Satellites on Balmer α due to H-H^+ collisions

M. Gerbaldi et al.
Institut d'Astrophysique de Paris, France

The spectrum of a plasma produced by a 300 mJ Nd:YAG 1064 nm laser focused into a cell containing 100 atmospheres of 99.999 % pure H_2 was recorded as a function of time after the plasma-forming laser pulse. At a delay of about 50 ns, while the plasma is highly ionized, a satellite appears in the far wing of H α. The experimental spectrum shown is corrected for scattering of the incident laser light, and for the instrumental response.

New theoretical calculations of the total profile of the atomic hydrogen Balmer α spectral line perturbed by collisions with protons have been made using accurate theoretical molecular potentials to describe the interaction between radiator and perturber. We point out the possible existence of quasi-molecular features due to H-H^+. Measurements of the main one in the spectrum of a plasma confirm the theoretical prediction.

Co-authors: *J.F. Kielkopf (Louisville, USA), N. F. Allard, S. Tremine, M. Gros (Paris, France), A. Decrette (Dijon, France)*

High Resolution IR, Visible, and UV Spectroscopy of the Sun and Arcturus

K. Hinkle et al.
National Optical Astronomy Observatory, U.S.A.

As part of our series of solar and stellar atlases, we have produced high-resolution atlases in the infrared and visible for both the sun and Arcturus. Samples of the spectra will be shown and information provided on obtaining the spectra in both electronic and printed formats. We are currently extending the spectral coverage of both atlases into the 1200-3000Å region of the ultraviolet. In this region line identification can be difficult due to both unidentified spectral features, some of which are modestly strong, and the transition of the spectrum from absorption to emission. Selected segments from the UV atlas will be shown. We will present a summary of atomic and molecular features identified in cool star spectra as well as suggestions for atomic and molecular species that need additional laboratory work.

Co-authors: *L. Wallace & D. Harmer (NOAO, U.S.A.), T. Ayres (CASA, U.S.A. & J. Valenti (STScI, U.S.A)*

High-quality HST/GHRS spectra of Vega: a laboratory for testing of atomic data

E. Niemczura et al.
Wroclaw University, Poland

In this paper we analyse high resolution ultraviolet spectra of Vega collected by the Goddard High Resolution Spectrograph (GHRS) aboard the Hubble Space Telescope (HST). These high signal-to-noise observations can be used for testing the atomic line parameters. However, the observed spectra are very rich in spectral lines, which often blending together produce strong spectral features. We therefore calculated synthetic spactra for different chemical composition of elements and compared them with the observations of the well-known star, Vega.
The theoretical spectra calculated for Kurucz's data base fit observations very good at near ultraviolet region (2339 Å $< \lambda <$ 2860 Å) where almost all observed lines can be identified and well reproduced addopting only small corrections to gf-values of some multipletes. The agreement is much worse at 1300 Å $< \lambda <$ 1340 Å, where about 45 % of observed lines remain unidentified.

Analysis of Fe I-II spectra of β Cassiopeiae

J. Daszynska et al.
Wroclaw University, Poland

We report an analysis of high resolution ultraviolet spectra of β Cassiopeiae collected during IUE satellite mission. In particular, we focus on Fe I-II spectra at wavelength region of 2575 - 2850 Å.
First, we made line identification by comparison of synthetic spectra calculated for different chemical composition of elements with observations. Lines corresponding to Fe I-II multiplets were then identified and their gf-values are discussed using Kurucz's and OP atomic data bases. Quality flags are assigned for the multipletes taking into account the agreement between theoretical spectra and the observations of β Cas. Finally, Fe-abundance for this star is derived from all Fe I-II lines located at the investigated spectral region.

Fourier transform spectroscopy of doubly ionised transition elements

J.C.Pickering et al.
Imperial College, London, UK

At Imperial College we are using our unique Fourier Transform (FT) spectrometer to record high resolution spectra of doubly ionised iron group elements down to a record short wavelength of 135 nm. Improvements in the quality of astrophysical spectra observed with the new generation of high resolution spectrographs on ground and space based telescopes have highlighted the inadequacies of the laboratory atomic data base needed to interpret these observations, especially in the VUV region (below 200nm) where the majority of absorption lines from hot stars are found. In these spectra lines from doubly and singly ionised species predominate. We are using a DC Penning discharge source to excite the doubly ionised 3*d*-group elements. Spectra of Fe III at visible through VUV wavelengthshave been recorded at Imperial College and have been complimented with IR spectra measured at NIST. The improvement in wavelength accuracy is an order of magnitude over previous work. Branching ratios from intensity calibrated spectra will be combined with level lifetimes to yield oscillator strengths. Work on Ni III and Mn III is also underway.

This work was supported in part by NASA Grant NAG5-4348 to Harvard University, and by PPARC of the UK. J.C.Pickering is supported as a Royal Society University Research Fellow

Co-authors: *A.P.Thorne (IC), and P.L.Smith (Harvard-Smithsonian CfA, USA)*

The Imperial College Laboratory Astrophysics Programme

J.C.Pickering et al.
Imperial College, London, UK

The Imperial College (IC) Fourier Transform Spectroscopy group has been focusing on improvements in the laboratory atomic data base for astrophysics. In recent years the group has made enormous improvements in the atomic data for neutral and singly ionised Fe, Co, Cr, V & Ti. We report a few examples of recent new measurements at IC which impact on a variety of astrophysical problems: Highly accurate wavenumber measurements of some lines of Cr II, Mg I & II, Ni II and Zn II for use in studies investigating a possible time variation in the fine structure constant α; Our extensive project of measurements of Ti II branching ratios and oscillator strengths is complete and represents a vast increase in the number of Ti II lines for which f-values are known to accuracy sufficient for astrophysical applications; Our projects on large scale term analyses of Cr I, V I & V II continue - and many new energy levels will be found, and lines will be identified for the first time. Improvements in wavelength and energy level accuracies are over an order-of-magnitude.

Co-authors: *A.P.Thorne , R.C.M.Learner & R.Blackwell-Whitehead*

Laboratory Studies of Atomic Ion VUV Emission Spectra of Astrophysical Interest

W.-Ü L. Tchang Brillet et al.
DAMAp, UMR 8588 du CNRS, Observatoire de Paris-Meudon, also University Paris 6

Laboratory studies of the emission spectra of multiply (two to five times) charged atomic ions are being carried out in the VUV wavelength region ($50-300nm$) motivated by the recent space missions (HST, SOHO and FUSE). The spectrogrammes are produced using vaccum spark sources and high resolution normal incidence vacuum spectrograph. The precision of $\Delta\lambda = \pm 0.0003-0.0005nm$ obtained on wavelengths lead to reliable identification of the spectral lines and to the determination of the atomic energy levels. The atomic configurations are interpreted by parametric calculations giving rise to improved transition probabilities. Ions of the iron (Mn, Fe) and platinum groups (Au, Os) have been investigated involving international collaborations (Institute of Spectroscopy of Troitsk, University of Amsterdam, University of Liège, University of Antigonish, NIST). Future projects concern ions of rare earth elements.

