

# des régions de formation stellaire

# à l'astrophysique de laboratoire







# **Star Forming Regions**

Reflexion Nebulae(NGC 2023, NGC 7023)Star Forming Regions(OMC1, M17)Dark Clouds(Barnard 68, BHR 71)

Extragalactic regions (N88 in the SMC)

Emission de H<sub>2</sub> dans l'IR, bandes J, H, K, L et M



# La tétralogie de l'Astrophysique

Buts: Interpréter les observations pour élucider les mécanismes en œuvre dans les "objets" étudiés.

Observational results X, UV, Visible, IR, Radio (submm, mm, cm) Complex conditions

> Laboratory simulations Simplified (?) conditions

Expériences au laboratoire simulant dans des conditions simplifiées certains milieux étudiés - mesurer les paramètres physiques et chimiques manquants pour une modélisation correcte Comparer leurs résultats à ceux des observations et déterminer ainsi de façon indirecte les caractéristiques des "objets"

#### **Theoretical modelling**

- Large chemical networks
- Physical processes
- Rate equations, numerical methods

Atomic and molecular data Basic physics and chemistry Laboratory spectroscopy

#### Importance in astronomy of the $H_2$ formation process on the star formation process

- stars form from the gravitational collapse of ISM clouds
- H<sub>2</sub> is the main constituent of the ISM
- the rate of gravitation collapse depends on a balance between:

gravitational forces compressing the material internal pressure of the clouds resisting to compression

- requires knowledge of the exothermicity disposal in the cloud to model realistically the gravitational collapse

(1 or 2 orders of magnitude depending on the mechanism)

Nascent H <sub>2</sub> with internal energy	-> H <sub>2</sub> will cool through radiation			
(rovibrational)	of IR photons			
Grain heating (no IR emission)	$-> \operatorname{cool} \dot{H}_2$			
	The molecular cloud collapse more readily			
Nascent $H_2$ with large translationa	-> Heating of the cloud			
and small internal energie	S			
Slow collapse				

### How to extract informations from the observations ?

### **Numerical models**

The main goal is to

-Deduce from the  $H_2$  line ratios, width, shift ... measured at different locations

- the *physical conditions* of the medium

- the likely associated *excitation processes*.

### Numerical shocks models

(Ref. Le Bourlot, Pineau des Forêts, Flower, Cabrit, 2002)

We use for this purpose interstellar medium evolution models with different shock types.

The planar, time-independent MHD equations (the magnetic field value is important to distinguish between J and C shocks) are solved in parallel with the chemical equations (self-consistent manner).

Complete set are also included of: chemical species, reactions, momentum and energy transfer processes, and grain properties

Shock models give (among many other results):

- The **absolute intensities** of many  $H_2$  emission lines over a wide wavelength range.
- The evolution of the **main physical parameters** in the shock-dominated region (temperatures, densities...)



### **Numerical PDR models**

(Ref. Le Petit, Roueff, Le Bourlot, 2002)

In PDRs (*Photon Dominated Regions*) H<sub>2</sub> excitation arises from *UV pumping*. The stationary, 1-dimension model computes the cloud structure at each point solving (in parallel): The radiative transfer equations The chemical equilibrium equations The collisional excitation and de-excitation equations for all the species The thermal equilibrium equations

Essential parameters are the cloud density and the incident radiation flux falling onto the medium (depending on the background sources).

Recent modifications now allow:

- to treat the problem of clouds illuminated onto their **two faces** 

- to use a **deuterium-based chemistry** in the calculations.

The set of species, grains properties and other various parameters are basically the same than in the shock models.

### **Photoionization code CLOUDY**

(Ref. Ferland, 2003)

To simulate non-equilibrium plasmas and predict their spectra.

