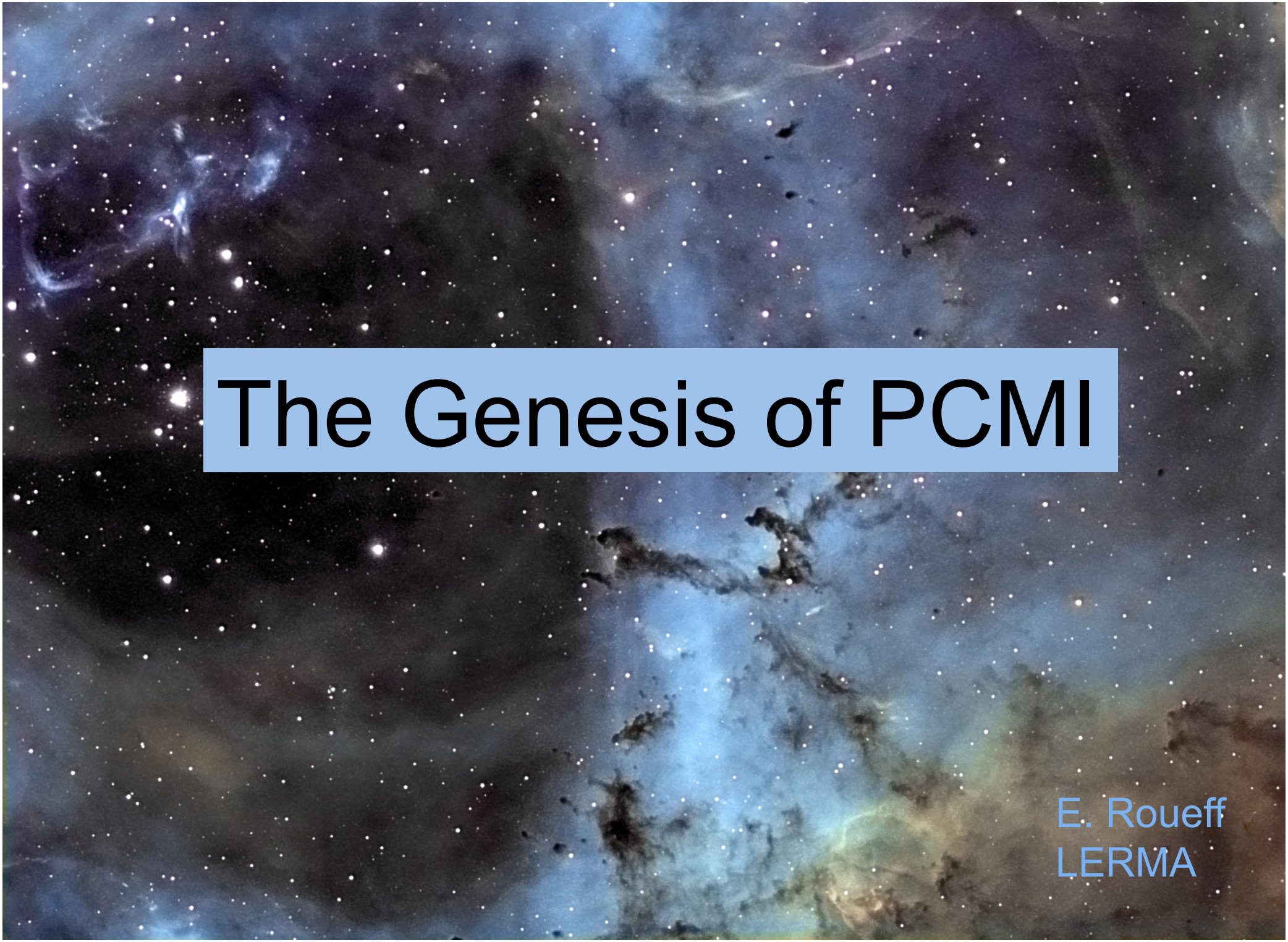


The Genesis of PCMI

E. Roueff
LERMA

The « pre-historical » time of PCMI

1974: Les Houches School on
"Atomic and Molecular Physics and the Interstellar Matter"
Proceedings edited by R. Balian, P. Encrenaz & J. Lequeux (1975)
C. Cesarsky, G.B. Field, D. Flower, P. Goldreich, S. Green, F. Kahn, R. McCarroll, M. Morris, H. Nussabumer, A. Penzias, H. Reeves, W. Watson