Co-author: *J.-F. Wyart, Laboratoire Aimé Cotton, CNRS II*

Doubly Hollow Lithium with Even Parity

J.-C. Chang et al.
National Hsinchu Teachers' College, Taiwan

The energy of double hollow lithium states with even parity are calculated with the saddle-point method. The energy shift and width of those resonance states are calculated with the saddle-point complex-rotation method. The partial Auger width is studied for each single open channel as well as for the fully coupled open channels. The predicted Li $[3s3p^2]\,^2P$ resonance energy and width are 176.294 and 0.3992 eV, respectively. The predicted Li $[3s3p^2]\,^2D$ resonance energy and width are 175.582 and 0.2626 eV, respectively. Some other resonances are studied as well.

Co-author: *Kwong T. Chung*

BelData - An Atomic Database for Astrophysical Purpose

L. Č. Popović et al.
Astronomical Observatory Belgrade, Volgina 7, 11000 Belgrade, Serbaia, Yugoslavia

In early-type stars like B and A stars and white dwarfs, Stark broadening is the main pressure broadening mechanism, and the corresponding Stark broadening parameters are of interest for a number of investigations related to stellar plasma. One may mention as examples calculation of stellar opacities, stellar atmospheres modeling and investigations, abundance determinations, interpretation and modeling of stellar spectra and investigation and modeling of subphotospheric layers.

In order to provide the Stark broadening parameters for astrophysical purposes extensive calculations of a large number of radiators have been performed at Astronomical Observatory in Belgrade. The BelData, the data base which contents this Stark broadening parameters, has as a goal to provide the faster and easier access to the data.

In the paper the present status and future plans of the BelData will be discussed.

Co-authors: *M. S. Dimitrijević and N. Milovanović*

The electron-impact broadening parameters for Pd II spectral lines.

D. Tankosić et al.
Astronomical Observatory Belgrade, Volgina 7, 11000 Belgrade, Serbia, Yugoslavia

Spectral lines of palladium in various ionization stages are observed in spectra of different type stars. For example spectral lines of neutral palladium are present in solar spectrum, while Pd II spectral lines are observed in Hg Mn star ξ Lupi spectra. Consequently, experimental and theoretical spectroscopic data are needed for the analysis and modeling of such lines, as well as for atmosphere investigation and modeling of such stars. Among the required spectroscopic data, Stark broadening data are of interest especially for hot stars as e.g. for Hg-Mn stars and white dwarfs.

There is not experimental data on the Stark broadening of ionized palladium. However, Stark broadening parameters for Pd II λ=136.33nm have been estimated by Lakićević (1983), based on regularities and systematic trends.

In order to provide Stark broadening data for singly ionized palladium we have calculated, by using the modified semiempirical approach, the corresponding data for Pd II lines, belonging to the $5s'''^2\mathrm{G}$-$5p'''^2\mathrm{F}^o$ multiplet. Calculation were performed for an electron density of $10^{23}\mathrm{m}^{-3}$ and within the temperature range of 5000K-50000K.

Co-authors: *M. S. Dimitrijević and L. Č. Popović*

Stark Broadening Effect in Hot Star Atmospheres: Tl II

N. Milovanović et al.
Astronomical Observatory, Belgrade, Yugoslavia

Electron-impact broadening is the main pressure broadening mechanism in the hot star atmospheres. Satellite ultraviolet spectral lines observations made by e.g. International Ultraviolet Explorer (IUE) and Goddard High Resolution Spectrograph (GHSR) installed at Hubble Space Telescope provided much better possibilities for the investigations of the trace elements spectral line in stellar atmospheres. Consequently, Stark broadening parameters data for such lines become of interest for stellar spectra interpretation, analysis and modelling as well as for abundance determination.

In order to provide the needed spectroscopic data for singly ionized Thallium spectral lines we present Stark broadening parameters for Tl II spectral lines calculated within the modified semiempirical approach. Calculations were performed within temperature range 5000K-50000K and for an electron density of $10^{23}\mathrm{m}^{-3}$.

These calculated data, together with other Stark broadening parameters for various elements, will be included in Belgrade Astronomical Database (BELDATA) on Internet address www.aob.bg.ac.yu.

Co-authors: *M. S. Dimitrijević and L. Č. Popović*

A Project for large-scale Stark broadening Data Calculation: Cd I

Milan S. Dimitrijević et al.
Astronomical Observatory, Belgrade, Yugoslavia

In order to complete as much as possible Stark broadening data needed for astrophysical and laboratory plasma research and stellar opacities calculations we are making a continuous effort to provide reliable Stark broadening data for a large set of atoms and ions. Our calculations are performed within the semiclassical - perturbation formalism, for transitions when a sufficiently complete set of reliable atomic data exist and the good accuracy of obtained results is expected. Extensive calculations have been performed, up to now for a large number of various radiators, and now we try to organize the obtained results in the BELDATA database (www.aob.bg.ac.yu). As the continuation of our project, we have calculated within the semiclassical-perturbation formalism, electron-, proton-, and ionized helium-impact line widths and shifts for 48 neutral cadmium lines, as a function of temperature and perturber density. Results are compared with other experimental and theoretical data. Besides the presentation of new results, our intention is to review our previous work as well.

Co-author: *Sylvie Sahal-Bréchot (Observatoire de Paris, Meudon, France)*

The CHIANTI atomic database: extension to the X-rays

G. Del Zanna et al.
DAMTP, University of Cambridge, UK

The CHIANTI atomic database consists of a critically evaluated set of atomic data (energy levels, radiative data, wavelengths, and electron collisional excitation rates) necessary to calculate the emission line spectrum of astrophysical optically-thin plasmas. IN the past few years, CHIANTI has been extensively used in the EUV for calibration and plasma diagnostics. This database has now been extended in the 1 - 50 Åwavelength region, to include all the significant emission lines (Dere et al., 2000). Comparisons of CHIANTI predicted line intensities with high-resolution X-ray solar (SMM/FCS, SOLEX) and stellar (Chandra HETG) spectra are presented here, to provide an assessment of the completeness and reliability of the most recent atomic data.

