THE HYDRIDE TOOLBOX

BOOK OF ABSTRACTS

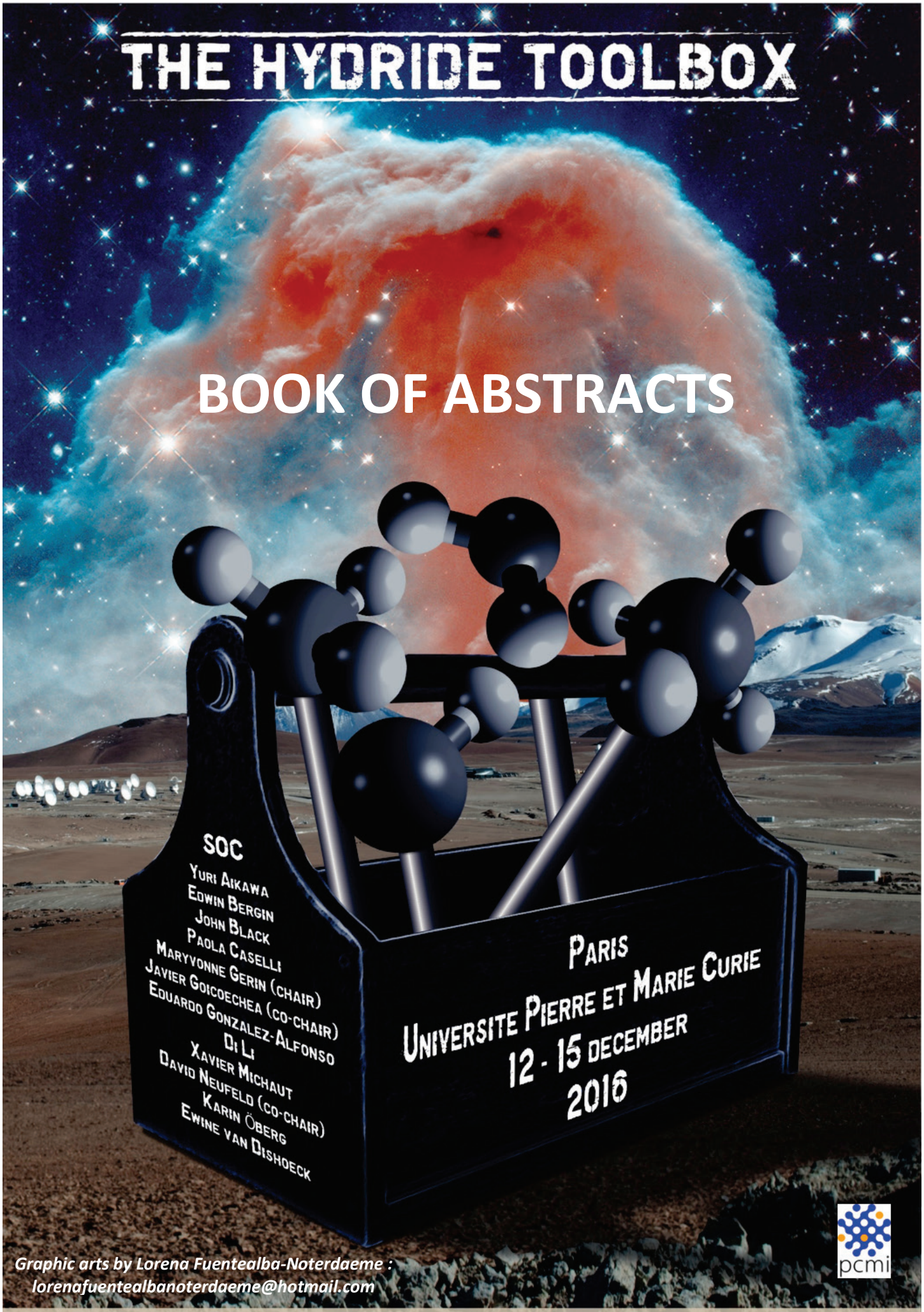

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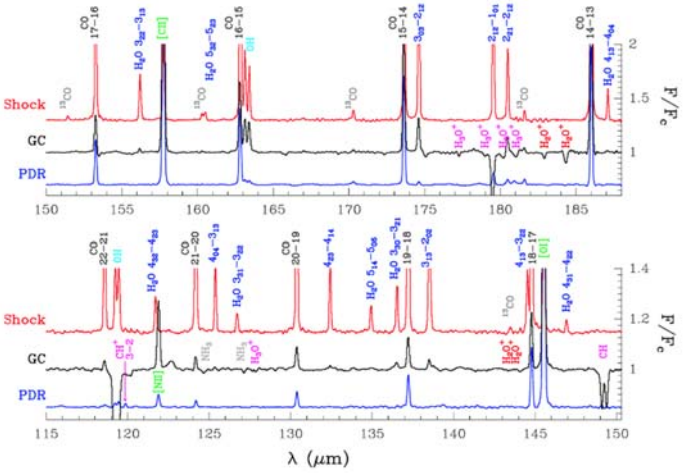
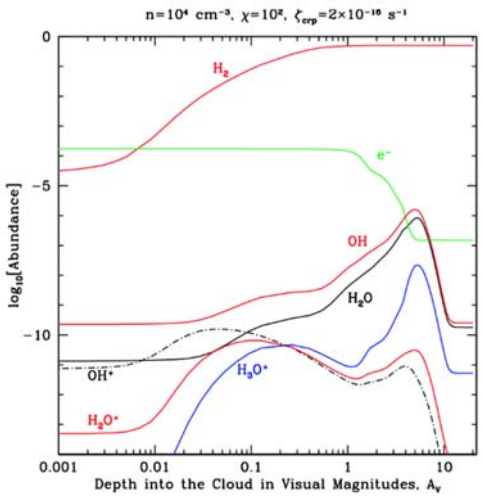
Table des matières

SCOPE

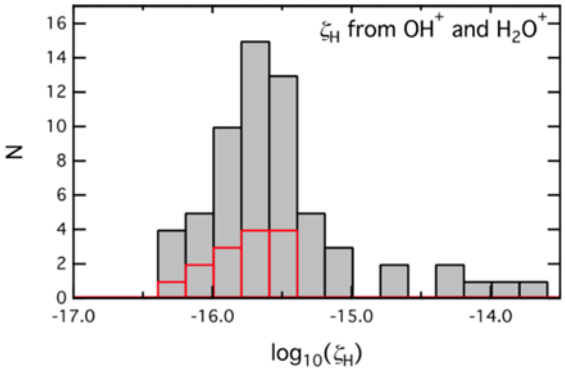
Hydrides are defined as molecules, radicals, and molecular ions containing one heavy atom (e.g., C, N, O, F, S, Cl, Ar, etc.) bound with one or several hydrogen atoms. Very abundant in the interstellar medium, these species were among the first molecules detected in space. With the recent development of submillimeter astronomy - in particular the Herschel satellite and the SOFIA stratospheric airplane - they are now observed in a wide range of environments, including low density diffuse matter, dense FUV illuminated interfaces of molecular gas and HII regions, cold and dense prestellar cores, molecular shocks, and even distant objects at high redshift.



Efficiently formed through hydrogenation of atomic gas, hydrides lie at the root of interstellar chemistry and of the formation of complex organic species. Despite the apparent simplicity of their chemistry, the development of models capable of explaining the observations of hydrides has required several decades. Many independent factors contributed to enhance the difficulty: i) the relative scarcity of astronomical data due to the limitation of observing from the ground, ii) the specific thermodynamic properties of a few hydrides of astronomical interest which raised issues regarding their formation timescales, and iii) the need for advanced modelling approaches combining fluid dynamics, gas phase and solid phase chemistries, as well as excitation processes including radiative and chemical formation pumping.



The improvements of state-of-the-art modelling combined with the recent progresses in theory and in laboratory data have led to a better understanding of astronomical hydrides, and have opened the possibility to use them as powerful diagnostics of the interstellar medium, both in our Galaxy or at cosmological distances. Indeed, hydrides have now been used in various ways to determine several important properties of the ISM such as, the density, the temperature, the molecular hydrogen content, the cosmic ray ionization rate, the turbulent dissipation rate, the magnetic field intensity, the ice condensation and evaporation processes, and the evolutionary time scale of matter. In parallel, they have become important probes of planet formation processes, tracing the role of the snow line in the growth of planet embryos, and the emergence of planet atmospheres.



Figures are taken from Goicoechea et al. (2013, 2015), Joblin et al. (in prep.), Hollenbach et al. (2012) and Indriolo et al. (2015). They are reproduced with permission from AAS managed by IOP publishing ©AAS

Main topics

- **Molecular physics and chemistry of hydrides**
- **Diffuse ISM, turbulence, and shocks**
- **Cosmic rays and magnetic field**
- **Extragalactic and AGN activity**
- **Solid phase processes and chemistry**
- **Stars and planet formation, exoplanets**
- **Future projects**

Invited Speakers

S. Aalto Chalmers UT-Sweden	**M. Agundez** ICMM-Spain	**J. Black** Chalmers UT- Sweden
P. Caselli MPI Extraterr. Phys.-Germany	**I. Cleeves** Harvard-Smith. CFA – USA	**E. Dartois** IAS – France
A. Faure IPAG – France	**S. Federman** U. Toledo- USA	**D. Galli** INAF – Italy
B. Godard Obs. Paris- France	**E. Gonzalez-Alfonso** U. Alcala-Spain	**T. Hama** Hokkaido U. – Japan
N. Indriolo Space Telescope Sc. Inst.-USA	**M. Kaufman** San Jose State U. – USA	**H. Kreckel** MPI Nuclear Physics-Germany
K. Menten MPI Radioastron.-Germany	**K. Öberg** Harvard-Smith. CFA – USA	**A. Omont** IAP-France
V. Ossenkopf Köln U.-Germany	**K. Pontoppidan** Space Telescope Sc. Inst.-USA	**E. Roueff** LERMA – France
J. Tennyson U. College London-England	**W. Ubachs** Vrije U.- Netherlands	**E. van Dishoeck** Leiden Obsevatory-MPE

Local Organizing Committee

Mathieu Bertin (UPMC)
Rémi Dupuy (UPMC)
Jean-Hugues Fillion (UPMC)
Benjamin Godard (Obs. Paris)
Darek Lis (Obs. Paris - UPMC)
Laurent Philippe (UPMC)
Nora Roger (UPMC)
Patrick Boissé (UPMC)
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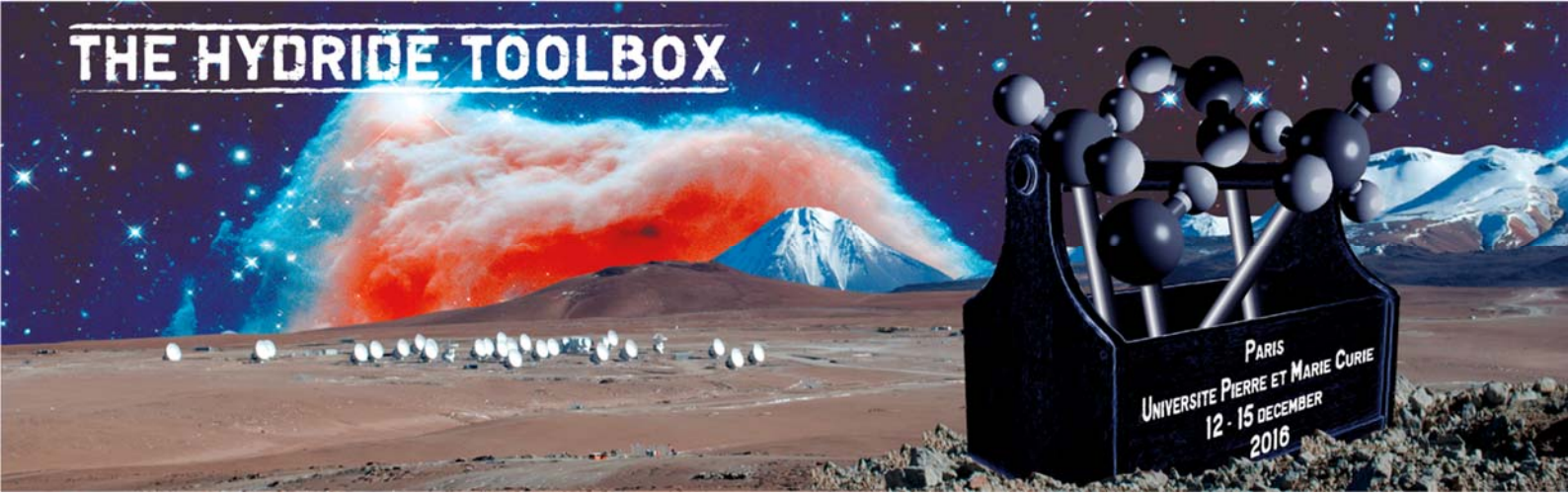
Maryvonne Gérin (ENS-Paris)
Pascal Jeseck (UPMC)
Xavier Michaut (UPMC)
Thomas Putaud (UPMC)



Monday, December, 12th

›8:30 **Registration (Tower 44- 1st Floor - Corridor 44-45 - Jussieu campus)**

›9:15 **Session: Molecular physics and chemistry of hydrides** *(Chair: P. Caselli)*

›9:15 **Review: Physics, chemistry and excitation of hydride molecules** *Evelyne Roueff*

›10:00 **Elastic and inelastic collisional processes** *Alexandre Faure*

›10:30 **Coffee break**

›11:00 **Hyperfine excitation of OH^+ by H** *François Lique*

›11:20 **Recombination, excitation and dissociation of hydride molecular cations in low energy electron collisions** *Ioan Schneider*

›11:40 **The high-resolution vibration rotation spectrum of HCl^+** *Jose Domenech*

›12:00 **Session: Stars and planet formation, exoplanets** *(Chair: P. Caselli)*

›12:00 **Review: Hydrides as tracers of the star and planet formation process** *Ewine van Dishoeck*

›12:45 **Buffet lunch**

›13:55 **Session: Stars and planet formation, exoplanets** *(Chair: E. Gonzalez-Alfonso)*

›14:00 **The Green Bank Ammonia Survey (GAS): First results of NH_3 mapping the Gould Belt** *Jaime Pineda*

›14:20 **Sunbathing around low-mass protostars - new insights from hydrides** *Agata Karska*

›14:40 **On the origin of C_4H and CH_3OH in protostars** *Johan Lindberg*

›15:00 **Hydride isotopologues** *Paola Caselli*

›15:30 **Coffee break**

›16:00 **Hydrides as tracers of dense shocked molecular gas** *Michael Kaufman*

›16:30 **The formation of H_2S in dark clouds** *Asuncion Fuente*

›16:50 **A three-dimensional model of the distribution and deuteration of water in SgrB2(M)** *Claudia Comito*

›17:10 **Flash advertisings & Poster session**

›19:00 **Cocktail in the panoramic room at the 24th floor of the Zamansky Tower (Jussieu Campus)**

Tuesday, December, 13th

›9:00 **Welcome Speech** *by Stéphane Régnier, Vice President of Université Pierre et Marie Curie*

›9:10 **Session: Solid phase processes and chemistry** *(Chair: X. Michaut)*

›9:10 **Hydrides in solid phases: physical processes and chemistry** *Emmanuel Dartois*

›9:40 **Radiolysis of Cosmic Ice Analogs of Ammonia, An Interstellar Hydride** *Leslie Gates*

›10:00 **Nuclear-spin dynamics of interstellar water ice** *Tetsuya Hama*

›10:30 **Chemistry of hydride-containing ices: UV photoprocessing of an H_2O:CH_4 ice analog** *Rafael Martin - Domenech*

›10:50 **Coffee break and poster session**

›11:30 **New binding energy calculations explain HF freeze-out observed in protostellar envelopes in NGC6334** *Matthijs van der Wiel*

›11:50 **VUV Photoionisation of CH_x radicals and reactivity of their cations CH_x^+** *Christian Alcaraz*

›12:10 **Search for a drifting proton-electron mass ratio from H_2** *Wim Ubachs*

›12:40 **Lunch**

›14:00 **Session: Stars and planet formation, exoplanets** *(Chair: K. Öberg)*

›14:00 **Hydrides in dense PDRs** *Volker Ossenkopf - Okada*

›14:30 **Ortho-to-para ratios of dihydride species** *Romane Le Gal*

›14:50 **Spectral mapping of CH, CH^+ and C^+ in Orion BN/KL: what they tell us about formation and excitation in shocks and PDRs** *Patrick Morris*

›15:10 **Origin and excitation mechanisms of OH and CH^+ in PDRs** *Anna Parikka*