1975: CECAM workshop on potential surfaces and processes
C. Moser, M. Elitzur, F. Fayard, Sheldon Green, J. Guibert, E. Herbst, A. Glassgold, W. Langer, J.M. Launay, E. Roueff, H. van Regemorter

1979 first attempt to PCMI: RCP, Michel Guélin + E. Roueff

The “historical“ time of PCMI

1981 : Action Thématique Programmée (James Lequeux)

ATP CNRS *Physico-Chimie des Molécules Interstellaires*

Top down

The first committee →

J. Lequeux
M. Guélin
L. Galatry
B. Macke
P. Bréchignac
A. Omont
E. Roueff

+ “eyes of CNRS“
S. Sahal
M. Gaillard
P. Charvin (INAG)

Courtesy of P. Bréchignac

The first Budget

- RECAPITULATION -

Projets	Crédits alloués (1981)	Responsable gérant les crédits	
MI 01	20.000 F	M. BERTHIER	Quantum chemistry Paris
MI 02	90.000 F	M. BAUDRY	radioastronomy observations Bordeaux
MI 03	15.000 F	M. ROUSSY	spectroscopy Nancy
MI 04	50.000 F	M. DEMAISON	spectroscopy Lille
MI 05	70.000 F	M. DESTOMBES	
MI 06	15.000 F	M. BARASSIN	chemical kinetics Orleans
MI 07	10.000 F	M. VIALA	Astro model Paris
MI 08	24.000 F	M. SCHAMPS	Quantum chemistry Lille
MI 09	2.000 F	M. ENCRENAZ	radioastronomy observations Paris
MI 10	8.000 F	Mme FALGARONE	??
MI 11	67.500 F	M. BERNARD	radioastronomy observations Paris
MI 12 et 13	29.500 F	M. GUELIN	Electronic spectroscopy (H_2, CO) Paris
MI 14	35.000 F	M. BRETON	Theoretical spectroscopy Orsay
MI 15	23.000 F	Mme LEFEBVRE-BRION	Theoretical dynamics Besançon
MI 16	10.000 F	M. ROBERT	
MI 17	16.000 F	M. ENCRENAZ	radioastronomy observations Paris
MI 18 et 20	27.000 F	M. NGUYEN QUANG RIEU	
MI 19	26.000 F	M. LUCAS	
Colloque	10.000 F		
Réserve missions astronomie	52.000 F	LEQUEUX	

Σ= 600 kF ≈ 91 k€

1983- 1988 ATP PCMI

President : E. Roueff
Scientific secretary : P. Bréchignac
Administrative secretary affected to the structure : M. Revillon

Implication of Chemical department of CNRS (P. Vermeulin)

“inter ATP“ group 1983, suggested by J.C. Lehman
ATP “Atmosphère“ M.L. Chanin, A. Chedin
ATP “Dynamique Réactionnelle“ R. Vetter
ATP PCMI

Opening towards IR suggested by M. Petit (INAG) : J.L. Puget in the comittee

ATP meeting sept 1983 IAP Paris

- Identification of new interstellar molecules in the ISM
- Excitation mechanisms of interstellar molecules
- chemical reactivity under interstellar conditions
- new perspectives of observation in the infra red
- Physical chemistry of molecules on grain surfaces

discussion issues with the regulating bodies

Reduce administrative intermediary in terms of credits affectation;

Keep incitations toward physicists and chemists
small vs large amount of funds

Attract new people into interstellar applications

Identify specific representative groups outside the astrophysical community

Millimiter spectroscopy : Lille LSH laboratory

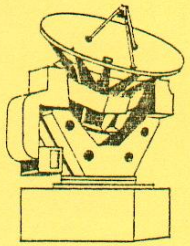
CRESU development in Meudon under B. Rowe's impulsion
(ion-molecule chemistry)

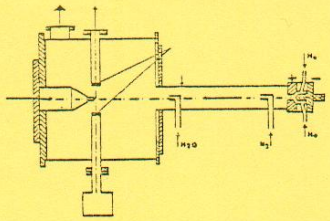
Involvement of quantum chemists (Berthier, Ellinger/Pauzat, …)
and quantum dynamics (J.M. Launay)

Opening to IR, preparation of ISO

discussion issues with the “tutelles“

More money !

