The role of laboratory experiments in the characterisation of cosmic material: critical analysis of past experience and guidelines for future developments

Bern - 6-8.10.1999

Report

1. Participants

L. Allamandola, L. Colangeli, P. Ehrenfreund, J.M. Greenberg, Th. Henning, E.K. Jessberger, J. Lequeux, V. Mennella, C. Reynaud, W. Schutte, T. Stephan, G. Strazzulla

2. Program

6.10.1999		
14.30 – 14.45	Welcome	V. Manno – J. Geiss
14.45 – 15.15	Introduction – Objectives	L. Colangeli – T. Henning
15.15 – 16.00	Evolution of organics and silicates in the ISM	J.M. Greenberg
16.00 – 16.30	coffee break	
16.30 - 17.15	Laboratory astrophysics – the near future	L. Allamandola
17.15 - 18.00	Interplanetary Dust Particles: cometary material in the laboratory	T. Stephan and E.K. Jessberger
7.10.1999		
9.00 - 9.45	Laboratory synthesis and spectroscopy of nanoparticles	T. Henning
9-45 – 10.30	The laboratory approach to the evolution of interstellar dust	V. Mennella
10.30 – 11.00	coffee break	
11.00 – 11.45	Solid-state nature of the cosmic dust responsible for the UIR and ERE bands	C. Reynaud
11.45 – 12.45	**Round table on cosmic dust**	All
12.45 – 14.30	Lunch Break	
14.30 – 15.15	Organics in the ISM and Solar System: open questions	P. Ehrenfreund
15.15 – 16.00	Processing of ices	G. Strazzulla
16.00 – 16.30	coffee break	
16.30 – 17.15	Laboratory Astrophysics: how to address current issues in solid-state astrochemistry by laboratory simulation ?	W. Schutte
17.15 – 18.15	**Round table on cosmic ices**	All
8.10.1999		
8.30 – 10.30	**Round table on:** • **Laboratory experiments to characterise cosmic dust and ice analogues. Techniques already used and lab. programs/wishes for the future** • **Identification/discussion of unsolved astrophysical problems and the role of laboratory experiments to clarify them**	All
10.30 – 12.00	**Operative session on:** - **Preparation of a report on the presentations and the discussion** - **Key problems/aspects to be addressed in detail during the second extended meeting** - **Distribution of actions for home work in preparation to the next meeting**	All
12.00 – 12.30	**SUMMARY of WORK**	
12.30 – 13.30	**Operative session on:** - **Involvement of other relevant colleagues in the second extended meeting** - **Preparation of a draft program and working groups**	All

3. Summary of discussion

3.1 Round table on cosmic dust

Points identified as key aspects for discussion and future studies are formation, evolution and destruction processes of cosmic dust and its relation to the molecular component.
It has been stresses the need of further measurements in laboratory to characterise materials and to determine the efficiency of various destruction processes. It is, however, necessary to guarantee that laboratory experiments are representative of actual space conditions.
The following aspects have been evidenced as critical aspects to clarify:

- the evolution from PAH's to carbon grains
- the role of precursors: molecules (e.g. acetylene) vs. PAH's
- the role of hetero-atoms during formation in space and in laboratory (e.g. H, N, ...)
- the relations between PAH's and grains in laboratory samples

3.2 Round table on cosmic ices

Experiments must be oriented to clarify the following points:

- Chemistry on-going during ice formation on a grain surface at low temperature
- Surface and bulk chemistry induced by ion/radical accretion vs. energetic processes
- Applicability of spectra of gas deposited on polished surface to actual space conditions
- Effects of polarisation and shape
- Discrepancies among results from different laboratories

A series of new experiments to be performed has been identified:

- Experiments in molecular cluster beams
- Photolysis processes
- Experiments at low UV doses
- Energetic processing in molecular formation on grain surfaces

Studies must also address the following points:

- Influence of isotopic effects on spectra
- Search for tracers of particle processing vs. UV irradiation and vs. thermal processing in space and laboratory ices
- What are the differences in ices in different environments ?
- Evidence of ion-UV processing in space vs. different environment properties ?
- Integrate grain and gas phase chemical processes into a realistic, inclusive IS chemistry model

3.3 Round table on laboratory experiments

The following table schematically identifies areas of interest for comparison of available results and future studies:

<table>
<tr><td>Aspect</td><td colspan="3">Materials</td></tr>
<tr><td></td><td>Silicates</td><td>Carbon</td><td>Ices</td></tr>
<tr><td rowspan="2">Production</td><td colspan="2">• from gas phase
• natural materials</td><td></td></tr>
<tr><td>• sol-gel reaction
• melting
• grinding</td><td>• from ices
• from solids</td><td>• condensation
• surface reactions
• cluster beams</td></tr>
<tr><td rowspan="2">Processing</td><td colspan="3">• thermal
• ion, UV, X-ray, shocks</td></tr>
<tr><td colspan="2">• H atoms</td><td>• H, C, N, O atoms</td></tr>
<tr><td rowspan="2">Assessment of characterisation methods</td><td colspan="3">• FUV-FIR spectroscopy
• TEM, SEM
• EDX
• Raman
• mass spectrometry
• PIXE
• neutron spectroscopy
• photoluminescence
• AFM</td></tr>
<tr><td></td><td>• depletion spectroscopy</td><td>• LC
• GC
• HPCL</td></tr>
<tr><td rowspan="2">Parameters</td><td colspan="3">• temperature (low to high)
• doses
• size
• porosity</td></tr>
<tr><td></td><td>• C/H
• hetero-atoms
• hybridisation ratio</td><td></td></tr>
<tr><td colspan="4">Relevance of techniques for samples returned from space</td></tr>
</table>

The following table summarises the open problems in different areas of laboratory investigation:

General problems	• Isotope effects • Size effects: single grains vs. clusters, spectral behaviour • Optical constants: comparison
Problems in sample production	• PAH's from organics et al. • Organic mantles • Silicates: chaotic vs. crystalline • Molecules on grain surface: methanol, CO_2, ... • Determination of stable nucleation structures
Problems in processing	• UV photon effects: two photon effects, ... • Shocks on grain mantles • Sputtering, chemi-sputtering • Time scale in laboratory vs. space • Chemical processing by UV, ions, X-rays, ... • Formation paths of crystalline silicates
Problems of characterisation	• Isolated grains and matrix effects • Gas phase spectroscopy of PAH's • Spectroscopy and luminescence of neutral and ionised PAH's, clusters, closed shell aromatic species
Problems with ices	• Detection of free radicals • Surface and bulk chemistry induced by ion/radical accretion vs. energetic processes

3.4 Round table on unsolved astrophysical problems

Here following is a list of key questions that deserve further investigation about the formation of materials in space:

1. Origin of PAH's and C-particles: which comes first ?
2. Crystalline silicates in comets and disks
3. Size distribution
4. Formation and processing of materials and mantles in space
5. Where are sulphur, Si, iron ?

Here following is a list of spectral features that still need observations and laboratory experiments for definite identification:

1. UV bump and FUV rise in extinction and the 3.4 μm band: search for correlation
2. The 3.4 μm band vs. environment (e.g.: post AGB stars, IS)
3. The FUV extinction rise: absorption or scattering ? PAH's vs. nano-particles vs. grains ?
4. Interpretation of "exotic" mid-IR spectra of CSM, ISM (ISO data)
5. ERE
6. DIB's vs. UIB's (limited agreement with PAH's)
7. Si-H non identification

Moreover, the detection of materials in space cannot be based only on the identification of spectral features. Other considerations, such as formation and survival of materials in space conditions, must be taken into account.

4. Results of operative sessions

4.1 Preparation of a report

The preparation of the present report has been agreed within the team according to the following time plan:

Activity	Person in charge	Deadline
Send list of items	LC, TH	end Oct. 99
Replies	All	end Nov. 99
Iteration	All	end Jan. 00

4.2 Key problems/aspects to be addressed during the following workshop

See program below.
Emphasis on:

a) Innovative experimental techniques
b) Visibility of laboratory astrophysics

4.3 Organisation of the following workshop

- When: 8-12.5.00
  1 week (9.00 a.m. Monday to 2 p.m. Friday)

- How: Few general presentations
  Few general presentations
  Sub-groups with chairmen to issue items to be discussed according to the program

4.4 Involvement of other colleagues in the workshop

GENERAL PRESENTATIONS (TBC)	
L.B.F.M. Waters (1/2 week, TBC)	Observations on silicates
A.G.G.M. Tielens	Observations on carbons
P. Ehrenfreund	Observations on ices

SILICON-BASED MATERIALS		
Core team members	Invited members	Solicited participants
Luigi Colangeli Thomas Henning *Mayo Greenberg*	F. Huisken J. Bradley L.B.F.M. Waters	A.Blanco *J.R. Brucato* L. D'Hendecourt *C. Jaeger* J. Nuth V. Pironello *T. Stephan (8/5 no, TBC)*

