ASTROFISICA MOLECULAR ASTROQUÍMICA : COMPLEJIDAD QUÍMICA EN EL ESPACIO



CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

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Outline of the talk:

Introduction to the physical properties of our "laboratories" THE ROLE OF MOLECULAR PHYSICS IN ASTROPHYSICS The interstellar and circumstellar media Gas, dust and PAHs

Evolved stars and Planetary Nebulae (AGBs and post-AGBs)

Our Tools, our needs, our observing machines

THE NANOCOSMOS PROJECT

Far-infrared spectral range (Space)

 $(\lambda \sim 30-350 \ \mu m)$ $(1/\lambda \sim 330-30 \ cm^{-1})$ (v~ 10 THz- 1000 GHz)

Submillimeter spectral range

 $(\lambda \sim 300-1000 \ \mu m)$ (v~ 1000 GHz- 300 GHz) ALMA

Millimeter spectral range

(λ ~1mm-10 mm) (v~ 300 GHz- 30 GHz) ALMA & single dish

The radio spectral range (microwaves)

($\lambda \sim 10mm$ -1 cm) (v~ 30 GHz- 3 GHz) Most ground based RT

 \Rightarrow "Transparent to dust" \Rightarrow Obscured dusty objects

 $(n, T_{\kappa}) \Rightarrow$ Molecular Universe \Rightarrow Gas and dust life-cycle

Properties of the diffe	<u>erent phase</u>	<u>s of the inte</u>	erste	<u>lar medium</u>
Phase	n [cm ⁻³]	Т [К]	f	M [10 9 M $_{\odot}$]
Hot ionised Medium	0.003	10 ⁶	0.5	-
Hot Neutral Medium	0.5	8000	0.4	1.4
Warm Ionized Medium	0.3	8000	0.1	1.0
Diffuse Clouds (HI)	50	80	-	2.5
Molecular Clouds	>300	10	-	2.5
HII Regions	1 – 10 ⁵	10 ⁴	-	-
Protoplanetary Systems	10⁴-10 ¹²	10-1000	-	-
Evolved Stars	10²-10 ¹⁴	10-2000	-	-
Earth Surface	2 10 ¹⁹	300		

f = Fraction of the galactic disk filled by each phase





Molecular clouds are filled with submicron dust grains ($\approx 0.5 \, \mu m$)



Complex organics formed on and in the ices

Thermal processing (inner envelope + disk)

Energetic processing (envelope + disk)







-G e -. . ALMA: a 20 km diameter telescope from interferometric observations Image of a planetary disk as observed with ALMA in the continuum emission at submm wavelenghts of dust grains. Synthetized telescope = 15 km.

The dust grains that will made rocky planets have been formed in evolved stars and SNe They have been processed (covered by ices) during several millions years in the evolution of molecular clouds. Learning about their formation is a crucial and key step in astrophysics Why observing molecules in Space

Molecular clouds are dark !! They contain H_2 and dust (gas/dust mass ratio ≈ 200 (all metals in grains !!)

Dust grains protect the inner part of molecular clouds against molecular photodissociation. Rich gas phase chemistry $H_2 + cosmic ray = H_2^+$ followed by $H_2^+ + H_2 = H_3^+$ and $H_3^{++}O$

Molecules are cooling agents=>dynamics=>star formation

Molecules aggregate on dust grains during gravitational collapse =>rich surface chemistry=>preparing the initial conditions for the composition of surface and atmosphere of rocky planets

Molecules => getting volume densities, kinematics, dynamics, and kinetic temperatures from their line profile and intensity

vibration rotation (a)

Microwave/millimeter/submillimeter/far IR

mid/near-Infrared

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asymmetric stretching vibrational motion







rotational motion

translational motion

Absorption of EM radiation



CH₃OH Internal rotation





MODELING ASTROPHYSICAL DATA: PRACTICALLY ALWAYS OUT OF EQUILIBRIUM

Lines arise from a region where temperature, abundance, and density can vary very fast



It is necessary to use sophisticated methods



e.g. LVG multishell or non-local codes



LVG multishell models



LVG multishell models



0.1

0.05

0

LVG multishell models





By selecting the appropiate molecule we can trace different physical parameters.

