resolve the very congested SO_2 spectrum. Our measurements are being undertaken at Imperial College, London, using an ultraviolet Fourier transform spectrometer. We present new room temperature SO_2 photoabsorption cross sections in the 190-220 nm region measured with an instrumental resolution of 0.0004 nm. These high-resolution cross sections are compared to previous, lower-resolution, data.

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A Product Study of the C_2H_3 + C_2H_3 and the C_2H_3 + CH_3 Reactions

R. P. Thorn, Jr., W. A. Payne, L. J. Stief and D. J. Bogan

Lab for Extraterrestrial Physics NASA/Goddard Space Flight Center, Greenbelt, MD 20771

F. L. Nesbitt

Department of Natural Sciences Coppin State College, Baltimore, MD 21216

X. Chillier

Astrochemistry Lab, M/S 245-6 NASA/Ames Research Center, Moffit Field, CA 94035

D. C. Tardy

Department of Chemistry University of Iowa, Iowa City, IA 52242

Low temperature vinyl radical reactions are important in the hydrocarbon photochemistry that occurs in the atmospheres of the outer planets and their satellites. Vinyl radical (C_2H_3) and methyl radical (C_2H_3) are products of hydrocarbon photochemistry and are found in the atmospheres of Jupiter, Saturn Titan, and Neptune. Reactions between free radicals take place on virtually every collision and there are multiple product paths, hence their study in the laboratory is very difficult. Both the total reaction rate constants and the fractional yields into the various product paths are needed as input information for models of planetary atmospheres. In the present work we have determined the product yields at low pressure (1 Torr He) and at T = 298K and 200K for the C_2H_3 + C_2H_3 and the C_2H_3 + C_2H_3 reactions.

The measurements were performed in a discharge flow system coupled with collision-free molecular beam sampling to a mass spectrometer operated at low ionizing energies. In both studies, atomic F was generated by microwave discharge of dilute F_2 in helium and entered the rear flow tube port. Vinyl was generated by the reaction of F with ethylene, and methyl by the reaction of F + methane. For the vinyl plus methyl studies a methane/ethylene mixture entered the flow tube through a movable injector. The parent molecule concentrations were adjusted so as to have methyl in 10 to 20 fold excess.

The results are:

$C_2H_3 + C_2H_3$	$\rightarrow C_4H_6$	not observed, detection limit = 1%	(1a)
	$\rightarrow C_2H_4 + C_2H_2$	100 %	(1b)

at 1 Torr and both 200K and 298K. For the vinyl plus methyl reaction:

$C_2H_3 + CH_3$	$\rightarrow C_3H_6$	10% at 298K, 30% at 200K	(2a)
	$\rightarrow CH_4 + C_2H_2$	90% at 298K, 70% at 200K	(2b)

These results are corroborated by a study of the CH_3D yield of the isotopic reaction, $C_2D_3 + CH_3$. The fractional yields determined at low pressure (1 Torr) in this study are an order of magnitude different from those observed at 100 Torr. This will impact the interpretation of observed product abundances on Titan as a function of altitude.

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Elastic Scattering of Electrons By Positive Ions

Clay S. Turner and Steven T. Manson
Department of Physics and Astronomy, Georgia State University

A program of study has been initiated for the calculation of differential cross sections for the elastic scattering of electrons from positive atomic ions of astrophysical interest. These angular distributions are applicable in two distinct manners: directly, to model astrophysical plasmas where elastic electron-ion scattering is an important process; and indirectly, as an aid in laboratory studies of differential cross sections for excitation in electron-ion collisions [1]. At present, the Rutherford cross section is routinely used in modelling; our results show that this can be an extremely poor approximation, especially for large angle scattering.

As a first step, the differential cross section (angular distribution) for elastic electron-ion scattering has been calculated for scattering from the ground states of all ions up to Zn (Z=30) using a relatively simple, but relatively accurate, Hartree-Slater central-field potential. The principal result of this study is that the Rutherford cross section, using the asymptotic charge, can be off at the larger angles by more than three orders of magnitude! In addition, it is generally (but not always) the case that the cross section at the larger angles is larger for the partially stripped ion than for the fully stripped, by as much as more than a factor of three, which shows that the process is not governed by the Z^2 dependence characteristic of Rutherford, but rather by the details of the complex interference among the various partial waves. The accuracy of our results are confirmed by direct experiment [2] and also by indirect results obtained from high-energy ion atom collisions where "quasi-elastic" scattering has been shown to be responsible for the so-called binary peak of ejected electrons [3]. But there is only a small amount of experiment of either type, so that theory and calculation are required.

Our intentions for the future are to increase the accuracy of the calculations by using all of the methodologies developed for atomic and ionic photoionization and apply them to the simpler problem of elastic scattering. We shall also extend this work by considering excited states, particular long-lived metastable states where the results could have astrophysical consequences.