CARBON-BASED MATERIALS		
Louis Allamandola (?) Elmar K. Jessberger Vito Mennella Cecile Reynaud	C.Joblin S. Wada H. Siegmann	*G. Baratta* P. Brechignac *O. Guillois* *H. Mutschke* *F. Salama*

ICES		
Pascale Ehrenfreund Willem Schutte Giovanni Strazzulla	M.H. Moore B. Schmidt A.G.G.M. Tielens St. Schlemmer	*M. Bernstein* *D. Hudgin* K. Hiraoka A. Kouchi *N. Watanabe* *M.E. Palumbo*

Yes
No
Core team member
No reply

5. Resolution from the working team meeting

As a follow up of the activities during the first meeting and the following iterations, the core team of the working group on the subject “**The role of laboratory experiments in the characterisation of cosmic material**” has decided to identify some key aspects of research in the field.
Objective of the Workshop in ISSI, Bern to be held on 8 – 12 May 2000 is to address as many as possible of the indicated subjects.

<u>5.1 Laboratory experiments to characterise cosmic dust and ice analogues</u>

The following Table summarises the principal aspects that are recommended to drive the exploration of cosmic material analogues in laboratory.

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The following considerations must be accounted for:

- It is important to distinguish between production techniques and processing that try to "simulate" the astrophysical conditions from those that are limited to "simulate" materials whose properties mimic those observed in space.

- The selection of laboratory materials as candidate to simulate cosmic dust must be based on a complete test of the spectral properties as well as on formation, evolution and elemental constraint considerations. Moreover, chemical matches allowed by meteorites and IDP's must confine the range of likely products. By this approach it is possible to identify most relevant materials.

- It is important to ascertain the degrees to which different possible formation mechanisms play a role in producing interstellar, cometary, and meteoritic materials. In so doing we understand better under which circumstances these various materials are formed (i.e. in the gas or on surfaces, for ice and refractories, or biotically).

- Since remote sensing is all we can hope for in most cases, spectral details are the most important probes. By combining information from different techniques it will be possible in differentiating between different material physical and chemical characteristics.

- When comet sample returns will become a reality, it will be possible to judge the relative importance of different interstellar/solar nebula processes (i.e., cosmic ray bombardment, UV photolysis, thermal processing etc.) that went into making up the primeval material that formed the Solar Nebula. It will be very important to exploit as many techniques as possible simultaneously, and further see if specific characteristics can be associated with spectral nuances. The techniques for the analysis of samples returned from space must be developed in contact with other scientific communities (e.g., glaciologysts). To this end actions towards relevant institutions (ESA, NASA) must be promoted.

- It is important to characterise the minor ice components and probe the surface versus bulk reactions of incoming radicals and atoms with the ice. It is important to truly understand the chemistry induced by energetic processing and to identify distinguishing characteristics of particle bombardment vs. photon processing vs. thermal processing. This is particularly important in unrevealing cometary processes for sample return missions. Lastly, a key challenge is to understand the interplay between ice surface/bulk chemistry and gas-phase chemistry.

5.2 Problems in laboratory experiments

The following Table summarises the identified open problems in different areas of laboratory investigation:

General problems	• Isotope effects • Size effects: single grains vs. clusters, spectral behaviour • Optical constants: comparison
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Problems with ices	• Detection of free radicals • Surface and bulk chemistry induced by ion/radical accretion vs. energetic processes

The following warnings have been issued:

- A large fraction of extraterrestrial dust is made of both carbonaceous and silicate materials. It is not yet clear if such a mixture is the result of aggregation of pure carbons and pure silicates or if the mixing already occurs at the microscopic level. Efforts should be done in the laboratory to produce particles containing Si, O, and C at the same time.

- A relevant question is to establish when laboratory spectra can be directly comparable with observations without the need to consider shape/size effects.

- Production of key ice species, such as methanol and carbon dioxide, on grain surfaces has to explain why carbon dioxide is more or less constant (with respect to water) in environments with very different physical conditions, while methanol seems to be formed only at high-T ($\leq$ 100 K) regions around massive stars. Is this related to some catalytic process of grain surfaces?

- Caution must be applied in UV irradiation experiments when UV flux is much higher than in space. The lifetime of UV produced radicals (at low T, in particular) must be addressed.

5.3 Unsolved astrophysical problems

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