Low dipole moment molecules are easily thermalized, even at moderate densities. These molecules can be used to trace the kinetic temperature.

High dipole moment molecules trace the gas density.

However, state to state collisional rates between the molecule and H_2 must be known in order to model the observed emission.

These collisional rates are only available for a few species (CO, HCN, HCO⁺, H₂CO, CH₃CN, SiO, NH₃, N₂H⁺, CS, HC₃N,...) and often they have been calculated with He rather than with molecular hydrogen as collider.

Molecules as probes of T and n_H



Based on figure by R. Genzel (1991)

MOLECULAR ASTROPHYSICS AS A MULTISDICIPLINARY FIELD



			N	umber of Atom	S		
2	3	4	5	6	7	8	9
H ₂	H_2O	NH ₃	SiH ₄	CH ₃ OH	CH ₃ CHO	CH ₃ CO ₂ H	CH ₃ CH ₂ OH
OH	H_2S	H_3O^+	CH ₄	NH ₂ CHO	CH ₃ NH ₂	HCO ₂ CH ₃	(CH ₃) ₂ O
SO	SO ₂	H ₂ CO	CHOOH	CH ₃ CN	CH ₃ CCH	CH ₃ C ₂ CN	CH ₃ CH ₂ CN
SO ⁺	HN_2^+	H ₂ CS	HC ≡CCN	CH ₃ NC	CH ₂ CHCN	C ₇ H	H(C≡C) ₃ CN
SiO	HNO	HNCO	CH ₂ NH	CH ₃ SH	HC₄CN	H_2C_6	$H(C \equiv C)_2 CH_3$
SiS	SiH ₂ ?	HNCS	NH ₂ CN	C₅H	C ₆ H		C ₈ H
NO	NH_2	CCCN	H ₂ CCO	HC ₂ CHO	c-CH ₂ OCH ₂		
NS	H_3^+	HCO_2^+	C₄H	$CH_2 = CH_2$	C ₇ ?		10
HCI	NNO	CCCH	$c-C_3H_2$	H ₂ CCCC			
NaCl	HCO	c-CCCH	CH ₂ CN	HC ₃ NH ⁺			CH ₃ COCH ₃
KCI	HCO+	ccco		acont datac	tion of spio	nc.	$CH_3(C \equiv C)_2 CN?$
AICI	ocs	CCCS	SiC ₄			115.	
AIF	CCH	HCCH	H_2CCC	$N^{-}, C_3 N^{-}, C_3$	₅ N ⁻ ,		11
PN	HCS ⁺	HCNH ⁺	HCCNC C	$_{1}H^{-},C_{6}H^{-}.C_{5}$	₃ H-		
SiN	c-SiCC	HCCN	HNCCC		,		H(C≡C)₄CN
NH	cco	H ₂ CN	H ₃ CO ⁺				
СН	CCS	c-SiC ₃	>]	15 cations			13
CH+	C ₃	CH ₃					
CN	MgNC	CH ₂ D ⁺ ?	>1	00 Carbon	Molecules		H(C≡C)₅CN
co	NaCN						
CS	CH_2					-	
C_2	MgCN		10	Metal-bea	ring Molec	ules	•
SiC	HOC+	CH, CH [*]	6	rings + C_{60}	$\& C_{70} + PA$	Hs	C ₆₀ ⁺
CP	HCN	CN	(8 00	70		
CO ⁺	HNC		I I				
HF	SICN	1940 5	50 60	70 80	90 2000		
	KCN?			Year			



AGBs and post-AGBs



Relative temperature fluctuations, with different amounts of transparency at different stages of the movie, showing either the surface features or the interior global dipole flow pattern.



http://www.lcse.umn.edu/research/RedGiant/

What is the structure of an AGB star ?

