Atelier PCMI - lundi 29 juin 2009 - programme préliminiaire

Interstellar dust: observational and laboratory insights

10h00 -10h25: Marie Godard - *Hydrogenated amorphous carbon photoluminescence and astrophysical implications for the extended red emission*

10h25-10h50*:* Yvain Carpentier - *Flame by-products as analogues of interstellar dust spectroscopic investigations*

10h50-11h15: pause

11h15-11h40: Michel Devel - *Bottom-up approach to study dielectric properties of carbon soot*

11h40-12h05: Pierre Guillard - *Dust emission in the Stephan's Quintet giant shock structure*

12h05-12h30: Caroline Bot - *Small scale infrared color variations in high lattitude cirrus clouds*

12h30-14h00 : Repas

14h00-14h25: Laurent Pagani - *Large-scale detection of micron-size grains towards L183 from Spitzer/IRAC observations*

14h25-14h50: Anne Coupeaud - *Dust silicate emission in FIR/submm*

14h50-15h15: Patrice Theulé - *Thermal reactions at low temperature in interstellar ices*

15h15-15h40: Evelyne Roueff - *Incorporation of stochastic chemistry on dust grains in the PDR code using moment equations. Application to the formation of H2 and HD*

15h40-16h00 : Pause

16h25-16h50: Céline Toubin - Theoretical investigation of the chemical reactivity at interstellar grain surfaces: Toward a new formation mechanism for Aminoacetonitrile Precursor of Glycine

16h50-17h15: Sylvain Picaud - *Atomistic modeling of ice particles and carbonaceous grains*

Hydrogenated amorphous carbons photoluminescence and astrophysical implications for the extended red emission - Marie Godard

Hydrogenated amorphous carbons (a-C:H) has proved to be excellent analogs of interstellar dust through IR vibrational absorption bands (3.4, 6.8 and 7.2 micrometers bands (respectively 2960 cm-1, 1460 cm-1 and 1380 cm-1)) widely observed in galaxies diffuse interstellar medium. a-C:H are candidates for one of the observed interstellar dust features : a large emission band in the red part of the visible spectrum, attributed to photoluminescence (PL) of interstellar dust, and called the extended red emission (ERE). The PL absolute quantum yield is one strong constraints set by such ERE observations. The PL relative quantum yield is known and measured for many a-C:H at discrete excitation wavelengths. The few absolute efficiencies determined are scattered and sometimes vary by orders of magnitude for supposedly identical a-C:H. We thus produce astrophysical a-C:H and analyze their PL and IR behavior, carefully accounting for thin film optical effects. By properly determining the excitation wavelength dependent PL absolute quantum yields for a wide variety of astrophysically relevant a-C:H, we can constrain these interstellar dust analogs as possible ERE candidates.

Flame by-products as analogues of interstellar dust : spectroscopic investigations - Yvain Carpentier

Carbonaceous materials are a widespread component of the interstellar medium. Especially, aromatic structures have been proposed to be the carriers of some interstellar features : the Aromatic Infrared Bands observed in emission, the non-linear UV rise and the UV bump of the extinction curve. A flat fuel-rich and premixed flame allow us to produce a wide variety of carbonaceous structures strongly depending on the combustion conditions (fuel, pressure, fresh gas velocity and C/O ratio). The produced species are either studied in the gas phase or deposited on a substrate. The free-flying PAH-like molecules are studied by mass spectrometry and laser spectroscopy. R2PI of small PAH species and derivatives have been performed in the spectral region of the UV bump. The solid particles are analysed by IR spectroscopy, Raman spectroscopy and UV absorption. Structural analysis by transmission electron microscopy is also performed. The main results will be presented and discussed in the astrophysical context.

Bottom-up approach to study dielectric properties of carbon soot - Michel Devel

Atmospheric carbon soot is mainly made of carbon nanoparticles arranged in fractal clusters of variable size. These nanoparticles are characterized by spherical geometries (with diameters ranging from a few to tens of nm) and by an onion-like arrangement of small carbon clusters. For our recent studies on this subject [1],[2], we have developed a bottom-up multi-step approach in which these soot nanoparticles are modeled by random distributions of various pure carbon chemical units (C13, C16, C19, C24) on concentric spheres. The frequency dependent dielectric susceptibility of these grain models have been computed in the optical and near-UV domain, thanks to a multi-step discrete dipole approximation (DDA) model[2], adapted to the typical geometry of the soot nanoparticles and to the use of true atomic anisotropic polarizabilities[1]. Because the nanoparticles are defined atomistically, the set of atomic point dipoles is distributed on an irregular grid and we cannot use traditional discrete-dipole approximation (DDA) codes. We thus developed an approximate multi-step method that allowed us to discuss scattering of light by both carbonaceous nanoparticles and aggregates of these nanoparticles. The resulting code is able to deal with more than 100 000 atoms (nanoparticles with 15 nm diameter, experimentally observed size) while keeping a very good accuracy compared to the exact modelisation. We find that the dielectric susceptibility of these nanoparticles is highly