›15:30 **Coffee break**

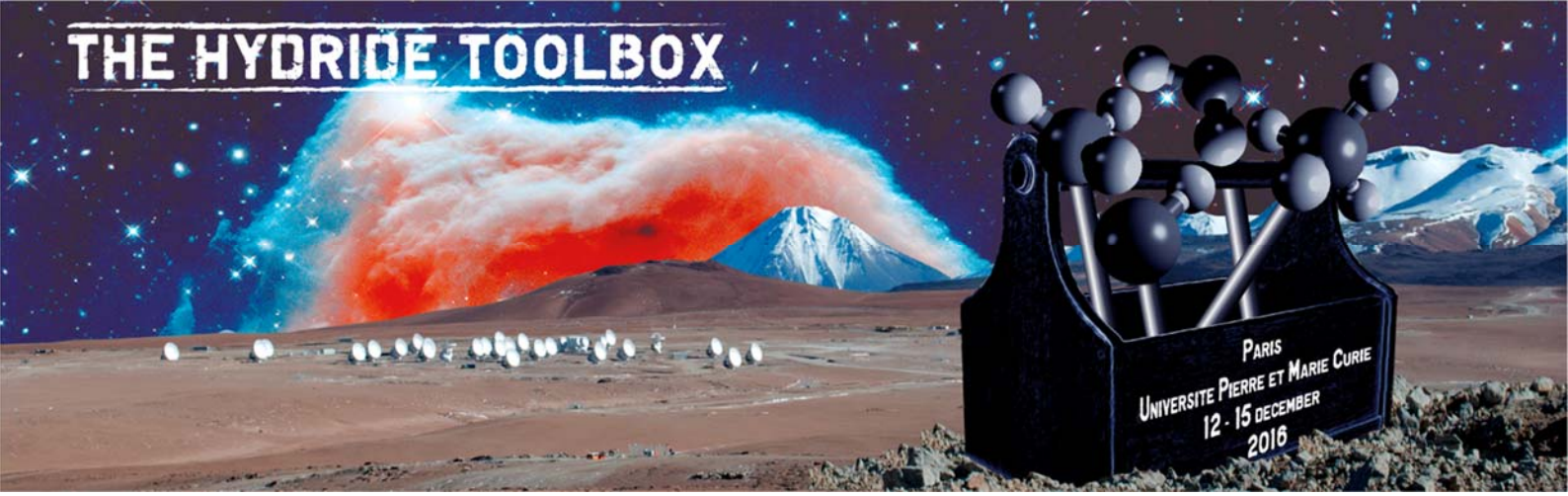
›15:55 **Session: Extragalactic and AGN activity** *(Chair: K. Öberg)*

›16:00 **Hydrides as probes of physical conditions and dynamics in galaxies: inflows and outflows** *Eduardo Gonzalez - Alfonso*

›16:30 **Herschel Legacy Survey of Hydrogen Fluoride Towards Nearby Galaxies** *Raquel Monje*

›16:50 **Probing the properties and evolution of galaxy nuclei with hydrides (and their friends)** *Susanne Aalto*

›17:20 **Flash advertisings & Poster session**



Wednesday, December, 14th

›9:00 **Session: Diffuse ISM, turbulence, and shocks** *(Chair: D. Neufeld)*

›9:00 **Hydrides in the Diffuse ISM: An Overview of Observations at Ultraviolet and Visible Wavelengths** *Steve Federman*

›9:30 **A far-infrared study of oxygen chemistry in diffuse clouds** *Helmut Wiesemeyer*

›9:50 **Evaluation of Molecular Hydrogen tracers** *Maryvonne Gérin*

›10:10 **Chemical probes of the turbulent diffuse ISM** *Benjamin Godard*

›10:40 **Coffee break**

›11:10 **Origin of CH^+ in diffuse molecular clouds** *Valeska Valdivia*

›11:30 **Session: Cosmic rays and magnetic field** *(Chair: D. Neufeld)*

›11:30 **H_3^+ physics and chemistry** *Holger Kreckel*

›12:00 **Protostars: Forges of Cosmic Rays?** *Marco Padovani*

›12:20 **Hydride Ions and Ionizing Irradiation in Young Stellar Objects** *Arnold Benz*

›12:40 **Lunch**

›13:55 **Session: Cosmic rays and magnetic field** *(Chair: J. Goicoechea)*

›14:00 **Molecular Ions as Tracers of the Cosmic-Ray Ionization Rate** *Nick Indriolo*

›14:30 **Analysis of ArH^+, H_3^+, OH^+ and H_2O^+ Observations to Estimate the Cosmic-Ray Ionization Rate Using Comprehensive Diffuse Cloud Models** *Mark Wolfire*

›14:50 **Extragalactic and AGN activity** *(Chair: J. Goicoechea)*

›14:50 **Herschel observations of OH and H_2O in compact obscured nuclei** *Niklas Falstad*

›15:10 **Coffee break**

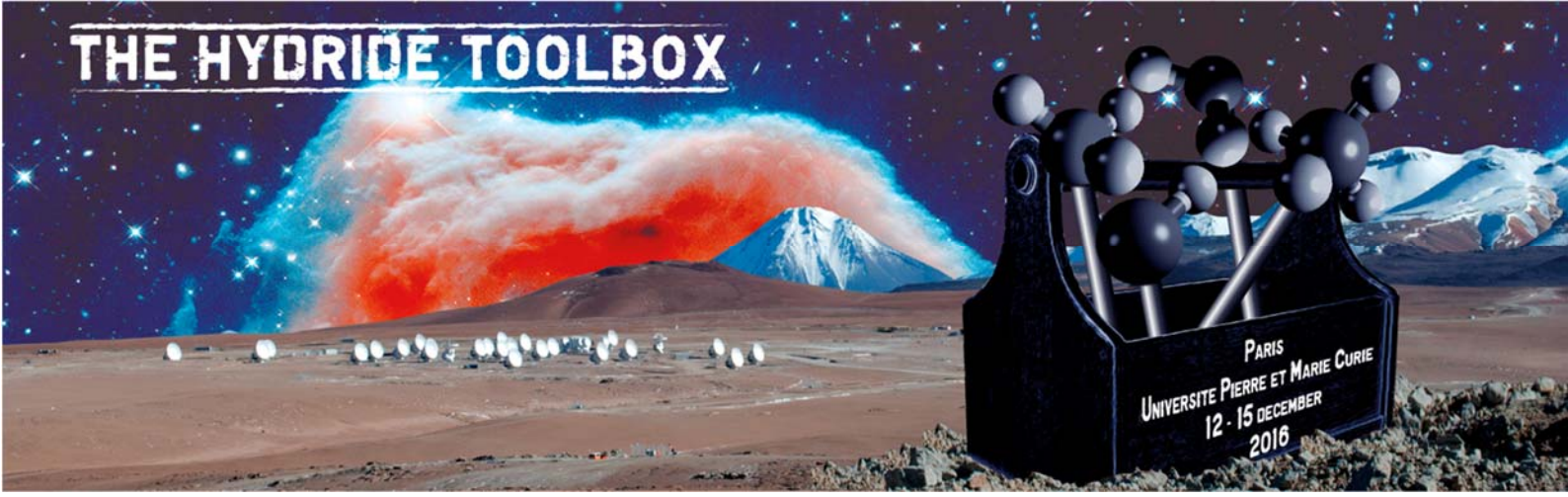
›15:40 **Detections of hydrides in high z sources, current analysis, and diagnostics** *Alain Omont*

›16:10 **Large turbulent gas reservoirs unveiled with CH^+(1-0) around starburst galaxies at z ~ 2.5** *Edith Falgarone*

›16:30 **The first hydrides** *Daniele Galli*

›17:00 **Hydrides toward PKS1830-211** *Sebastien Muller*

›20:00 **Conference Dinner at the Observatory of Paris (Cassini Room)**



Thursday, December, 15th

›9:00 **Session: Stars and planet formation, exoplanets** *(Chair: J. Black)*

›9:00 **Observations of hydrides in disks** *Klaus Pontoppidan*

›9:30 **Physical and Chemical Evolution of Hydrides in Disks and Implications for Planet Formation** *Ilse Cleeves*

›10:00 **Hydrides in Circumstellar Envelopes** *Marcelino Agundez*

›10:30 **Coffee break**

›11:00 **Molecular Emission in Planetary Nebulae as Seen by the Herschel Planetary Nebula Survey (HerPlaNS)** *Isabel Aleman*

›11:20 **Molecular physics challenge for exoplanet studies** *Jonathan Tennyson*

›11:50 **Hydrides in 2D hydrodynamic turbulence** *Pierre Lesaffre*

›12:10 **Lunch**

›13:50 **Poster prize**

›14:10 **Session: Future projects** *(Chair: M. Gérin)*

›14:10 **Future Observations of Hydrides with Ground-based, Air- and Space-Borne Telescopes** *Karl Menten*

›14:40 **FAST Telescope: Current Status, Planned Capabilities, and Upcoming Projects** *Marco Krco*

›15:00 **A Probe Mission to Trace Water from Interstellar Clouds to the Solar System** *Paul Goldsmith*

›15:20 **Laboratory astrophysics challenges** *Karin Öberg*

›15:50 **Theoretical & modeling challenges / Summary of the meeting** *John Black*

›16:20 **Wrap up**

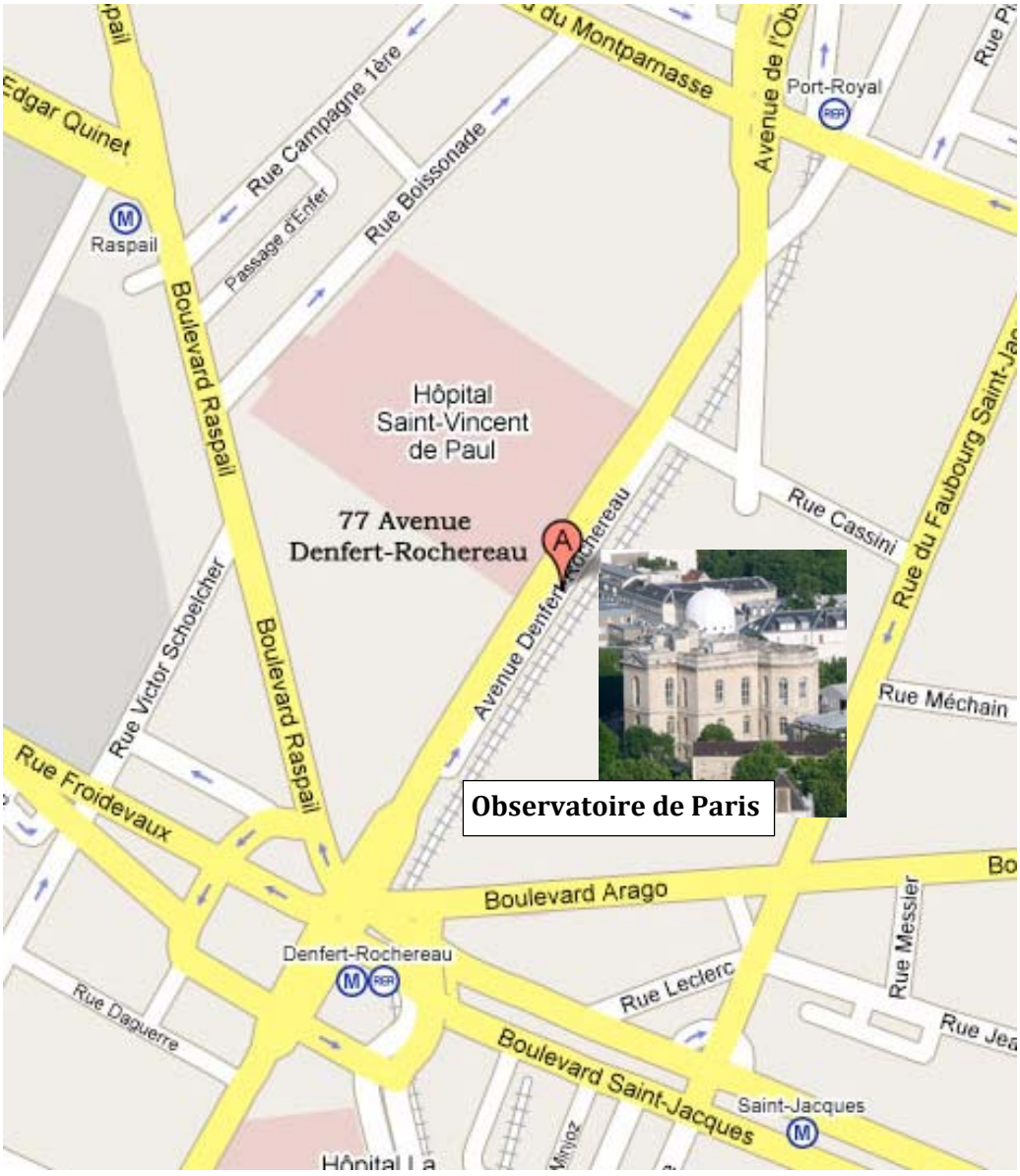
PRACTICAL INFORMATION

Registration, **conferences**, **poster sessions** will take place at the **1st floor** of the **44 tower** (corridor 44-45) at the University Pierre et Marie Curie (Jussieu Campus).

O**n Monday, December 12th**, a **lunch buffet** will be served at conference place at 12:45pm.

On Monday, December 12th, in the **evening,** the participants are invited to a **welcome cocktail** in the panoramic room at the **24th floor** of the **Zamansky Tower** (central tower of Jussieu Campus). (Scheduled time **7:00 pm**)

On Wednesday, December 14th, in the **evening,** the **conference dinner** will be given in the **"Cassini room"** at the **Observatoire de Paris** in the historical center of the city. The entrance of the Observatoire is located at the address: 77, avenue Denfert Rochereau, 14th arrondissement Paris. (Scheduled time **8:00 pm**)



Nearest Metro stations and RER stations:
Denfert-Rochereau (Metro lignes 4, 6, RER B)
Port Royal (RER B)

Access by city bus : Observatoire-Port Royal (Lignes 38, 83, 91)

Contact: xavier.michaut@upmc.fr Phone number: ++33-(0)6-80-68-78-34

Molecular physics and chemistry of hydrides

Physics, Chemistry and Excitation of Hydride Molecules

Evelyne Roueff[1]

[1]*LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universités, UPMC Univ. Paris 06, F-92190, Meudon, France*

Interstellar hydrides, molecular compounds where one heavy atom is chemically bound to one or several hydrogen atoms, have been comprehensively discussed in a recent review [1]. Table 1 reports the presently detected hydride molecules in the interstellar medium, according to their elemental families.

Table 1: Detected interstellar hydrides.

C	**N**	**O**	**S**	**F**	**Cl**	**Ar**
CH	NH	OH	SH	HF	HCl	ArH^+
CH_2	NH_2	H_2O	H_2S		HCl^+	
CH_3	NH_3	OH^+	SH^+		H_2Cl^+	
CH_4	NH_4^+ *	H_2O^+				
CH^+		H_3O^+				
CH_3^+ *						

* Species reported under their monodeuterated substitute.

The present talk will summarize the structural and thermochemical properties of these hydride molecules. I also will discuss how those features can be linked to astrophysical diagnostics through energy and chemical kinetics considerations, providing plausible gas phase chemical reaction schemas under a variety of interstellar conditions.
Some specific examples will be discussed at the light of recent observational, theoretical and/or experimental studies.

References

[1] Gerin M., Neufeld D.A. and Goicoechea J.R., ARAA, 2016, 54, 181

Reactive and inelastic collisions involving hydrides

Alexandre Faure[1,2]

[1] *Univ. Grenoble Alpes, IPAG, F-38 000 Grenoble, France*
[2] *CNRS, IPAG, F-38 000 Grenoble, France*

Hydrides play a central role in molecular astrophysics as significant reservoirs of heavy elements. Excitation studies of interstellar hydrides deserve a particular attention because the reactive processes with H and H_2, negligible at low temperature for most interstellar molecules, can compete with or even dominate the energy transfer processes. This challenging problem was adressed by theory only recently [1, 2, 3]. We will review recent theoretical results on closed-shell, radical and ionics hydrides due to H_2, H and electron collisions. The competition between inelastic, exchange and reactive channels will be examined and the relative importance of these processes in radiative transfer studies will be illustrated. Comparisons with experimental results will be presented for benchmark (closed-shell) systems, at the state-to-state level, demonstrating that interaction potential calculations have now reached a high level of accuracy. The ortho-to-para ratios of hydrides, as derived from Herschel observations (see e.g. [4] and references therein), will be also discussed and the role of nuclear-spin selection rules in the gas-phase will be emphasized. Perspectives will be finally given regarding the expected major developments in the field of molecular excitation.