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Laboratory investigations of molecular hydrogen formation on dust grain analogues

Gianfranco Vidali. J. Roser, C.Liu
Syracuse University, Physics Department, Syracuse, N.Y. 13244-1130

Valerio Pirronello
Universita' di Catania, Istituto di Fisica (Sicily)
Ofer Biham
The Hebrew University, Physics Department (Israel)

We report results on molecular hydrogen formation on surfaces of realistic analogues of dust grains under astrophysically relevant conditions. Experiments were conducted using two low energy hydrogen and deuterium beams impinging on samples kept at 6 to 20 K in an ultra-high vacuum chamber. Most of the results reported here are for molecular hydrogen formation on olivine (a silicate), but preliminary results on amorphous carbon and other materials will be presented as well.

Our main results are:

a) Recombination kinetics depends quadratically on reactants concentration at low coverage;

b) Mobility is dominated by thermally activated processes;

b) Recombination depends strongly on surface temperature between 8 and 15 K, depending on sample material.

Based on these results, we propose a model consisting of a set of rate equations for the recombination of molecular hydrogen in different astrophysically environments.

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A New Molecular Model for the Carrier of the 2175 Å Interstellar Extinction Feature

Thomas J. Wdowiak
Astro and Solar System Physics Program Department of Physics University of Alabama at Birmingham Birmingham, AL 35294-1170

Luther W. Beegle
Jet Propulsion Laboratory California Institute of Technology 4800 Oak Grove Drive M/S: 183-601 Pasadena, CA 91109-8099

The constancy of the wavelength of the peak of the interstellar ultraviolet extinction feature (2175 Å 1 10 Å) can be explained by the presence of a repeating substructure in the form of an aromatic double ring, throughout a hydrocarbon molecular aggregate which is a component of interstellar grains. The quantum mechanical origin should make this aspect of the feature independent of grain size, unlike other models such as plasmon resonance. Other aspects of the overall molecular aggregate would explain the observed variation in breadth of the feature (the "bump"). This model was inspired by experiments where the simple polycyclic aromatic hydrocarbon (PAH) naphthalene ($C_{10}H_8$) is subjected to the energetic environment of a plasma, resulting in the synthesis of a molecular aggregate that has ultraviolet spectral characteristics that suggest it provides insight into the nature of the carrier of the 2175 Å interstellar extinction feature and may be a laboratory analog. Ultraviolet, visible, infrared, and mass spectroscopy, along with gas chromatography, indicate that it is a molecular aggregate in which an aromatic double ring ("naphthalene") structural base serves as the electron "box" chromophore that gives rise to the envelope of the 2175 Å feature. This chromophore can also provide the peak of the feature or function as a mantle in concert with another peak provider such as graphite. The molecular base/chromophore manifests itself both as a structural component of an alkyl-aromatic polymer and as a substructure of hydrogenated PAH species. Its spectral and molecular characteristics are consistent with what is generally expected for a complex molecular aggregate that has a role as an interstellar constituent, including infrared spectral character and realistic schemes for complex molecule formation in post AGB stars.

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Critical Evaluation and Compilation of Atomic Transition Probability Data Relevant to Space Astronomy

W. L. Wiese and D. E. Kelleher
National Institute of Standatds and Technology

With partial support from NASA, we are in the process of critically re-evaluating transition probabilities of H - Ca (Z=1-20), elements published about 30 years ago in Vols. I and II of "Atomic Transition Probabilities by W. L. Wiese et al. Much work has been done since then, mostly theoretical, with the most extensive results being provided by members of the Opacity Project (OP). In 1996, Atomic Transition Probabilities of Carbon, Nitrogen, and Oxygen was published by W. L. Wiese, J. R. Fuhr, and T. M. Deters. Work on updating the other elements is continuing. Our new compilations rely heavily on OP results because they are so extensive and are reasonably accurate in many cases. Accurate experiments and other accurate computations are of course also essential to evaluation.

H-Ne (Z=1-10), plus Fe I: During FY 97, we have continued critically evaluating and compiling transition probability data for the light elements H, He, Li, Be, and B. In addition, we have worked on Fe I. We expect to complete these elements during FY 98. As part of out data evaluation process, we have included neutral species and all stages of ionization. Our table for neutral helium is essentially complete. The tables for Li I and II will be finished as soon as relevant energy-level data become available, which should be in FY 98. A new relativistic code for transition probabilities of hydrogenic spectra, with treatment of QED effects, has been written. During FY 98, our group plans to complete f-value tables for hydrogenic spectra of H-Ni (Z= 1-28), for transitions up to principal quantum number n=20. Much of the data for beryllium and boron have been taken from the Opacity Project (OP), and we have included other data sources whenever we deemed to be of comparable or greater accuracy than OP values. We expect to complete our tables on Fe I during FY 98. This table will include vastly improved transition probabilities, incorporating new energy levels and term designations, thereby superseding our previous publication from 1988. We will continue our work on fluorine and neon.