#### Shock model program (Pineau des Forêts, Flower, Roueff, Le Bourlot)

```
!---- shock parameters ------
С
                    ! shock type : 'C' or 'J', Steady state : 'S'
3
                    ! Nfluids : 1, 2 ou 3
1.0D0
                    ! Bbeta -> Bfield = Bbeta * sqrt(nH)
30
                    ! Vs -> shock speed (km/s)
                    ! Vn - Vi initial (cm s-1)
1.0e3
0.01
                    ! op H2 -> initial H2 ortho/para ratio (999.9 -> ETL)
4.650
                    ! T(n,i,e) -> initial gas temperature (K)
1.0D6
                    ! nH init -> initial value for n(H) + 2.0 n(H2) + n(H+) (cm-3)
15
                    ! Tgrains -> initial grain temperature (K)
                    ! Cool KN -> 1: Kaufman & Neufeld cooling
0
!---- environment ------
5.0D-17
                    ! Zeta -> cosmic ray ionization rate (s-1)
                    ! RAD -> flux radiation (multiplicative factor)
0.D0
0.D0
                    ! Av -> initial extinction (magnitudes)
!---- numerical parameters -----
10000
                     ! Nstep max -> max number of integration steps
5
                    ! Nstep_w -> number of steps between 2 outputs
49
                     ! NH2 lev -> Number of H2 levels included
150
                     ! NH2 lines out -> Max number of H2 lines in output file
BOTH
                     ! H_H2_flag -> H-H2 collisions : DRF, MM or BOTH
1
                     ! iforH2 -> Formation on grain model (1, 2, 3, 4)
2
                     ! ikinH2 -> Kinetic energy of H2 newly formed (1, 2)
1.00D09
                    ! XLL -> caracteristic viscous length (cm)
1.00D-7
                    ! Eps V -> precision of computation
3.00D8
                    ! timeJ -> shock age (years)
2.0008
                     ! duration max -> max. shock duration (years)
1
                     ! Force_I_C -> 1: Force Ion Conservation
!---- output specifications ------
FD
                     ! species: 'AD' (cm-3), 'CD' (cm-2) or 'FD' (n(x)/nH)
                    ! H2 levels: 'AD' (cm-3), 'CD' (cm-2) or 'ln(N/g)'
AD
local
                    ! H2 lines: 'local' (erg/s/cm3) or 'integrated' (erg/s/cm2/sr)
1-----
 INTEGER:: iforH2 = 1 ! Flag : H2 formation on grains
                     ! 0: 1/3 of 4.4781 eV in internal energy (=> 17249 K) (Allen, 1999)
                     ! 1: Proportional to Boltzman Distrib at 17249 K
                     ! 2: Dissociation limit : v = 14, J = 0,1 (4.4781 eV)
                     ! 3: v = 6, J = 0,1
                     ! 4: fraction = relative populations at t, initialised as H2_lev%density
                                    and changed during integration
 INTEGER:: ikinH2 = 1 ! Flag : H2 formation energy released as kinetic energy
                     ! 1: 0.5 * (4.4781 - internal)
                     ! 2: Inf(1.4927 eV, 4.4781 - internal)
```







Energie (cm<sup>-1</sup>)

Fro. 2—Simulated low-resolution spectra of H<sub>2</sub> emission in reference model 14. The model spectra have been convolved with Gaussians of width  $\Delta \lambda = 0.02 \ \mu m$  (*left*) and  $\Delta \lambda = 0.015 \ \mu m$  (*right*). Line positions in various vibration-rotation bands are indicated below each spectrum, and the major contributors to each strong feature are identified. The intensity is shown as a percentage of the total fluorescent intensity per resolution element; i.e., the intensity scale is in units  $0.011_{wind}/\Delta \lambda$ , or  $3.835 \times 10^{-4} \text{ ergs s}^{-1} \text{ cm}^{-2} \ \mu m^{-1} \text{ sr}^{-1}$  for the left panel and  $5.113 \times 10^{-4} \text{ ergs s}^{-1} \text{ cm}^{-2} \ \mu m^{-1} \text{ sr}^{-1}$  for the right panel.

