Grains in Astronomy: An Overview

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This review will examine the principal astrophysical processes associated with grains in a variety of cosmic environments, ranging from interplanetary space of the Solar System to the interstellar medium of the hosts of high-z QSOs and starburst galaxies in the early Universe. As the dominant source of opacity in the UV/optical continuum, grains play pivotal roles in the reprocessing of radiation. With a huge surface area per unit mass, grains also interact strongly with gas-phase matter, serving as a catalyst for molecule formation and as a sink for refractory species being depleted from the gas. Of particular recent interest are grains at the small-size end of the size distribution, nanometer-sized clusters of atoms, which form an almost continuous transition between classical grains and large molecules and which give rise to astrophysical phenomena of particular diagnostic value. A wide range of basic data are needed for the successful interpretation of grain-related astronomical observations.

The formation and reformation of interstellar dust.

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The formation of new interstellar dust is primarily associated with stars nearing or at the the end of their lifetime. Depending on their mass, this can either be when they reach the Asymptotic Giant Branch (AGB) phase of their evolution or, in the case of massive stars, when they explode as supernovae (SNe). The contribution of SNe to the Galactic dust budget is not yet clear, but that due to AGB stars is evident and can include amorphous and crystalline silicates, amorphous carbon, SiC, graphite, etc. However, not all of these AGB stardust grains are detected in these circumstellar regions or in the interstellar medium. In this presentation I will summarise the dust sources and their relative contributions to the Galactic dust budget. I will discuss dust formation in circumstellar environments, and the associated unresolved problems, in the light of observational evidence and the direct and indirect detection and analysis of presolar and interstellar dust in the Solar System. I will also discuss the grain lifetime problem and the fact that it is apparently necessary to re-form and grow grains in the interstellar medium through the processes of accretion and coagulation in order to explain the observations of interstellar dust.

Laboratory analogues of cosmic dust

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We present laboratory experiments aimed at the simulation of solid grain formation and processing in space. Especially, we report on condensation studies of silicon carbide grains from the gas phase, and on annealing experiments investigating amorphous-crystalline phase changes in silicate grains by heat treatment and ion irradiation. An important aspect of these experiments is the investigation of the chemical and crystallographic structure of the grains. For spectroscopic studies of isolated grains we apply matrix isolation spectroscopy in noble gas matrices.

The question of presolar components within interplanetary dustparticles (IDPs) collected in the stratosphere.

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Interplanetary dust particles (IDPs) are from asteroids and comets, and they are the smallest and most fine-grained meteoritic objects available for laboratory investigation. Cometary IDPs are of special significance they are the only available samples of comets, and comets expected to be enriched in preserved solar nebula and presolar components. These components may include not only cosmically rare refractory grains (e.g. SiC, Al2O3) that are recovered from meteorites but, more importantly, cosmically abundant interstellar silicates and carbonaceous grains that were the fundamental building blocks of the solar system. Apparently these less refractory grains may not have survived alteration on the parent bodies of meteorites. Some cometary IDPs contain GEMS (glass with embedded metal and sulfides) whose exotic properties match those of astronomical amorphous silicates that are ubiquitous throughout interstellar space. Furthermore, measured D/H ratios as high as 0.01 in some (GEMS-rich) IDPs suggest the preservation of pristine organic material from cold interstellar molecular clouds, and crystalline (Mg-rich) silicates in GEMS-rich IDPs resemble circumstellar silicates detected by the Infrared Space Observatory (ISO). These observations raise the prospect that some IDPs may be composed either in part or entirely of pristine assemblages of presolar interstellar and circumstellar material

Overview of mid-infrared observatories

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An overview of past and future space-borne observatories at mid-infrared wavelengths is given. The Infrared Space Observatory (ISO) was operational from November 1995 – April 1998 and provided the first opportunity for spectroscopic observations over the complete 2.4–200 μm wavelength range above the atmosphere. This wavelength range is very rich in atomic and molecular lines as well as solid-state features, and some examples of exciting new results will be given, with special attention to molecular data needs. Future observatories such as SIRTF, SOFIA and FIRST will build and improve on the ISO results, either in sensitivity, spectral resolution and/or wavelength coverage. The complementarity with the ground-based Atacama Large Millimeter Array (ALMA), which will become operational in the same time-frame, will be discussed as well.