References

[1] Lique F., Faure A., J. Chem. Phys, 2012, 136, 031101

[2] Zanchet A. et al., ApJ, 2013, 766, 80

[3] Motapon O. et al., Phys. Rev. A, 2014, 90, 012706

[4] Persson C. et al., A&A, 2016, 586, A128 012706

Hyperfine excitation of OH^+ by H

François Lique[1], Niyazi Bulut[2], and Octavio Roncero[3]

[1] *LOMC - UMR 6294, CNRS-Université du Havre, Le Havre, France*
[2] *Firat University, Department of Physics, Elazığ, Turkey*
[3] *Instituto de Física Fundamental, CSIC, Madrid, Spain*

The OH^+ ions are widespread in the interstellar medium and play an important role in the interstellar chemistry as they initiates the oxygen chemistry. The OH^+ abundance could also be a valuable tracer of cosmic ray and X-ray ionization rates in photon dominated regions (PDR's). Since OH^+ is very reactive and rapidly destroyed after its formation, its rotational populations is expected to be out of local thermodynamic equilibrium and may be driven the chemical state-to-state pumping mechanism:

$$O^+ + H_2 \rightarrow OH^+ + H \quad (1)$$

State-to-state rate constants for the chemical pumping mechanism together with radiative and approximate collisional coefficients were used in radiative transfer models to simulate the rotational emission of OH^+ from PDR's [1]. Surprisingly, it was found that the inelastic collisions dominate over the chemical pumping for determining the emission from low rotational states of OH^+. It clearly indicates that accurate collisional data with the H collisional partner are needed for modeling the abundance of OH^+.

In this talk, we present the calculation of OH^+–H fine and hyperfine resolved rate coefficients for temperatures ranging from 10 to 1000 K using quantum wave packet and recoupling approaches [2, 3]. The calculation of OH^+–H rate coefficients were extremely challenging since (i) in OH^+–H collisions, there is a reactive channel corresponding to the hydrogen exchange that may affect the inelastic rate coefficients (ii) there are two electronic states correlating to OH^+ and H reactant, each one having different rate coefficients (iii) the OH^+–H collisions can be reactive, leading to a competition between inelastic and reactive processes at high energies. The new rate coefficients should help significantly in the interpretation of OH^+ spectra and enable the OH^+ molecule to become a powerful astrophysical tool.

References

[1] Gómez-Carrasco et al., ApJ, 2014, 794, 33

[2] Bulut N., Lique F., Roncero O., J. Phys. Chem. A, 2015, 119, 12082

[3] Lique F., Bulut N., Roncero O., MNRAS, 2016, submitted

Recombination, excitation and dissociation of hydride molecular cations in low energy electron collisions

J. Zs. Mezei[1], F. Colboc[1], D. O. Kashinsky[2], D. A. Little[3], M. D. Epée Epée[4], S. Niyonzima[5], N. Pop[6], C. M. Coppola[7], K. Chakrabarti[8], O. Motapon[4], A. Bultel[9], K. Hassouni[10], D. Talbi[11], A. P. Hickman[12], A. Faure[13], J. Tennyson[3], and I. F. Schneider[1]

[1]*Laboratoire Ondes et Milieux Complexes UMR6294, Université du Havre, France*
[2]*Department of Physics and Engineering, US Military Academy, NY, USA*
[3]*Department of Physics and Astronomy, University College London, UK*
[4]*Faculty of Sciences, University of Douala, Cameroon*
[5]*Faculté des Sciences, Université du Burundi, Bujumbura, Burundi*
[6]*Politehnica University of Timisoara, Romania*
[7]*INAF-Osservatorio Astrofisico di Arcetri, Bari, Italy*
[8]*Department of Mathematics, Scottish Church College, Calcutta, India*
[9]*CORIA UMR6614, Université de Rouen, Saint-Etienne du Rouvray, France*
[10]*LSPM UPR3407, Université Paris 13, Villetaneuse, France*
[11]*Laboratoire Univers et Particules de Montpellier, UMR5299, France*
[12]*Department of Physics, Lehigh University, PA, USA*
[13]*Institut de Planétologie et d'Astrophysique de Grenoble, CNRS-INSU, France*

Accurate state-to-state rate coefficients have been computed for electron-impact dissociative recombination, ro-vibrational excitation and dissociative excitation of hydride molecular cations [1]:

$$XH^+(N_i^+, v_i^+) + e^- \rightarrow X + H, \quad XH^+(N_f^+, v_f^+) + e^-, \quad X + H^+ + e^- \qquad (1)$$

Detailed studies, based on the Multichannel Quantum Defect Theory , have been achieved for H_2^+ [2], HD^+ [3], BeH^+ [4], BeD^+, CH^+ and SH^+, species relevant for interstellar media and for cold natural or laboratory plasmas, the comparison with storage-ring measurements resulting in good agreement.

References

[1] Schneider I. F., Dulieu O., and Robert J. (editors), EPJ Web of Conferences, 84, 2015

[2] M. D. Epée Epée et al, MNRAS 455, 2015, 276

[3] K. Chakrabarti et al, Phys. Rev. A 87, 2013, 022702

[4] S. Niyonzima et al, Phys. Rev. A 87, 2013, 022702

The high resolution vibration rotation spectrum of HCl^+

José L. Doménech[1], Brian Drouin[2], José Cernicharo[3], Víctor J. Herrero[1], and Isabel Tanarro[1]

[1] *Instituto de Estructura de la Materia CSIC, Serrano 123. 28006 Madrid, Spain*
[2] *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA*
[3] *Grupo de Astrofísica Molecular, Instituto de Ciencia de Materiales de Madrid CSIC, Sor Juana Inés de la Cruz 3, Cantoblanco, 28049 Madrid, Spain*

The chloroniumyl cation, HCl^+, has been identified in space from *Herschel*'s spectra [1]. A joint analysis of extensive vis-UV spectroscopy emission data together with a few high resolution and high accuracy mm-wave data provided the necessary rest frequencies to support the astronomical identification [2]. Now that the *Herschel* mission is over, there are few alternatives to continue the study of this and other hydrides. The instrument GREAT onboard SOFIA can, in principle, cover the frequency region of the lowest frequency rotational transitions of $H^{35}Cl^+$ and $H^{37}Cl^+$, but telluric lines centered at 1441.1 and 1444.0 GHz overlap some of the hyperfine components of the transitions, and that could hinder the detection. IR observations from ground platforms at high spectral resolution can be an alternative and complementary tool to the mm and sub-mm observations, and way to build up in the study of HCl^+. However, the fit mentioned above did not contain any rotationally resolved data from vibrational transitions in the ground state. Adding that information to the global fit improves the accuracy of the predictions of the model for other transitions and can facilitate possible observations in the infrared region of the spectrum. In this work we have accurately measured the frequencies of an extensive set of vibration-rotation lines of the $v = 1 \leftarrow 0$ band of $H^{35}Cl^+$ and $H^{37}Cl^+$ in the mid-IR at high spectral resolution, using a difference frequency spectrometer and a hollow cathode discharge reactor. We have also performed an extended and improved isotope independent fit with mm-wave, optical and infrared data.

References

[1] DeLuca, M., Gupta, H., Neufeld, D. et al. Astrophys. J. Lett., 2012, 751,L37

[2] Gupta, H., Drouin, B. & Pearson, J.C., Astrophys. J. Lett., 2012, 751,L38

Stars and planet formation, exoplanets

Hydrides as tracers of star- and planet formation

Ewine F. van Dishoeck[1]

[1]*Leiden Observatory / MPE*

Interstellar hydrides are excellent diagnostics of the physical and chemical processes in star-forming regions because of the sensitivity of their abundances to temperature and UV radiation. This talk will summarize new insight that has been obtained from various programs on the Herschel Space Observatory, especially the 'Water in Star-forming Regions with Herschel' (WISH) and 'Dust, Ice and Gas in Time' (DIGIT) Key Programs. H2O and OH are two key hydrides whose emission originates from shocks associated with star formation, and is strongly observed for many low- to high-mass protostars with remarkably similar line ratios. However, existing dense shock models overestimate the H2O/CO and H2O/OH line ratios. This points to the need of a new class of UV irridiated shock models along the outflow cavity walls. Other hydrides such as CH+, OH+ and H2O+ are also detected and are good diagnostics of dissociative shocks, the UV radiation field and cosmic ray ionization rate. H2O emission from protoplanetary disks is surprisingly weak, suggestings strong grain growth and settling of icy grains to the midplane, the first steps of planet formation.

The Green Bank Ammonia Survey (GAS): First results of NH_3 mapping the Gould Belt

Jaime E. Pineda[1], Rachel K. Friesen[2], and the Green Bank Ammonia Survey team[1]

[1]*Max-Planck-Institut für extraterrestrische Physik, Giessenbachstrasse 1, 85748 Garching, Germany*
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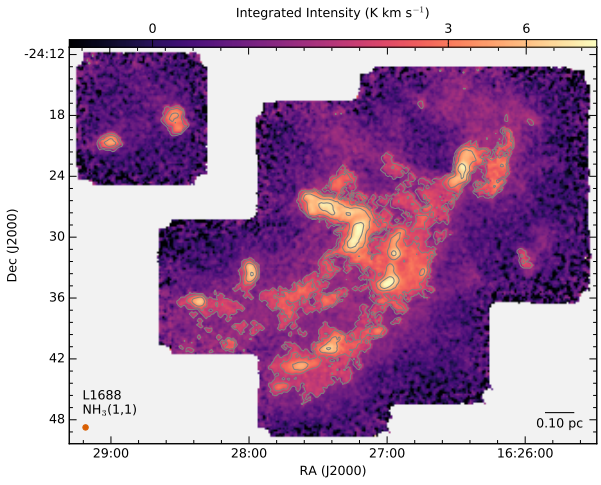
We present an overview of the first data release (DR1) and first-look science from the Green Bank Ammonia Survey (GAS). GAS is an ambitious Large Program at the Green Bank Telescope to map all Gould Belt star-forming regions with $A_v \gtrsim 7$ visible from the northern hemisphere in emission from NH_3 and other key molecular tracers. This first release includes the data for four regions in Gould Belt clouds: B18 in Taurus, NGC 1333 in Perseus, L1688 in Ophiuchus, and Orion A North in Orion. We find that the NH_3 emission is generally extended beyond the typical 0.1 pc length scales found in dense cores. Thanks to these observations we can finally explore the sharp transition between the supersonic turbulence in molecular clouds and the subsonic turbulence inside cores in a systematic fashion across different environments. We also present the initial analysis of the abundance variation of NH_3 at different column densities, a comparison of the gas and dust temperatures across the clouds different clouds in this release and how they vary with increasing star formation activity.



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Sunbathing around low-mass protostars - new insights from hydrides

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Stars form in dense molecular clouds, where gas and dust are typically well-shielded from the interstellar UV radiation. Nonetheless, UV photons can be produced in situ in the surroundings of young protostars, either by the accretion of material onto the protostar or powerful shocks driven by the protostellar jets. Recent observations with *Herschel* reveal that even relatively small UV fields dramatically alter the chemical composition of the gaseous envelopes, as best seen in the observations of light (ionised) hydrides (e.g. OH, CH, OH^+, CH^+), thus providing new insights into a UV-driven chemistry.

I will show how the observations of hydrides allow us to interpret the origin of far-IR spectra from low-mass protostars. In particular, I will demonstrate that hydrides in velocity-resolved HIFI profiles pin-point the location of UV dissociated gas in the immediate surroundings of protostars [1]. The same physical component is isolated in the H_2O and high$-J$ CO lines and quantitatively explains the shape of the CO ladders towards those sources. Furthermore, the observed H_2O / OH ratio is *only* explained by employing new models of UV-irradiated shocks [2]. In conclusion, observations of hydrides and related species provide new insights into how protostars feed back on their parental material, potentially altering the initial conditions for how planets form.

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On the origin of C_4H and CH_3OH in protostars

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Warm carbon-chain chemistry (WCCC) sources are a subset of deeply embedded low-mass protostars [1], but unlike the *hot corino* sources with high abundances of complex organic molecules (COMs) evaporating at high ($T \sim 100$ K temperatures), these sources are instead characterised by unusually high abundances of unsaturated hydrocarbon molecules, often with long carbon chains, such as HC_3N, HC_5N, and C_4H, but low abundances of COMs. The carbon-chain molecules are thought to form from the hydride CH_4 (methane) reacting with C^+ in the gas phase, first leading to acetylene and then more complex species [2].

The CH_4 is in turn thought to form from grain-mantle hydrogenation of C atoms, and is known to thermally evaporate at ~ 30 K, enabling WCCC in a warm region ~ 1000 AU around the protostar, sometimes referred to as a *lukewarm corino*.

Recently, a correlation was found between the COM species CH_3OH and the WCCC molecule C_4H towards a sample of embedded protostars [3], suggesting that the molecules have a common origin in this environment. This is surprising, given that CH_3OH has a much higher evaporation temperature and that non-thermal evaporation of CH_3OH cannot explain the observed abundances [4].

We here present new data from a larger survey of C_4H and CH_3OH in embedded protostars to evaluate this proposed correlation [5]. An accurate understanding of the origin of carbon chains and complex organics is crucial to explain the physical properties of the youngest low-mass protostars.

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Hydride isotopologues

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Deuterated molecules are the best tracers of cold and dense regions in molecular clouds. In this talk I shall focus on the diagnostic power of the deuterated forms of H_3^+ and NH_3 for pre- and proto-stellar cloud cores at the dawn of star formation.

Hydrides As Tracers of Dense Shocked Molecular Gas

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When supersonic flows occur in molecular gas, the resulting shock waves heat and chemically modify the ambient gas. The resulting molecular line emission can be used to probe the underlying shock physics as well as to constrain the conditions in the preshock gas. The important hydrides OH and H_2O are formed in warm, dense molecular gas heated above several hundred Kelvin though the reactions:

$$H_2 + O \rightarrow OH + H \quad (1)$$

$$H_2 + OH \rightarrow H_2O + H \quad (2)$$

Emission from H_2O, OH and related molecules is key to understanding the shock physics.

I will discuss the role that initial conditions can play on the resulting shock structures that arise in dense molecular gas. In particular, I will show that the effects of ultraviolet radiation, grain surface reactions, and shielding are important for determining the preshock conditions as well as the degree to which various hydrides are able to survive in the downstream, UV-illuminated gas[1]. The resulting absolute and relative amounts of hydride emission provide key diagnostics, in particular, of the UV field strength. This presence of UV may explain, for instance, the lower-than-expected H_2O abundance measured by WISH[2].

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The formation of H_2S in dark clouds

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Sulfur is one of the most abundant elements in the Universe (S/H$\sim 1.5\times10^{-5}$) and plays a crucial role in biological systems on Earth, so it is important to follow its chemical history in space. Surprisingly, sulfurated molecules are not as abundant as expected in the interstellar medium. Sulfur is thought to be depleted in molecular clouds by a factor of 1000 compared to its estimated cosmic abundance. Because of the high hydrogen abundances and the mobility of hydrogen in the ice matrix, sulfur atoms impinging in interstellar ice mantles are expected to form H_2S preferentially. By now, OCS is the only S-bearing molecule unambiguously detected in ice mantles [1],[2] and, tentatively, SO_2 [3]. Upper limits of the solid H_2S abundance could be derived by [4]. Gas phase and gas-grain chemical models have increased in complexity and now we can have a hint of the composition of the ice mantles from the comparison of high sensitivity molecular data with state-of-the-art chemical models [5]. Particularly important is the study of the 2-10 mag visual extinction range where the icy mantles are formed. We present systematic H_2S observations in seven molecular filaments in Taurus and Perseus. These filaments are selected to include regions with different environment conditions (incident UV field, turbulence, dust temperature). For $A_v < 10$ mag, the H_2S abundance changes by more than an order of magnitude from one region to the other. We do not find any evidence of a possible correlation between the H_2S abundance and the UV field. We find, however, some correlation between the H_2S abundance and the non-thermal linewidths. These results are discussed in the context of state-of-the-art gas-phase and surface chemistry.