Atomic data for Astrophysics: Internet Centre of Atomic Data

A.F.Kholtygin
Astronomical Institute of St.Petersburg University

A concept of the Internet Center of Atomic data for astrophysics is discussed. This Center includes three parts: Atomic data collection; Atomic data guide and Atomic data news. The Atomic Data Collection contains the tables of atomic data (mainly referred to excitation of atoms and ions by electron impact) and a vast list of atomic databases. The short descriptions of these databases are given. The Atomic data guide presents a description of the atomic data dispersed in the Internet and gives a convenient tools to find the data you need. The information on the various collections of atomic data, not included in regular journal and Internet databases are given. The Atomic data news is an updated page, including the information on the scientific meetings relevant to obtaining and using atomic data and new methods, programs and atomic data collections and databases. The preliminary working version of such center [1] is described.

1. http://www.astro.spbu.ru/staff/afk/AdDatCenter/adc.html

NIST Databases on Atomic Spectra

W. C. Martin et al.
National Institute of Standards and Technology, USA

Several NIST atomic and molecular databases of astronomical interest are accessible at the URL: physics.nist.gov. The *Atomic Spectra Database (ASD)* offers evaluated data on energy levels, wavelengths, and transition probilities for atoms and atomic ions. Data are given for some 950 spectra and 70,000 energy levels. About 91,000 spectral lines are included, with transition probabilities for about half of these. Additional and improved data resulting from our ongoing critical compilations will be included in successive new versions of *ASD*. Our other atomic databases include the *Ground Levels and Ionization Energies for Neutral Atoms*, and bibliographic databases on transition probabilities and line broadening. An upcoming new database will give wavelengths and intensities for the stronger lines of all neutral and singly-ionized atoms, along with energy levels and transition probabilities for the persistent lines. This work is supported by the U.S. National Aeronautics and Space Administration and the U.S. Department of Energy.

Co-authors: *J. Fuhr D. Kelleher, P. Mohr, A. Musgrove, K. Olsen. L. Podobedova, J. Reader, E. Saloman, C. Sansonetti, J. Sansonetti, W. Wiese*

Grain Formation in the Stellar Environment: Low vs. High Luminosity Stars

T. Tsuji
Institute of Astronomy, Univ.Tokyo, Japan

Presence of dust in cool luminous stars has been known for a long time and its mechanism of formation is relatively well understood by a non-equilibrium process at relatively low temperature of the circumstellar envelope. The same mechanism of dust formation cannot be applied to cool low luminosity stars such as brown dwarfs in which dust forms in the photosphere. For the dust to be sustained in the photosphere for a long time, the dust in cool dwarf stars should be in detailed balance (LTE) with the gas. Such a situation is realized only when dust cannot grow too large because of the destructive efect of the surface tension force and hence at relatively high temperature near the condensation temperature. Then, dust exists only deep in the photosphere, but cannot in the cool surface layers. For this reason, the photosphere of brown dwarfs should be hybrid of deeper layers dominated by dust grains and surface layers dominated by volatile molecules. Recent observations show the presence of the two distinct groups of brown dwarfs: L dwarfs apparently dusty and T dwarfs showing strong bands of methane (CH_4) but little evidence for dust. We show that a unified understanding of the observed spectra and colors of L and T dwarfs can be provided by our hybrid models, and this fact in turn confirm that the dust of brown dwarfs forms in LTE deep in the photosphere.

Dust formation in C-rich AGB stars

P. Cau
UMIST, U.K.

We use a detailed chemical and physical model of the inner wind of the carbon-rich star IRC-10216, which includes the effects of periodic shocks, to model the nucleation of PAHs, their aggregation and the further growth of these structures. We show that once dimers of PAHs are formed in the wind, they efficiently stick together giving rise to a population of grains with an average diameter of several Angstroms. We also consider deposition of acetylene on these grains and show that, assuming certain values for the rate of the involved reactions, observational constraints on the size of grains and on the depletion of acetylene can be met.

A Laboratory Investigation of the Formation of Pre-Solar Oxide Grains and Grains in the Early Solar System

B. D. Leskiw et al.
Penn State University and Goddard Space Flight Center, USA

Our research on the stoichiometry, structure, and nucleation of silicon oxide clusters and their application to cosmic oxide grain formation and nucleation will be presented. The role of clusters in the chemical pathways leading to the formation of grains in cooling outflows of circumstellar shells in evolved stars, and possible oxygen isotope effects in grains will be illustrated. Our recent experimental data on silicon oxide clusters have implications relevant to recent observations by the Infrared Space Observatory (ISO) indicating the presence of crystalline forms of oxide grains in oxygen-rich shells of evolved late- type stars. The silicon oxide clusters were produced in a laser vaporization source and either the cationic or anionic clusters were investigated by pulsed field extraction in a time-of-flight mass spectrometer, or the neutral clusters were probed by multiphoton ionization with a femtosecond laser (50 fs @ 800 nm). This is the first detailed specific experimental study of the role of clusters on the formation of cosmic grains. The study has become feasible as a result of long-term investigation of the development of atomic and molecular beam methods. The experimental results have implications for the chemical origin of the formation of our solar system.

Co-authors: *S. E. Kooi and A.W.Castleman, Jr.*

Silicon-Carbon chemistry in carbon stars: Spectral modelling of SiC_2

B.L. Duigan et al.
University of Nottingham, U.K.

Silicon dicarbide (SiC_2) and other silicon containing molecules have been detected in various astrophysical environments, the former being particularly abundant in the atmospheres and circumstellar envelopes of carbon stars[1]. The chemical composition, coupled with the cool surface temperatures of these stars, provide ideal conditions for the formation of exotic chemical species[2].

In one of the first high resolution studies of carbon stars, data were recorded for three nights at the William Herschel Telescope, La Palma, Spain. The main aim of this study was to provide rotationally resolved spectra of the Merrill-Sanford bands of SiC_2. Computational modelling of the SiC_2 origin band was performed. Comparison of modelling with observational data has allowed a preliminary identification of the location of SiC_2 in these stars. These may be divided into stars with circumstellar (low temperature) SiC_2 or photospheric (high temperature) SiC_2. The application of a detailed knowledge of SiC_2 spectroscopy therefore yields insight into the physical and chemical conditions in the circumstellar environments of carbon stars.

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Co-authors: *T.R. Kendall, P.A. Couch & P.J. Sarre*

TiO in the optical spectra of AGB stars: Spectral modelling

T.R. Kendall et al.
University of Nottingham, U.K.

Absorption features due to TiO are are prominent in the optical spectra of cool, evolved, oxygen-rich stars. Recent advances in spectroscopic studies [1,2,3] of this molecule allow, for the first time, modelling of the TiO bands. We present simultaneous modelling of the α, γ and γ' bands between 5400 and 7200 Å in a number of high resolution (R=39000) spectra of M-type AGB stars. Observational data were obtained using the GIRAFFE echelle spectrograph at the 1.9m Radcliffe reflector, Sutherland, South Africa. The computational code uses three-dimensional radiative transfer and non-LTE techniques and takes into account line saturation. This spectral synthesis yields temperature information and column densities for the TiO molecule in these environments.