Infrared Observations of Interstellar Ices

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The research on ices in dense molecular clouds has made great progress since the launch of the Infrared Space Observatory. For the first time, full 2–200 μm infrared spectra of highly obscured protostars were obtained, showing a multitude of broad absorption bands. Laboratory simulations of interstellar ices are crucial to identify the carriers of these bands, and to derive the physical and chemical history of interstellar ices and their relationship to cometary ices.

It is found that the observed bands can be primarily explained by 'simple' ices such as CO, CH_3OH, CO_2, and CH_4 embedded in an amorphous H_2O–rich environment. The formation of these ices is best explained by grain surface chemistry models, rather than direct accretion of species formed in the gas phase. Accurate fitting of the band profiles reveals that the composition and structure of these ices are also affected by the heat of nearby massive protostars. Interestingly, this appears not to be the case for low mass protostars.

In this talk, I will indicate which laboratory experiments are needed to make further progress in the identification of the absorption bands toward protostars, and to better understand the formation and evolution of interstellar ices.

Various Aspects of the Spectroscopy of PAHs (Polycyclic Aromatic Hydrocarbons)

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The recent observations of the near infrared emission bands (UIBs), obtained by pointing ISO to a large variety of astrophysical objects, have revealed both the ubiquity of the carriers and some interesting variations in the relative intensities of the various bands.
The full exploitation of these results needs a good understanding of the physical mechanisms responsible for the formation of these emission bands. This requires in particular a detailed knowledge of the spectroscopic properties of the Polycyclic Aromatic Hydrocarbons (PAHs) proposed carriers, in a very wide spectral range (from far IR to far UV), as well as their intramolecular dynamical behaviour upon electronic excitation. Indeed, they are expected to be present as free-flying macromolecules, and to act as efficient UV/visible to infrared light converters.
The charge state of the interstellar PAHs is an important aspect of this problem, since going from neutral to charged PAHs seriously modifies their spectroscopy : infrared intensities are affected, and strong electronic transitions of very small energy appear. The laboratory study of these electronic transitions in PAH cations, when achieved in the gas phase, can address questions such as the possible contribution of these species to the Diffuse Interstellar Bands (in the visible and near-IR), and the electronic to vibrational intramolecular energy conversion mechanism, which is an essential feature of the UIB emission process in space.

Silicates

R. Waters.
SRON, Groningen, The Netherlands.

Abstract not available.

Infrared Observations of Gas-Phase Molecules

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Infrared observations of vibrational transitions of interstellar molecules, although more difficult than mm-wave observations of rotational transitions, have resulted in detections of several important molecules, notably CH_4, C_2H_2, and CO_2, and study of numerous others, including H_2, CO, and HCN. They also provide a selective probe of molecules very close to forming and evolved stars, and nearly simultaneous observations of many rotational states.

Ground-based observations have been hampered by lack of sensitivity and by telluric absorption. By observing from above the atmosphere, ISO was able to detect CO_2 and observe new sources, but most of its observations were made at too low of resolution to measure line shapes or even separate closely spaced lines. SIRTF will have much improved sensitivity, but quite low spectral resolution, making it of limited use for gas-phase molecular observations. SOFIA will be very well suited for study of molecules, with submm heterodyne instruments and R=100,000 grating spectrometers, although it will suffer from telluric CO_2 and H_2O.

Surface Reactions in Interstellar Space

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There is a large body of evidence indicating that chemical reactions on the surfaces of dust particles occur in interstellar clouds. Although chemical models of interstellar chemistry have included surface reactions since the late 1970's, it is only recently that detailed experimental and theoretical evidence concerning the rate of the most important of these reactions – the formation of molecular hydrogen by recombination of two neutral atoms – has become available. The rate determined for this reaction on several types of surfaces is much smaller than anticipated by astrochemists. These results raise the question of whether the rates of other surface reactions are similarly smaller than anticipated. We have recently run models in which smaller rates are assumed for all surface reactions and have found some significant differences from earlier model results. The necessity of measuring these rates in the laboratory will be emphasized. We have also recently included photodissociation processes ocurring on grain surfaces in our models. Preliminary results of these models will be discussed as will the need for more laboratory information.