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A three-dimensional model of the distribution and deuteration of water in SgrB2(M)

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One of the main science rationales behind blasting off a submm/far-infrared, high-resolution spectrometer to space (see the HIFI instrument on board Herschel) is the unique capability of studying the emission and absorption of water molecules in the gas phase towards astronomical objects, without the water vapour in our own Earth atmosphere acting as a screen in between. This was also one of the goals of the HEXOS Key Project, or Herschel observations of EXtraordinary Sources, which included the high-mass star-forming region Sgr B2. In this work we have concentrated on Sgr B2(M). The HIFI unbiased line survey of this source contains tens of spectral lines from H_2O, its ^{18}O and ^{17}O isotopologues, and its deuterated counterpart HDO, plus self-consistent information on the strong dust emission from 500 GHz to 2 THz. At the same time, HDO observations carried out with ALMA at 1-mm wavelength provide an insight into the small-scale, hot-core emission of the cloud. Schmiedeke et al. (2016) have developed a 3D full radiative transfer model of the continuum emission towards the Sgr B2 cloud. We build on this extensive description of the source to include a 3D modeling of the distribution of H_2O and HDO (see Comito et al. 2003, 2010), towards the Sgr B2(M) core.

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Hydrides in dense PDRs

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In the last years, heterodyne instruments at far-infrared wavelengths provided a first access to the ground-state transitions of numerous light hydrides allowing for a first reliably assessment of their column densities. While in diffuse clouds a rich hydride chemistry is goverened by the cosmic ray rate and the molecular hydrogen density, dense photon-dominated regions (PDRs) provide a more complex scenario due to efficient collisional destruction processes and the sensitivity of the photodissociation rates on the details of the spectral distribution of the impinging UV field.

Because of the nonlinear interaction of many processes, the diagnostic value of any particular abundance ratio is very limited. Large model grids are needed to quantify the dependence of the different species on parameters such as elemental abundances, dust-to-gas ratio, PAH size and abundance, hardness of the UV field, cosmic ray rate, and of course, density and self-shielding.

By reviewing some recent observations we will introduce current questions such as: What are the sources of non-thermal excitation of many hydrides? What drives the endothermic formation of hydrides in regions without vibrationally excited H_2? Why do many observations contradict the model predictions on the chemical stratification of the PDRs? To what degree can we separate the different effects governing the ionization balance in an irradiated cloud by identifying diagnostic reaction chains?

For all those questions it becomes quickly clear that a full understanding of the relevant processes is only possible when combining the information from hydrides with complementary data on dust and PAHs, [CII], H_2 vibrational lines, and other reactive ions.

Ortho-to-para ratios of dihydride species

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With the *Herschel* Space Observatory, ortho-to-para ratios (OPRs) of several species have been measured in the envelopes of high- and low-mass star-forming regions, such as H_2O, NH_3, NH_2 as well as ions such as H_2O^+ and H_2Cl^+, with values often different from their expected thermal values. As an example, the OPR of NH_2, recently measured towards four different high-mass star-forming regions, was found to lie either below the high temperature limit of three ($2.2 - 2.9$) or above this limit (~ 3.5, $\gtrsim 4.2$, and $\gtrsim 5.0$) [1].

Measuring molecular OPRs in such environments can give crucial information about the prevailing physical conditions, such as the temperature of the gas, but can also bring new constraints on the interstellar chemistry. Hence, determining how these OPRs formed becomes an important issue. This determination involves a comprehensive analysis of the processes governing the interstellar nuclear-spin chemistry of these simple polyatomic species including the formation and the plausible conversion of the different spin symmetries, both in the gas phase and on the grain surfaces.

Since the NH_2 thermal OPR ranges from the statistical limit of three at high temperatures to infinity as the temperature decreases towards zero, lower values than the statistical limit are strictly forbidden in thermal equilibrium. Nevertheless, at low interstellar gas temperatures, where H_2 is highly para-enriched, abnormally low observed NH_2 OPR values can be explained by astrochemical models including nuclear-spin chemistry. Regarding the OPR values found above three, partial NH_2 spin thermalization processes could elucidate these unexpected results. For instance, H-atom exchange reactions between NH_2 and atomic hydrogen can possibly occur, thus increasing the OPR with decreasing temperature. This reaction has indeed been shown to proceed without a barrier, meaning that the H-exchange will be efficient in the temperature range of interest [2]. These and other interesting and novel modeling results will be presented.

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Spectral mapping of CH, CH^+ and C^+ in Orion BN/KL: what they tell us about formation and excitation in shocks and PDRs.

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The methylidyne ion CH^+ has a high formation energy barrier, $\sim$0.46 eV, and is thus a good tracer of non-equilibrium processes in diverse environments where shocks and intermittent dissipation of turbulence may sufficiently excite H_2 to react with C^+ in the standard reaction pathway. The CH^+ ion can also form in PDRs under the right conitions of UV field strength and availability of vibrationally-excited H_2. Similarly the C^+ cooling line is a tracer of PDRs, and also believed to be a tracer of shocked gas. Thus in a warm, dense, and energetically varied star-forming environment of Orion BN/KL, irradiated by numerous nearby young hot stars and containing a well-known eruptive outflow from a massive YSO near the center the complex, the signatures of gas heated from the shocks and UV irradiation should both be present and distinguishable in sensitive spectroscopic observations. We summarize the results (Morris et al. 2016 ApJ, 829, 15) of velocity-resolved spectral mapping observations of sub-mm CH lambda-doubling lines, CH^+ rotational ground and first excited state lines, and C^+ taken with Herschel/HIFI over the inner $3' \times 3'$ region centered on the BN/KL complex, allowing us to assess the roles of shocks and UV irradiation in the formation and excitation of these species. The kinematic properties and surprising lack of shock-related signatures in any species leads us to believe that UV irradiation is the principle (in fact the only evident) mechanism leading to steady state production of CH^+ in this region, which we support with PDR models, and sets conditions on the physical properties of the gas in the shocked outflow. Despite the availability of excited H_2 in the outflow, the lack of C^+ and CH^+ there may indicate an alternative set of reactions involving the removal of C^+ that skips CH^+ production altogether, possibly in the production of CO through CO^+ in different velocity flows, which we explore with new APEX observations of CO^+ rotational transitions.

Origin and excitation mechanisms of OH and CH^+ in PDRs

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Photodissociation regions (PDRs), where physics and chemistry are driven by FUV photons, show an extremely rich and warm photochemistry. The rotationally excited lines of OH and CH^+ probe the warmest PDR gas layers, providing strong constraints for understanding the physics and chemistry in strongly FUV-irradiated interstellar clouds. The far-IR OH emission lines have been associated with the presence of unresolved dense structures and high pressure gas [1, 2]. Excitation of highly reactive CH^+ is driven by collisions and by chemical pumping after reaction of C^+ with vibrationally excited H_2 [3, 4].

We present fully sampled PACS maps (110"×110") of the OH 84 and 119 μm and CH^+ J=3-2 lines in the Orion Bar. The spatial distribution of these lines confirms the clumpy structure of the Bar and constrains the origin of OH and CH^+ to the dense clumps. It is clear that the vibrationally excited H_2 is the key in the formation and excitation of CH^+. To a lesser extent, excited H_2 is also relevant for OH formation. Interestingly, the peak OH emission corresponds with a bright young object identified as a proplyd, which confirms that this line is tracing dense irradiated structures.

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Observations of hydrides in disks

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Hydrogen-bearing simple molecules, and hydrides in particular, are powerful tracers of chemistry in planet-forming disks. They are also thought to carry a large fraction of the volatile, solid mass beyond the snow line. This makes hydrides a critical ingredient for the formation of planets as well as of habitable environments. Direct observations of hydrides on all size scales are therefore needed for understanding planet formation at a very fundamental level, and for answering the question of how chemically common the Earth is among exoplanets. In the past years, great progress has been made in observing protoplanetary chemistry with Spitzer, Herschel, ALMA and ground-based large infrared telescopes. I will review the current state of observations of hydrides in planet-forming disks, as well as our best understanding of what the data tell us about the chemistry of planets. Finally, I will discuss the role the James Webb Space Telescope and other future observatories may play in our understanding of the evolution of hydrides in planet-forming disks.

Physical and Chemical Evolution of Hydrides in Disks and Implications for Planet Formation

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Observations from infrared to radio wavelengths with facilities such as *Spitzer* and *Herschel* (and soon ALMA) have revealed interesting puzzles regarding both the abundances and distributions of key hydrides, including water and NH3, present in protoplanetary disks. Open questions include deriving spatial abundances, the role of interstellar inheritance vs. disk reprocessing, and the role of the local physical environment within the disk. We discuss some of the proposed physical and chemical drivers of the observed molecular distributions, along with challenges for future modeling efforts. We also discuss future avenues with ALMA to shed light on hydride chemistry in protoplanetary disks.

Hydrides in Circumstellar Envelopes

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Circumstellar envelopes around evolved stars are well known molecular sources. Among the variety of molecules they harbor, hydrides constitute an interesting scientific case. To understand how chemistry works in these environments it is neccessary to underline that the circumstellar material is ejected by the evolved star, a process that becomes especially important during the Asymptotic Giant Branch (AGB) phase, and thus, the chemical composition is largely established at the surroundings of the stellar photosphere, where thermochemical equilibrium holds. Thus, unlike in the case of interstellar chemistry, here the initial chemical composition consists of stable neutral molecules and the starting physical conditions at the base of the envelope are relatively well constrained.

At the typical temperatures (2000-3000 K) and densities ($>10^{10}$ cm^{-3}) of AGB photospheres, thermochemical equilibrium predicts that some elements should be nearly locked in the corresponding fully saturated hydride. This is the case of the halogens fluorine and chlorine, which should be nearly in the form of HF and HCl, respectively, something that has been confirmed by *Herschel* observations [1]. However, for most abundant heavy elements, such as carbon, nitrogen, oxygen (in the case of C-rich stars), silicon, phosphorus, and sulfur, only a tiny fraction is predicted to be in the form of the corresponding hydrides CH_4, NH_3, H_2O, SiH_4, PH_3, and H_2S. Observations, however, have found that all these hydrides have abundances much higher than predicted [2, 3, 4, 5]. Hydrides are, therefore, challenging our view of the chemistry of circumstellar envelopes around evolved stars.

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Molecular Emission in Planetary Nebulae As Seen by the Herschel Planetary Nebula Survey (HerPlaNS)

Isabel Aleman[1] and the HerPlaNS team

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The Herschel Planetary Nebula Survey (HerPlaNS) obtained far-infrared broadband images and spectra of 11 well-known planetary nebulae (PNe) using the PACS and SPIRE instruments aboard the *Herschel Space Observatory* [1]. A line survey in these PNe over the entire spectral range between 51 and 672 μm (far-IR to submillimeter) revealed the emission of CO, OH, OH^+ and CH^+ in a few objects. In my presentation I will report the results of the spectroscopy analysis of these emission. Among the results is the first detection of OH^+ emission in PNe [2]. The emission of the molecules above in the Herschel spectra is observed only in PNe with hot central stars (T_{eff} $>$ 100000 K), with ring-like or torus-like structures. The fact that we do not detect the molecular emission from objects with low star effective temperature suggests that the hardness of the ionizing central star spectra (i.e. the production of soft X-rays, $\sim$ 100 – 300 eV) could be an important factor in the production of molecular emission in PNe.

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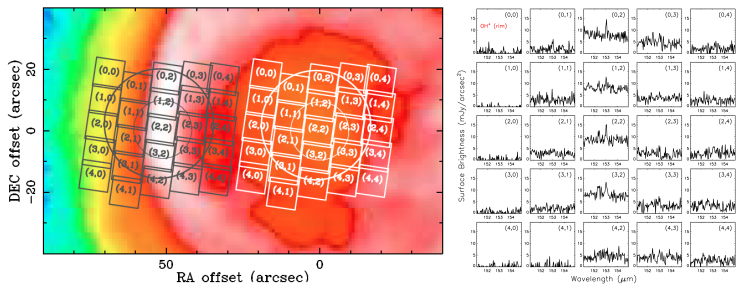

Figure 1: OH^+ in the *PACS/HerPlaNS* spectra of the PN NGC 6781. *Left:* PACS footprints (boxes) for the rim (grey) and center (white) pointings. The figure on the background is the PACS 70 μm image. *Right:* Spatial variation of the OH^+ 152.99μm line emission for the rim pointing. No emission is seen from individual spaxels in the center pointing spectra.

Molecular physics challenge for exoplanet studies

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Hydrides in 2D hydrodynamical turbulence

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We present CHEMSES, a multi-dimensional code which couples hydrodynamics and chemistry. CHEMSES results from the interface between RAMSES (a widely used MHD solver) and the Paris-Durham shock code (which models a large range of detailed physical and chemical processes relevant to the interstellar medium). In particular, CHEMSES is the first hydrodynamical model able to follow H2 levels population in a time-dependent manner.

With this tool, we examine the chemical outcome of a decaying turbulent 2D field for which we resolve the dissipation scales. Our simulation domain is thus very small, of order 10^{16} cm. The initial r.m.s. velocity is 2 to 4 km/s, of the order of the average r.m.s. energy of the interstellar medium, but much larger than what would be predicted at these small scales: this is to account for the potential intermittency of the interstellar medium. In these simulations, the turbulence dissipation releases enough energy to overcome the photo-dissociation of some hydrides of interest (H2O, OH, CH).

We show that a significant fraction of dissipation occurs first in shocks and then in shearing layers when the kinetic energy has decayed significantly. We focus on the shocks and present a method to carefully extract shock fronts. We attempt to quantify to what extent these shock fronts yield hydride molecules, and whether steady-state models such as those produced by the Paris-Durham shock code can be used to reproduce these results.

Solid phase processes and chemistry

Hydrides in solid phases: physical processes & chemistry

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Interstellar ice mantles constitute an interface between ISM solids that built the first grains with a rich chemistry that takes place in the gas phase. Molecules, atoms and radicals condense, react on icy surfaces, and are subjected to UV radiation and cosmic rays at low temperatures, participating in the evolution toward more complex molecules. Each characteristic band of ice observed by spectroscopy is an important species, with abundance in the range of 10^{-4}-10^{-7} compared to H_2. These high abundances represent a considerable reservoir of matter that, when released, impacts the gas phase and supplies the ladder of molecular complexity. After complete volatiles sublimation, the refractory remaining evolved complex residues may be incorporated in planetesimals during protostellar disks evolution. In this presentation, we will focus specifically on the early observed abundances, processes and physico-chemistry of potential hydrides parents in interstellar ice.

Radiolysis of Cosmic Ice Analogs of Ammonia, An Interstellar Hydride

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The goal of our experiments is to elucidate mechanisms of electron-induced radiolysis in cosmic (interstellar, planetary, and cometary) ice analogs of ammonia which is the most abundant nitrogen-containing hydride in the interstellar medium (ISM). Astrochemical processes were simulated under ultrahigh vacuum conditions by high-energy (1keV) and low-energy (10eV) electrons incident upon nanoscale thin films of condensed ammonia deposited on cryogenically cooled (∼90 K) metal substrates (Mo(110)/Ta(110)). Post-irradiation temperature-programmed desorption (TPD) was used to analyze the irradiated films. Experiments with isotopologues of ammonia provided strong evidence for the electron-induced formation of hydrazine (N_2H_4) and diazene (N_2H_2) from condensed ammonia. To understand the dynamics of condensed ammonia radiolysis, we investigated the dependence of these reaction products' yields on irradiation time, film thickness, electron flux, and electron energy. Radiolysis yield versus irradiation time/film thickness results are consistent with a one-step bimolecular mechanism for the formation of both hydrazine and diazene. The production of hydrazine and diazene at electron energies as low as 10 eV is qualitatively consistent with the hypothesis that condensed phase radiolysis is mediated by low-energy electrons produced by the interaction of high-energy radiation with matter. These results provide a basis from which we can begin to understand the mechanisms by which ammonia can form more complex species in cosmic ices.

Nuclear-spin dynamics of interstellar water ice

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Like electrons, molecular nuclei have spin angular momentum. Because a proton is a fermion with a nuclear spin angular momentum of $I_p = 1/2$, nuclear spin isomers exist for molecules which contain identical protons in symmetric geometry. For two-spin systems such as H_2O, there are ortho ($I = 1$, triplet) and para ($I = 0$, singlet) molecules [1].

Nuclear-spin conversion (NSC) between ortho- and para-molecules by radiation or nonreactive collisions is extremely slow in the gas phase, because NSC requires a simultaneous transition of the rotational and nuclear-spin states of the molecule [2]. In contrast, NSC on/in condensed phase can be drastically accelerated by intermolecular interactions inducing rotational hindrance and nuclear-spin state mixing [3]. Thus, understanding the nuclear-spin dynamics of molecules both in the gas and condensed phases is important to extract the physical and chemical processes behind astronomical observations.

We review recent experimental progress towards understanding the mechanisms controlling the nuclear-spin state of interstellar H_2O ice. We are also going to discuss the importance of considering gas-phase chemical processes to understand the origin of anomalous OPRs observed for interstellar H_2O [4].