### **BHR71**

3 colors composite image in the visible showing:

-The dark cloud which absorbs the light from the background stars

- A proto-star (IRS1) in formation inside the dark cloud and the associated ejecta to the South

- spectrograph slit positions used for this study are indicated

- Alves and Lada The ESO Messenger n°103 March 2001

- Lemaire, Field, Pineau des Forêts, Callejo Near infrared emission from a protostar in BHR71, ApJ in preparation





 $H_2$  emission in the K band

**BHR71** 

3 colors composite image in the visible showing:

-The dark cloud which absorbs the light from the background stars

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### BHR 71 Spectroscopy

K Band spectrum (1.8 à 2.5  $\mu m)$  obtained at VLT (ESO) with the ISAAC instrument

The spectral image to the right corresponds to the slit position on the picture



#### Integrated spectrum on the brightest spot.

Absolute and relative observed intensities of the 3 molecular hydrogen (H<sub>2</sub>) lines are compared to the values calculated by sophisticated theoretical models, 3 adjusting their parameters.

This leads to the determination of the physical and chemical (density, temperature, velocity, turbulence, nature of the exciting sources (shocks, UV radiation...) reigning in the object(s) under study.



### **OMC1** ORION Molecular Cloud 1

- Giant molecular clouds where high mass stars form trigger the formation of low mass stars
- Located at 450 pc
- Lying between
  - BN-KL (fast outflows, shocks)
  - Trapezium stars (intense UV field)

Composite image obtained by using Adaptative Optics (AO) at ESO & CFHT 3.6m telescopes

Spatial resolution: 0.15 '' Wavelength: 2.121  $\mu$ m Spectral resolution  $\lambda/\Delta\lambda$ =100 Infrared H<sub>2</sub> emission v=1-0 S(1) line + continuum



### **OMC1** Velocity field around BN-KL

# Integral field spectral movie obtained at CFHT using:

- 3.6 m mirror
- The adaptative optics (PUEO)
- A Fabry-Perot (GRIF)
- Gives access to the velocity field in this explosive region
- Reveals internal shocks associated with protostars within some clumps of gas

#### Spatial resolution: 0.15 " Infrared emission of H<sub>2</sub> around the v=1-0 S(1) transition from 2.106 to 2.136 µm Spectral resolution: 100 km.s<sup>-1</sup> (R=3000)







**Trichromie (R,G,B)** 2.12 μm, 2.24 et 2.27 μm (ESO-VLT NAOS-CONICA) L'hydrogène moléculaire apparaît en rouge tandis que le continu est rose





#### Pure H2 emission: 2.12µm – 2.24µm



The width of the filaments (40-50 AU) appears to be actual shock width. This put important constraints on shock models in which - density - magnetic field - shock velocity determines the shock width.

## **Barnard 68**

#### **Bok globule**

composite image: visible + infrared

Looking for H<sub>2</sub> formation using VLT ISAAC in spectroscopic mode

5 hours integration no  $H_2$  detection



# Interstellar clouds, from the diffuse nebula to the sites of ongoing star formation

	K	cm <sup>-3</sup>
Diffuse molecular clouds	<b>50-100</b>	$n \sim 10^{2}$
Cirrus clouds	10-100	$n \sim 10 \text{ to } 10^3$
Dense molecular clouds	10-20	$n > 10^{3}$
Giant molecular clouds	15-40	$n > 10^{3}$



Mauna Kea volcano summit 4200 m (Hawaï) CFHT Observatory ...and many others 20



# Laboratory Astrophysics

Interstellar Grains Spectroscopic Signatures

Laboratory experiment on H<sub>2</sub> formation

on grains analogues



### Formation of molecules on interstellar grains

 $H_2$  does not form efficiently in the gas phase by radiative association of neutral H atoms

- 3 body reaction H+H+H -> H<sub>2</sub>

only with n>10<sup>12</sup> cm<sup>-3</sup> 10<sup>9</sup> years in the ISM conditions

- 2 body reaction  $H+H \rightarrow H_2$ 

cannot get rid of the 4.5 eV bond energy via photon emission

-> Interstellar grains of dust act as catalysts

but very few known on the physics/chemistry of the processes

# Surfaces, H<sub>2</sub> formation Retrospective

The gas-grain surface interaction is the main route for the molecule formation in the ISM - Gould and Salpeter (1963)

Interstellar grains acts as catalysts

- from the very simple H<sub>2</sub> formation
- to the more complex chemistry



Figure 1.10-. H atoms interacting with an interstellar dust grain. The surface of the grain is uneven, and the atoms travel on it, can recombine or be released into the gas phase.