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Co-authors: *P.A. Couch & P.J. Sarre*

Nonadiabatic effects in the photodissociation of SiO

F. Dayou et al.
Observatoire de Paris-Meudon, France

This study concerns the photodissociation of SiO by absorption from the first vibronic state of the ground electronic surface $X^1\Sigma^+$. In this photodissociation process, the contributing states must have a large transition moment with the ground state. Thus the most likely candidate is the $E^1\Sigma^+$ state. The non adiabatic interaction between E and the upper $F^1\Sigma^+$ state near R=4.5 bohr should lead to perturbations in the photodissociation cross sction for energies ranging in the region of the avoided crossing. All the relevant ab initio electronic potentials and the transition moments involved in the X-E and X-F transitions, as well as the E-F non adiabatic radial coupling matrix element, have been calculated at the MCSCSF level, using the MOLPRO package. Then, two different approaches (time-independent and time-dependent methods) have been used to obtain the photodissociation cross section.

Co-authors: *W.-Ü L. Tchang Brillet, A. Spielfiedel, N. Feautrier (Meudon) & M. Monnerville (Université de Lille)*

Theoretical modeling of optical spectra of L-dwarfs - semiempirical approach

Ya. Pavlenko
Main Observatory, Kyiv-127, 03680 Ukraine

Problems of theoretical modeling of the optical spectra ($\lambda\lambda$ 600 - 950 nm) of L-dwarfs (1000 < Tef < 2200 K) are discussed. To fit the observed features in the visible part of the spectra of the coolest objects we use some additional suggestions: a) there are *extra* depletions of molecular species absorbed in the visible region of L-dwarf spectra; b) there are (a few?) additional (dusty?) opacity κ sources in their atmospheres; c)dditional opacity κ depends on wavelength.
We found:
a) the overall shape of the optical spectra of L-dwarfs are governed by the wings of K I and Na I resonance doublet lines. Their profiles show a strong dependence on Tef and gravity; b) The comparison of the observed and computed spectra allows us to determine the yield of the depletion of molecular species into the dust and parameters of the additional opacity; c) the (0-0) band of the $A^6\Sigma^{(+)}$-$X^6\Sigma^{(+)}$ system of CrH molecule is fitted in the red part of the spectrum (λ 860 nm) of the coolest L-dwarfs.

Water vapour in cool dwarfs

H.R.A. Jones et al.
Liverpool John Moores University, U.K.

M dwarf spectra beyond 1.35 microns are dominated by water vapour yet terrestrial water vapour makes it notoriously difficult to make accurate measurement of the water vapour bands from ground-based observations. We have used ISO spectra to cover the 2.5–2.9 micron region in a range of M dwarfs. Our strategy is to construct a small grid of well-studied M stars with different conditions of temperature, and metallicity: spectral types M2V, M4V, M6V and M8V, M4Vsd and two M6III. The observations give much better coverage of the the strong absorption bands around 2.6 and 2.7 microns and are at higher resolution than ground-based studies. We find excellent agreement with the predictions of the latest ab intio calculations for water vapour. These comparisons will be presented together with a new scale of bolometric magnitudes for the M dwarf regime.

A HCN and HNC Rotational-Vibrational Line List and Spectroscopic Data for Astronomy.

G. J. Harris et al
Department of Physics and Astronomy, UCL, U.K.

The linear triatomic molecule HCN is known to be abundant in the atmosphere of carbon stars with Teff less than 3000K. Jorgensen et al found that including an opacity from just the 8 strongest infrared HCN vibrational bands caused their model atmosphere to expand by 5 times whilst the surface pressure dropped by one or two orders of magnitude. The temperatures within the type of carbon star in which HCN is a significant source of opacity are such that energy levels up to 20 000 cm-1 above the ground state will be significantly populated. Hence hundreds of vibrational levels will be significantly populated and there will be more than just the 8 vibrational bands contributing to the overall HCN/HNC opacity. Neither theoretical nor experimental data exists to the extent needed to fully model the opacity of HCN and HNC within carbon star atmospheres. We present here new ab initio global HCN and HNC potential and dipole surfaces and spectroscopic data. These form a starting point for calculating an extensive ab initio HCN/HNC rotational- vibrational line list and hence a new HCN/HNC opacity function to aid the modeling of carbon star atmospheres.

Co-authors: *O. Polyansky, J. Tennyson, T van Mourik*

Oscillator Strengths for B–X, C–X, and E–X Transitions in Carbon Monoxide

S.R. Federman et al.
University of Toledo, USA

Oscillator strengths for transitions in CO were obtained at the Synchrotron Radiation Center of the Univ. of Wisconsin-Madison. Our focus was on transitions that will be observed in interstellar spectra with the *Far Ultraviolet Spectroscopic Explorer*; these transitions are also important in studies of selective isotope photodissociation where fractionation among isotopomers can occur. Absorption from the ground state ($X\ ^1\Sigma^+\ v'' = 0$) to $B\ ^1\Sigma^+$ ($v' = 0, 1$), $C\ ^1\Sigma^+$ ($v' = 0, 1$), and $E\ ^1\Pi$ ($v' = 0, 1$) was measured with the 4 m Normal Incidence Monochomator. The instrumental resolution was approximately 0.10 Å. As in our earlier experiment, fits to the A–X (5,0) band, whose oscillator strength is well known, yielded the necessary column density and excitation temperature. These parameters were used in the least-squares fit of the transitions of interest to extract their band oscillator strengths. The results will be compared with other recent determinations.

Co-authors: *S. Cheng, M. Fritts, and D.C. Knauth (Univ. of Toledo) and K.M. Menningen and K. Fulk (Univ. of Wisconsin-Whitewater)*

Line by Line Spectra of the Intersystem Bands of CO in the 130-160 nm Range

M. Eidelsberg et al.
Observatoire de Paris-Meudon, 92195 Meudon, France

When dense interstellar regions are observed in the VUV, the allowed CO A-X bands may become strongly saturated. In such cases, the weak spin forbidden intersystem bands which borrow their intensity by mixing with the $A^1\Pi$ state provide an interesting alternative.

The line by line spectra of the intersystem transitions relating the $e^3\Sigma^-(v')$, $d^3\Delta(v')$, and $a'^3\Sigma^+(v')$ levels to the fundamental $X^1\Sigma^+(v''=0)$ level have been calculated up to J'=34. The calculations take into account for the first time the interaction of a given level of the triplet state with several vibrational levels of the $A^1\Pi$ state.

