

PROGRAM		
8 May 2000		
9.00 – 9.20	Welcome	V. Manno – J. Geiss
9.20 – 9.40	Objectives of the workshop	L. Colangeli – Th. Henning
9.40 – 10.00	Working group formation	
10.00 – 10.30	Coffee break	
10.30 – 11.00	New methods for making amorphous icy grains	A. Kouchi
11.00 – 13.00	Splinter WG's on: "Laboratory experiments – approach and problems"	Short presentations: 1.5 h Open discussion: 0.5 h
13.00 – 14.30	Launch break	
14.30 – 15.00	Experiments on carbon-based macro-molecules	C. Joblin
15.00 – 16.00	Coffee break	
16.00 – 18.00	Splinter WG's on: "Laboratory experiments – approach and problems"	Identification of key points: 1 h Open discussion: 1 h
9 May 2000		
9.00 – 9.30	Laboratory constraints on Mg-rich and Fe-rich silicate evolution	J.R. Brucato
9.30 – 10.30	Splinter WG's on: "Laboratory experiments – approach and problems"	Open discussion: 1 h
10.30 – 11.00	Coffee break	
11.00 – 13.00	Splinter WG's on: "Laboratory experiments – approach and problems"	Conclusions: 1 h Preparation of report: 1 h
13.00 – 14.30	Launch break	
14.30 – 15.00	Status of laboratory research on carbonaceous particles	H. Mutschke
15.00 – 15.20	Working group 1 report	
15.20 – 15.40	Working group 2 report	
15.40 – 16.00	Working group 3 report	
16.00 – 16.30	Coffee break	
16.30 – 18.00	Open discussion and resolutions	
10 May 2000		
9.00 – 9.30	Observational evidences on carbon properties	A.G.G.M. Tielens
9.30 – 10.30	Splinter WG's on: "Astrophysical problems and laboratory role"	Identification of key points: 1h
10.30 – 11.00	Coffee break	
11.00 – 13.00	Splinter WG's on: "Astrophysical problems and laboratory role"	Open discussion: 2 h
13.00 – 14.30	Launch break	
14.30 – 15.00	Silicates in circumstellar environments	L.B.F.M. Waters
15.00 – 16.00	Splinter WG's on: "Astrophysical problems and laboratory role"	Conclusions: 1 h
16.00 – 16.30	Coffee break	
16.30 – 18.00	Splinter WG's on: "Astrophysical problems and laboratory role"	Preparation of report: 1.5 h
11 May 2000		
9.00 – 9.30	Observational evidences on ice properties	P. Ehrenfreund
9.30 – 9.50	Working group 1 report	
9.50 – 10.10	Working group 2 report	
10.10 – 10.30	Working group 3 report	
10.30 – 11.00	Coffee break	
11.00 – 13.00	Open discussion and resolutions	
13.00 – 14.30	Launch break	
14.30 – 16.00	Splinter WG's: Preparation of documents	
16.00 – 16.30	Coffee break	
16.30 – 18.00	Splinter WG's: Preparation of documents	
12 May 2000		
9.00 – 10.00	Splinter WG's: Preparation of documents	
10.00 – 10.30	Summary	
10.30 – 11.00	Coffee break	
11.00 – 13.00	Summary and conclusions	

Overview presentations	
New methods for making amorphous icy grains	A. Kouchi
Experiments on carbon-based macro-molecules	C. Joblin
Laboratory constraints on Mg-rich and Fe-rich silicate evolution	J.R. Brucato et al.
Status of laboratory research on carbonaceous particles	H. Mutschke, et al.
Observational evidences on carbon properties	A.G.G.M. Tielens
Silicates in circumstellar environments	R. Waters
Observational evidences on ice properties	P. Ehrenfreund

WG on silicon-based materials	
Participants: J.R. Brucato, L. Colangeli , A. Jones, Th. Henning , F. Huisken, C. Jaeger , E.K. Jessberger, F. Molster, V. Pirronello, L.B.F.M. Waters	
The chemical composition of silicate dust around evolved stars and protostars	A. Jones et al.
Light-emitting silicon nanoparticles as potential carriers of the Extended Red Emission (ERE)	F. Huisken and G. Ledoux
Spectral properties and crystallisation behaviour of amorphous magnesium silicates produced by the sol gel method	C. Jaeger
Heterogeneous catalysis on solids of astrophysical interest as a method to characterise their surface	V. Pirronello et al.