The kinetics of the reaction under interstellar conditions is still not well understood

- experimental aspects

what is an interstellar grain ? how to work in the lab under interstellar conditions ?

> **Low flux** (<10<sup>12</sup> atoms/cm<sup>2</sup>/sec) **and E**<sub>k</sub> (10-300 K) **of H atoms Low sample temperature** (5-40 K), **Low background pressure** (10<sup>-10</sup> torr)

- theoretical aspects

what are the physical and chemical mechanisms involved ? what formalism to use to give account of them ?

# **Essential questions**

At least 2 unanswered essential questions regarding H<sub>2</sub> formation in the ISM

$$H+(H - grain) \longrightarrow \underbrace{H_2(v,j) + K.E}_{GAZ \ PHASE} + grain$$

1 - On what surfaces and over what range of temperature can H atoms combine efficiently enough to form  $H_2$  observed in the ISM

2 – What is the energy partitioning of the exothermicity of  $H_2$ formation into the grain surface, into internal energy of  $H_2$  and into kinetic energy of the product  $H_2$ 

# Composition and physical/chemical state of the interstellar grains

Class bare material

- Silicates Olivine Mg<sub>0.8</sub>Fe<sub>1.2</sub>SiO<sub>4</sub>
- Graphite the more active to form H<sub>2</sub>

Material

- Amorphous carbon and HAC active catalyst
- PAHs
- Sic
- MgS

core + ice mantle material (UV processed or not)

- Ice covered grains

CO,  $H_2O$ ,  $NH_3$ ,  $CH_4$ ,  $CO_2$ ,  $N_2$ Methanol

- Refractory organics covered grains

Signatures (abs., emi.)

9.7 and 18 μm bands217.5 nm bump7.6 μm bands

3.3, 6.2, 7.7 and 11.3 μm
11.4 μm
30 μm

3.1, 4.6, 6.0, 6.85 μm 3.4, 6.0 μm

Grains origin: Novae, Supernovae, ejected stellar matter

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# Surfaces, H<sub>2</sub> formation Experimental aspects

**Surface science:** 

\* Crystalline material

\* Catalysis

#### state specific detection of H<sub>2</sub> desorbing from surfaces

ZareKubiak et al (1985) $H_2$  / Cu(110) and Cu(111)ZachariasSchröter et al (1991), Rutkowski et al (2001) $H_2$ , D2, HD / Pd(100)Kolasinski et al (1992) $H_2$  / Si(100) and Si(111)WinklerPozgainer et al (1994) $H_2$  / Ni polycrystalline

#### Astrophysical surface science:

\* polycrystalline

\* amorphous

desorption experiments

- doped Si bolometer surface Govers et al (1980)

- silicates and carbonaceous material

Vidali, Pirronello Vidali, Pirronello et al (olivine: 1997, amorphous carbon: 1999)

- ice covered material (amorphous solid water)

Manico et al (2001), Roser et al (2002), Ek: Roser et al (2003)

Baurichter, Luntz Hornekaer et al (2003, 2005)

Dulieu et al (2005)

- HOPG Zecho et al (2002)

# Surfaces, H<sub>2</sub> formation Experimental aspects

#### **Diagnostics methods without state specific resolution:**

 \* TPD-QMS (thermally programmed desorption)
 \* TOF-QMS





#### **Diagnostics methods with state specific resolution:**

\* REMPI-TOF (λ scan)
\* REMPI-TOF-TPD (λ fixed)