Band integrated oscillator strengths have been calculated and compared to the values obtained by Federman et al. at 4.2K from interstellar absorption spectra recorded with the HST and with low resolution laboratory spectra obtained at room temperature on the LURE Synchrotron facility at Orsay. Excellent agreement is found. Recent high resolution spectra obtained at 77K by Yoshino et al. on the KEK Photon Factory facility and by us on the new SU5 line at Orsay are successfully simulated with these synthetic spectra. An Atlas of these intersystem transitions is in preparation.

Co-authors: *F. Rostas and J.L. Lemaire*

The UMIST database for astrochemistry 1999

Y. H. Le Teuff et al.
UMIST, U.K.

We report a new version of the UMIST database for astrochemistry. The previous (1995) version has been updated and its revised format is revealed here. It now comprises of 4170 gas-phase reactions between 397 species important in astrophysical environments. The database now also contains the temperature ranges and – where available – the temperature dependence of all its reactions. New data on photo process cross sections (ionisation, dissociation, fragmentation) for a few species are also available. Finally, a new online Java applet for data extraction has been created and its use is explained in detail.

Co-authors: *T. J. Millar & A. J. Markwick*

Line f-values for the $d(7)$-$X(0)$ intersystem band of CO

P. L. Smith et al.
Harvard-Smithsonian CfA, Cambridge, MA USA

Because of the high abundance of interstellar CO, absorption lines of the allowed A-X bands (110 to 156 nm) are often saturated and thus difficult to use for ISM studies. Therefore, we have studied the absorption spectrum of 5 weaker intersystem (spin-changing) bands in order to provide line oscillator strengths (f-values) for some absorption features seen with HST. Line oscillator strengths can be difficult to calculate for these weak bands because each is perturbed by a number of vibrational levels of the A state.

For the measurements, the gas studied was cooled to 77 K; the resolving power was about 200,000. Line f-values were determined from an equivalent width analysis of absorption spectra obtained at a number of column densities. We present line oscillator strengths for some of the lines of the $d\ ^3\Delta_i(7)$ - $X\ ^1\Sigma^+(0)$ band and compare to results from calculations.

This work was supported in part by NASA Grant NAG5-4348 to Harvard University.

Co-authors: *G. Stark (Wellesley College), K. Yoshino (Harvard-Smithsonian CfA), and J. R. Esmond (Harvard-Smithsonian CfA; deceased)*

Radiative Association in $Li^+ + H^-$ collisions

A. S. Dickinson et al.
Physics Dept., Univ. of Newcastle upon Tyne, NE1 7RU U.K.

Radiative association is one of the ways of forming LiH in low density environments. Its formation in collisions of Li(2p) +H(1s) has been shown to be about five orders of magnitude faster than for Li(2s) + H(1s) [1]. We investigate LiH formation in $Li^+ + H^-$ collisions, considering association on both the C and D $^1\Sigma^+$ states as about 96% of the mutual neutralization is to these states at low energy [2]. A quantal description of the process [3] has been used. The potentials are from ref. [4] and the dipole moments from ref. [5]. Similar results were obtained from both the C and D states. At 1000 K the total radiative association rate coefficient from the D state is 9.2×10^{-15} cm^3/s, compared to 2.1 $\times10^{-20}$ cm^3/s in Li(2s) + H(1s) collisions [6].

British Council support is gratefully acknowledged.

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Co-author: *F X Gadéa (I.R.S.A.M.C., Toulouse, France)*

Gas heating and cooling in normal late–type galaxies

D. Pierini et al.
Max-Planck-Institut für Kernphysik, Germany

We present observational evidences on the mechanism of gas heating and on its location within the different phases of the interstellar medium (ISM) of normal (i.e. non–starburst) late–type galaxies. The analysis refers to a sample of 19 Virgo cluster galaxies of different massive star–formation activity, where the dust, gas and stellar components are rather well characterized via multi–wavelength observations. In particular, we make use of recent ISO LWS and CAM measurements. We confirm the theoretical expectations that the gas heating is due to electrons photoelectrically ejected mainly from the carriers of the Aromatic Infrared Bands (AIBs), whatever the nature of the latter is. The photoelectric effect is due only to the far–ultraviolet component of the Interstellar Radiation Field, which, instead, heats, as a whole, the carriers of the AIBs and the other dust components. This explains both the behaviours of the gas cooling–line-to-dust mid–infrared emission ratio and of the gas cooling–line-to-dust total far–infrared continuum emission ratio with the mass normalized star–formation rate of the galaxy. Finally, we show that the gas heating takes place in both the "compact" (i.e. associated to HII regions and giant molecular clouds) and "diffuse" (i.e. associated to the HI gas) components of the ISM.

Co-authors: *Boselli A., Leech K.J., Lequeux J., Tuffs R.J. and Völk H.J.*

HI Shells in the Large Magellanic Cloud

S. Kim et al.
MSSSO, Australia; UIUC, USA

A recent high-resolution HI survey of the Large Magellanic Cloud (LMC) shows that the structure of the neutral atomic interstellar gas is dominated by numerous shells and holes as well as complex filamentary and spiral-type structure. We present an up-to-date catalog of candidate HI *supergiant* and *giant* shells in the LMC. The candidates are visually selected from the HI data cube using selection and classification criteria which are described. 23 supergiant shells, defined as those regions whose extent is much larger than the HI scale height, are catalogued. 103 giant shells (radii less than the scale height of the HI gas) are catalogued. We further classify the HI shells into five different types, based on the comparison of the HI with their associated Hα emission. The size distribution of HI shells follows a crude power law, $N(\log R) \propto R^{-1.5}$. For constant energy input to the HI shells and a constant shell creation rate, a shell luminosity spectrum of the form $\phi(L) \propto L^{-\beta}$, where $\beta = 1.75 \pm 0.2$, is obtained. This agrees well with the observed HII region luminosity spectrum for the LMC (Kennicut, Edgar & Hodge 1989) which has $\beta = 1.75 \pm 0.15$. HI shells containing HII regions and OB associations seem to expand more rapidly than those without, providing direct evidence for substantial input of mechanical energy from regions of star-formation.

Co-authors: *M.A. Dopita (MSSSO, Australia), L. Staveley-Smith (ATNF, Australia), & M.Bessell (MSSSO)*

H_2O Masers as a Product of Turbulence

V. Strelnitski et al.
Maria Mitchell Observatory, U.S.A.

We further develop the new conceptual model of H_2O masers in regions of star formation proposed recently by the present and other authors. According to this model, the H_2O masers are produced in slightly supersonic, small-scale shocks, in which the energy of turbulence caused by the interaction of the outflow from a young star with its surroundings is dissipated. The turbulent nature of H_2O masers is confirmed by the coincidence of the observed sizes of the masers with the predicted scale of the shocks, the fractal structure of the maser clusters, and the Kolmogorov spectrum of the observed velocity field. We discuss a theoretical model of supersonic turbulence, which can reconcile the observed combination of Kolmogorov spectrum with a low fractal dimension of the set on which turbulence dissipates. Comparison of a computer simulation of the propagation of maser radiation through a turbulent medium, with the observed interferometric maps of H_2O masers leads us to conclude that these masers are saturated.