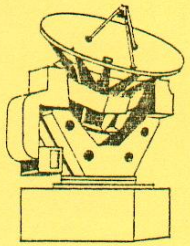


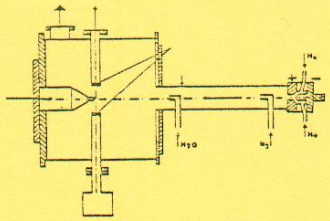


COLLOQUE ATP 1987

PHYSICO-CHIMIE DES MOLECULES INTERSTELLAIRES

5 et 6 mai 1987
à Grenoble





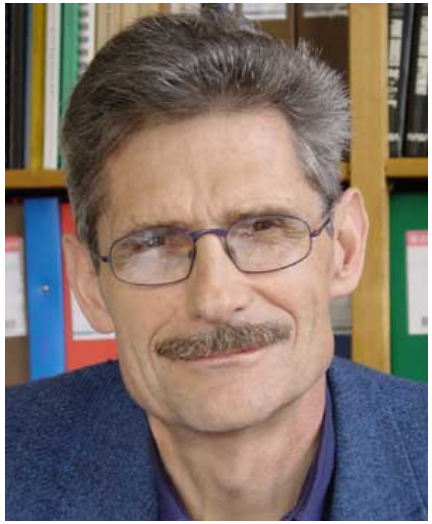
The end

COLLOQUE ATP 1987

PHYSICO–CHIMIE DES MOLECULES INTERSTELLAIRES

5 et 6 mai 1987
à Grenoble

The second period



A. Omont

1988 GDR PCMI

Physico-Chimie des Molécules Interstellaires

Bottom – up

1989 meeting in Orsay

1991 workshop Paris Observatory on chemical mechanisms on grain surfaces

1991 meeting IAP: recognition of the importance of surface physics and chemistry; perspective of ISO

1992 GDR PCM**G**I

*Physico-Chimie des Molécules et des **Grains** Interstellaires*

1995 : launch of ISO

A new area : the PAH hypothesis (Leger + Puget 1984, 1989)

Debate between coal model and models involving transient heating of free very small grains

The third period

1996 Programme National PCMI, negociated between G. Lelièvre (INSU), P. Bréchignac and ER to keep the opportunity of collaborative work in the frame of ISM. Additional support from CNES (ISO) and CEA; top – down

Budget ≈ 1600kF (CNRS 1200, CEA 300, CNES ≈ 1000k€

A great input from François Boulanger as deputy director : the need for hydrocarbonated nanoparticles

New experimental setups

PIRENEA (Toulouse)
Nanograins (Orsay)
PAHs in CRESU (Rennes)

CRESU experiment for neutral-neutral reactions (Rennes)

merged beam experiment for neutral radical reactions (Bordeaux)

Formolism (Cergy Pontoise)