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Chemistry of hydride-containing ices: UV photoprocessing of an H_2O:CH_4 ice analog.

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Methane is the only hydride confirmed to be present in interstellar ice mantles. In prestellar cores, ice mantles are energetically processed by the secondary UV field, inducing chemical reactions that lead to the formation of more complex species [1]. Laboratory simulations under astrophysically relevant conditions are used to understand these processes. We present UV-irradiation experiments of an H_2O:CH_4 ice analog. Formation of CO, CO_2, CH_3OH, and H_2CO was observed [2]. In particular, CH_3OH and H_2CO are detected toward cold regions in the interstellar medium with abundances that cannot be explained with pure gas-phase chemical models (see, e.g., [3]). Therefore, an origin in the solid phase and a subsequent nonthermal desorption needs to be invoked. Photon-induced desorption of these species from pure methanol ice (and presumably from pure formaldehyde ice) has been found to be negligible [4]. However, formation and inmediate desorption of formaldehyde has been observed during our experiments, probably thanks to the excess energy in the parent photofragments after photodissociation. This demonstrates that photodesorption can take place through more than one mechanism when ice molecules are photodissociated upon UV irradiation, leading to different patterns in the evolution of the photodesorption yields.

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New binding energy calculations explain HF freeze-out observed in protostellar envelopes in NGC 6334

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The hydrogen fluoride (HF) molecule has a remarkably stable abundance with respect to hydrogen in various phases of the interstellar medium [1]. HF is therefore an excellent tracer of overall column density, particularly in low-density clouds. It is expected, however, that the steady HF/H_2 ratio breaks down in denser regions, where HF may condense from the gas phase onto surfaces of dust grains, as occurs with other molecules. The desorption behavior of HF from interstellar dust grains has not been studied experimentally or theoretically so far, and predictions of freeze-out conditions have thus been impossible.

We present ab initio calculations for the binding energy of HF molecules onto various types of ice-covered and bare grains, representative for those found in the ISM. Using these values, we are able to explain the differences in HF column densities observed in two neighboring, dense ($>10^4\,cm^{-3}$), star-forming cores embedded in the Galactic NGC 6334 complex. HF is observed in the gas phase in one core, but appears to be absent in the other, somewhat younger core [2].

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VUV Photoionisation of CH_x radicals and reactivity of their cations CH_x^+

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We report on the VUV photoionization of CH_x radicals (x=1-3) produced in a pyrolysis [1] and a fast flow tube reactor [2] sources on the DESIRS beamline at the French synchrotron SOLEIL. Vibrational and electronic states of the CH^+ and CH_3^+ cations have been caracterized. Beside the interest for their spectroscopy, one motivation is also to study the state-selected reactivity of these ions to provide data to planetary ionospheres and ISM modellers.

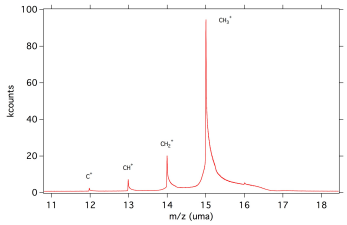

Figure 1: TOF-MS of CH_x^+ ions produced by photoionisation of CH_x radicals

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Search for a drifting proton–electron mass ratio from H_2

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An overview is presented of the H_2 quasar absorption method to search for a possible variation of the proton–electron mass ratio $\mu = m_p/m_e$ on a cosmological time scale [1]. The method is based on a comparison between wavelengths of absorption lines in the H_2 Lyman and Werner bands as observed at high redshift with wavelengths of the same lines measured at zero redshift in the laboratory. For such comparison sensitivity coefficients to a relative variation of μ are calculated for all individual lines and included in the fitting routine deriving a value for $\Delta\mu/\mu$. Details of the analysis of astronomical spectra, obtained with large 8–10 m class optical telescopes, equipped with high-resolution echelle grating based spectrographs, are explained. The methods and results of the laboratory molecular spectroscopy of H_2, in particular the laser-based metrology studies for the determination of rest wavelengths of the Lyman and Werner band absorption lines, are reviewed. Theoretical physics scenarios delivering a rationale for a varying μ will be discussed briefly, as well as alternative spectroscopic approaches to probe variation of μ, other than the H_2 method. Also a recent approach to detect a dependence of the proton-to-electron mass ratio on environmental conditions, such as the presence of strong gravitational fields, will be highlighted. Currently some 56 H_2 absorption systems are known. Their usefulness to detect μ-variation is discussed, in terms of column densities and brightness of background quasar sources, along with future observational strategies. The astronomical observations of ten quasar systems analyzed so far set a constraint on a varying proton-electron mass ratio of $|\Delta\mu/\mu| < 5 \times 10^{-6}$ (3-σ), which is a null result, holding for redshifts in the range $z = 2.0 - 4.2$. This corresponds to look-back times of 10–12.4 billion years into cosmic history. Attempts to interpret the results from these 10 H_2 absorbers in terms of a spatial variation of μ are currently hampered by the small sample size and their coincidental distribution in a relatively narrow band across the sky.

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Extragalactic and AGN activity

Hydrides as probes of physical conditions and dynamics in galaxies : inflows and outflows

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The far-infrared spectra of most Ultra-Luminous Infrared Galaxies, as seen by *Herschel*/PACS, is characterized by strong molecular absorption by light hydrides, mostly lines of H_2O and OH, but also lines of NH, NH_2, NH_3, CH, HF, CH^+, OH^+, H_2O^+, and H_3O^+. These detections will be reviewed, with special emphasis in H_2O and OH. It will be shown that OH is an excellent tracer of galaxy-scale molecular outflows through P-Cygni profiles and high-velocity blueshifted wings observed in absorption, showing outflowing velocities which exceed in some cases 1000 km s^{-1}. In addition, the [O I] 63 μm line and the OH doublets show evidence for inflows in some sources with extremely buried nuclei, through inverse P-Cygni profiles and/or redshifted absorption.

Radiative transfer models for the outflows seen in OH will be presented, with the main goal of estimating the involved energetics. Our analysis is based on fitting the spectra of the OH 119, 79, 84, and 65 μm doublets through a superposition of model components from a library. The molecular outflows indicate mass outflow rates of at least several times 100 $M_\odot$/yr and momentum fluxes $10^{35.5-37}$ dyn. With time depletion scales of a few times $< 10^8$ yr, the outflows have a strong impact in the evolution of these merger ULIRGs. The buried AGNs in some of these galaxies have the strongest feedback effect on the surrounding ISM, likely responsible for limiting the growth of the SMBH and quenching the circumnuclear star formation.

Herschel Legacy Survey of Hydrogen Fluoride Towards Nearby Galaxies

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Based on the importance of the hydrogen fluoride (HF) studies in the Milky Way, we conduct a comprehensive survey of the HF molecular line in nearby galaxies obtained with reliable archival Herschel/HIFI and SPIRE molecular spectra from the High Energy Astrophysics Science and Analysis Data Center (HEASARC). The objective of this survey is to probe the chemistry of fluorine and to determine to what extent HF can be used as diagnostics of the physical process at play in the ISM of the host galaxy. With our studies we will determine the main excitation mechanism of HF - collisions with electrons, IR or chemical pumping - in nearby galaxies and provide steady templates of the chemistry and physical conditions of the ISM to be used in the early universe, where observations of hydrides are more scarce.

Probing the properties and evolution of galaxy nuclei with hydrides (and their friends).

Susanne Aalto[1]

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Molecular gas plays a fundamental role in feeding and regulating star formation and growth of supermassive black holes (SMBH) in galaxy nuclei. Particularly powerful activity occurs when interactions of gas-rich galaxies funnel large amounts of molecular gas and dust into nuclei of luminous and ultra luminous infrared galaxies (LIRGs/ULIRGs).

(U)LIRGs are of fundamental importance to galaxy mass assembly over cosmic time. Some (U)LIRGS have deeply embedded galaxy nuclei that harbour a very active evolutionary stage of AGNs and/or starbursts. The nuclear activity will often drive mechanical feedback in the form of molecular winds, jets and outflows.

Far-infrared (FIR) telescopes, such as the Herschel Space Observatory, are powerful instruments for studying galaxy evolution using molecules as diagnostic tools - exploiting their ability to trace dynamical, chemical and physical conditions. Emerging new ground based mm and submm arrays, most notably ALMA and NOEMA, allow for observations of molecules with exquisite spatial resolution - revealing pc-scale details in galaxy nuclei.

I will review the use of hydrides (e.g. H_2O, H_3O^+, OH, OH^+, HF) for studying dusty nuclei and the nature of the embeeded activity. We can, for eample, investigate ionization rates and the impact of Cosmic ray-, X-ray- and PDR-chemistry and the onset of feedback in the form of outflows and winds. Interestingly, in some deeply oscured nuclei the chemistry shows strong similarities to that of Galactic hot cores. I will present ALMA results on the hydride H_2S and discuss how it can be used to both study IR-irradiated nuclei and search for shocks in molecular outflows. Finally I will show very recent ALMA observations at resolutions of tens of milli-arcseconds (few pc) of opaque nuclei. These regions offer both challenges and opportunities for FIR and submm studies of the nature of the buried activity – which we suggest is a deeply buried accreting SMBH or an extreme, high-temperature, burst of star formation.

Herschel observations of OH and H_2O in compact obscured nuclei

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The high infrared (IR) luminosities of luminous infrared galaxies (LIRGs) are supplied by warm dust heated by star formation or a central active galactic nucleus (AGN). Due to these large amounts of gas and dust surrounding the central regions, direct observations of the nuclei are often impossible at many wavelengths, a problem that is aggravated in especially compact and dusty cores. An indirect way to study the nuclei in such objects is offered by the light hydrides OH and H_2O which couple well to the IR radiation field and therefore can be used to probe the warm dust itself.

We present the results and analysis of Herschel observations of the compact obscured nuclei in the extremely H_2O luminous LIRG Zw 049.057 and the merger component Arp 299A. The molecular lines and continuum are modeled using a spherically symmetric radiative transfer code. We find that the far-IR absorption lines in both galaxies are primarily formed in Compton-thick, warm ($T_{\rm dust} > 100$ K) cores with high columns of H_2O and OH (similar to the nuclear regions of the ULIRG Arp 220). A surprising difference between the two sources is that we find a strong enhancement of ^{18}O in Zw 049.057, but not in Arp 299A. A possible explanation is that the activity in Zw 049.057 is in a later evolutionary phase, where its ISM over time has been enriched by ejecta from massive stars.

Detections of hydrides in high z sources, current analysis, and diagnostics

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High redshifts, typically z $\sim$ 2-4, move submillimeter lines of hydrides, up to $\nu_{rest} \sim 1.2$ GHz, into good millimeter atmospheric windows, which makes easy their detection by large millimeter arrays. Most features of the Herschel heritage about hydrides in local galaxies may thus be studied at high redshift with ALMA, especially in bright ULIRGs ($L_{IR} >\sim 5\ 10^{12}$ Lo), also known as submillimeter galaxies. They may even be studied with IRAM/NOEMA thanks to strong gravitational lensing. Such studies are already well advanced for the strongest emission lines, especially those of H_2O in a large sample of lensed galaxies discovered by Herschel. They confirm that the intensities of H_2O lines are almost comparable to those of high-J CO lines and show that the H_2O line luminosities are roughly proportional to L_{IR}, reflecting the dominance of IR pumping in the excitation of H_2O in the ULIRG starburst cores. The comparison of line profiles and high angular resolution studies show that H_2O and high-J CO lines are emitted by the same gas of these cores. Multi-line H_2O studies provide an estimate of the dust temperature inside these cores as well as of the H_2O abundance there. The extension of these studies to other strong emission lines, such as H_2O^+, is in progress, as well as for absorption lines connected to the ground state of various hydrides such as CH^+, OH^+, H_2O and H_2O^+. These absorption lines are key tracers of extended diffuse gas and of powerful outflows. A spectacular very broad emission of CH^+ is also observed in a number of sources resulting probably from shocks in the extended gas. Such studies should be rapidly extended, including mapping at high angular resolution, detailed line profiles, and various other situations such as H_2O excitation by strong shocks or by AGN, inflows, etc.

Large turbulent gas reservoirs unveiled with CH^+(1-0) around starburst galaxies at $z \sim 2.5$

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Starburst galaxies at redshift $z \sim 2$–3 are among the most intensely star-forming galaxies in the universe. How do they accrete their gas to form stars at such high rates is still a controversial issue. We report ALMA Cycle 2 detections of CH^+(1-0) emission and absorption lines from six gravitationally lensed starburst galaxies at $z \sim 2.5$ with star-formation rates in the range 300–1400 $M_\odot\ yr^{-1}$. The unique conjunction of its spectroscopic and chemical properties allows CH^+ to highlight the sites of most intense dissipation of mechanical energy. The absorption lines reveal highly turbulent reservoirs of diffuse molecular gas, extending far out of the galaxies. The emission lines, with line widths, up to 1300 $km\,s^{-1}$, much broader than those of CO, arise in myriads of shocks propagating in dense gas with a velocity dispersion fed by large scale high-speed collisions. The CH^+ lines therefore probe the fate of prodigious energy releases, primarily stored in turbulence before being radiated away. The turbulent reservoirs of diffuse gas act as sustained mass and energy buffers over timescales up to a few hundreds of Myr. Their ultimate energy supply is likely to be the release of gravitational energy from galaxy mergers, combined with stellar- and/or AGN-driven galactic winds.

The first hydrides

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Hydrides were the first molecular species to appear in the Universe about 400,000 yr after the Big Bang [1]. Their formation was severely hindered by the low density of the expanding Universe, the intensity of the cosmic radiation field, and the absence of solid catalyzers. Despite the low abundance of atomic constituents other than H and He, significant amounts of HD, LiH and their ionic counterparts HD^+, H_2D^+ and LiH^+, as well as HeH^+, were formed in the primordial gas from redshift $z \approx 1000$ to $z \approx 10$. In this talk I will review the chemical pathways leading to the formation of the first hydrides, their role in controlling the cooling of the gas, and their potential as observational probes of the Dark Ages of the Universe [2].

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Hydrides toward PKS 1830−211

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The radio molecular absorber at $z = 0.89$ toward the lensed quasar PKS 1830−211 is a prime target to investigate interstellar hydrides and use them as powerful diagnostic tools of the interstellar medium in the disk of a distant galaxy, as well as powerful cosmological probes (e.g., of invariance of fundamental constants of Nature).

Thanks to the absorber's redshift, most of the hydrides ground transitions are redshifted into ALMA bands, allowing us to obtain high-sensitivity, high-quality (spectral baseline), and pure absorption (no contamination by emission) spectra. The sightlines toward the two lensed images of the quasar intercept the disk of the foreground lensing galaxy at galactocentric radii ~ 2 kpc and ~ 4 kpc, either side of its center. The ALMA observations of hydrides such as H_2O, ArH^+, HF, OH^+, H_2O^+, H_2Cl^+, ..., reveal with unprecedented details the characteristics of each line of sight. The detection of some of their rare isotopologues allows us to measure isotopic ratios at half the present age of the Universe.

The time variability of the absorption profiles (due to intrinsic morphological changes in the background quasar) adds even more to the interests of this unique source, since it can reveal the small scale structures (at ∼pc scale) of the absorbing gas and the chemical correlation of different species.

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Diffuse ISM, turbulence, and shocks

Hydrides in the Diffuse ISM: an Overview of Observations at Ultraviolet and Visible Wavelengths

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I will present an historical overview of studies on simple hydrides detected via their absorption lines at ultraviolet (UV) and visible wavelengths. The focus will be on observations of H_2, CH, CH^+, OH, and OH^+ and on models developed to interpret the molecular abundances. Because UV radiation penetrates diffuse molecular clouds, photodissociation plays a key role in chemical models, but dynamical effects are important, too. The status of efforts to explain the observations will be highlighted. Continued progress is possible by incorporating complementary results at longer wavelengths into the analyses.

A far-infrared study of oxygen chemistry in diffuse clouds

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The synthesis of OH and H_2O in diffuse clouds involves ion-neutral reactions whose educts and products are all accessible to observations. Here we focus on the ground-state transitions of OI, OH^+ and OH [1], which allow us to determine column densities from first principles. Thanks to the high spectral resolution of HIFI and GREAT, absorption features from various spiral arm crossings can be distinguished, at distances beyond those traced by optical or UV spectroscopy. We re-determined the oxygen abundance in diffuse atomic and molecular clouds on several sightlines. With 310-350 ppm, the result does not differ markedly from values obtained from UV spectroscopy. This precludes an excessive gas-phase depletion of oxygen in favor of refractory carriers [2][3]. The abundance analysis of OH produced an estimate of the branching ratio of the dissociative recombination of H_3O^+ into OH and H_2O, in reasonable agreement with experimental determinations [4][5].