Co-author: *B. Holder*

Strong Unidentified Emission Line at 2.8935 μm from ISO Observations

R.H. Rubin et al.
NASA/Ames, Orion Enterprises, U.S.A.

We have detected anunidentified (uid) strong emission line in an ISO/SWS spectrum of the Orion Nebula. The line has a rest wavelength 2.89350$\pm$0.00003 μm and is a factor of 3.6 weaker than the nearby, H I 11–5 line (2.8728 μm). The $14'' \times 20''$ aperture was centered at the position 1SW, observed by us with HST, that is $26.2''$ W and $18.5''$ S of θ^1Ori C (Rubin et al. 1997, ApJ, 474, L131). The average surface brightness in this aperture is 3.9E-18 W m^{-2}arcsec^{-2}. We do not detect the uid line in our SWS02 spectra of any of the several bright planetary nebulae, which we observed for a comparable time. We have also examined many of the ISO archival spectra taken by others of the Orion Nebula and find no indication of the uid line. Unlike our 1SW position (well in the heart of the ionized region), most of these other Orion spectra were taken at positions where molecular/ photodissociation (PDR)/neutral species would be expected to dominate. Recent spectra of Orion taken at UKIRT confirm the presence of this strong uid line. A long-slit observation ($80'' \times 1''$) centered at 1SW and pointing through θ^1Ori C showed that the emission is spatially extended and appears to be coincident with the brightest part of the H II region. A second observation with the slit passing through the proplyd P159-350 shows no significant enhancement of the line at that location.

Co-authors: *T.R. Geballe (Gemini Obs.), S.W.J. Colgan (NASA Ames), R.J. Dufour (Rice Univ.)*

H_2 IR Emission and the Formation of dense Structures in the Orion Molecular Cloud (OMC1)

L. Vannier et al.
Observatoire de Paris-Meudon, France

Observations are reported of IR emission of H_2 from a region of OMC1 between the BN object and IRc2 to the north and the Trapezium stars to the south. Data were obtained using the ESO 3.6m telescope in the K-band around 2μm with the ADONIS adaptive optics system. Images of H_2 v=1-0 S(1) show a spatial resolution of $\sim$ 0.15".
Detailed investigations of the distribution of sizes of structures in our images have been performed by area-perimeter analysis, Fourier analysis and brightness distribution studies. These demonstrate that structure is not fractal but shows preferred scales at sizes of 2" and 0.3" (1"$\sim$ 2.1x10^{-3}pc). In an attempt to estimate the density in observed structures, predictions of both shock and photodissociation region models have been compared with measured emission brightness in the H_2 v=1-0 S(1) line. Magnetic (C-type) shocks with velocities of 30 kms^{-1} and preshock densities of 10^6cm^{-3} yield the best representation of our data, notwithst anding significant discrepancies for the brightness ratio between v=2-1 S(1) and v=1-0 S(1) lines. Our results show that post-shock densities are several times 10^7cm^{-3}. This is sufficiently high that the passage of C-type shocks in Orion yields gravitational instability which may in turn trigger star formation in the post-shock gas.

Co-Authors: *Lemaire J.L., Pineau des Forêts G., Rouan D., Rostas F. (France), Field D., Pijpers F. (Denmark)*

Diffuse Interstellar Bands (DIBS) - Spectroscopic laboratory data relevant to astronomical observations.

Fred M. Johnson
California State University, Fullerton, USA.

Results from an extended literature survey and a 35 year experimental spectroscopic program will be presented. These results enable the unraveling of the underlying code necessary for the identification of the dominant chromophores responsible for the DIBs. The main chromophores are the thermodynamically stable tetrabenzoporphyrins (MgTBP and H_2TBP). The large amount of spectroscopic data includes low temp. supersonically cooled vapor and quasaline matrix isolation spectra, as well as Raman and FTIR data. Electron bombardment (70 eV) of MgTBP and analysis via mass spectrometry of the resulting molecular fragments, reproduced 19 out of a possible 24 presently identified interstellar "CHN type" interstellar molecules, including the enigmatic MgNC radical! The lifting of the otherwise degenerate electronic S_1 state of MgTBP in a Shploskii matrix results in a 36 cm^{-1} splitting, seen in about a dozen DIBs as well as lab spectral transitions. Virtually all observed and newly discovered DIBs can now be readily assigned to vibronic transitions in MgTBP, whose dominant SORET band coincides exactly with the strongest DIB at 4428 Å. The identification of porphyrins in the interstellar medium has obvious implications for the origin of life.

Mapping observations of large organic molecules in massive star-forming regions

M. Ikeda et al.
National Astronomical Observatory, Japan.

We carried out mapping observations of O-bearing molecules (CH_3OH, C_2H_5OH etc) and NH-/NH_2-bearing molecules (CH_2NH, CH_3NH_2 etc). Such a molecule, which is saturated or nearly saturated, has been believed to be prodcued on dust grain. We found difference between distributions of O-bearing molecules and those of NH-/NH_2-bearing molecules. O-bearing molecules are concentrated to H II regions. If these molecules are produced on the dust grain, many embedded OB-stars in H II regions can heat the dust grain, and produced molecules can be evaporated. This indicates that dust chemistry may be important for formation mechanisms of these molecules. On the other hand, intensity peaks of NH-/NH_2-bearing molecules are shifted to the west of H II regions. This resut indicates that formation mechanisms of NH-/NH_2-bearing molecules may be different from those of O-bearing molecules.

Co-author : *M. Ohishi*

Shocked molecular gas seen through OH absorption towards the supernova remnant W28

A. J. Green et al.
University of Sydney, Australia

When a supernova remnant drives a shock wave into an adjacent molecular cloud, collisionally excited OH (1720 MHz) masers may be detected at the interaction site. These masers are expected to form only under restricted ranges of gas density and temperature. Many bright masers have been detected in the supernova remnant W28. We present OH absorption measurements towards the remnant, confirming the presence of shocked molecular gas. Measurements of this type are able to examine the structure and kinematics of shocked molecular clouds, and test models for the production of OH and the excitation of the masers.