Population distribution of molecules desorbed from the surface

Pulsed tunable dye laser: 190-205 nm

# Surfaces, H<sub>2</sub> formation

adsorption of gas on grains $\rightarrow$	collision H-grain thermal accommodation sticking in surface (or volume)
diffusion →	mobility on surface
reaction $\rightarrow$	recombination and $H_2$ formation
desorption $\rightarrow$	ejection of excited H <sub>2</sub>

slow process  $\sim 1$  atom/day

 $E_{v,J}$   $E_k$  grain heating



# Surfaces, H<sub>2</sub> formation Experimental aspects

#### Grain surface characteristics:

Atoms or molecules characteristics and interaction with the surface:

- \* morphology (crystalline, micro- or poly- crystalline, amorphous)
- \* role of the defects
- \* porosity (dense / fluffy), area/unit vol.
- \* bare grain size distribution (0.01 to  $0.5 \ \mu m$ )
- \* surface temperature
- \* adsorption processes
- \* type of interaction with the surface (physi- vs. chemi-sorption)
- \* binding sites and energies
- \* ice morphologies and surface coverage (ice mantles, mixtures)
- \* flux of incoming atoms, kinetic temperature
- \* sticking coefficient
- \* mobility, time scales: residence time, migration time  $(10^{-12} \text{ to } 10^{-3} \text{ s})$
- \* formation processes
- \* recombination efficiency
- \* desorption kinetics (thermally activated mobility?)
- \*  $E_{v,j}$  &  $E_k$

# Surfaces, H<sub>2</sub> formation Theoretical aspects

#### **Reaction mechanisms**

#### -Eley-Rideal

prompt mechanism occur at high H atom coverage rate  $\rightarrow$  create "hot" H<sub>2</sub>

#### -Langmuir-Hinshelwood

migration mechanism by tunneling or thermal hooping occur at low and high H atom coverage rate  $\rightarrow$  create H<sub>2</sub> at surface temperature

#### - Interaction of atoms and molecules with surfaces:

\* physisorption (vdW interaction)

- \* chemisorption (covalent bond)
- Desorption from grains results from:

pulsed heating (collisions, cosmic rays)
sputtering (CR, photo-induced desorption)
penetration length (CR vs. UV)
chemical reactions (exothermicity, stored energy)



# Surfaces, H<sub>2</sub> formation Theoretical aspects

Data analysis Modelling of surface chemistry on interstellar grains Theoretical and computational methods:

> \* Polanyi-Wigner equation analysis of TPD experiments

$$n^{th} \text{ order: } \frac{dN(t)}{dt} = -k_n N^n e^{\left(-\frac{E_{des}}{k_B T_S}\right)}$$
  
n, k and E : empirically derived parameters

 $\rightarrow$  activation energy barriers for diffusion and desorption processes

- \* Rate equation model → production rate of H<sub>2</sub>
  \* Modified rate equations
- \* Master equation

#### → O. Biham

\* Stochastic approaches of the surface chemistry  $\rightarrow$  S. Charnley Master equation, Monte-Carlo methods





### RÉACTIVITÉ CHIMIQUE HÉTÉROGÈNE

Formation d'hydrogène moléculaire et de petites molécules

sur des surfaces d'intérêt astrophysique à très basse température (FORMOLISM)

#### Etude de la formation de la molécule d'hydrogène sur une surface de glace d'eau amorphe (GEA)

- Compte tenu de la grande diversité des formes amorphes et cristallines de la glace d'eau et de leur intérêt actuel, il nous a semblé intéressant de commencer notre programme scientifique dans cette voie.

- De plus les mesures effectuées sur des surfaces couvertes d'un manteau de glaces ( $H_2O$ , CO...) sont en principe relativement plus simples à interpréter que celles menées sur des surfaces sèches.

- En effet, la couverture d'un solide par une glace est homogène et dès que quelques monocouches ont été déposées, le substrat et ses défauts de surface ne jouent plus aucun rôle.