Theoretical Simulations of Fundamental Processes of the H_2 Formation Reaction on an Icy Surface

Junko Takahashi
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To understand fundamental processes of gas-surface reactions is very important to develop astrochemical models in the interstellar medium. A classical molecular dynamics (MD) computer simulation was performed to investigate the whole fundamental processes of the H_2 formation reaction on the surface of dust grains. Amorphous water ice slabs were generated at 10 K and 70 K as a model surface of icy mantles of dust grains, and two incident H atoms were successively thrown onto the surface to reproduce the H_2 formation reaction, $H + H \rightarrow H_2$, on the dust surface. The following fundamental processes were studied in detail; 1) sticking of an H atom onto the dust surface from gas phase, 2) diffusion of an H atom on the dust surface, 3) reaction of two H atoms on the dust surface, 4) ejection of a product H_2 from the dust surface back into gas phase. The internal energy distribution of the product H_2 molecules was also examined, and it was found that H_2 formed on an icy surface will be in highly vibrationally excited states.

Probing the Nature of Grain Surface Chemistry and Ice Photochemistry by Laboratory Simulation

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The current status of laboratory results concerning the simulation of grain surface chemistry and photochemistry of instellar ices will be reviewed. A limited number of species observed in interstellar ices have now been successfully reproduced by simulating surface chemistry. However considerable uncertainty remains whether laboratory yields are sufficient to reproduce the observed abundance. Solving this problem is essential since it would allow a reconstruction of the chemical conditions responsible for the formation of interstellar ices.

Present data on the energetic modification of interstellar ice analogs mainly concern infrared spectroscopy which is primarily sensitive to simple products. In the ISM, such species may be produced by many processes. To constrain the importance of energetic processing, future laboratory studies should focus on more complex products. These could than be searched in hot core regions, where minor constituents of interstellar ices can be observed in the gas phase.

H_2 in Space

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From 28 September to 1 October 1999, an international conference entitled 'H_2 in Space' was held at the Institut d'Astrophysique in Paris. The meeting reviewed the current state of knowledge of the theoretical, experimental and observational properties of molecular hydrogen, with a view to obtaining a better understanding of H_2 in Galactic and extragalactic environments. Molecular hydrogen may be excited by collisions with other particles (as in shock waves), by ultraviolet pumping (as in photon-dominated regions: PDR's), through its formation on the surfaces of dust grains (in interstellar clouds), or by absorption of the cosmic background radiation (in the primordial gas). We shall summarize the adequacy, or otherwise, of our knowledge of H_2 (and HD), from the viewpoint of being able to reliably predict the spectrum arising from each of these excitation mechanisms.

Water in Sunspots and Stars

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At the 5800 K the surface of the sun is too hot for the formation of water. Water vapour exists, however, in the umbrae of cool (3200 K) sunspots. We will discuss our laboratory infrared emission spectra of water in the 400-6000 cm^{-1} region as well as sunspot absorption measurements in 600-1000 cm^{-1} (N band), 2500-3200 (L band) and 4200-5000 cm^{-1} (K band). In addition water observations from the ground and from orbit for other stellar sources such as Mira variables will be discussed.

Astronomy, Physics, and Chemistry of H_3^+

Takeshi Oka
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The recent discovery of the infrared spectrum of H_3^+ in dense molecular clouds as well as in the diffuse interstellar medium has demonstrated the ubiquity of this molecular ion which plays the pivotal role in the cosmic ray driven ion-neutral reaction scheme of molecular formation. The spectrum is also observed in outer planets as strong and pure emission and has become a powerful probe for monitoring plasma activities in planetary ionospheres. These astronomical observations have introduced several questions whose solution requires the understanding based on laboratory experiments and theory, and provided new incentives for researchers in the fields. A Royal Society Discussion Meeting was assembled in February this year where astronomers, physicists and chemists discussed a variety of problems from different perspectives. The fundamental nature of the molecular ion has made such interdisciplinary discussions possible and fruitful. The topics included: laboratory spectroscopy and theory, electronic recombination and ion-neutral chemistry, remote diagnostics of Jovian magnetosphere, the role of H_3^+ in planetary atmosphere, observations of H_3^+ in dense and diffuse clouds especially the surprising abundance in diffuse clouds, interstellar chemistry and deuterium fractionation, bistability etc. Many new findings were reported and ideas proposed in this and two accompanying meetings. Some highlights of the discussions will be reported.