dependent on the type of chemical units used to construct the particles, but almost independent of their distribution in the various shells of the nanoparticle. This points to the possibility to gain information on the atomic structure of soot by means of EELS or optical measurements. Our results also confirm the importance of further studying atmospheric carbon soot in order to understand their optical and infrared effects and to give a definite balance sheet of their radiative properties. Acknowledgments The "Région de Franche-Comté" is thanked for its financial support for M.R. Vanacharla. References [1] F. Moulin, M. Devel and S. Picaud, Optical properties of soot nanoparticules, JQSRT, 109, 1791-1801 (2008) [2] R. Langlet, M.R. Vanacharla, S. Picaud and M. Devel F. Moulin, Bottom-up multi-step approach to study the relations between the structure and the optical properties of carbon soot nanoparticles, to be published in JQSRT, available online at http://dx.doi.org/10.1016/j.jqsrt.2009.03.015 [3] D. Alexander, J. Anderson, P. Crozier, Improved determination of aerosol optical properties from the EEL spectrum, Microsc. Microanal. 13 (Suppl 2), 1254–1255 (2007).

Dust emission in the Stephan's Quintet giant shock structure - Pierre Guillard
Spitzer observations emphasized surprisingly bright mid-IR H2 rotational line emission from the Stephan's Quintet (SQ) X-ray emitting giant shock structure (~ 30 kpc long). Guillard et al. 2009 proposed an interpretation where the H2 gas forms out of the multiphase shocked gas. In this scenario, dust is a key-element because its presence is required for H2 to form. Therefore we expect that some of the dust emission comes from molecular gas. Dust observations can also constrain the physical structure of the H2 gas, in particular the unknown amount of cold molecular gas. I will present new Spitzer observations - where faint PAH and dust continuum emission from the SQ shock is detected - and modelling of the dust spectral energy distribution. I will show that the data are consistent with the expected emission from dust associated with the warm (> 150 K) H2 gas and a Galactic dust size distribution. The low flux ratio between the PAH 7.7 and 11.3 micron bands and the detection of strong SiII 35 micron line emission can be both interpreted as evidence for a high electron density (ne >~ 0.3 cm-3). Present data do not allow to decide whether the molecular gas is diffuse or fragmented into clumps that are optically thick to UV radiation. Our model calculations show that far-IR Herschel observations would allow us to answer this question.

Small scale infrared color variations in high latitude cirrus clouds - Caroline Bot
High galactic latitude cirrus are thought to be one of the simplest characterized environment: clouds are optically thin and away from star forming regions. Indeed, on large scales, the infrared emission shows very limited variations of the dust temperature and dust emissivity, and infrared colors are constant. However, I will present the discovery of small scales variations in the infrared colors (60/100 and 160/100microns colors) observed in high galactic latitude fields. These variations were first observed in a serendipitous analysis of the Spitzer Infrared Nearby Galaxies Survey (SINGS) and are now confirmed for cirrus observed around the Small Magellanic Clouds (SAGE-SMC survey). A trend is observed between these two IR colors that can not be accounted for by current dust models. Different interpretations will be discussed.

Large-scale detection of micron-size grains towards L183 from Spitzer/IRAC observations : a new window to explore the realm of grains - Laurent Pagani
Grain growth in the cold and dense interstellar medium is predicted and sometimes advocated from the modeling of far infrared and submillimeter observations and in some cases from near infrared extinction measurements but never directly witnessed. We

present Spitzer/IRAC mid-infrared (MIR) images of L183 which show scattered light on tens of square arcminutes. This scattered light can only be explained by micron-size grains. With the help of a preliminary 3D modeling, a first tentative quantification of the dust properties will be discussed. This is the first time that big grains are directly observed. Because scattering is much more sensitive to the grain size than absorption and because MIR radiation goes deeper into molecular cloud cores than shorter wavelengths, we suggest that this MIR window is an excellent tool to study grain growth in dark clouds, a tool which will become effective with the future James Webb Space Telescope (JWST).