- Il s'agissait au départ de calibrer les résultats de notre expérience par rapport aux résultats obtenus récemment par Roser et al (ApJ 2002 et 2003) et Hornekaer et al (Nature 2003) en les complétant grâce à notre appareillage qui possède des diagnostics plus complets (TPD + REMPI/TOF).

- Si la majorité de nos premiers résultats concordent avec les leurs, quelques autres jettent des doutes sur certaines des mesures déjà publiées tandis que de nouveaux les complètent sur des aspects très importants négligés ou non observés auparavant.

#### PERSPECTIVES 2005-2009

1. Diagnostic supplémentaire sur l'énergie de translation des molécules formées, projet d'imagerie ionique IONIM (ACI) en cours de test.



#### 2. Diagnostic RAIRS sur les glaces: spectroscopie IR (10000-400 cm<sup>-1</sup>) par TF

(spectroscope complet acquis, adaptation à l'enceinte ultra-vide courant 2005) diagnostic des multiples états physiques des glaces d'eau dans les bandes à 3µm, diagnostic d'espèces nouvelles formées dans des réactions à basses températures

**3. Préparation et caractérisation des échantillons solides in situ** (C amorphe, graphite, silicates ...) (projet programmé pour le second semestre 2005)

4. Développements théoriques en relation avec l'équipe de Meudon (recrutement ?)

**5. Nouvelle enceinte ultra-vide** (projet 2006 ...)

# L'équipe d'astrophysique à l'Université de Cergy-Pontoise

Astrophysique	Jean Hugues FILLION	MdC
	François DULIEU	MdC
	Hanouchah MOMENI	MdC
de	Saoud BAOUCHE	Doctorant $\rightarrow$ Postdoc
	Lionel AMIAUD	Doctorant
i	Eric SOMSON	AI
Laboratoire	Tahar AMORI	ITA
	1 year postdoc ??	
Astronomie et Astrophysique	Jean Louis LEMAIRE	Pr
	Gonzague CALLEJO	Doctorant → ATER
	Lars KRISTENSEN	Doctorant
	Stephan DIANA	IE Informatique

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de	V. Pirronello	Universita de Catania	It	
Laboratoire	G. Vidali	Syracuse University	USA	
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	<b>D. Field</b>	<b>Aarhus Universitet</b>	Dk	
	M. Gustafsson, F. Pijpers			
Astronomie	<b>D. Rouan</b>	<b>Observatoire de Paris</b>	LESIA	
et	Y. Clénet	Clénet GriF (CFHT), NACO (VLT)		
Antrankara	<b>G.</b> Testor	<b>Observatoire de Paris</b>	LUTH	
Astrophysique	G. Pineau des Forêt	s Université Paris-Sud, IA	S, Orsay	
	M. Gérin, E. Falgarone ENS Paris			
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Laboratoire d'Étude du Rayonnement et de la Matière en Astrophysique

### L'astrophysique à l'Université de Cergy-Pontoise Laboratoire LERMA/LAMAp UMR 8112 CNRS & MEN

#### L'astrophysique observationnelle

Sujets d'étude:

#### Le Milieu Interstellaire. Etoiles en formation Observation – Interprétation



Visite du laboratoire: http://wwwusr.obspm.fr/~lamap/

> Contributions: CGVO CRIdF MEN CNRS

### L'astrophysique de laboratoire

Sujets d'étude:

# Formation de H<sub>2</sub> sur des surfaces simulant les grains interstellaires



Buts:

#### **Comprendre l'Univers**

Mesurer les caractéristiques physico-chimiques de réactions intervenant dans le milieu interstellaire.

2) Expériences au laboratoire simulant, dans des conditions simplifiées, certains milieux étudiés

- mesurer les paramètres manquants permettant une modélisation correcte des observations.

Buts:

Comprendre l'Univers Interpréter les observations pour élucider les mécanismes en œuvre dans les "objets" étudiés.

1) Modélisations théoriques basées sur les lois de la Physique et de la Chimie

- comparer leurs résultats à ceux des observations et déterminer ainsi de façon indirecte les caractéristiques des "objets".