Astrophysical Ices in the Lab (*AILab*)

Workshop, 7-8 March 2016

Instituto de Estructura de la Materia, IEM-CSIC

Serrano 121, Madrid (Spain)

Comité
de
Espectroscopía
SEDOPTICA

Program

Schedule	Monday 7 March	*Schedule*	Tuesday 8 March
9:00-9:15	Documentation and Opening remarks		*Session 4* *Chair: M.A. Satorre*
	Session 1 *Chair: V.J. Herrero*	*9:00-9:45*	P4: G. Muñoz Caro CAB-CSIC: Properties of interstellar ice analogs: composition, structure, and photon-induced desorption
9:15-10:00	P1: N. Watanabe ILTS Overview of our works focusing on tunneling reactions, H-diffusion, and H2 spin conversion, etc.	*9:50-10:10*	O6: R. Escribano IEM: Modelling CO/H2O ice mixtures
10:10-10:30	O1: I. Tanarro et al. IEM : Infrared spectroscopy of carbonaceous interstellar dust analogues deposited by PECVD: effects of processing by high energy electrons	*10:15-10:35*	O7: M.L. Senent et al IEM: Weakly intramolecular interaction effects on the structure and low temperature spectra of ethylene glycol, an astrophysical species
10:35-11:00	*Coffee break*	*10:35-11:00*	*Coffee break*
	Session 2 *Chair: A. Kouchi*		*Session 5* *Chair: I. Tanarro*
11:00-11:45	P2: J. Cernicharo ICMM-CSIC: Nanocosmos	*11:00-11:45*	P3: Y. Kimura ILTS : Nucleation experiment to understand formation of cosmic dust
11:55-12:15	O2: T. Hama ILTS : Tunneling H addition to benzene and its control via surface structure	*11:55-12:15*	O8: B. Maté et al. IEM: Stability of glycine to energetic processing under astrophysical conditions investigated via infrared spectroscopy
12:20-12:40	O3: M.A. Satorre et al. UPV : Experimental studies of density and refractive index for astrophysical ices	*12:20-12:40*	O9: Y. Oba ILTS : Formation of chiral glycine by surface reactions of normal glycine with deuterium atoms at 10 K
13:00-14:30	*Lunch*	*13:00-14:30*	*Lunch*
	Session 3 *Chair: Y. Kimura*		*Session 6* *Chair: G. Muñoz Caro*
14:30-15:15	P3: V.J. Herrero IEM Laboratory astrophysics at IEM: overview of recent results	*14:30-15:15*	P6: A. Kouchi et al. ILTS : Development of an UHV transmission electron microscope for in-situ observation of ice
15:25-15:45	O4: H. Hidaka ILTS : Observation of amorphous solid water by non-contact atomic force microscopy	*15:25-15:45*	O10: J.L. Doménech IEM : Infrared spectroscopy of protonated ions
15:50-16:10	O5: V. Timón IEM : Theoretical calculations on HACs	*15:50-16:10*	O11: G. Molpeceres IEM Methane/Ethane binary mixtures under astrophysical

			conditions
16:15-16:45	*Coffee break*	*16:15-16:45*	*Coffee break*
16:45	Visit to IEM laboratories	*16:45*	*Closing remarks: N. Watanabe*
19:00	Optional: dinner in downtown Madrid	*19:00*	

Abstracts

P1: Naoki Watanabe

Institute of Low Temperature Science, Hokkaido University, Sapporo 060-0819, Japan

Overview of ILTS works focusing on tunneling reactions, H-diffusion, and H_2 spin conversion, etc.