We conclude our study with an outlook on signposts of endothermic production paths in the spectroscopy of OH and H_2O, and comment about the contrast ratio between spiral arm and interam gas as seen in the ground-state lines of OH and OH^+.

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Evaluation of Molecular Hydrogen tracers

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HF and CH are known to be good tracers of the presence of molecular hydrogen in the diffuse interstellar gas, including regions where atomic and molecular hydrogen coexist, or where CO emission is not detectable. We have compared CH and [CII] absorption spectra obtained with *Herschel* with CO emission [1] along the line of sight towards the massive star forming region W31C. For this particular sight-line, the CO emission per H_2 column density is consistent with the standard value. However CH or HF absorption spectra are difficult to obtain from ground based observatories. Therefore, we have undertaken an absorption survey with ALMA and NOEMA, towards a sample of continuum sources including objects studied with *Herschel*. The target species are molecular ions whose abundance relative to H_2 is expected to be relatively constant in the diffuse ISM, HCO^+, CF^+, HOC^+. [2] discuss a pilot project towards W49N. We present a more extensive comparison of the hydride and molecular ion spectra which provides further support for using HCO^+ as a probe of H_2 in the diffuse ISM. We show a serendipitous detection of HCO^+ and HCN in the Galactic bulge, which indicates the presence of diffuse molecular gas within 1kpc of the center of the Galaxy in agreement with existing determinations of extinction towards bulge stars.

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Chemical probes of the turbulent diffuse ISM

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Because it is predominantly heated by the UV radiation field, the diffuse interstellar medium (ISM) has long been thought to behave like a photo-dissociation region (PDR). Yet, for the last 30 years, absorption spectroscopy has revealed a gas with a chemical richness that was unexpected from the sole predictions of static PDR-type models. This problem has recently been deepened by the detection with the Herschel, SOFIA, and ALMA telescopes of large abundances of small hydrides with highly endo-energetic formation routes. It has been proposed that these species are nothing else but a signature of another powerful energy reservoir of the diffuse ISM, its supersonic turbulence.

Two processes have been invoked: the turbulent mixing between the warm neutral medium and cold neutral medium and the turbulent dissipation through viscous friction and ion-neutral decoupling. The presence of these hydrides in the cold diffuse ISM is therefore much more than a chemical riddle : it is rooted in the physics of the diffuse ISM, the intermittency of the turbulent cascade and the rate of its dissipation, and it connects with the broader issues of star formation and galaxy evolution.

The absorption spectra were interpreted in the framework of the TDR (Turbulent Dissipation Regions) model, the Paris-Durham shock code, and recent biphasic simulations of magnetized turbulence. Comparing the predictions of these models with multiwavelength observations of atomic and molecular species (e.g. CH^+, SH^+, SH, H, H_2, HCO^+ and CO) may lead to the measurements of essential properties of interstellar turbulence, including its dissipation rate, the scale of the dissipative structures, their timescales, and the dominant dissipative process.

Origin of CH^+ in diffuse molecular clouds

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CH^+ ubiquity and abundance has been a long-standing problem and most of numerical approaches fail to reproduce the observations. Different works point out that the observed abundances of CH^+ are likely produced in warm layers of gas resulting, for instance, from turbulent mixing or turbulent dissipation processes. Molecular clouds are turbulent and complex structures, where the warm and cold phases of the ISM are tightly interwoven forming clumpy and filamentary structures, providing a variety of physical conditions for the development of the chemistry. In a previous work we have shown that the multiphase structure and the turbulence boost the presence of H_2 in warm regions [1]. This warm H_2 can enhance the abundances of molecules with high energy barriers, such as CH^+.

We present results obtained for a MHD simulation of a turbulent molecular cloud, where we included the H_2 formation, which we post-processed using a steady-state chemical solver that we developed. We explored the consequences of the presence of warm H_2 and the role of the multiphase structure of the ISM on the abundance of CH^+, analyzing also the role of the ion-neutral drift velocity on the effective formation rates for CH^+.

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Cosmic rays and magnetic field

Physics and chemistry of H_3^+

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The triatomic hydrogen ion H_3^+ takes a special role in the chemistry of the interstellar medium. It acts as a universal proton donor, and initiates a network of ion-neutral reactions that can lead to the formation of water or organic species in the gas phase. Observations of H_3^+ have been used to infer information on important parameters like the cosmic ray ionization rate [1] and physical properties in the central molecular zone of the galactic center [2]. In this context a good understanding of the H_3^+ formation and destruction processes is essential.

In the first part of my talk I will review the laboratory efforts to shed light on the destruction of H_3^+ by free electrons [3] and the thermalization in collisions with H_2 [4]. Furthermore, I will discuss the non-thermal nuclear spin populations of interstellar H_3^+ and attempts to model their origin [5].

In the second part I will address open questions and outline future experiments involving H_3^+ and some other light hydride molecular ions at the new Cryogenic Storage Ring [6] at the Max Planck Institute for Nuclear Physics.

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Protostars: Forges of Cosmic Rays?

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It is largely accepted that Galactic cosmic rays, which pervade the interstellar medium, originate by means of shock waves in supernova remnants. Cosmic rays activate the rich chemistry that is observed in a molecular cloud and they also regulate its collapse timescale, determining the efficiency of star and planet formation, but they cannot penetrate up to the densest part of a molecular cloud, where the formation of stars is expected, because of energy loss processes and magnetic field deflections. Recently, observations towards young protostellar systems showed a surprisingly high value of the ionisation rate, the main indicator of the presence of cosmic rays in molecular cloud. Synchrotron emission, the typical feature of relativistic electrons, has been also detected towards the bow shock of a T Tauri star. Nevertheless, the origin of these signatures peculiar to accelerated particles is still puzzling. Here we show that particle acceleration can be driven by shock waves occurring in protostars through the diffusive shock acceleration mechanism. We find that shocks in protostellar jets can be strong accelerators of protons, which can be easily boosted up to relativistic energies. Another efficient acceleration site is located at the protostellar surface, where shocks caused by impacting material during the collapse phase are strong enough to accelerate protons. Our results demonstrate the possibility of accelerating particles during the early phase of a proto-Solar-like system and can be used as the argument to support available observations. The existence of an internal source of energetic particles can have a strong and unforeseen impact over the stellar and planet formation process as well as on the formation of pre-biotic molecules.

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Hydride Ions and Ionizing Irradiation in Young Stellar Objects

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We report on *Herschel*/HIFI observations of ionized hydrides observed toward young stellar objects (YSO) of high, intermediate and low mass (Class 0 and I) in twelve star-forming regions. They were observed as part of the 'Water in star-forming regions with *Herschel*' (WISH) program in 6 spectral settings providing fully velocity-resolved line profiles. The YSOs include objects with luminosities ranging from 4 $L_\odot$ to 2×10^5 $L_\odot$ [1].

The lines of CH^+, OH^+, H_2O^+, and C^+ are detected mostly in blue-shifted absorption. All these lines except H_2O^+ are occasionally also detected in emission. H_3O^+ and SH^+ are only detected in emission and only toward some high-mass objects. The velocity shift relative to the star-forming region is of the order of 2 – 10 km/s and the line widths are 1 – 10 km/s. We search for emission at off-positions and distinguish genuine absorptions by the YSO from interstellar diffuse foreground lines. The observed line parameters and correlations suggest two different origins, related either to gas entrained by the outflow or to the circumstellar envelope of YSOs.

The abundances of ionized hydrides are estimated from chemical slab models, assuming far UV (FUV) and X-ray irradiation. The intensity of irradiation was estimated by comparing with observations and using a density model. If the FUV flux required for low-mass objects originates at the central protostar, a substantial FUV luminosity, up to 1.5 $L_\odot$, is required. There is no molecular evidence for X-ray induced chemistry in the low-mass objects on the observed scales of a few 1000 AU. For high-mass regions, the FUV flux required to produce the observed molecular ratios is smaller than the unattenuated flux expected from the central object(s) at the scale of the *Herschel* beam radius.

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Molecular Ions as Tracers of the Cosmic-Ray Ionization Rate

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The fast ion-molecule chemistry that occurs in the interstellar medium (ISM) is initiated by cosmic-ray ionization of both atomic and molecular hydrogen. Species that are near the beginning of the network of interstellar chemistry such as H_3^+ , OH^+, and H_2O^+ can be useful probes of the cosmic-ray ionization rate. This parameter is of particular interest as, to some extent, it controls the abundances of several molecules. Using observations of these species we have inferred the cosmic-ray ionization rate of hydrogen throughout the Milky Way disk. OH^+ and H_2O^+ also allow us to determine the molecular hydrogen fraction (amount of hydrogen nuclei in H_2 versus H) as their abundances are dependent on the competition between dissociative recombination with electrons and hydrogen abstraction reactions involving H_2. Our observations of OH^+ and H_2O^+ indicate environments where H_2 accounts for less than 10% of the available hydrogen nuclei, suggesting that these species primarily reside in the diffuse, atomic ISM. Average ionization rates in this gas are on the order of a few times 10^{-16} s^{-1}, with most values in specific clouds above or below this average by about a factor of 3. This result is in good agreement with the most up-to-date determination of the distribution of cosmic-ray ionization rates in diffuse molecular clouds as inferred from observations of H_3^+.

Analysis of ArH^+, H_3^+, OH^+ and H_2O^+ Observations to Estimate the Cosmic-Ray Ionization Rate Using Comprehensive Diffuse Cloud Models

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We have obtained estimates for the cosmic-ray ionization rate (CRIR) in the Galactic disk, using a detailed model for the physics and chemistry of diffuse interstellar gas clouds to interpret previously-published measurements of the abundance of four hydride molecular ions: ArH^+, OH^+, H_2O^+ and H_3^+. Within diffuse atomic clouds observed along the sightlines to bright submillimeter continuum sources, measurements of ArH^+, OH^+, H_2O^+, and H column densities imply a mean logarithm of the CRIR of $< \log_{10}[\zeta_{\rm p}({\rm H})/n_{50}] > = -15.40 \pm 0.04$, corresponding to a CRIR of $(4.0 \pm 0.5) \times 10^{-16}\, n_{50}\, {\rm s}^{-1}$, where $\zeta_{\rm p}({\rm H})\, {\rm s}^{-1} \sim [\zeta_{\rm t}({\rm H})/1.5]\, {\rm s}^{-1}$ is the primary ionization rate per H atom, $\zeta_{\rm t}({\rm H})\, {\rm s}^{-1}$ is the total ionization rate per H atom, $50\, n_{50}\, {\rm cm}^{-3}$ is the density of H nuclei, and the quoted errors are standard errors on the mean. The intrinsic dispersion of $\log_{10}[\zeta_{\rm p}({\rm H})/n_{50}]$ is estimated as 0.21, corresponding to a factor 1.7. Within diffuse molecular clouds observed toward stars in the solar neighborhood, measurements of H_3^+ and H_2 imply a mean logarithm of the CRIR of $< \log_{10}\, \zeta_{\rm p}({\rm H}) > = -15.66 \pm 0.10$, corresponding to a CRIR of $(2.2 \pm 0.6) \times 10^{-16}\ {\rm s}^{-1}$ and a total ionization rate per H_2 molecule of $\zeta_{\rm t}({\rm H_2}) \sim 2.3\, \zeta_{\rm p}({\rm H}) = (5.1 \pm 1.1) \times 10^{-16}\ {\rm s}^{-1}$, in good agreement with previous estimates [1]. Here, the intrinsic dispersion of $\log_{10}\, \zeta_{\rm p}({\rm H})$ is estimated as 0.11, corresponding to a factor of only 1.3.

We gratefully acknowledge the support of a grant from NASA's Astrophysical Data Analysis Program (ADAP).

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Future projects

Future Observations of Hydrides with Ground-based, Air- and Space-Borne Telescopes

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FAST Telescope: Current Status, Planned Capabilities, and Upcoming Projects

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The Five-Hundred Meter Spherical Aperture Telescope (FAST) is quickly approaching operational status. It will soon begin to contribute significantly to our understanding of Hydrides in the galaxy through observations at L-Band. In this talk we will describe FAST's current status, planned capabilities, and upcoming projects with special focus on how those relate to the study of HI, and Hydrides at L-Band.

We will present the results of OH and CH observations across a boundary region in Taurus [2]. Comparison with extinction across the boundary yields estimates of the "dark gas" fraction. The CH abundance is nearly constant, with less dispersion than that of CO, or OH across the $0.8 < A_v < 2.1$ region. The overabundance of CH at lower extinctions is consistent with the presence of a C-shock.

Observations of the four OH lines, combined with CO, and HI data along 51 sightlines of Galactic Observations of Terahertz C+ (GOTC+) reveal that approximately 18% of OH clouds have no associated CO emission at a sensitivity of 0.07K [1]. We examine the differences between CO-dark, and CO-bright clouds in the survey.

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A Probe Mission to Trace Water from Interstellar Clouds to the Solar System

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In addition to its biogenic importance, water is a valuable probe of many key processes in astrophysics from interstellar shocks to the formation of habitable planets. This Probe Mission will address the following questions.

What is the relationship between gas-phase water and ices in different environments? Water is mainly produced on grain surfaces in quiescent regions with Av $>$ 2 mag and in hot, shocked gas, but is largely frozen on dust grains in cold, quiescent clouds. Submm water transitions can provide a better understanding of the gas-phase H_2O abundance.

What is the velocity field in collapsing dense cores that are moving to form new stars? Water, being kept in the gas phase at a low abundance by cosmic-ray produced UV photons, is a uniquely powerful tracer of kinematics of the inner parts of dense cores, due to its high excitation requirement.

What is the distribution of cold water in protostellar disks? Rotational transitions are a unique probe of gas-phase water in cold, outer disks, and the high sensitivity of the low-lying H_2O lines to the gas dynamics will allow us to establish the radial distribution of the water emission.

What are the reservoirs of water in the Solar System and how did the Earth acquire its water? Measurements of hydrogen (D/H) and oxygen isotopic ratios in water in comets and other Solar System objects, together with the investigation of water outgassing from main-belt asteroids such as Ceres, will provide clues to the origin of terrestrial water.

All of the above measurements would be enabled by a 7–10 m dia. telescope. Preliminary design work has shown that a segmented telescope of this size can be folded into a Falcon 9 Heavy shroud and directly launched to a L2 orbit. The scientific program requires very high spectral resolution on the order of 10^6. The Probe Mission will include small heterodyne arrays covering the key lines of water and its isotopologues at 509, 548-557, 1107-1113, 1153, and 1228 GHz. Low-noise receivers have been developed at all of these frequencies. Recent advances in ASIC digital spectrometers will allow processing all of the array elements in all bands simultaneously. The data volume and downlink are not problematic. The performance of heterodyne spectrometers is not significantly affected by the temperature of the reflective telescope optics, and the temperature achieved by the purely passively-cooled telescope will be $\simeq$ 100 K.

Laboratory astrophysics challenges

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Theoretical and modeling challenges / Summary of the meeting

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I will try to summarize the conference with a view toward the future. During the conference, I will listen to the presentations with reference to several questions. What are some of the issues that seem most promising for future work? What are the principal weaknesses in existing theoretical models of hydride chemistry? For example, how can unresolved or overlapping systems of PDRs in galaxies best be described? What is needed to improve the usefulness of models of circumstellar envelopes and of stratified disks? How can the treasures hidden in archives (Herschel, HST, ALMA, and others) best be exploited?

Poster session

Electronic structure and reactivity of astrochemically relevant inorganic hydrides

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Understanding the electronic structure of metal hydrides provides important quantitative information about stellar composition and formation, and origin-of-life reactivity. Two examples of hydride chemistry studied in our laboratory will be discussed: (a) the multireference gas phase electronic structure of iron monohydride (FeH), computed at an extraordinarily accurate level of coupled cluster theory [1], and (b) gas phase reactions of H and H_2 with large transition metal-siliceous grain models [2], computed using DFT and explicitly correlated MP2 levels of theory. These two studies of inorganic hydrides each provide a wholly different type of challenge for computational chemistry.