COMPOSITION du CONSEIL SCIENTIFIQUE
du PROGRAMME NATIONAL sur la
PHYSIQUE ET CHIMIE DU MILIEU INTERSTELLAIRE

1996-2000

Dominique BOCKELEE-MORVAN, représentant le PNP SDU
François BOULANGER, Directeur-adjoint SDU (14)
Philippe BRECHIGNAC, Directeur SPM (04)
Claude BREMARD, représentant le Département SC
Fabienne CASOLI, représentant l'INSU
Gilberte CHAMBAUD, expert SC (17)
Odile DUTUIT, expert SC (17)
David FLOWER, expert Grande-Bretagne (astro)
Maryvonne GERIN, représentant la Section 14 du Com. National SDU
Dieter GERLICH, expert Allemagne (chimie)
Elizabeth GIACOBINO, représentant le Département SPM
Bertrand GIRARD, représentant la section 04 du Comité National SPM
Michel GUELIN, expert SDU (14)
Louis d'HENDECOURT SDU (14)
Martine JOUBERT, représentant le CNES
Thierry MONTMERLE, expert CEA (astro)
Irène NENNER, représentant le CEA
Alain OMONT, expert SDU (14)
Cécile REYNAUD, expert CEA (physicochimie)
Evelyne ROUEFF, expert, Présidente SDU (14)
Anne ZEHNACKER, représentant la section 17 du Com. National SC

Since 1997 : New structuration of the astrophysical french community in national programs - 1 director + 1 president

present astronomical landscape

"Programme national"

PNCG INSU, CNES, CEA, IN2P3, INP	V. Hill, M. Arnaud
PNHE IRFU, CNES, INSU, IN2P3	G. Dubus, B. Gibbels
PNPS INSU, CNES, CEA	B. Dintrans, Y. Lebreton
PNP INSU, CNES	A. Morbidelli, F. Robert
PNST INSU, CNES	D. Delcourt, L. Klein
PCMI INSU, CNES, INP, INC	M. Gerin, C. Joblin, A. Canosa J. Pety, K. Demyk, J.H. Fillion

+

"Actions spécifiques"

ASA (ALMA) INSU
ASHRA (Haute Resolution Angulaire) INSU, CNES
ASOV (Observatoire Virtuel) INSU, CNES
GAIA INSU
JMMC INSU
ASGRAM INSU, CNES, INP
AS SKA LOFAR INSU

1997 : New structuration of the astrophysical french community in national programs
1 director + 1 president

"Programme national"

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+

"Actions spécifiques"

ASA (ALMA) INSU
ASHRA (Haute Resolution Angulaire) INSU, CNES
ASOV (Observatoire Virtuel) INSU, CNES
GAIA INSU
JMMC INSU
ASGRAM (Gravitation, metrology) INSU, CNES, INP
AS SKA LOFAR INSU

A double challenge

→ PCMI has significant interfaces with other INSU programs

- Participation to the elaboration and science exploitation of ground-based telescopes (ex: IRAM) and space missions (ex: ISO, Herschel/Planck).
Exploit the gain in sensitivity and spatial resolution of new instrumentation (ALMA, NOEMA)

- Expertise in the analysis of astronomical data: *from molecules and grains to the physics and chemistry of interstellar and circumstellar environments*

  link with solar system (isotopic composition)

  link with stellar formation

  link with interstellar extragalactic and primordial environments

- Stay open!

→ PCMI should maintain and extend its interdisciplinar expertise in Physics and Chemistry.

- running and development of spectroscopic studies and microphysical processes in connection with the opening of new spectral windows and new astrochemical questions;

- preserve the fundamental interest of physicists and chemists ?

- other areas (dynamics, turbulence, …)

Extragalactic Molecules (as of 07/2014)

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	>8 atoms
OH	H_2O	H_2CO	c-C_3H_2	CH_3OH	CH_3CCH	HC_6H	c-C_6H_6 *
CO	HCN	NH_3	HC_3N	CH_3CN	CH_3NH_2		C_{60}* (?)
H_2 *	HCO^+	HNCO	CH_2NH	HC_4H *	CH_3CHO		
CH	C_2H	C_2H_2 *	NH_2CN	$HC(O)NH_2$ 2013			
CS	HNC	H_2CS ?	l-C_3H_2				
CH^+ **	N_2H^+	$HOCO^+$	H_2CCN				
CN	OCS	c-C_3H	H_2CCO				
SO	HCO	H_3O^+	C_4H				
SiO	H_2S	l-C_3H					
CO^+	SO_2						
NO	HOC^+						
NS	C_2S						
NH	H_2O^+						
OH^+	HCS^+ 2013						
HF	H_2Cl^+ 2014						
SO^+	NH_2 2014						