WG on carbon-based materials	
Participants: G. Baratta, P. Brechignac, M. Greenberg, O. Guillois, C. Joblin, V. Mennella, H. Mutschke, C. Reynaud , F. Salama , S. Wada	
Raman and Photoluminescence studies of ion irradiated carbon-based materials	G.A. Baratta et al.
Laboratory spectra of cold gas phase PAH cations	Ph. Bréchignac
Progress and open questions in the problem of the identification of the Unidentified Infrared (UIR) bands carriers in the frame of the solid state hypothesis	O. Guillois
Synthesis and properties of carbon materials of astrophysical interest	C. Reynaud
Solid and gas-phase spectroscopy of PAHs: results and perspectives	F. Salama
Analysis of molecular components in QCC: laboratory analog of interstellar carbonaceous dust	S. Wada et al.

WG on ices	
Participants: M. Bernstein, P. Ehrenfreund , A. Kouchi, M.H. Moore, M.E. Palumbo, St. Schlemmer, W. Schutte, G. Strazzulla , A.G.G.M. Tielens, N. Watanabe	
Ice Photochemistry and Deuterium Enrichment of PAHs	M. P. Bernstein et al.
Infrared spectra of processed ices containing H ₂ O, CO ₂ , CH ₄ , and CH ₃ OH: photolysis vs. ion bombardment	M. H. Moore et al.
On the comparison between laboratory and astronomical spectra	G.A. Baratta et al.
Experiments with Trapped Nanoparticles	S. Schlemmer et al.
Ammonium BiCarbonate, A new candidate for the 6.8 micron absorption band towards embedded Young Stellar Objects	W. Schutte
Measurements of photonic and atomic surface reactions at 10K	N. Watanabe

New methods for making amorphous icy grains

Akira Kouchi

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We have developed new methods for making amorphous icy grains: 1) CO sublimation-induced disruption method and 2) continuous production method by fast codeposition of CO₂ and H₂O. These method enables us to perform better comet nucleus simulation experiments than hitherto performed.

We further report new results of experiments demonstrating that the heat of crystallization of impure amorphous ice is not exothermic like pure amorphous ice, but endothermic. This result clearly shows that the runaway crystallization of cometary ice never occurs.

Finally, perspective of new experiments will be discussed: i) Surface structure observation of amorphous ice using a low temperature ultrahigh vacuum AFM, and ii) Formation of amorphous ice by surface reaction using oxygen and hydrogen atoms.

Experiments on carbon-based macro-molecules

C. Joblin

CESR-CNRS – Toulouse – France

The presence of polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium was suggested in the mid 80es. Since then, a lot of laboratory studies have been devoted to these species. Concerning spectroscopy, I will review the main results that have been obtained from the far UV to the far IR in different environments: gas phase, rare gas matrices, supersonic jets. The contribution of PAHs to the UIR emission bands, the UV extinction curve, and the DIBs can then be discussed in the light of these laboratory results.

Although there is strong evidence for the presence of PAHs in interstellar space, the PAH model is faced with the difficulty to identify individual species. It is likely that the interstellar PAH population is not dominated by the rather small size and fully hydrogenated species which are usually studied in the laboratory. This raises new questions such as the formation process of interstellar PAHs and their physical and chemical evolution in the ISM. New experimental set-ups are clearly required for these studies. Some interesting results have been recently obtained in ionic cyclotronic cells. The PIRENEA experiment is based on this technique with the special aim of approaching the interstellar conditions of high vacuum and cold temperature. The capability of this experiment to produce laboratory analogues of interstellar PAHs and study their role in interstellar chemistry will be presented.

Laboratory constraints on Mg-rich and Fe-rich silicate evolution

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(2) Istituto Universitario Navale, Napoli, Italy

Cosmic dust grains are one of the main component in various astronomical environments of our galaxy. The life of the dust grains starts with their condensation in the outflows of evolved red giant, supergiant, nova, and supernova stars. Once formed the cosmic grains enter the interstellar medium where they suffer transformation processes. Finally, they become the building blocks of a new generation of stars and planetary system. During this life cycle the cosmic dust is the object of chemical, morphological and structural changes which are responsible for optical properties transformations and influence the size and shape distributions of the grains.