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Spectroscopic survey of electronic transition of C_6H, $^{13}C_6H$, and C_6D

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Electronic spectra of C_6H are measured in the $18\,950 - 21\,100$ cm^{-1} domain using cavity ring-down spectroscopy of a supersonically expanding hydrocarbon plasma. In total, 19 (sub)bands of C_6H are presented, all probing the vibrational manifold of the $B^2\Pi$ electronically excited state. The assignments are guided by electronic spectra available from matrix isolation work, isotopic substitution experiments (yielding also spectra for $^{13}C_6H$ and C_6D), predictions from ab initio calculations, and rotational fitting and vibrational contour simulations using the available ground state parameters as obtained from microwave experiments. Besides the 0_0^0 origin band, three nondegenerate stretching vibrations along the linear backbone of the C_6H molecule are assigned: the ν_6 mode associated with the C-C bond vibration and the ν_4 and ν_3 modes associated with C≡C triple bonds. For the two lowest ν_{11} and ν_{10} bending modes, a Renner-Teller analysis is performed identifying the $\mu^2\Sigma(\nu_{11})$ and both the $\mu^2\Sigma(\nu_{10})$ and $\kappa^2\Sigma(\nu_{10})$ components. In addition, two higher lying bending modes are observed, which are tentatively assigned as $\mu^2\Sigma(\nu_9)$ and $\mu^2\Sigma(\nu_8)$ levels. In the excitation region below the first nondegenerate vibration (ν_6), some $^2\Pi$-$^2\Pi$ transitions are observed that are assigned as even combination modes of low-lying bending vibrations. The same holds for a $^2\Pi$-$^2\Pi$ transition found above the ν_6 level. From these spectroscopic data and the vibronic analysis a comprehensive energy level diagram for the $B^2\Pi$ state of C_6H is derived and presented [1].

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Inner-shell photoexcitations as probes of the molecular ions CH^+, OH^+, and SiH^+: Measurements and theory

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The ion-photon merged-beam technique at the SOLEIL synchrotron was used to record the photoionization (ion yield) spectra in the K-shell and L-shell photon energy regions of the molecular hydride ions CH^+ (~ 290 eV), OH^+ (~ 550 eV) and SiH^+ (~110 eV) [1]. The corresponding absolute cross-section spectra of the parent atomic ions C^+, O^+ and Si^+ were also recorded under identical experimental conditions. From a comparison between the molecular and atomic spectra, estimations of the oscillator strengths of the Kα (CH^+ and OH^+) and Lα (SiH^+) transitions, respectively, were obtained.
Ab initio calculations of the core-excited molecular energy level structures and corresponding dipole transition moments, based on the configuration-interaction single approach, were performed. The results crucially interpret the experimental data in terms of contributions from ground and excited valence electronic states.
The CH^+, OH^+, SiH^+ molecular hydride and C^+, O^+, Si^+ atomic ions are known to play significant roles in astrophysical [2] and laboratory plasma processes [3]. The present experimental and theoretical data will facilitate identification of these molecular ions in astronomical and laboratory plasma sources [4] and will also aid the modeling of their species abundance and dynamics [5].

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Quantum calculations on diatomic hydrides for stellar atmosphere modelling

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We report full quantum scattering calculations of inelastic cross sections and rate coefficients for Mg or Ca in collision with H atoms. Transitions between the ground and several excited atomic states are considered, as well as transitions involving mutual neutralisation and ion-pair production. These calculations are based on new highly accurate ab initio potential energy functions and non adiabatic couplings, obtained for the $^2\Sigma^+$ and $^2\Pi$ lowest electronic states of MgH and CaH, with extended active spaces and basis sets [1]. The collision energy range is from threshold up to 10 eV. The main mechanisms underlying the scattering processes are discussed. An extension of these calculations is performed by means of a multichannel model approach based on an approximate treatment of the ionic-covalent interactions [2]. The agreement between the model estimates with the quantum rates found for the upper states allows to extend the number of channels involved in the dynamics calculations. Rate coefficients are thus obtained for all processes between the 12 lowest atomic states of Mg as well as for the processes involving the Mg^+ ion. Those molecular data are important to model spectral lines in stellar atmospheres. Their impact on statistical equilibrium of Mg populations through the non-LTE departure coefficients is investigated for two stellar atmospheres: the Sun and the HD122563 metal-poor star.

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Sensitivity from frequency splittings in the molecular spectra to a variation of the fundamental constants

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Microwave spectra of simple molecules provide a testground for astrophysical searches for a possible variation of the fundamental constants [1]. The approach based on the comparison of the radial velocities of two molecular lines with different sensitivity coefficients to a variation of the proton to electron mass ratio constant μ [2] is extended to frequency intervals between molecular transitions [3]. The frequency interval in the molecular spectra between two near resonant transitions defines a frequency splitting with an enhanced value of the sensitivity coefficient compared to that of one transition. Such degeneracies in the rotational spectra of the diatomic molecules arise from the cancellation of rotational intervals with frequency shifts associated to the isotopic effect and the rotation-vibration interaction. The sensitivity coefficients of rotational transitions in different vibrational levels of the electronic ground state for LiH and CO isotopic species are accurately calculated for J=0-30 and v=0-3 using a Dunham expansion model. Sensitivity coefficients with values ranging up to $K_{splitt} \sim \pm 10^3$ are derived for different frequency splittings. Alternatively, the frequency interval defined by a rotational transition of isotopic CO and an ammonia inversion transition provides a frequency splitting with a sensitivity coefficient in the range $K_{rot-inv} \simeq -1$—0.
The comparison of frequency intervals between rotational lines of isotopic CO and LiH with ammonia inversion lines detected in the microwave spectra of B0218+357 quasar is discussed. The constraint derived on $\Delta\mu/\mu$ is $4 \times 10^{-6}(1\sigma)$ with observational data from [4].

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Formation of cationic hydrides of noble gases in the proto-solar nebula

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Observations of noble gases in space most often rise questions. The following couple of examples is illustrative: the deficiency of the noble gases (Ar, Kr, Xe) observed in the atmosphere of Titan or in comets [1], and the non-observation of any noble gas complexes formed with the two more abundant species He and H, in particular HeH+ whose spectroscopy is well documented in the laboratory. It should be reminded that ArH+ was only identified two years ago in the Crab Nebula [2]. In every cases, the reactivity with H3+ seems to play a key role, and the chemical process implied is a radiative association.

The reactivity of the noble gases, Helium to Xenon, with H3+ has been studied with quantum simulation methods, dynamics included. All of them give stable complexes via radiative associations, with a reasonable efficiency for the heaviest elements. Astrophysical consequences are discussed.

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Temperature dependence of H_2D^+ and HD_2^+ recombination with electrons: a spectroscopic study

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H_3^+, the simplest polyatomic ion, plays a crucial role in the chemistry of interstellar medium and stands as a precursor for the formation of complex molecules including hydrides [1]. For example reaction of H_3^+ with oxygen atoms is considered an important pathway for creation of OH^+ ions [2]. The deuterated isotopologues of H_3^+ (especially H_2D^+ and HD_2^+) are thought to be important species involved in deuteration chemistry in interstellar clouds [3] and dissociative recombination of these ions with electrons is a key process in astrochemical models [4].

We present an experimental study on recombination of H_2D^+ and HD_2^+ ions with electrons. A stationary afterglow apparatus equipped with near infrared cavity ring down spectrometer (SA-CRDS) was used to probe the time evolutions of H_3^+, H_2D^+, HD_2^+ and D_3^+ in discharge and afterglow plasma. By changing the H_2/D_2 ratio we were able to determine the binary an the ternary recombination rate coefficients for H_2D^+ and HD_2^+ in the temperature range of 80 - 145 K. The resulting rate coefficients are within experimental error the same as those previously reported for H_3^+ and D_3^+ [5, 6].

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Small-scale physical and chemical structure of diffuse molecular clouds along the line of sight to Sgr B2

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We take advantage of a spectral line survey performed with ALMA in the direction of the giant molecular cloud Sgr B2 [1] to probe the small-scale physical and chemical structure of diffuse clouds along the line of sight. The survey covers the frequency range from 84.1 to 114.4 GHz at an angular resolution of 1.6". Many important and abundant molecular species have transitions in this frequency regime that are suitable for absorption studies.

This line survey provides an excellent opportunity to study molecular and isotopic abundances not only on sub-parsec scales in the diffuse envelope of Sgr B2 itself, but also in the diffuse clouds located along the whole 8 kpc long line of sight to the Galactic Center. The high angular resolution of the survey also allow us to investigate the kinematic structure of the individual diffuse clouds using linewidth and velocity centroid information. I will present the first results of these analyses.

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Exploring Molecular-Cloud formation with OH 18 cm transition

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Recently, we found that the OH 18 cm transition can be used as an excellent thermometer of the molecular gas in a wide range of the H_2 density from 10^2–10^7 cm^{-2} ([1] Ebisawa et al. 2015). The OH 18 cm transition consists of the four hyperfine components (1612, 1665, 1667 and 1720 MHz), and their relative intensities are sensitive to the gas kinetic temperature. For instance, we found a clear absorption feature of the 1612 MHz line against the cosmic microwave background (CMB) toward the translucent cloud eastward of Heiles Cloud 2 (HCL2). By using a statistical equilibrium analysis, we determined the gas kinetic temperature to be 53–60 K in this source, which is apparently higher than that of dense cores. This method was also applied to the dark molecular cloud L134N and the photodissociation region of the rho-Ophiuchi molecular cloud, and the existence of the warm molecular gas surrounding the dense cores were revealed. All these results suggest that the OH 18 cm transition traces a new class of warm molecular gas, which is possibly related to the formation processes of molecular and/or the CO-dark molecular gas recently traced by Herschel in the [C II] fine structure line.

We also applied this technique to the remarkable straight structure in the northern part of HCL2 to explore its origin. Interestingly, we detected the 1720 MHz line in absorption toward the structure. According to our statistical equilibrium analysis, the 1720 MHz line absorption traces a dense and cold ($T_k < 30$ K) part of the cloud surrounded by warm envelope gas. Combined analyses of OH, ^{13}CO and C^{18}O suggest that the straight structure may be formed by compression of a warm envelope gas extending to the southwestern part of HCL2. These results demonstrate that the OH 18 cm transition can be used to study molecular-cloud formation.

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Extragalactic molecular complexity: opportunities and new challenges in the ALMA era

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Until recently, the study of the molecular interstellar medium of galaxies has been mostly focused on a few, relatively abundant, molecular species. Recent attempts at modeling the molecular emission of active galaxies [2] have shown that standard high-density tracers do not provide univocal results and are not able to discriminate between different relevant environments (e.g., star-formation vs AGN). Spectral lines surveys [1] allow us to explore the richness of the molecular spectrum of galaxies, provide tighter constrains to astrochemical models, and find new more sensitive tracers of specific gas properties. What started as a time-consuming pioneering work has become now routinely accessible with the advent of ALMA. Here I will report some recent results of molecular line observations in local galaxies, focusing on the use of non-standard molecular tracers as diagnostics of the ISM properties in extremely obscured galactic nuclei.

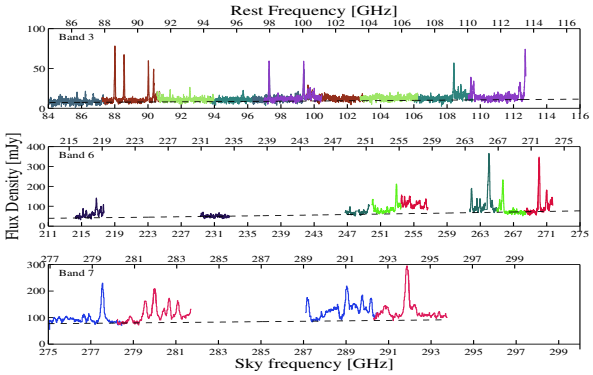

Figure 1: ALMA spectral scan of the obscured luminous infrared galaxy NGC4418 from [1].

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Chemistry of Hydroxyl (OH) Radicals in the ISM Molecular Clouds: Gas-phase Reaction with H_2CO between 22 and 107 K

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The modeled abundances of HCO are about two orders of magnitud lower than the observed ones in prestellar cores [1]. In this work we determine the rate coefficient (k_{OH}) of the gas phase reaction OH + H_2CO → HCO + H_2O at temperatures between 22 and 107 K, using the pulsed CRESU technique. This technique and the experimental setup employed have been described in detail by Jiménez et al. [2]. It is based on the isentropic gas expansion through a Laval nozzle from a high pressure region to a low pressure region. This adiabatic expansion cools down the gas and forms a uniform jet in temperature and total gas density over several tens of cm. This uniformity is essential for performing reaction chemical kinetic studies in the timescale of hundreds of microseconds. Latest advances have allowed us to extend the explorable temperature range up to 107 K. A great increase in the rate coefficient (k_{OH}) at ultralow temperatures has been observed compared to the room temperature values. The implications on the modeled abundances of HCO radicals from the gas-phase reaction of OH with formaldehyde in molecular clouds will be discussed.

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Herschel /HIFI spectral line survey of the Orion Bar: Evidence for temperature and density gradients

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Photon Dominated Regions (PDRs) are interfaces between the mainly ionized and mainly molecular material around young massive stars. Analysis of the physical and chemical structure of such regions traces the impact of far-ultraviolet radiation of young massive stars on their environment.

We present results on the physical and chemical structure of the prototypical high UV-illumination edge-on Orion Bar PDR from an unbiased spectral line survey with a wide spectral coverage.

A spectral scan from 480-1250 GHz and 1410-1910 GHz at 1.1 MHz resolution was obtained by the HIFI instrument onboard the *Herschel* Space Observatory. We obtained physical parameters for the observed molecules. For molecules with multiple transitions we used rotational diagrams to obtain excitation temperatures and column densities. In case of species with available collisional rates, we also performed a non-LTE analysis.

About 115 lines corresponding to 28 molecules (including isotopologues) have been detected in the line survey. Most species trace kinetic temperatures in the range between 100 and 150 K and H_2 volume densities in the range between 10^5 and 10^6 cm^{-3}. The species with temperatures and / or densities outside of this range include the H_2CO transitions tracing a very high temperature (315 K) and density (1.4×10^6 cm^{-3}) component and SO corresponding to the lowest temperature (56 K) measured as a part of this line survey.

The wide range of temperatures and densities is most likely the result of the stratification of the PDR, as confirmed by the abundance profiles of an isobaric high-pressure PDR model. A few line intensities however require very high densities probably resulting from clumpiness for their interpretation, such as the high-pressure and temperature gas traced by C_2H and H_2CO, which may be related to very dense, unresolved structures at high temperatures (probably close to the ionization front of the Orion Bar).

Low energy electron induced processes in ammonia pure ice

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NH_3 is a major component of ice mantles in molecular clouds [1] (up to $\sim 15\%$ of H_2O) and is involved in the grain surface chemistry route to form complex molecules. In the life cycle of NH_3, the formation step is mostly attributed to the hydrogenation of trapped nitrogen on dust grains.[2] However, abundances measured are below the model predictions [3], showing that desorption and destruction by conversion to other compounds have to be determined. Among the thermal and non-thermal mechanisms responsible [4], we have focused our attention on processes induced by low energy electrons (LEE, Energy < 20 eV). LEEs interactions with matter are indeed hypothesized to be the primary driving force in a wide variety of radiation-induced chemical reactions.[5]

NH_3 ice multilayers (~ 5 ML) are deposited under ultra-high vacuum (UHV) at a controlled temperature between 28 and 110 K, and are irradiated using a low energy electron gun. Vibrational High Resolution Electron Energy Loss Spectroscopy (HREELS) is used for the chemical characterization of the layer before and after electron processing.[6] Desorption yields of neutral species are followed by mass spectrometry as a function of the electron incident energy, in order to understand the involved mechanisms and the resulting processes (reaction, desorption, ...).

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Scaling the Collisional Rate Coefficients of Hydrides

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Collisional rate coefficients play an important role as fundamental data needed to accurately model astrophysical environments such as circumstellar envelopes, molecular clouds, and photodissociation regions (PDRs). In environments like these where gas behaves non-thermally, collisional excitation and de-excitation processes must be accounted for as well as radiative processes to determine the molecular quantum level populations. In cold regions, the main collision partners are H_2 and He due to their great abundance, so inelastic collisional rate coefficients with these species are required to produce accurate models. While some relevant scattering measurements have been obtained in the laboratory, the complexity of direct experimental methods causes most astrophysical systems to be studied only theoretically. Furthermore, scattering calculations for collisional systems with H_2 are computationally demanding, and ultimately, the rate of molecule detection in astrophysical environments is faster than the rate at which we can compute scattering data. Here, rate coefficients for collisions of H_2 (and He [1, 2]) with rotationally excited HF [3] and HCl [4] are compared to those of long linear molecules [5] to see if hydrides can be used to estimate unknown rate coefficients. Predicted H_2 and He molecular rotational excitation rate coefficients can help interpret observations of non-thermal interstellar gas.