* rotation-vibration
** : electronic spectrum

From http://www.astro.uni-koeln.de/cdms/molecules

the required expertise to analyse the spectra is in the PCMI community

Chemical complexity in the ISM

- about 200 identified interstellar molecules (without isopologues) + D, ^{13}C, ^{18}O, ^{15}N, ^{34}S, … substituted molecules

  → identify chemical formation / destruction processes

  → possible state to state chemistry (ortho/para)

- exotic character (radicals, reactive species, isomers, molecular ions (positive and negative)

  spectroscopic identification, role of theoretical chemistry

  debate between C_3H^+ / C_3H^- in the Horsehead: instructive

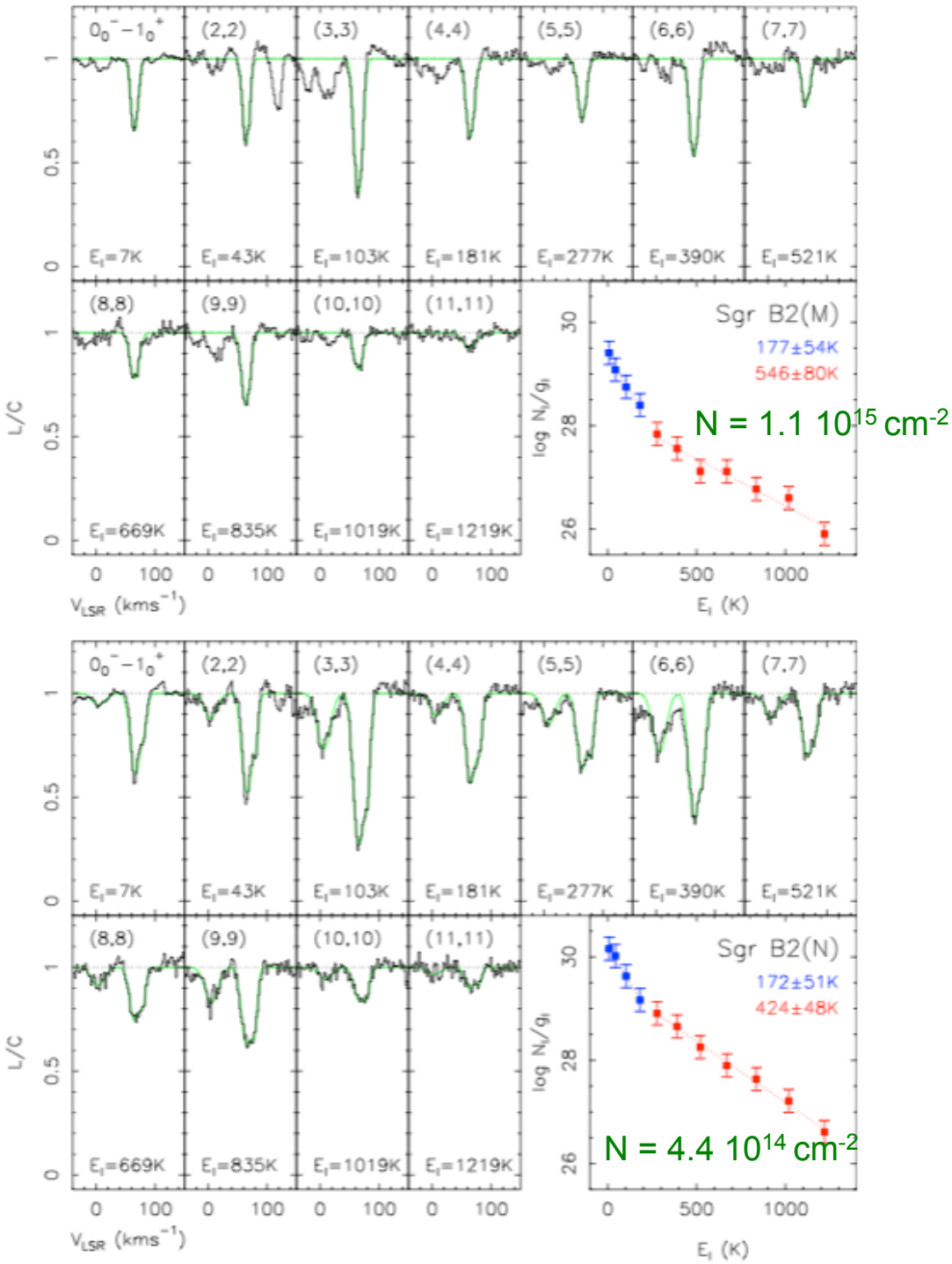
- how complex? Link to exobiochemistry?