O1: Isabel Tanarro, Miguel Jiménez-Redondo, Germán Molpeceres, Belén Maté, Víctor J. Herrero

Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Infrared spectroscopy of carbonaceous interstellar dust analogues deposited by PECVD: effects of processing by high energy electrons

Carbonaceous compounds are found in very diverse astronomical media. A significant amount is found in small dust grains, which show characteristic IR absorption bands revealing the presence of aliphatic, aromatic and olefinic functional groups. Among the various materials investigated as possible carriers of these bands, hydrogenated amorphous carbon has led to the best agreement with the observations. Carbonaceous grains are processed by UV radiation and collisions with high energy particles in their passage from asymptotic giant branch stars to planetary nebulae and to the diffuse interstellar medium. The mechanisms of their production and evolution in astronomical media are presently a subject of intensive investigation. In this work we present a study of the stability of carbonaceous dust analogues generated in He+CH4 RF discharges. To simulate the processing of dust in the interstellar environments, the samples have been subjected to electron bombardment. IR spectroscopy is employed to monitor the changes in the structure and composition of the carbonaceous films.

P2: José Cernicharo

Instituto de Ciencias de Materiales, CSIC, Madrid, Spain

Nanocosmos

O2: Tetsuya Hama

Institute of Low Temperature Science, Hokkaido University, Sapporo 060-0819, Japan

Tunneling H addition to benzene and its control via surface structure

This talk shows that the amorphous or crystalline structure of a solid benzene surface controls its chemical reactivity toward hydrogen. In situ infrared reflection-absorption spectroscopy revealed that H atoms can add to an amorphous benzene surface to form cyclohexane by quantum tunneling. However, hydrogenation is greatly reduced on crystalline benzene. We suggest that the origin of the high selectivity of this reaction is the large difference in intermolecular steric hindrance between the amorphous and the crystalline surfaces.

O3: Manuel Domingo; Ramón Luna; Carlos Millán; Carmina Santonja and Miguel Ángel Satorre

Escuela Politécnica Superior de Alcoy, UPV, 03801 Alicante, Spain

Experimental studies of density and refractive index for astrophysical ices

The talk will describe how density and refractive index are determined, in our laboratory, by means of double laser interferometry and quartz crystal microbalance (QCMB) techniques.

Some results will be shown to relate these parameters with values used in astrophysics or spectroscopy (i.e. band strength, optical constants, etc.) and to show the relationship of them with the structure of ices (i.e. crystalline-amorphous structure, porosity, etc.).

P3: Víctor José Herrero

Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Laboratory astrophysics at IEM: overview of recent results

The activity of the Laboratory Astrophysics group at IEM will be illustrated with representative examples from its main research lines. The results reviewed will deal with molecules (CO_2, CH_4) and ions (NH_4^+, $HCOO^-$) in ice, as well as with ion-molecule chemistry leading to H_3^+, N_2H^+, NH_4^+ and ArH^+ in hydrogen-rich cold plasmas. Both experimental measurements and theoretical calculations will be presented.

O4: Hiroshi Hidaka[1], Yoshiaki Sugimoto[2], Syunichi Nakatsubo[1], Naoki Watanabe[1], Akira Kouchi[1]

[1]Institute of Low Temperature Science, Hokkaido University, Sapporo, 060-0819, Japan.

[2]Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, 277-8561, Japan.

Observation of amorphous solid water by non-contact atomic force microscopy

Amorphous solid water (ASW) is abundant material of interstellar ice and is mainly present so as to cover the interstellar dust grains which are mineral particles with sub-micron size. Morphology of ASW is known to affect the physical and chemical phenomena occurring on ASW. However, the morphology of ASW in nano-scale range depending on the growth conditions is still unknown. Recently, we performed the real-space observations of surface structure of ASW formed by the oblique and the background vapor deposition method by using atomic force microscopy at several temperatures. In our presentation, the temperature and the deposition method dependence of surface morphology of ASW will be presented.

O5: Vicente Timón

Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Theoretical calculations on HACs

Cosmic carbonaceous nanoparticles present in the interstellar medium are a very important component of interstellar dust as hydrocarbon polymers. In fact a large amount of interstellar carbon is locked into polycyclic aromatic hydrocarbons and carbonaceous dust grains. The composition of these grains is believed to be similar to that of hydrogenated amorphous carbon (HAC), which is a complex disordered form of carbon consisting of diamond-like sp^3 and graphite-like sp^2 bonded carbon that can exhibit diverse properties depending on its formation conditions. A usual way of preparing HAC films in our laboratory is through plasma enhanced chemical vapor deposition (PECVD) of suitable gas precursors. Small hydrocarbons (CH_4, C_2H_2) reproduce reasonable well the main absorption bands of interstellar carbonaceous dust.