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Theoretical *ab-initio* calculations of photoabsorption spectra of XH_2^+ (X =C, O, Si) molecular ions: comparison with experimental data

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Molecular hydride ions are ubiquitous in the interstellar medium (ISM). Accurate knowledge of their corresponding spectroscopic lines therefore enables a detailed diagnosis of the ISM. However, laboratory experiments and *ab-initio* calculations of such molecular data remain challenging.
In this context, we present a combined theoretical and experimental work on the x-ray photoabsorption spectroscopy of diprotonated molecular ions of Carbon, Oxygen and Silicon generally labelled as XH_2^+ (X=C, O, Si). In a previous work we have investigated the singly protonated XH^+ species [1]. A combination of *ab-initio* post Hartree-Fock and nuclear dynamics method provides a remarkable tool to simulate the x-ray photoabsorption spectra. In detail, we use the Configuration Interaction (CI) method to compute the potential energy surfaces of hundreds of inner shell excited states. The spin orbit coupling is taken into account through the Breit-Pauli operator. Finally, the photoabsorption spectra are computed with a nuclear wave packet propagation method which includes the core-hole lifetime.
The theoretical results compare quantitatively with the experimental ones and allow the attribution of the experimental spectroscopic lines. In order to elucidate the spectra structure of the studied systems, we investigate the nature of the electronic dipolar transitions.

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ALMA observations of SH^+ emission in the Orion Bar photodissociation region

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The molecular ion SH^+ is unique probe of energetic processes in the ISM. In particular, SH^+ is expected to be detectable in significant amounts if the very high endothermicity (0.86 eV or ∼9860 K) of the gas-phase reaction:

$$S^+ + H_2(v{=}0) \rightarrow SH^+(X^3\Sigma^-) + H \qquad \text{(R1)}$$

can be overcome. Compared to reactive ions such as CH^+, SH^+ rotational lines can be detected from the ground (at ∼345.9 GHz, with accurate line frequencies and spectroscopic parameters recently revisited by us [1]).

At the edge of strongly UV-irradiated molecular clouds, temperatures can reach ≃500-1000 K, and H_2 is collisionally excited and UV-pumped to vibrationally excited levels [2]. Indeed, reaction R1 becomes exothermic when H_2 molecules are in v=2 or higher energy vibrational levels [3]. We present high angular resolution images of SH^+ 1_0-0_1 lines obtained with ALMA toward the the Orion Bar [4]. The resulting images resolve a narrow SH^+ emission filament at the very edge of the photodissociation region. These observations allow us to better understand the formation and excitation of SH^+.

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Primordially hydridic Earth

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Analysis of available material of the Earth's crust, samples from the Moon and meteorites with Sun's photosphere show the correlation of relative abundances of elements with their first ionization potential (IP) [1]. This means that in one early moment of the Solar System formation there was strong dipole magnetic field and the matter was ionized and was moving perpendicular to the field lines. This cosmological theory was proposed by F. Hoyle to explain angular momentum transfer from the Sun to planets. Ionized particles were trapped by Lorenz forces, what caused the separation of elements by their IP [1]. Recent re-examination of this idea (including new data from space probes on Mars and Venus) confirmed and expanded it [2].

Taking the trend of the correlation it is possible to calculate initial bulk mass fractions for Earth. The results show very high initial content in hydrogen, making it first element in mole fraction. Unbonded hydrogen may have escaped, leaving up to 5.1 wt % chemically stored in form of hydrides [1, 2]. Indeed, hydrides were proposed as suitable candidates for the Earth's core to resolve its density problem. Progressive decomposition of hydrides may sustain observed hydrogen flow from the Earth's surface.

Primordially hydridic composition of the Earth provides new geochemical model for the planet [1] with strong consequences on radial differentiation of elements, mineral systems, climate events and many others. This topic requires closer attention of the scientific community.

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Non-Ionizing UV (< 7 eV) Photochemistry of Cosmic Ice Analogs of Ammonia

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While gas-phase reactions and surface reactions on bare carbonaceous or silicaceous dust grains contribute to cosmic chemistry, energetic processing via photochemistry and radiation chemistry of cosmic ices is thought to be the dominant mechanism for the cosmic synthesis of prebiotic molecules. Radiation chemistry is defined as the "study of the chemical changes produced by the absorption of radiation of sufficiently high energy to produce ionization." Ionizing radiation in cosmic chemistry include high-energy particles (e.g., cosmic rays consisting mostly of protons) and high-energy photons (e.g., extreme-UV (12.4 –124 eV), X-rays and - rays). In contrast, photochemistry is defined as photon-induced electronic excitation not involving ionization. In addition to photochemistry, vacuum-UV (6.2 –12.4 eV) light may initiate radiation chemistry because the condensed matter work function is lower than the gas phase ionization energy for a given molecule. For example, the work function of amorphous ice (the main constituent of cosmic ices) is ~ 8.7 eV, which is smaller than the gas phase ionization energy of 12.6 eV for water. Because most previous astrochemical studies have used light sources that produce > 8 eV photons, discerning the role of photochemistry vs. radiation chemistry in astrochemistry is challenging. By using a source whose photon energy does not exceed 7 eV, we have studied ammonia cosmic ice reactions attributable solely to photochemistry. We will compare and contrast these results to those obtained in the same ultrahigh vacuum chamber with 1 keV electrons which initiate radiation chemistry in condensed ammonia.

Effect of the dipolar interaction *via* the three-body problem of Bose Einstein condensate

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We present our numerical calculation of the dipolar interaction for the three-body problem of Bose Einstein condensate by using the Hartree-Fock-Bogoliubov-Popov (HFBP) method.

We study the effect of this dipolar interaction on the stability of the condensate. We determine the different densities: condensate and the thermal cloud at finite temperature.

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Theoretical study of Rydberg states of HeH^+ ion using the Halfium model

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The Halfium code was developed to investigate the excited states of diatomic molecules with two active electrons. The theoretical method is based on the combination of the R-matrix variational method and the multichannel quantum defect theory. While the initial applications of the theory focused on the hydrogen molecule H_2 [1], we report here the first application of the Halfium code to study Rydberg states of heteronuclear diatomic molecular ion HeH^+.

In this contribution [2, 3], we present systematic study of the Rydberg spectrum of HeH^+ ion for the $^{1,3}\Lambda$ ($\Lambda = 0 - 4$) symmetries over the bond length interval [1−5] a.u.. Furthermore, We compare our results with those of other authors [4, 5, 6] and discuss the agreements/disagreements with them.

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Chemistry of oxygen and nitrogen hydrides studied in a low temperature ion trap

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We have studied a number of astrophysically relevant reactions of (hydrated) oxygen and nitrogen cations with molecular hydrogen. These include, in particular, hydrogen abstraction reactions

$$\mathrm{NH^+ + H_2 \rightarrow NH_2^+ + H}, \quad (1)$$
$$\mathrm{NH^+ + H_2 \rightarrow H_3^+ + N}, \quad (2)$$
$$\mathrm{NH_2^+ + H_2 \rightarrow NH_3^+ + H}, \quad (3)$$
$$\mathrm{O^+ + H_2 \rightarrow OH^+ + H}, \quad (4)$$

and proton transfer

$$\mathrm{NH^+ + H_2 \rightarrow H_3^+ + N}. \quad (5)$$

We will present the measured rate coefficients of these reactions at temperatures in the range 10–300 K. We will focus on the reaction of $\mathrm{O^+ + H_2}$, discussing the possible role of $\mathrm{O^+}$ internal excitation on the reaction kinetics. We will also report on our progress in studying the $\mathrm{O^+ + H}$ charge transfer reaction.

An investigation of the origin of the argonium emission from the Crab Nebula

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We present a study of the OH^+ and ArH^+ (argonium) emission discovered by Herschel in the Crab Nebula ([1]). A photodissociation region (PDR) code, UCL_PDR, modified to account for the unusual conditions in the Crab Nebula, with a chemical network including ArH^+ reactions from [2] and X-ray chemistry, has been used to model one of the Crab Nebula knots, with the inputs provided by photoionisation modelling using the MOCASSIN code. It is found that, as with the interstellar case considered by [2], ArH^+ requires a low molecular hydrogen fraction to form in these conditions. Models with the standard interstellar cosmic ray ionisation rate ($\zeta_0 = 1.3 \times 10^{-17}$ s^{-1}) fail to reproduce the OH^+ and ArH^+ line ratios from the Herschel observations, with significantly higher values ($> 10^4\zeta_0$) giving better results. This is consistent with the intense charged particle environment of the Crab. We have also investigated the effects of the strongly enhanced X-ray flux. We report the results of our attempts to reproduce the observed molecular emission from the Crab Nebula, in order to investigate the underlying physical conditions.

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Formation of Solid H_2-Bodies

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Introduction We study the formation of cold, substellar sized bodies due to the fragmentation of gravitationally unstable fluids in a phase transition. The main interest is the potential formation of solid H_2 bodies in molecular clouds.

Context Observations of various ices and the existence of comets suggest that phase transition processes are happening in cold regions. H_2 condensation conditions can be reached in dense substellar structures such as cometary knots and during the plane-parallel contraction, where the temperature rise is only of a factor 2.

Physics Linear analysis shows that fluids in a phase transition are gravitationally unstable at any scale, because compression does not increase pressure, but the condensed phase fraction. Using the inter-molecular Lennard-Jones potential, the virial equilibrium study shows that there is an unvirializable density domain where H_2 clumps can form at temperatures $\leq 600\,\mathrm{K}$.

Simulations The non-linear dynamics of fluids in and out of a phase transition are studied using the molecular dynamics code LAMMPS. Supermolecules are used to combine the Lennard-Jones and gravitational potential. The simulations confirm that fluids presenting a phase transition are gravitationally unstable, independent of the strength of the gravitational potential. The instabilities produce a wide spectrum of ice clumps, from small multimers, to comets, to gravitationally bound planetoids.

Conclusions Our work shows that the physics of cold self-gravitating fluids such as dark molecular clouds is much richer than usually assumed. The segregation in a gravitational field of small grains towards larger bodies such as comets and planetoids cannot be simulated with traditional hydrodynamical codes, but is possible with a super-molecular approach. Observations, linear and virial analysis as well as computer simulations suggest the possibility of the formation of substellar H_2 bodies due to the combination of phase transition and gravity in cold regions. H_2 phase transition is reached easily during plane-parallel collapses if the initial temperature is $\leq 15\,\mathrm{K}$.

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MgH_2 in space and interaction with H

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Magnesium hydrides are of two kinds: MgH, that is a gas existing at very high temperature conditions, and MgH_2, that is an alkali metal hydride with cristalline structure. The most commonly studied hydride in astrophysical applications is MgH, especially in the context of cool stellar atmospheres modelling (e.g. [1, 2, 3, 4]) and insterstellar medium[5].

On the other hand, the magnesium dihydride in form of nanoparticle could allow for 3-body recombination when interacting with H and, in principle, influence the hydrogen kinetics itself. For this reason it is usually adopted in the hydrogen storage community. Eventually, although not easily detectable[6], it is worth to investigate in which conditions it can form and which effects are expected on the hydrogen kinetics.

In this contribution we will enquire the chemo-physical conditions at which MgH_2 could form, according to its formation enthalpy. In particular, we will investigate the values of temperature and pressure, together with available radiation field, at which such hydride could be found and the force-field adopted to describe the interaction with H.

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Optical observations of IR bubbles S73 and S74

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Infrared bubbles S73 and S74 [1] are the infrared — i.e. the dusty — counterpart of the HII region RCW98. This region contains at least three massive O or early B stars [2]. This is probably a very young HII region and is associated with the bright-rimmed cloud SFO 75[3]. We present new optical observations (FEROS, 2.2m MPG/ESO) of the HII region RCW 98 located inside the two distinct infrared bubbles. We show that the two bubbles differ kinematically, which might be connected to different ages of structures. More detailed description of observations and results can be found in [4].

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The IMPETUS project: Using ABACUS for the high performance computation of radiative tables for accretion onto a galaxy black hole, in active galactic nuclei

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Intensive calculations of digital tables for the radiative terms that appear in the energy and momentum equations used to simulate the accretion onto supermassive black holes (SMBHs) in the center of galaxies, are presented. Cooling and heating rates are presented, calculated with a Spectral Energy Distribution constructed from an accretion disk plus an X-ray power-law. In addition a detailed comparison between Blondin's analytical formulas and our photoionization calculations shows some differences up to factors of a few when the gas gets close to the SMBH. The electronic structure of atoms, the photoionization cross-sections, and the recombination rates are treated in great detail. With the discovery of outflows originating at sub-parsec scales, these tables may provide a useful tool to model gas accretion processes onto a SMBH.

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UV photodesorption of CH_4 from pure and CO-rich ices

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In cold and dense regions of the interstellar medium (ISM), molecules are found either in gas phase or accreted at the surface of insterstellar dust grains. UV irradiation of the ice mantle of these grains is the motor for a rich solid-phase chemistry, but also provides a non-thermal pathway for the desorption of molecules. This photodesorption process is believed to account for a significant part of the gas-to-ice abundance ratio of some molecules. In recent years, laboratory studies have aimed at determining absolute photodesorption rates of molecules commonly found in the ISM (CO, H_2O, N_2, CO_2...) and at understanding the underlying desorption mechanisms.[1][2][3]

Here we report an experimental study of the photon-induced desorption of CH_4, one of the most abundant molecules in ice mantles. We obtained the energy-resolved photodesorption rates between 7 and 13.6 eV for both a pure, thick CH_4 ice and for CH_4 deposited on top of a thick CO ice. The latter confirms results from a previous study [1] that showed the ability of CO to induce desorption of other molecules, significantly changing the energy-resolved profile and overall photodesorption yield of CH_4 compared to the case of the pure ice.

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Ortho-para ratio of H_2O in molecular clouds: development of enrichment techniques to investigate the role of cold grains

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Recent improvements of algorithms and calibration files of *Herschel* data processing, bring more accurate measurements of the *Ortho-to-Para* Ratios (OPR) of H_2O and its excitation temperature. Toward W49n [1] and W51, *Herschel* observations show, for some velocity components, OPR of H_2O lower than the value expected at the thermal equilibrium in diffuse interstellar clouds. It is assumed that OPR of water could bring information about the temperature of formation of water molecules.

As the molecules are presumably formed on icy mantles of interstellar grains, at very low temperatures, before being released into the gas phase, we develop laboratory experiments to investigate the role of the solid-gas interface on the Nuclear Spin Conversion (NSC) from very diluted matter [2] to condensed phases [3]. We work now on the preparation of *ortho*-enriched icy films to investigate this 'spin-memory' in the ice during UV and IR photodesorption.

In this communication, we focus on the recent progress concerning nuclear spin conversion of H_2O trapped in cryogenic matrices under infrared LASER irradiation. We show numerical results of optical pumping on water trapped in argon matrix at low temperature and future prospects concerning nuclear spin states equilibration during UV photodesorption [4, 5] of ice.

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Complete Hydrogenation of a PAH cation

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The H_2 molecule is the most important in the Universe. The polycyclic aromatic hydrocarbons (PAH) are well known to be catalyst of the H_2 formation [1]. In this work [2], experimental and theoretical studies have been performed on the hydrogenation of a coronene cations as prototypical PAH molecules. The main results show the existence of magic numbers in the sequential hydrogenation process. The quantum chemistry calculations show that hydrogenation follows a site-specific sequence leading to the appearance of cations having 5, 11, or 17 hydrogen atoms attached, in agreement with the magic numbers found in the experiments. Furthermore, these calculations also allow to propose a complete hydrogenation sequence (figure 1).

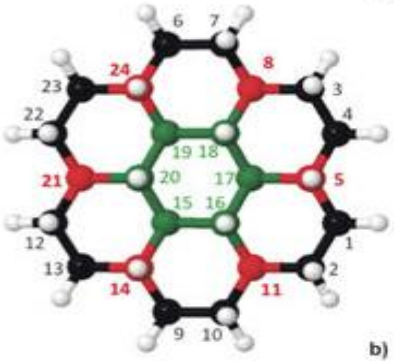

Figure 1: Fully hydrogenated coronene cation and the sequence, followed for the addition of each hydrogen atom. The colors correspond to the location of the carbon, outer edge (black), inner edge (red) center ring(green)

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— Van Der Wiel Matthijs
— Van Dishoeck Ewine
— Walker Kyle
— Wiesemeyer Helmut
— Wolfire Mark
— Wootten Henry
— Zanon Thomas
— Zgonnik Viacheslav

Index