Dust silicate emission in FIR/submm - Anne Coupeaud
The observations of PRONAOS and Archeops in the submillimeter wavelengths range revealed a dependence with temperature of the spectral index of the dust emissivity beta. This parameter is of a great importance for astrophysical people who used it for the estimation of the dust mass. Our goal is to explain the unusual optical properties of the big silicate grains in this domain of long wavelengths. With the experimental set-up Soirs d'ete (Studies On InfraRed and Submillimeter Dust interstEllar Thermal Emission) we performed some experiments on absorption properties of analogues interstellar grains in function of the temperature (300K to 4K).

Thermal reactions at low temperature in interstellar ices - Patrice Theulé
Different types of chemical reactions are occurring in interstellar ices. New and more complex molecules are formed and eventually desorbed into the gas phase when the ice is submitted to energetic processes, thermal or not. This is especially the case in star formation regions. I will give three examples of thermal reactions occurring at low temperature and correlate the work done in laboratory with IR spectra taken by ISO or Spitzer.

Prise en compte des fluctuations dans les processus chimiques a la surface des grains. Application a la formation de H2 et HD - Evelyne Roueff
Unlike gas phase reactions, chemical reactions occuring on interstellar dust surfaces cannot be always modeled by rate equations. Due to the small grain sizes and low fluxes, large fluctuations may take place in the number of adsorbed atoms during the gas-grain interactions and stochastic methods are then required. We have used the moment equations formalism introduced by the Hebrew University group (Barzel and Biham) within the Meudon PDR (Photon Dominated Regions) code and derived the formation rates of H2, HD and D2 on grain surfaces. We discuss the validity of the rate equations formalism for the grain formation rate of these molecules within a range of dust temperatures. We will also report on the extension of this method to compute methanol, formaldehyde and water formation on grains.

Theoretical investigation of the chemical reactivity at interstellar grain surfaces: Toward a new formation mechanism for Aminoacetonitrile Precursor of Glycine
- Céline Toubin
The origin of amino acids in the prebiotic chemistry of the early Earth has been a topic of long standing interest. Interestingly, proton relay mechanisms have previously been found theoretically in heterogeneous reactions on ice in connection with stratospheric ozone depletion, and for an initial step in the Strecker synthesis. In this context, calculations have been carried out for the reaction between methanimine, CH2NH, and the two isomers HNC/HCN leading to aminoacetonitrile---a known precursor of glycine--- in both gas phase and on a model icy grain surface. Three mechanisms are evidenced in the reference gas-phase calculations: for CH2NH reacting with HCN, there are two routes referred to as indirect and direct, and for CH2NH reacting with the isomer HNC, a one-step mechanism

is found. All these reaction paths have quite high barriers, but on a model interstellar grain icy surface, very considerable barrier reduction results, due to a concerted proton relay mechanism. Explicit water molecules in a reaction ring are shown to participate in this relay mechanism in the reactions of CH2NH both with HCN and with the HNC isomer. The significance of these results for glycine or other complex organic molecules production in the ISM is discussed. D. M. Koch, C. Toubin, S. Xu, G. H. Peslherbe, J. T. Hynes, J. Phys. Chem. C 111 15026-15033 (2007) D.M. Koch, C. Toubin, G. Peslherbe, J.T. Hynes, J. Phys. Chem. C 112 2972 (2008)

Atomistic modeling of ice particles and carbonaceous grains - Sylvain Picaud

In the present work, atomistic simulations have been used to model ice surfaces and carbonaceous grains of atmospheric interest and their interactions with surrounding molecules such as water and polycyclic aromatic hydrocarbon (PAHs). In particular, Grand Canonical Monte Carlo simulations have been performed to calculate the adsorption isotherms of various partially oxidized methane derivates, such as methanol, formaldehyde, formic acid and acetone, on ice surfaces in tropospheric conditions. The GCMC method has also been used to simulate the adsorption isotherms of water molecules around carbonaceous particles of spherical shape modeling soot emitted by aircrafts, as a function of the size and chemical composition of these particles. Moreover, because soot is also suspected to modify the atmospheric chemistry by providing surfaces for heterogeneous reactions, we have modeled chemical reactions at the surface of carbonaceous grains. However, because ab initio calculations on the corresponding large systems are not computationally tractable, we have developped mixed classical/semi-empirical calculations to characterize, as a first application, the oxidation process of small PAHs by the OH radical at the surface of small graphite clusters. Although these studies have been performed in the context of atmospheric sciences, we will show that such atomistic simulations could also be used to give insigths on processes occuring on grains of interstellar interest.