H_2O in Young Stellar Objects

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Water plays a fundamental role during the first stages of the star formation process being one of the main gas coolant in the warm environment of very young stars. Absorption features from water frozen on the icy grain mantles are commonly observed towards massive protostars. Radio maser lines of H_2O are also a typical signature of the first stages of the star formation. Recently, thanks to the ISO satellite, many thermal lines in emission have been detected in the mid and far infrared around young low mass protostars. They probe warm gas (T>100 K) originating from a variety of different environments: from the protostar disk/envelopes, from warm regions exposed to the far ultraviolet photons of the young star or from gas heated by the shocks driven by protostellar outflows. In all these conditions, the water fractional abundance as well as the relative abundance between solid and gaseous H_2O are very sensitive both to the warm chemistry characterizing the star formation process and to its temporal evolution. Such emission provides therefore a valuable diagnostic tool for the interaction between newly formed Young Stellar Objects and their environment.
In this contribution, I will review the main physical and chemical processes influencing the formation and evolution of the water molecule in star formation environments, giving particular emphasis to what has been learned through the observations obtained by ISO and, more recently, by SWAS.

Water in comets, observations and models

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Water is believed to be the main constituent of ices in cometary nuclei. Its sublimation is driving cometary activity at short distances from the Sun. It is difficult to observe directly water in comets, however, because of absorption by the earth's atmosphere. Recent breakthroughs — in comets C/1996 B2 (Hyakutake), C/1995 O1 (Hale-Bopp), 103P/Hartley 2, and C/1999 H1 (Lee) — were made using new-generation, high-resolution ground-based infrared spectrometers, the Infrared Space Observatory (ISO) and the Submillimeter Wave Astronomy Satellite (SWAS). The deuterated species HDO was also observed by ground-based submillimetre telescopes.

The infrared fundamental and combination vibrational bands of H_2O are emitted by fluorescence excited by the Sun, which can be modelled using available spectroscopic data bases. Their observation gives us access to the rotational distribution of water and its physical conditions. The ortho-to-para ratio of water is observed to be significantly smaller than 3, its high-temperature equilibrium value, but the meaning of this measurement is still controversial. The rotational lines of water were observed for the first time in comets by ISO and SWAS. The [D]/[H] ratio of cometary water is higher that the "cosmic" value, but smaller than observed in interstellar molecular clouds. This puts stringent constraints to the formation scenarios of the Solar System.

Atomic and Molecular Data Needs in the 900–1200 Å Spectral Region

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The Far Ultraviolet Spectroscopic Explorer is presently producing high resolution (R $\sim$ 20,000) absorption-line spectra of astronomical objects ranging from solar system planets to quasars. The 900–1200 Å wavelength region observed by FUSE is exceedingly rich in atomic and molecular transitions arising out of the ground state. It is already clear from early FUSE observations that the atomic data (e.g., oscillator strengths) for some transitions are considerably different than those predicted by theoretical calculations.

In this talk, I will briefly discuss the most pressing atomic and molecular data needs for this wavelength range. I will also describe astronomical experiments that are being conducted to improve the accuracy of atomic oscillator strengths for ionic species such as Fe II. Finally, I will provide a list of those transitions for which laboratory measurements would be useful in interpreting FUSE absorption-line measurements of the interstellar and intergalactic media.

Chandra and XMM-Newton:
Atomic Data Needs for X-ray Astronomy

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With the launches of the Chandra X-ray Observatory and XMM-Newton, high resolution X-ray spectra of cosmic sources are broadening our understanding of the physical conditions, such as temperature, density, ionization state, and elemental abundances. X-ray emitting astrophysical plasmas can be generally classified by their dominant ionization mechanism, either collisional ionization or X-ray photoionization. The atomic data needs are significantly different for these two cases; however, for both cases it is important that we identify robust and accurate diagnostics and that we verify completeness of the broadband models. We discuss the status of the atomic data currently used in atomic databases for X-ray astronomy, in view of theoretical and experimental atomic physics considerations. We will also discuss the application of these models to new astrophysical data.

The FERRUM Project

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The FERRUM project aims at improving the database for oscillator strengths in iron group elements with an emphasis on astrophysically important ions. The international collaboration includes experts on experimental, theoretical and observational data. The first results concern Fe II.
Experimental radiative lifetimes (LIF technique) for some particular levels of Fe II are combined with experimental (FT spectroscopy) and theoretical branching fractions to obtain absolute oscillator strengths, which are then compared with new theoretical data (orthogonal operator technique). Depending on the agreement complementary theoretical data are included. The new data are tested in stellar spectra (HST, NOT).
We have obtained f-values for Fe II lines in the UV and optical regions originating from lower levels with excitation energies in the range 3-10 eV. The lines belong to four different transition arrays. The difference between experimental and theoretical data is of the order of 10%. The new data provide independent and new lines for abundance analysis and a test of LTE conditions in stellar atmospheres.
Lifetimes of metastable states are measured at a storage ring, providing the first experimental data for forbidden lines, [Fe II].