Infrared Space Observatory satellite obtained infrared spectra showing high crystallisation degree in the silicate grains both in the outflows surrounding oxygen rich evolved stars and in short and long period comets. Moreover, observations of dust in the interstellar medium and in regions of active star formation show that the structure of silicates remains essentially amorphous.

In this work we present laboratory results concerning amorphous and crystalline magnesium and iron rich silicates, which have been detected as principal components of the cosmic dust grains.

Status of laboratory research on carbonaceous particles

H. Mutschke, Th. Henning, C. Jaeger, M. Schnaiter, A. Braatz

*Astrophysical Institute and University Observatory,
Friedrich Schiller University Jena, Germany*

We give a short review of the present status of our knowledge about the structure and the optical properties of (hydrogenated) amorphous carbon particles. Recent results from astrophysical and other laboratories on formation and modification processes of amorphous carbon structures as well as on the relations between electronic structure and spectral features will be summarized and open questions will be highlighted.

Especially, we discuss the influence of structural parameters such as the sp^2/sp^3 ratio and the hydrogen content on the appearance of the π -electron UV-feature, the far infrared absorption cross section, and the photoluminescence properties. The effect of the particle morphology on optical properties will be emphasized and temperature effects will be discussed. Further, we note current progress in the study of special carbon structures such as onion-like particles and nanodiamonds.

Observational evidences on carbon properties

A.G.G.M. Tielens

Kapteyn Astronomical Institute – Groningen (NL)

Silicates in circumstellar environments

Rens Waters

Astronomical Institute “Anton Pannekoek”, Amsterdam (NL)

Silicates are one of the main components of solid material in space. The properties of circumstellar and interstellar silicates are important diagnostics of their formation history. These properties can be studied using infrared spectroscopy, and by comparing observed spectra to laboratory data. The spectra taken with the Infrared Space Observatory (ISO) constitute a very rich database, and have revealed a remarkable variety of silicates in circumstellar and interstellar environments. In particular, the presence of crystalline silicates in many different classes of objects has been found. So far, crystalline silicates have been found in circumstellar environments, while they are lacking in the interstellar medium. The ISO spectra for the first time allow mineralogy of the silicates, and present us with a new tool to study dust formation and evolution in space.

Observational evidences on ice properties

*P. Ehrenfreund
Leiden Observatory*

Interstellar dust and gas have been recently revisited with the Infrared Space Observatory (ISO) and ground based observations. These results allowed the discovery of several new molecules, as well as accurate abundance measurements of solid species and their gaseous counterparts. ISO-SWS and ground-based data show that the major species in interstellar ices toward high mass star forming regions are H_2O , CO_2 and CH_3OH . Additionally organic species such as OCS , H_2CO , HCOOH , CH_4 and OCN^- are observed toward massive protostars in small abundances. A comparison of laboratory data with recent ISO results shows extensive ice segregation in the vicinity of protostars and evidence for acid-base reactions occurring on interstellar grain surfaces. Thermal processing seems to be a dominant factor in interstellar ice chemistry. The role of UV energetic processing of interstellar ices remains uncertain. Likely the UV radiation field of a young protostar is strongly attenuated within its close environment. To study the formation and evolution of the key molecules CO_2 and CH_3OH in the laboratory may help to reconstruct the temperature and irradiation conditions in protostellar environments. The chemical and physical processes in dense clouds strongly influence the ice properties which can be monitored by infrared spectroscopy. Therefore future ground-based observations investigating the changes in the ice abundance and structure toward high massive protostars, low mass protostars, and field stars should strongly enhance our knowledge on grain surface reactions and energetic processes in such environments. Grain surface chemistry and subsequent evaporation of simple molecular mantles drive the gas phase complexity. In this review a schematic outline on the solid state chemistry in the protostellar environment is presented and processes which lead to the chemical diversity of interstellar ices and the formation of complex molecules in ice and gas are discussed.