- competition / complementarity between gas phase and surface chemistry

- nature of the excitation (collisional, photon or/and chemistry driven?) example of H_3O^+ detected by Herschel (Lis et al. 2014)

- ionisation diagnostics: example of H_3^+ in the Central Molecular Zone of the galactic center (reconcile high energy physics diagnostics and chemical analysis)

→ Take part to the Virtual Observatory and databases efforts (VAMDC, VO theory services : PDR, STARFORMAT).



A nice example

Herschel observations of metastable absorption transitions of H_3O^+ (isoelectronic with NH_3) towards GC and W51 by Lis et al. ApJ 785, 135, 2014

Signature of "hot" chemical formation : $H_2O^+ + H_2 \Rightarrow H_3O^+ + H$

Assuming steady state:

$$\mathcal{F} = \mathcal{D} = N(H_3O^+)\, n_e\, k_e\, (H_3O^+) / L$$
$$\approx 10^{-11}\, (1pc/L)\, (n_e/0.1)\ cm^{-3}\ s^{-1}$$
$$\approx \zeta\ n_H\ \varepsilon$$

$\zeta\, n_H < 10^{-11}/\ \varepsilon$ assuming $L \approx 1pc$, and $n_e < 0.1\ cm^{-3}$

compatible with $\zeta = 10^{-15}\ s^{-1}$ with $n_H\ \varepsilon = 10^4\ cm^{-3}$

In agreement with derivation from H_3^+ by Goto 2013, JPCA 117, 9919 (see talk by F. Le Petit)

Some vocabulary hobbies

(Thermo)chemistry

- Kilojoule per mole
- Hartree
- Pressure
- Timescale ≈ s
- Lengthscale ≈ cm
- Mass ≈ g
- MCSCF CI ,MBPT, ….
- Close-coupling, IOS, CS, …
- Extinction cross sections
- H^+ , α particles

Astronomy

- K
- Electron-volts
- Density
- Timescale ≈ yr
- Length scale ≈ parsec
- Solar mass = $M_\odot$
- Abundances
- Column density
- Magnitude
- Cosmic ray
- Depletion

Share the units!

Energy / enthalpy	kJ $mole^{-1}$	1kJ $mole^{-1} \approx$ 120K
Energy	Hartree	1 Hartree = 27.2 eV
Pressure	bar	1 bar = 7.25 10^{21} cm^{-3} K
time	second	year : 1 yr = 3.16 10^{7}s
length	cm	1AU = 1.5 10^{13} cm, 1pc $\approx$ 3 10^{18} cm
mass	g	1 solar mass : $1M_{\odot}$= 2 10^{33} g
Surfacic mass	g/cm^2	$1M_{\odot}$/ pc^2 : 2.1 10^{-4} g/cm^2
Linewidth / shift	Hertz	dv (km/s) = 300000 • dν / ν
extinction	σ (cm^2)	A_{λ}= 2.5loge * σ * n_gx (magnitude)
Column density	cm^{-2}	$\langle N_H / A_v \rangle \approx$ 1.9 10^{21} cm^{-2} mag^{-1}

A_v=1 ≈ 1.9 10^{21} x 1.67 10^{-24} x 1.4 g/cm^2 ≈ 4.4 10^{-3} g/cm^{-2} = 21 $M_{\odot}$/ pc^2

Needs of molecular astrophysics

- Opening of new spectroscopic windows
- Thermodynamic equilibrium is seldom achieved in ISM
- Information needed on the various intermediates