In the present work, we report through the use of theoretical quantum DFT methods and IR spectroscopy the determination of the most stable HAC's structures. Aromatic ring structures that are extracted from hydrogenated and methylated polycyclic aromatic hydrocarbons published in the literature are studied as solids. Their infrared spectra are expected to be coincident with the experimental data recorded in the laboratory and measured in the interstellar medium.

P4: Guillermo Muñoz Caro

Centro de Astrobiología, INTA-CSIC, Carretera de Ajalvir, km 4, Torrejón de Ardoz, 28850 Madrid, Spain

Properties of interstellar ice analogs: composition, structure, and photon-induced desorption

At the Center of Astrobiology (CAB) near Madrid, experiments are performed using the ISAC set-up for the simulation of ice processes. The ice is monitored by transmittance-FTIR and vacuum-UV spectroscopy, while the gas phase is analyzed using a QMS. Our main interest is the study of the ice properties during UV-irradiation and/or controlled warmup. Our group also collaborates on heavy ion and X-ray irradiation of ice experiments in large facilities.

Recent results on the photon-induced desorption and warm-up of molecular ices will be presented.

In addition to chemical processes in the ice, it is also important to study the ice structure.

O6: Rafael Escribano

Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Modelling CO/H_2O ice mixtures

With the purpose to simulate ice mixtures generated at the ILTS laboratories, a number of models have been designed for amorphous CO/H_2O mixtures of various proportions. The method used involves several steps: first, a crystalline CO ice is built; next, some CO molecules are replaced by H_2O molecules; then, the system is made amorphous in a molecular dynamics run; finally, the amorphous structure is optimized and the spectra are predicted at the minimum of the potential energy surface. The static pressure inside the sample cell is also monitored in the process. Calculations are performed using Materials Studio and Siesta packages.

O7: María Luisa Senent and Rahma Boussessi

Departamento de Química y Física Teóricas, IEM-CSIC, Serrano 121, Madrid 28006

Weakly Intramolecular Interaction Effects on the Structure and Low Temperature Spectra of Ethylene Glycol, an Astrophysical Species.

Even as its most popular application is as antifreeze, Ethylen Glycol (EG) is a relevant astrophysical species. It is rather abundant with respect to other medium-sized organic molecules in comets and meteorites where it is considered the most frequent of the sugar-related alcohols. Together with glycolaldehyde and ethanol, it represents a key species to understand the composition of extra-terrestrial ices. EG was identified in the Murchison and Murray meteorites and very recently, in ices in the hot core of Orion. In 2002, the molecule was detected in emission toward the galactic center source Sagittarius B2(N-LMH).

The successfully detection in gas phase have motivated laboratories studies of the rotational spectra which interpretation is not straightforward given the presence of unexpected tunnelling effects. An elaborate variational procedure of reduced dimensionality based on explicitly correlated coupled clusters calculations (CCSD(T)-F12) is applied to understand the far infrared spectrum.

P3: Yuki Kimura

Institute of Low Temperature Science, Hokkaido University, Sapporo 060-0819, Japan

Nucleation experiment to understand formation of cosmic dust

Nucleation is an initial process to form a particle by self-assembly of matter from a mother phase. In case of mineral formation in space, nanometer sized particles, called dust, have been nucleated from a supersaturated vapor, which is ejected from evolved stars, such as asymptotic giant branch star and supernova. However, details of the formation processes of cosmic dust have not been understood. Here, I will show our recent experimental studies to comprehend the detail of the mineral formation in space.