Raman and Photoluminescence studies of ion irradiated carbon-based materials

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Solids objects in space (interstellar grains, comets, interplanetary dust particles, etc.) are continuously exposed to energetic physical agents such as cosmic rays and/or UV photons. For several years our and other groups have been involved in the experimental study of the effects induced by fast ions colliding with solids (frozen gases, carbonaceous and organic materials, silicates, etc.) of astrophysical interest. Among the effects induced by ion irradiation, the formation of an organic residue evolving at higher doses towards an hydrogenated amorphous carbon with decreasing optical gap is particularly interesting. This has been observed in several kinds of carbon containing targets, both frozen (C_6H_6 , CH_4 , C_4H_{10} , etc.) and refractory (polystyrene, polypropylene, etc.). Both fast ions (low energy cosmic rays, galactic protons, fast solar protons, solar wind particles) and carbon containing solid targets (interstellar grains, comet mantles, interplanetary dust particles, etc.) are present in space. Thus under certain circumstances, materials similar to that produced in laboratory may form in space. In addition ions could have a role in space in modifying (disordering) the structure of pre-existing refractory (i.e. amorphous carbon grains with relatively high degree of order, graphite, etc.).

Here we present an experimental Raman and photoluminescence study, carried out “in situ”, of the effects induced by ion irradiation of carbon containing frozen gases, amorphous carbon grains and graphite.

Ice Photochemistry and Deuterium Enrichment of PAHs.

Max P. Bernstein,(1) Jason Dworkin,(1) Scott A. Sandford, and Louis J. Allamandola
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Polycyclic aromatic hydrocarbons (PAHs) are common in carbonaceous chondrites, and IDPs, and are probably the most abundant and widespread class of organic compounds in the universe. In dense molecular clouds where temperatures are low (<50 K) PAHs condense along with most gas-phase species into ices dominated by H₂O. Indeed, the presence of PAHs in interstellar ices have been demonstrated by recent astronomical observations and emission from PAHs were reported in comet P/Halley. Our previously reported laboratory studies of UV processing of PAHs in H₂O showed that PAHs undergo reactions in interstellar ice grains which could be the source of certain hydrocarbons in carbonaceous chondrites and IDPs (2).

At this workshop we will present the results of our more recent studies on the UV processing of aromatic molecules in ice under astrophysical conditions including: (i) regio-chemistry of these reactions which allow us to make specific predictions about what structures should be seen if this process is the source of polar aromatic hydrocarbons seen in meteorites and (ii) isotopic studies showing that such reactions may explain the deuterium enrichments in these meteoritic hydrocarbons. In addition, we briefly address possible implications of these compounds for the evolution of life since naphthaquinones are ubiquitous in living systems and perform a fundamental role in biochemistry.

This work pertains to questions regarding the origin and fate of organic materials in the ISM, comets, meteorites and IDPs, the distribution of deuterium in organic molecules, and the role of UV radiation in the formation and modification of molecules in space.

- (1) Drs. Bernstein and Dworkin are with the SETI Institute, Mountain View CA.
- (2) M. P. Bernstein, S. A. Sandford, L. J. Allamandola, J. S. Gillette, S. J. Clemett, and R. N. Zare. "Ultraviolet Irradiation of Polycyclic Aromatic Hydrocarbons (PAHs) in Ices: Production of Alcohols, Quinones, and Ethers." *Science* 283, 1135-1138 (1999), and references therein. See also the Perspectives piece by Pascale Ehrenfreund pp 1123-1124.

LABORATORY SPECTRA OF COLD GAS PHASE PAH CATIONS

Ph. Bréchnignac

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Based on their plausible abundances estimated from the intensity of the infrared emission aromatic features, the PAH cations have been proposed as plausible candidates for DIBs carriers identification, because of their expected spectroscopic properties throughout the visible and near infrared range..

Extensive work has been undertaken to build up a database with spectra of these species using rare gas matrix isolation spectroscopy. However it is not accurate enough to allow any DIB assignment, because:

- 1) the bands are shifted by the interaction with the host matrix in an unpredictable way.
- 2) The bands exhibit a matrix induced broadening, which -most of the times - hides the actual bandwidth

We have developed in Orsay a novel technique which allow to obtain the gas phase spectra of cold PAH cations, i.e. under the proper conditions to mimic the interstellar medium. We will present the principle, the present achievements, and the prospects of this technique as a tool to help to elucidate the DIBs mystery.

Bréchnignac Ph. and Pino T., 1999, A&A **343**, L49-L52

T. Pino, N. Boudin and Ph. Bréchnignac, , J.C.P. **111**, 7337 (1999).

The chemical composition of silicate dust around evolved stars and protostars

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Although this meeting is entirely devoted to chemical evolution of ices upon bombardment of energetic particles (UV photons and/or cosmic-rays particles), one must not forget that these particles may severely affect the "core" of the grains, i.e. the silicates, largely observed in the Interstellar Medium. We present in this poster an analysis of the chemical composition of silicate dust around various objects, namely evolved stars and protostars.