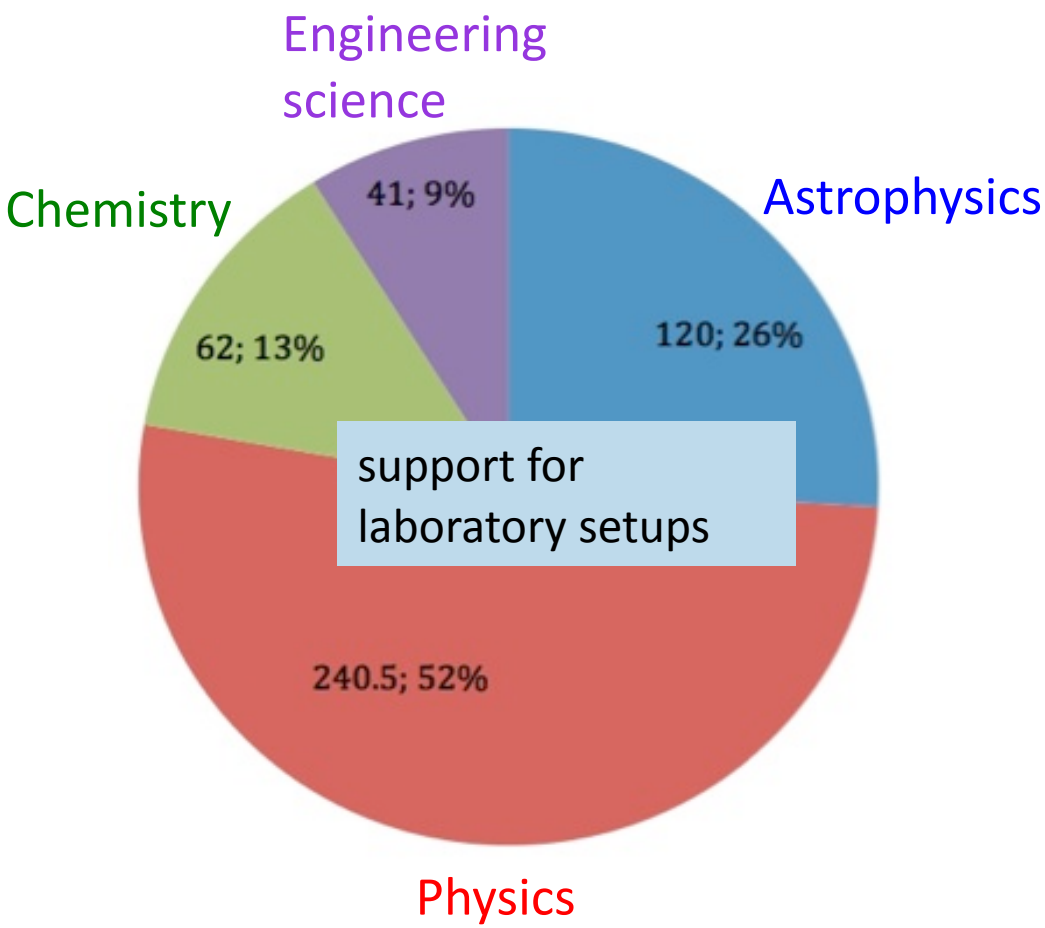
- Spectroscopic properties
- Chemical synthesis
- reaction rate coefficients for $10 \leq T \leq 3000$ K
- formation enthalpies of various isomers
- Photoprocesses
- Collisional excitation rate coefficients
- Sensitivity analysis welcome!
- Numerical aspects
- Surface processes
- Chemical modelling

Shared interest between physicists, chemists and astrophysicists can be found

Are young people prepared?

PN PCMI – Budget 2005-2008 (courtesy of C. Joblin)

Origin of financial support: Astrophysics (53%) – CNES (15%) – Physics (19%) - Chemistry (6%) - CEA (7%)



~ 1 Million Euros – 250 k€/year. Call issued each year

74 projects supported (most on a pluri-annual basis)

44 Institutes involved - ~120 researchers (>200 on the email diffusion list)

~ 500 articles – more than 100 invited conferences

~ 14 workshops, schools, conferences (co-organisation of 4 international conf.)