Co-authors: *M. Wardle, J. Lazendic*

Absorption against the cosmic 2.7 K background: A technique for detection of asymmetric top molecules in cosmic objects

S. Chandra et al.
School of Physical Sciences, S.R.T.M. University
Nanded 431 606, India

Observation of an interstellar line in absorptionagainst the cosmic 2.7 K background is an unusual phenomenon. Up to now, onlytwo lines have been reported in absorption against the cosmic 2.7 Kbackground: (i) the 1_{10} - 1_{11} transition of formaldehyde, and (ii) the 2_{20} - 2_{11} transition of cyclopropenylidene.

In the present investigation, we discuss about the conditions under which the transitions 2_{20} - 2_{11} and 2_{20} - 2_{21} in asymmetric topmolecules may be observed in absorption, even against the cosmic 2.7 K background. Observing these lines in absorption may be used as a technique for detection of some asymmetric top molecules in cosmic objects.

Co-authors: *W.H. Kegel (Institut für Theoretische Physik der J.W. Goethe Universität, Frankfurt am Main, Germany) and A.K. Sharma (Nanded, India)*

High resolution UV absorption studies of N_2, SO_2

Peter L. Smith et al.
Harvard-Smithsonian CfA

The most prominent EUV emission features in the airglows of Titan and Triton, where N_2 is the major atmospheric constituent, originate from the $N_2 c_4' \ ^1\Sigma_u^+(v=0)$ level. We report new photoabsorption measurements of 43 rotational line oscillator strengths in the $c_4'(0) - X(0)$ band of N_2. These are the first measurements of individual line f-values for this band. Such values, which are important for models of atmospheres at various temperatures, cannot be reliably calculated from band f-values and Hönl-London factors because of perturbations. A summation over the integrated cross sections of the measured lines yields a room temperature band f-value of 0.132 ± 0.020.

SO_2 is an important constituent of the atmospheres of Io and Venus. Accurate photoabsorption cross section data at the temperatures of these planetary atmospheres are required for the interpretation of SO_2 observations and for reliable photochemical models. Our high-resolution ($\lambda/\Delta\lambda \approx 450,000$), room-temperature measurements of SO_2 absorption cross sections in the wavelength region 198 to 220 nm [Stark et al., JGR Planets, 104, 16,585 (1999)] are being extended to lower temperatures.

This work was supported in part by NASA Grant NAG5-6222 to Wellesley College.

Co-authors: *G. Stark, J. Rufus, K. Yoshino, K. P. Huber, K. Ito, A. P. Thorne*

Spectral Survey of the Orion Molecular Cloud Core in the Region of 455-505 GHz

M. Araki et al.
Fukui University

A spectral survey in the region of 455-508 GHz has been carried out toward the Hot Core region at the center of the Orion Molecular Cloud using the JCMT 15 m telescope. Beam size of this observation is 10", which agree with size of the core. 313 spectral lines were observed in this survey. The lines are numerically dominated by rotational transitions of large organic molecules. Using an LTE rotational temperature abundance analysis, some of the derived column densities show a systematic increase over previously calculated values. Particularly, $(CH_3)_2O$, C_2H_3CN and C_2H_5CN are extremely abundant. For SO_2, two lines in detected 35 lines were assigned to the vibrational excited state. The two lines have a Boltzmann distribution in the inside of vibrational excited state, i.e. the Boltzmann distribution is independent from that of the vibrational ground state. This phenomenon indicates that this vibrational excited state was not made by collision and was made by excitation with emission from IRc2.

Co-Authors: *M. Ohishi, Glenn J. White, N. S. Higginbottom, and J. S. Greaves*

ATOMIC AND MOLECULAR SPECTROSCOPIC DATA FROM KECK SKY SPECTRA

T. G. Slanger et al.
SRI International, USA

The 4000-9000 Å sky spectra from the W.M. Keck 10-meter telescope and the associated HIRES crossed-grating echelle spectrometer on Mauna Kea are generating atomic and molecular spectra of unparalleled quality from the terrestrial night airglow. In some instances, e.g. the N-atom lines near 5200 Å and the newly-discovered $K(D_1)$ nightglow line at 7699 Å, these spectra significantly improve literature line positions. Molecular spectra of OH and O_2 show many new features. For the OH Meinel band system, a large range of rotational levels is seen, exhibiting a quasi-two-temperature thermal distribution, in addition to isotopic lines, and satellite lines. The O_2 Atmospheric Band system, O_2(b-X), is prominent, showing vibrational development up to v 15 in the upper state, far higher than any previous observations. The vibrational distribution is strongly bimodal, a clue to its origin that is not yet understood. Observations of the O_2(A'-a) Chamberlain system in the blue spectral r egion is similarly leading to characterization of a large range of vibrational levels in the O_2(a) state.

These studies have been supported by NSF Aeronomy, NASA Planetary Atmospheres, and NASA Sun-Earth Connection. The W. M. Keck Observatory is operated by the California Institute of Technology and the University of California.

Acetylene and Ammonia low temperature Mid-UV spectra for planetary atmospheres.

A. Jolly et al.
LISA, Université Paris 12, France.

The detection of C2H2 and NH3 features above 190 nm should allow determination of the acetylene and ammonia distribution to deeper levels in the jovian atmosphere than had previously been possible. To achieve this task, we have measured the UV absorption coefficient of both species in the 190-235 nm range at 293 and 173 K. The temperature dependence of the coefficient is very pronounced in this wavelength range mostly due to the appearance of hot bands. In order to have a better understanding of these effects and to extrapolate variation to lower temperatures, we have undertaken a spectroscopic modelling of the acetylene and ammonia absorption bands. This will enable to use synthetic spectra at the jovian temperature range 110-150 K to analyse the HST observations.

Co-authors: *Y. Benilan, F. Shindo and F. Raulin*

Comparison of Low Temperature NH_3 Collisions with He and H_2 via Pressure Broadening

D. R. Willey et al.
Allegheny College, USA

We have observed pressure broadening of NH_3 by both He and H_2 (normal and para) at kinetic temperatures of 10 - 40 K. These measurements were accomplished using the collisional cooling technique which allows quasi-equilibrium spectroscopy to be performed at temperatures far below typical molecular condensation points. Pressure broadening was observed for three NH_3 inversion transitions, $(J, K) = (1, 1), (2, 2)$ and $(3, 3)$. Normal H_2 pressure broadening cross sections were found to be up to eight times larger than corresponding He cross sections while para- H_2 cross sections were intermediate between normal- H_2 and He. We have also compared our experimental results to calculated cross sections derived from *ab initio* and semi-empirical NH_3 - He and NH_3- para- H_2 potential surfaces.