Differences between these two lines of sight are obtained not only in the physical structure of the silicates (large proportions of crystalline silicates are present in evolved stars whereas those observed in protostars are totally amorphous but also in the chemical nature of the silicates (olivine in evolved stars and orthopyroxene and aluminosilicates in protostars). This poster describes in detail ISO spectra from these objects. Since the observed silicates relate to each other following a certain pattern of evolution of the grains, we postulate that most observed differences may be the result of fast particles bombardment of interstellar grains that modify their structure and chemical composition. Experiments at IAS are undertaken to test this hypothesis in order to retrace with quantitative arguments, the life of a grain in the ISM.

Progress and open questions in the problem of the identification of the Unidentified Infrared (UIR) bands carriers in the frame of the solid state hypothesis

Olivier Guillois

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In this contribution, using some of the high quality published SWS spectra exhibiting the UIR bands, we present improvements in the understanding of these features in terms of solid state particles. The discussion will be mostly based on comparisons obtained between laboratory measured properties of solid carbonaceous materials and ISO spectra for the three different classes of UIR sources, A, B and C as labelled in the simple classification proposed by Geballe (1997) and Tokunaga (1997). We will also discuss recent advances in the field of solid state physics in the nanometric range which seem to us relevant in the astrophysical context.

Light-emitting silicon nanoparticles as potential carriers of the Extended Red Emission (ERE)

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High-purity silicon clusters and nanoparticles ($d = 1 - 8$ nm) are produced by CO₂-laser-induced gas phase reactions in a flow reactor. The particles are transferred into a molecular beam apparatus where they are analyzed *in situ* with a time-of-flight mass spectrometer. Our finding that the particles' velocity is strongly correlated with their mass enables us, by introducing a chopper into the cluster beam, to considerably reduce the dispersion of their size distribution and to perform size-selected low-energy cluster deposition on various substrates. High resolution transmission micrographs demonstrate the capabilities of the new apparatus and reveal the perfect monocrystalline structure of the silicon nanoparticles. The monodispersed silicon films have been further characterized by studying their photoluminescence (PL) behavior. As predicted by the quantum confinement model, the peak of the PL curve shifts with decreasing particle size to smaller wavelengths (higher energies). A careful analysis of the PL efficiencies yields extraordinary high values near 100%. These results provide strong arguments to attribute the origin of the Extended Red Emission (ERE) to crystalline silicon nanoparticles. The spectral variations observed so far can be explained just by invoking different size distributions of the crystalline cores of the Si particles involved.

Spectral properties and crystallisation behaviour of amorphous magnesium silicates produced by the sol gel method

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Mid- and far-infrared spectra gained by the Short Wavelength Spectrometer (SWS) of the ISO satellite have clearly shown the coexistence of amorphous and crystalline silicates in circumstellar envelopes around young stars, in evolved stars and planetary nebulae, and in comets. Since optical properties of amorphous magnesium silicates of the system $\text{MgO} \cdot \text{SiO}_2$ are still lacking in the literature we will provide mass absorption coefficients (MACs) for a wide range of compositions. Optical constants of the amorphous magnesium silicates have been determined for different Mg/Si ratios covering the astrophysically relevant spectral range. The magnesium silicates have been produced by the sol gel method. The chemical compositions vary from nearly pure silica up to $\text{Mg}_{2.6}\text{SiO}_{4.6}$. The absorption maximum of the Si-O stretching band of the silicates depends on the composition and will be shifted from 9.0 to 10.25 μm , respectively. One of the main questions in astrophysics is the transition of the silicates from the amorphous to the crystalline state. Former investigations of the annealing behaviour of these silicates have shown the need of a temperature of more than 1000 K for starting crystallisation. In our work we can show that magnesium silicates with a slightly modified structure can start to crystallise at temperatures of about 700 K.