Na-Ca (Z=11-20): Revision and extension of Vol. II also relies heavily on OP results. Thus far weve focused on Na, Mg, Al, and Si (Z=11-14). Currently available OP calculations do not, however, include the effects of the Spin-Orbit interaction, and only multiplet values are reported. For most transitions and most spectra, OP results compare favorably with experiments and other accurate calculations which include Spin-Orbit effects, except for halogen-like and noble-gas-like spectra. Spin-Orbit effects account for the bulk of the noble-gas-like discrepancies, but the origin of the large discrepancies between OP and CIV-3 in Fluorine-like spectra is not yet known. Agreement is good only for the largest line-strengths, S, and rapidly deteriorates for S ¡ 1. K. Berrington and his colleagues at the Belfast OP group have recently developed the capability to incorporate Spin-Orbit effects perturbatively. Early results for F-like Na III indicate that the major part of this discrepancy is not due to this effect.

Photoluminescence by Interstellar Grains: A New Constraint on Dust Models

Adolf N. Witt
The University of Toledo

The recent detection of extended red emission (ERE) in the diffuse interstellar medium on a Galaxy-wide scale, in addition to the earlier ERE detections in reflection nebulae, planetary nebulae, dark nebulae, HII regions, and extragalactic systems supports the conclusion that a major component of interstellar dust is a highly efficient photoluminescent material. I will review the existing astronomical data related to the spectral characteristics of the ERE and the photon conversion efficiency of the ERE process and will derive a set of requirements which laboratory analogs proposed as ERE sources must meet. These include a broad emission band of 60 nm $<$ FWHM $<$ 100 nm with variable peak wavelengths W(pl) in the range 610 nm $<$ W(pl) $<$ 850nm, correlated with the density and hardness of the exciting radiation, high cosmic abundance, high photoluminescence quantum yield ($\gg$ 10%), a broad unstructured UV/visible absorption spectrum, and stability in a wide range of interstellar radiation and density environments. I will discuss how possible candidates, including variants of hydrogenated amorphous carbon (HAC), polycyclic aromatic hydrocarbons (PAHs), refractory organic residues derived from photolysis of ices, fullerenes, and silicon nanocrystals, meet these requirements. Based on existing laboratory evidence, the characteristics of silicon nanocrystals come closest to reproducing the astronomical ERE. Such particles should therefore be considered as a possible new component of interstellar dust.

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Temperature-Dependent Photoabsorption and Emission Studies of Atmospheric Gases, with Application to Planetary Atmospheres

C. Y. Robert Wu[1], F. Z. Chen[1], T. Hung[1], D. L. Judge[1], J. Caldwell[2]
[1] *University of Southern California, Los Angeles, CA*
[2] *York University, North York, ON Canada*

One of our recent laboratory efforts is concerned with the interaction of ultraviolet (UV) and extreme ultraviolet (EUV) photons with planetary, interplanetary, and cometary gases under various temperature conditions. The temperature-dependent measurements include absolute absorption cross sections and absolute cross sections for the production of fluorescence through photodissociation of molecules.

In recent years, we have obtained temperature-dependent absolute absorption cross sections of molecules at temperatures between 140 K and 400 K using a closed absorption cell and up to 650 K using a windowless high-temperature absorption cell. Our temperature-dependent photoabsorption cross sections for CO, C_2H_2, NH_3, H_2S, CS_2, and SO_2 have been applied in modeling optical albedos of Venus, Mars, Saturn, Jupiter, Titan, Io, and Jupiter after the collision of Comet Shoemaker-Levy 9. Future work in this area includes C_6H_6, which is of interest on Jupiter.

For higher temperature measurements, a windowless absorption cell allows us to measure absorption cross sections throughout the UV and EUV spectral region, free of troublesome outgassing problems encountered while using high temperature closed cells. In a windowless absorption cell, however, accurate absolute pressure measurements are difficult to achieve. To resolve this difficulty, we directly calibrate the column density for given experimental flow and temperature conditions of the molecule of interest, and in specific wavelength regions where the absorption cross sections are known to be continuous and nearly constant with wavelength.