O8: Belén Maté, Víctor J. Herrero, Isabel Tanarro and Rafael Escribano

Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Stability of glycine to energetic processing under astrophysical conditions investigated via infrared spectroscopy

We have studied, via infrared spectroscopy, the effect of 2 keV electrons bombardment on amorphous and crystalline glycine layers at low temperatures to determine its destruction cross section under astrophysical conditions. Moreover, we have probed the shielding effect of water ice layers grown on top of the glycine samples at 90 K. These experiments aim to mimic the conditions of the aminoacid in ice mantles on dust grains in the interstellar medium or in some outer Solar System objects, with a water ice surface crust. A residual material, product of glycine decomposition, was found at the end of the processing. A tentative assignment of the infrared spectra of the residue will be discussed in the presentation.

O9: Yasuhiro Oba, Naoki Watanabe, Akira Kouchi

Institute of Low Temperature Science, Hokkaido University, Sapporo 060-0819, Japan

Formation of chiral glycine by surface reactions of normal glycine with deuterium atoms at 10 K

Glycine (NH_2CH_2COOH) is the simplest amino acid and does not have a chiral center among 20 protenoic amino acids. However, if one of the carbon-bound hydrogens is replaced with its isotopic counterpart deuterium (D), glycine becomes chiral. We experimentally demonstrated that chiral glycine ($NH_2CHDCOOH$) is formed by surface reactions of NH_2CH_2COOH with D atoms at temperatures as low as 10 K, which is the typical temperature of interstellar molecular clouds. Although no chiral molecules have been observed in interstellar medium, chiral glycine may be one of the most primordial chiral molecules in the Universe.

P6: Akira Kouchi, Naoki Watanabe, Hiroshi Hidaka, Tetsuya Hama, Yuki Kimura,

Shunichi Nakatubo, Kazuyuki Fujita, Kunio Sinbori, and Masayuki Ikeda

Institute of Low Temperature Science, Hokkaido University, Sapporo 060-0819, Japan

Development of an UHV transmission electron microscope for in-situ observation of ice

An ultrahigh vacuum (UHV) transmission electron microscope for in-situ observation of ice has been developed. A column of the microscope is evacuated by 5 ion pumps, two Ti-sublimation pumps, and two turbomolecular pumps. The pressure of the specimen chamber is lower than 1x10-7 Pa. We use a single tilt liquid He cooling holder for specimen cooling to 4 K. Three ports are directed to the specimen surface for in-situ studies: gas-inlet, UV irradiation, and a quadrupole mass spectrometer. Results of preliminary observation will be presented: formation of high-density amorphous ice by matrix sublimation method and UV-induced formation of ice XI.

O10: José Luis Doménech

Instituto de Estructura de la Materia, IEM-CSIC, Serrano 123, 28006 Madrid, Spain

Infrared spectroscopy of protonated ions

Molecular ions are key elements in the chemistry of the ISM. Even though their concentration is much smaller than that of neutrals in molecular clouds, their high reactivity makes them important intermediates in the formation of more complex molecules. Much of the information available for their identification in the ISM comes from rotational spectroscopy. Our recent work at the IEM aims at producing vibration-rotation spectroscopic data with high enough accuracy to be able to predict or guide searches for the rotational transitions of these ions both in space and in the laboratory.

O11: Germán Molpeceres[1], Miguel Ángel Satorre[2], Juan Ortigoso[1], Carlos Millán[2], Rafael Escribano[1], and Belén Maté[1]

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Methane/Ethane binary mixtures under astrophysical conditions

Spectroscopy of small hydrocarbons has taken renewed attention due to the recent missions surveying Pluto's surface (New Horizons) or the 67P/Churyumov–Gerasimenko comet (Rosetta). Laboratory data of plausible molecules present in these environments is needed in order to unambiguously assign spectroscopic features obtained by these missions.

In this work we present the results obtained in our laboratories for a series of binary mixtures composed of methane and ethane, providing information about the spectroscopic effects arising from the mixture of the components and giving also numbers for the optical constants of these materials. An atomistic interpretation of these mixture effects will also be given using quantum chemistry tools.