Processing of carbon grains in space and in the laboratory

Vito Mennella

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Several evolutionary factors can modify the composition of carbon grains in the interstellar medium. Grain transformation is mainly driven by UV and cosmic ray irradiation, as well as by interaction with atomic hydrogen. To get more insight into the properties of interstellar carbon grains and to outline their evolution, laboratory simulations of processes active in space are of fundamental interest. We discuss laboratory research involving processing of nano-sized carbon particles under simulated interstellar medium conditions. The results provide constraints for more solid identifications of the aromatic and aliphatic carbon materials responsible for the UV interstellar extinction bump and of the 3.4 micron band, respectively.

**Infrared spectra of processed ices containing H₂O, CO₂, CH₄, and CH₃OH:
photolysis vs. ion bombardment**

M. H. Moore (1), P. A. Gerakines (2), R. L. Hudson (3)

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(2) NRC/NASA/Goddard Space Flight Center

(3) Eckerd College/NASA/Goddard Space Flight Center

In our laboratory, ices condensed within one cryogenic system can either be irradiated with MeV protons or photolyzed (~ 10 eV photon⁻¹). New data will be presented comparing results from proton and UV-photolysis experiments of H₂O+CO₂, H₂O+CH₄, H₂O+CO₂+CH₃OH, and H₂O+CO₂+CH₄. The yield of products detected using mid-IR spectroscopy will be compared. In irradiated H₂O+CO₂ ices, it was known that H₂CO₃ is the dominant product. For the first time, H₂CO₃ has now been identified in photolyzed H₂O+CO₂ ice. This result is consistent with our general finding that these two processes result in the same type of product species. The amount of product formed in these ices is determined by the total energy dose not by the type of processing.

On the comparison between laboratory and astronomical spectra

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It is well known that particle shape and size can have very important effects on the profile of icy absorption features. In fact Mie-scattering calculations show that absorption features can be shifted with respect to laboratory (bulk) spectra of thin films and subpeaks appear. The difference between bulk spectra and small particle extinction spectra depends on the optical constants (n , k) of the sample and in particular it is not negligible for those species with "strong transitions" and at high concentration in the ice mixture.

In order to know whether a band profile in a specific ice mixture would be affected by particle shape and size effects it is necessary to have the optical constants of that mixture and perform small particles cross-section calculations. However if in principle optical constants can always be measured in practice this is not straightforward. After several years of experiments and IR spectroscopy of icy mixtures we have found an experimental method to know whether particle shape and size would affect the profile of an absorption feature and hence whether laboratory spectra of thin films are representative of small particles extinction spectra. In particular, we have found that some instances exist in laboratory spectra for which the profile of absorption bands depends on the inclination of the ice film with respect to the infrared beam of the spectrometer. Furthermore when this is the case if the spectrum is taken at oblique incidence the band profile depends on the polarisation of the infrared beam as well.

Here we show that when a band profile in a laboratory spectrum depends on the inclination of the sample or, equivalently, on the polarisation of the electric vector of the IR beam, it cannot be directly compared to astronomical observations.

**Heterogeneous catalysis on solids of astrophysical interest
as a method to characterize their surface**

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It is proposed that the experimental investigation of the catalytic synthesis of molecules by surface reactions on amorphous and polycrystalline solids (that can be considered realistic analogues of interstellar grains) together with a careful theoretical simulation of the process as an accurate method able to characterize the surface via the distribution of energies determining the adsorbate dynamics. A specific case that has been thoroughly performed will be shown.

Synthesis and properties of carbon materials of astrophysical interest

Cecile Reynaud

Service des Photons, Atomes et Molecules, CEA-Saclay, France

I will present the experimental development done in our laboratory to determine the nature of the carbon component of the cosmic dust in order to progress in the identification of the carriers of the Unidentified Infrared (UIR) bands. We have synthesised nanoparticles of hydrogenated carbon using the gas phase laser pyrolysis method. I will introduce this method and its application to the understanding of the growth of carbon particles from a hot gas phase as a function of temperature and residence time. Infrared spectroscopy and electron microscopy techniques have been used to correlate the particles properties with the growth conditions. We have also formed thin films of hydrogenated amorphous carbon by heavy ions irradiation of carbonaceous compounds. I will discuss the optical properties of these films as a function of the irradiation dose and their interest for the understanding of the carbon cosmic dust.

Solid and Gas-Phase Spectroscopy of PAHs: Results and Perspectives

F. Salama

NASA-Ames Research Centre

The laboratory studies of interstellar carbon materials analogs (PAHs) will be discussed with their advantages and limitations from the point of view of the application to astrophysical processes. The discussion will focus on the newest generation of laboratory experiments that are currently being developed in order to provide a closer simulation of space environments and a better support to space missions. The astrophysical implications and future perspectives will be stressed.