We also plan to extend our work on dissociative excitation processes for application to planetary atmospheres. A windowless high-temperature flow cell that is capable of achieving temperatures from 300 to 900 K has been used to determine fluorescence excitation functions of excited atomic and molecular species produced through photon excitation of atmospheric molecules such as N_2 (relevant to the atmospheres of the Earth, Titan, and Triton), CO, and CO_2 (Venus and Mars). Absolute fluorescence cross sections have been measured for the production of specific NI and NII EUV emissions resulting from photodissociation of N_2 at room temperature and 650 K. The dissociative photoionization excitation of N_2 has also been studied at several selected wavelengths shortward of 360 Å, using a coincidence technique to detect the NI 1200 Å fluorescence photon and the N^+ ion. The maximum quantum yields for these processes are of the order of 0.06. Thus, the neutral dissociative excitation processes can be competitive with dissociative ionization excitation for the multiple-electron transition states of N_2. The NI and NII results are important in the interpretation of the ultraviolet airglow emissions of the Earth, Titan, and Triton.

Typical results of both the photoabsorption and photon emission studies will be presented.

High-Resolution, High-Temperature Cross Section Measurements of N_2 and O_2 in the 834 and 917 Å Regions

C. Y. Robert Wu[1], T. Hung[1], D. L. Judge[1], T. Matsui[2], K. Ito[3]
[1] *University of Southern California, Los Angeles, CA*
[2] *Tsukuba University, Tsukuba, Japan*
[3] *Photon Factory, KEK, Tsukuba, Japan*

This paper reports the temperature-dependent ultrahigh-resolution photoabsorption cross section measurements of N_2 and O_2 in the extreme ultraviolet (EUV) region, and their atmospheric modeling implications. One of the important issues regarding the interpretation of the NII 916 Å extreme ultraviolet airglow emissions of the Earth, Titan, and Triton, and the OII 834 Å EUV airglow emission of the Earth, is the effect of temperature on the atmospheric extinction due to absorption by N_2 and O_2. Since the temperature of the upper atmosphere of the Earth is typically in the 200 to 1000 K range it is therefore important to know these molecular cross sections at such temperatures.

We have carried out high resolution photoabsorption cross section measurements of (1) N_2 with a resolution of 0.003 Å and 0.008 Å in the 915.0-917.28 Å and the 833.1-834.5 Å regions at temperatures of 555 and 295 K and (2) O_2 with a resolution of 0.008 Å in the 830-835 Å region at a temperature of 295 K. The 6VOPE (6.65-m vertical off-plane Eagle spectrograph) spectrometer available at the Photon Factory, KEK, Tsukuba, Japan, was employed in the present study.

We are currently carrying out N_2 modeling calculations using our measured data as constraints. Interpolation of the data within the measured temperature range, i.e., 295 and 555 K, will follow. After that, we plan to extend our calculation/modeling using N_2 measurements extended to temperatures as high as 900 K, the temperature of the upper atmosphere of the Earth. This would thus provide a complete set of measured/modeled high-temperature high-resolution data of N_2 for NII and OII airglow modeling of the Earth's upper atmosphere where the temperature profile ranges from 200 to 1000 K. Similar measurements and modeling on O_2 will be performed in the near future.

We also plan to measure the high-temperature absorption cross section of S_2 in the 2600-2800 Å region with a resolution of 0.08 Å. The cross section data thus obtained will allow modelers to better determine the temperature ranges, resolution, and specific vibrational progressions of S_2 which are particularly important to a significant improvement of the determination of the column abundance of S_2 in the observed SL9/Jupiter spectra.

Experimental Verification of Multisphere Light-Scattering Calculations: I) Rigorous Solution and II) the DDA

Yu-lin Xu and Bo Å. S. Gustafson
Department of Astronomy, University of Florida

Because much of the light throughout the solar system is due to sunlight scattered by dust particles and surfaces of larger structures, and because these are commonly believed to be aggregates of complex morphology, there is a need to develop practical solutions to the scattering problem. Currently, numerical techniques are most often used. Best known are the DDA (Discrete Dipole Approximation) originally developed by Purcell and Pennypacker in 1973 [1,2] and the T-matrix method developed by Waterman in 1971 [3]. As more computer power becomes available, the flexibility and conceptual simplicity of the DDA allow users to adapt it to an increasing range of problems encountered in astronomy and astrophysics. We therefore like to know if the DDA yields reliable solutions when applied to solar system problems and find out if a more suitable solution currently exists.

We present comparisons of calculations for the scattering by aggregates of spheres, using respectively the DDA method and our rigorous solution developed recently [4,5], to experimental data from our microwave analogue scattering laboratory [6]. While all tests of the rigorous theory made so far are satisfactory, the approximate solution works well only for the small volume structures that it has been applied to in the past. We show that the validity of the approximate solution is questionable, at least as it is currently implemented, when used on larger structures.

Besides the advantages of the exact solution in reliability and convergency, timing-test results also indicate its superior efficiency to the approximate DDA solution. Our calculations are all carried out on a DEC 600 5/333 AlphaStation. Practical examples show that the exact solution method is approximately ten times faster than the DDA method and that the scattering calculations can be extended to significantly larger aggregates using the exact method.

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