→ an indicator of interdiciplinarity

PN PCMI 2005/14– Laboratory astrophysics

Main supported experimental set-ups – Gas-phase

	PhLAM, Lille	G. Wlodarczak	Microwave and THz spectroscopy
SOLEIL	LPPM, Orsay	O. Pirali	Far-IR spectroscopy (AILES beamline, SOLEIL)
CRESU	IPR, Rennes	A. Canosa	Gas kinetics (15-500 K) Neutral-neutral reactions
PIRENEA	CESR, Toulouse	C. Joblin	Photodissociation, Spectroscopy and reactivity of PAHs and derived clusters/ complexes (40–300K)
NANOGRAIN	LPPM, Orsay	P. Bréchignac T. Pino E. Dartois	Production and characterisation of laboratory analogues of interstellar carbonaceous matter

PN PCMI 2005/14 – Laboratory astrophysics

Main supported experimental set-ups – Solid-phase

	PIIM, Marseille	T. Chiavassa G. Danger	Reaction mechanism on ices Application to Prebiotic chemistry, interstellar and cometary ice analogs
	LSPES, Lille	H. Leroux	Gas-silicate interactions
SONATE	CEA, Saclay	N. Herlin-Boime	Nanograin synthesis by laser pyrolysis
SICAL + MICMOC	IAS, Orsay	E. Dartois L.d'Hendecourt	Processing of Amorphous Carbons Chirality studies
CoSpiNu SPICES	LPMAA/ LERMA Paris	X. Michaut J.-H. Fillion	Nuclear spin conversion
FORMOLISM	LERMA, Cergy	J.L. Lemaire F. Dulieu	H_2 formation on grains Reactions on grain surfaces

The international dimension

1993 *Physical Chemistry of Molecules and Grains in Space,* LE MONT SAINTE-ODILE
1995 1st Franco-British Meeting on the *Physics and Chemistry of the Interstellar Medium*, LILLE
2008 Arcachon "Molecular Universe" international joined conference with PCMI

1996 - 2000 FP5 "ASTROCHEMISTRY" Research Training Network (RTN)
2003 - 2008 FP6 "Molecular Universe" RTN
2005 - 2009 FP6 "JETSET" RTN
2010 - 2014 FP7 "LASSIE" RTN
2009 – 2013 Astronet STARFORMAT , CATS projects
2014 - : SYNERGY grant (Madrid – Toulouse)

Similar experiences with higher fundings (including PhD and postdoc positions)

2002 - spanish Consolider-Ingenio project "Molecular Astrophysics for Herschel and Alma era"
2010 - Netherlands Organisation for Scientific Reasearch (NWO) Astrochemistry Programme
2011 - 2017 SchwerPunkt Program (SPP) DFG "Physics of the interstellar medium" including galactic + extragalactic communities
UK? , Italy?

Conclusions and prospects

PCMI has been a wonderful opportunity to broad my personal knowledge and meet fantastic colleagues. I am thus very grateful to many of you for such an achievement.

A real interdisciplicary community is gathered. The structuration has taken time and short term politics priorities may break it much quicker.

A lot of results from IRAM, Herschel, ALMA present and to come and some pioneering chemical physics studies (CRESU, ….), original opportunities (LURE, SOLEIL)

Some concern about student formation. In the astrophysical cursus, limitation to bases of spectroscopy. Nothing about reactivity. 2nd year cursus? Physico-chemical cursus?

Budget has considerably increased since beginning. Yet, the dedicated amount may appear somewhat unreasonably limited. Other sources of funding (ANR, ERC grants, …) are there but they do not favor the gathering of the community.

Despite non spectacular budget perspectives, maintain the aperture politics both towards astrophysical "Extrasolar Cosmochemistry" (Jura & Young, AREPS 42, 45, 2014) and physico-chemical domains. However, stay rigorous in the referring of the projects (relevance of the vocabulary, check of the experimental setups, numerical aspects, …); keep regular meetings and workshop and do not forget the international .

All my best wishes to the new team in charge