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UV studies related to the physico-chemistry of planetary and cometary environments

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A better understanding of the complex organic chemistry involved in comets and methane-rich planetary atmospheres can be achieved via the comparison of observations with results obtained by models. Available observations are still few and their reduction, analysis and interpretation requires the knowledge of a large set of data. Unfortunatelly, some of them are totally unknown especially if one takes into account the extreme physical conditions of the studied objets. Furthermore, this methodology makes sense only if the theoretical descriptions of both physical and chemical phenomena are really accurate. We will point out some lacks and sources of uncertainties in the chemical schemes used in models. Then, we will present UV studies (coupling experimental and theoretical approaches) developped in our laboratory in order to determine fundamental parameters (absorption cross sections, quantum yields and rate constants) in the accurate conditions of temperature and pressure. Implication for observations and models will be emphasized.

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Laboratory chemical dynamics and outer planets

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Reactions of CN ($^2\Sigma^+$) and C_2H ($^2\Sigma^+$) radicals with unsaturated hydrocarbons are of fundamental relevance to form complex nitriles and polyynes in hydrocarbon rich atmospheres, planets, and moons. Here we present results on crossed molecular beams experiments combined with electronic structure calculations on the reactions of C_2H and CN radicals with acetylene, methylacetylene, allene, and benzene. Our investigation show that both radicals attack the unsaturated bond without entrance barrier in exothermic reactions. The collision complex decomposes to form the hydrocarbon and a H atom or shows a H atom migration prior to hydrogen atom loss. The identification of this C_2H /CN - H exchange opens a versatile route to form unsaturated nitriles and polyynes and predicts their formation in hydrocarbon rich planetary atmospheres. Further, our studies provide a solid database on reaction products and shall guide chemical investigation of the NASA-ESA Cassini-Huygens mission to identify unsaturated hydrocarbons in Titan. Most important, these experiments verify unambiguously that the knowledge of reaction rate constants only is insufficient for detailed chemical models of planetary atmospheres. Reaction products and most important reactive intermediates MUST be included to get a plausible chemical model of planetary atmospheres.

Infrared Spectroscopy of Jupiter and Saturn

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Infrared spectroscopy is a powerful tool to study planetary atmospheres, which are emitting most of their internal energy at infrared wavelengths. Vibration -rotation bands of molecules are present in the IR planetary spectra, which give access to constraints on thermal structure, composition in minor elements, and cloud structure of the giant planets. The benefits of high accuracy database for molecules of planetary interest has accompanied the progresses in our knowledge of these atmospheres, as exemplified with CH_4 and NH_3 recent measurements, which were used recently for Galileo NIMS and ISO data reduction. In particular, some important results have been recently obtained on the water vapor distribution on Jupiter (NIMS/Galileo), on the identification of ammonia ice feature at 2.7 micron (NIMS/Galileo), and with the detection of CH_4 fluorescence on Jupiter and Saturn from ISO spectra.
Some guidelines on the expected future prospects in planetary atmospheres will be presented here, in the context of the future work in planetary atmospheres.

Clouds and Chemistry of Jupiter's Atmosphere:
A Post-Galileo, Post-ISO Perspective

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Observations of Jupiter by the Galileo probe and orbiter and the Infrared Space Observatory during the past four years have significantly enriched our knowledge of the composition in the gaseous and the condensed phases, and the structure of the atmosphere of this planet. At the same time, they have posed unprecedented challenges to our understanding of the thermodynamic, cloud microphysical and the chemical processes which are central to the question of the origin of the atmospheres of Jupiter and the other giant planets. In this paper, we will illustrate this point by examples of the relevant phenomena, including the volatile depletion and enhancement at varying depths, presence of water vapor in the "stratosphere", but the enigmatic behavior of this species in the deep troposphere, and the speculations about the nature of the "multi-layered" cloud structure. Finally, we will make recommendations for certain key laboratory measurements which could enhance the scientific interpretation of the observations.

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