Photodissociation of H_2O and D_2O using VUV Laser or Synchrotron Radiation

J.H. Fillion et al.
Observatoire de Paris-Meudon, France

A complete determination of the rotational and vibrational population distributions of the OH/OD($A^2\Sigma^+$) fragments resulting from the VUV photodissociation of H_2O/D_2O in the 132-119 nm range is presented. Gas-phase H_2O/ D_2O has been photolyzed by means of a tunable vacuum ultraviolet laser or by synchrotron radiation. Spontaneous fluorescence spectra from the OH/OD($A^2\Sigma^+$) transition have been recorded with partially resolved rotational structure. The rovibrational population distributions of the OH/OD($A^2\Sigma^+$) photofragments were obtained for 15 excitation wavelengths, using an original analysis method based on the solution of an overdetermined set of linear equations. The experimental rotational populations and vibrational branching ratios are compared with Phase Space Theory results, recent ab-initio calculations by van Harrevelt et al. (2000) and with previously available experimental results. This study provides an improved understanding of the H+OH($A^2\Sigma^+$) dissociation channel of H_2O excited in the B $^1A_1$ state which should benefit to the interpretation of the OH observations in comets.

Co-authors: *A. Zanganeh, J.L. Lemaire, N.Shafizadeh, F. Rostas (France), M. Castillejo and J. Ruiz (Spain)*

Spectroscopy of NH_2 in Comet Hale-Bopp: Nature of the Non-LTE Rotational Distributions

R. J. Glinski et al.
Tennessee Technological University, USA

The recent bright comet Hale-Bopp has provided an excellent opportunity toperform detailed spectroscopy on molecules under astrophysical conditions. We have obtainedmoderate resolution spectra of NH_2 radical using the fiber-fed multi-objectspectrometer on the 3.5-m. WIYN telescope. We have obtained spectra of the 030 NH_2 band on several nights when the comet was 2.6 au and 1.0 au from the sun. The emission spectra show marked differences at the two heliocentric distances but almost no differences with nucleocentricdistance. A greater contribution from lines of high rotational J levels at distances nearer the sunwas observed. A photostationary state model was required to model the appearance of selectivelypopulated levels. The changes in the lower state rotational populations are essentiallycontrolled by the competition between rotational radiative cooling and up-pumping throughabsorption of optical solar radiation. We use these data along with our previous work (Bucher and Glinski, 1999, MNRAS 308, 29) on non-LTE energy distributions to formulate an analytical meansfor obtaining energy level populations under astrophysical conditions. We seeksolutions to the grand canonical Boltzmann equation that will allow direct extraction ofinformation on the physical conditions from spectra of molecules in non-thermal environments suchas comets, the ISM, and PDRs.

Co-author: *C. M. Anderson, University of Wisconsin, USA*

The carbon monoxide CO molecules and the C_2^- ions in comet C/1989 Y1 (Scoritchenko-George)

K.I.Churyumov et al.
Kyiv National University, Ukraine

We present the results of investigation of spectra of comet C/1989 Y1 (Scoritchenko-George) obtained by K. Churyumov et al. Feb. 26.7 UT, 1990 with the 6-m BTA telescope (Nizhny Arkhyz, Mount Pastukhov, the SAO of the RAS). 311 of emission lines of the molecules C_2, C_3, CN, NH, CH, Na, NH_2, CO, CO^+, CH^+, N_2^+, C_2^- and other were identified. Main peculiarities of the comet spectra were the presence of emission lines of negative carbon C_2^- ions and numerous emission lines of neutral molecules of carbon monoxide CO (triplet and Asundi bands). We identified the following transitions of CO: $d^3\Delta - a^3\Pi_r$ 15-3, 13-2, 11-2, 9-1, 8-1, 7-1, 7-0, 5-0, 4-0; $e^3\Sigma^- - a^3\Pi_r$ 7-0, 6-0, 5-0; $a'^3\Sigma^+ - a^3\Pi_r$ 11-1 (with subbands K=2, 3); 16-4 (with subbands K=0, 1, 2, 4); 9-0 (with subbands K=0, 1, 2); 8-0 (with subbands K=0). In the first time the emission lines of the carbon negative C_2^- ions (electron transitions $B^2\Sigma_u^+ v'$ - $X^2\Sigma_g^+ v''$) and the neutral carbon monoxide CO molecules (electron transition $e^3\Sigma^-$-$a^3\Pi_r$) were found. Calculation of molecular negative ions of carbon C_2^- column density with a cross-section 1 cm^{-2} $N = 9.22 \cdot 10^{11} cm^{-2}$ have been made.

Co-author: *V.V. Kleshchonok*

Modeling Chemistry in Cometary Comae: Sensitivity of Results to Uncertainties in Basic Data

D.C. Boice
Southwest Research Institute, USA

A model of cometary comae is presented for the gas, dust, and plasma flow in the near-nucleus environment for interpreting observations and *in situ* measurements of comets. The simulations are based on a multifluid, gas dynamic model with a detailed photo and gas-phase chemical reaction network, dust entrainment by the gas, and separate flow of the neutral gas, plasma, and fast neutral atomic and molecular hydrogen.

A case study using automatic differentiation is carried out to investigate the sensitivity of model results to uncertainties in input parameters, including basic atomic and molecular data, a variety of ionization sources, compositions, and properties of the cometary nucleus. Automatic differentiation is a powerful technique for performing accurate estimates of the errors associated with numerical results that depend on large numbers of parameters, each with its own uncertainty. It is applied to the cometary coma model to estimate errors associated with abundances, isolate critical reaction pathways, and determine the sensitivity of model results to temperature, flow speed, and other physical quantities.

Infrared Vibrations of Some HCN Polymers

Shantanu Rastogi et al.
Physics Department, Gorakhpur University, INDIA.

The observation of cyano (CN) group stretching at 4.5 μm and its overtone at 2.25 μm in several outer solar system bodies; the yellow-orange-red coloration of Jupiter and Saturn and the orange haze of Titan's atmosphere; solid X-(CN) molecules detected by IR absorption in the vicinity of protostars in molecular clouds; all point to the widespread astrophysical presence of Hydrogen Cyanide and its polymers. Laboratory simulations yield 'tholins', having significant components of HCN polymers.

We report a complete vibrational dynamics study of important HCN polymers - Polyaminocyanomethylene and Polyaminomalononitrile. The band position of CN stretching mode, important in the identification of X-(CN) structures, changes as a result of variation in its chemical environment. Both intra and inter molecular interactions effect its vibration. The dispersion features have been analyzed to understand the influence of molecular size and chain length on this and other important modes. The lower frequency data will be useful in analyzing high resolution spectra from ISO or other Space missions. The density of states, obtained from dispersion curves, has been used to obtain Heat Capacity Vs. Temperature. Heat Capacity information can be used in studying the thermal behavior, stability and effect of UV radiation and subsequent degradation or transitions of HCN polymers in ISM and in planetary atmospheres.

Co-authors: *V.D. Gupta (Lucknow,INDIA)*