Experiments with Trapped Nanoparticles

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In our laboratory we developed specific traps for studying ions, molecules and dust particles under astrophysical conditions. This contribution will concentrate on the description of our newest device, the nanoparticle trap. Here single, isolated and due to the quadrupolar trapping field, well localized nanoparticles can be monitored by optical means over very long times. A first application of this trapping technique is based on the high mass resolving power in a mass range which is otherwise not accessible (NPMS: nanoparticle mass spectrometry). In several examples we will show how a combination of NPMS and in-situ preparation of the particle leads to a fundamental understanding of basic processes such as sticking, desorption and charging. In the last part we will introduce our present activities related to catalytic processes on dust analogues on a molecular level.

References

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Ammonium BiCarbonate, A new candidate for the 6.8 micron absorption band towards embedded Young Stellar Objects

*Willem Schutte
Leiden University*

UV irradiation of ice mixtures containing H₂O, CO₂, NH₃ and O₂ produce a strong feature at 6.8 micron. Comparison to literature data shows that this feature can be ascribed to the NH₄⁺ ion, while the countercharge is provided by HCO₃⁻. Indeed, irradiation of H₂O, CO₂, and O₂ produces carbonic acid (H₂CO₃), showing that the Ammonium Bi Carbonate (NH₄⁺.HCO₃⁻) is produced by the "classical" cryogenic acid-base reaction scheme, as first proposed by Grim et al. in 1991. The 6.8 micron band provides a good match to the interstellar 6.8 micron feature associated with icy mantles in dense clouds. No definite spectral structure is associated with the HCO₃⁻ ion in water-rich ices, indicating that NH₄⁺ may produce the 6.8 micron band even in the absence of spectral structure of the counterion. It is shown that the ion assignment is consistent with the systematic red-shift with line-of-sight temperature of the interstellar 6.8 micron band as observed by ISO-SWS (Keane et al. 2000).

**Analysis of Molecular Components in QCC:
Laboratory Analog of Interstellar Carbonaceous Dust.**

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Quenched Carbonaceous Composite (QCC) is product of a hydrocarbon plasma that has been shown previously to have a 220 nm absorption as well as infrared absorption bands that are close in wavelength to the infrared emission bands in the interstellar medium (Sakata et al., Nature, 301, 493, 1983, Sakata et al., ApJ, L51, 1984).

We have analyzed the molecular components of QCC using mass spectroscopy. The mass spectrum of the gas evaporated by a CO₂ laser shows two envelopes peaking around 200 and 500 amu. In the high mass envelope, many peaks which fit to compact type PAH molecules are present, for example, 374 amu (C₃₀H₁₄, naphtocoronene), 386 amu (C₃₂H₁₄, ovalene), 472 amu (C₃₈H₁₆, circodiphenyl), 496 amu (C₄₀H₁₆, circumanthracene), and 520 amu (C₄₂H₁₆, circopyrene). In the low mass envelope, the highest peak is found at 228 amu which corresponds to the peak of benzo[c]phenanthrene, chrysene, benz[a]anthracene, triphenylene, and naphthacene.

Clusters with about 130 carbon atoms are evaporated from the QCC by heating. All of these carbon clusters are composed of carbon atoms with even number and they have very little hydrogen.

We have previously shown that the QCC is composed of onion-like spherules with 5-15 nm in diameter (Wada et al, A&A, 345, 259, 1999). It appears that the PAH molecules detected by mass spectroscopy are adsorbed to or included in the onion-like structure.

This indicates that onion-like carbonaceous spherules and PAH molecules are formed simultaneously by the cooling process of plasmic gas containing of hydrogen and carbon.

Measurements of photonic and atomic surface reactions at 10K

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We will report results of our experiments on photo-induced productions of H_2 and CO_2 (if possible) from amorphous ice. There have been several works to observe these molecular productions mainly from interstellar analogue ice mixed with several molecules. Using simpler ice, that is, pure and CO-doped ice, we tried to gain more information such as cross sections, reaction channels, reaction site (on the surface or in bulk), desorption mechanism. We will also mention problems and difficulties in our experiments. We may present our preparing experiments of atomic surface reactions.