Parameters for some	Max	Min	Period
well known AGB stars	Magnitud	Magnitud	days
Mira (o Ceti)	2	10,1	331,996
χ Cygni	3,3	14,2	408,5
R Hydrae	3,5	10,9	388,87
R Carianae	3,9	10,5	308,71
R Leonis	4,4	11,3	309,95
S Carinae	4,5	9,9	149,9
R Cassiopeiae	4,7	13,5	430,46
R Horologii	4,7	14,3	407,6
U Orionis	4,8	13	368,3
RR Scorpii	5,0	12,4	281,45
R Serpentis	5,16	14,4	356,41
R Centauri	5,3	11,8	546,2
R. Trianguli	5,4	12,6	266,9
R Leporis	5,5	11,7	427,1
R Aquilae	5,5	12	284,2
R Aquarii	5,8	12,4	386,96
U Cygni	5,9	12,1	463,24



Many AGBs are optically visible : low mass loss rate (10⁻⁷ solar masses /year) others are very dusty : high mass loss rate (10⁻⁴ solar masses/year) All them are pulsating

CHEMISTRY IN SPACE

How Molecules are formed ?

Physical conditions very different from those in the Earth Laboratories

Interstellar gas is far from thermodynamical equilibrium

MODELS UNDER THERMAL EQUILIBRIUM

Reaction rates and the path to form molecules are not important. Molecular abundances are determined by their value at thermodinamical equilibrium.

That means that two and three body reactions must be much faster that the time scale for dinamic evolution.

Of course, these models will provide reasonable results only for the most dense and warm regions. In the external layers of the envelope molecular abundances will be strongly dependent on the chemical kinetics and on the UV photons entering the envelope. The formation rate of the molecule AB, assuming that the activated complex reaches an equilibrium between formation and destruction is given by

 $\frac{dn(AB)}{dt} = n(AB^*) \times n(M)k_2$ $\frac{dn(AB^*)}{dt} = n(A) \times n(B) \times k_1 - n(AB^*) \times n(M) \times k_2 - n(AB^*) \times k_3$

 $dn(AB^*)/dt = 0$

 $n(AB^*) = \frac{n(A) n(B) k_1}{(k_3 + k_2 n(M))}$

and

 $dn(AB)/dt = \frac{k_1 k_2 n(A) n(B) n(M)}{k_3 + k_2 n(M)}$

If A, B y M are neutral species then $k_1 \approx 10^{-11} \text{ cm}^3 \text{s}^{-1}$ and $k_2 \approx 10^{-10} \text{ cm}^3 \text{s}^{-1}$, but $k_3 \ 10^{+11} \text{ s}^{-1}$, and

 $dn(AB)/dt \approx 10^{-32} n(A) n(B) n(M) cm^{-3}s^{-1}$

The best case in the ISM/CSM occurs for A=B=M= H

 $H + H + H \Leftrightarrow H_2 + H$

For hydrides (BH) the optimal case will correspond to A=H, M=H and B \in (C,N,O), i.e., n(B) \approx 10⁻⁴ n(H) and

 $dn(BH)/dt \approx 10^{-36} n^{3}(H) cm^{-3} s^{-1} B \in (C,N,O)$

EXAMPLE:

Let us consider an atomic cloud without dust grains and without radiation field. For t=0 the density of atomic hydrogen is n and that of molecular hydrogen is 0. The formation of H_2 occurs through the reaction

 $H + H + H = H_2 + H$

with a rate $K = 10^{-32} \text{ cm}^{6} \text{ s}^{-1}$

The formation rate of H₂ is given by $\frac{dn(H_2)}{dt} = K n_{H}^3(t); \quad f(t) = \frac{2 n_{H2}(t)}{n_{H}(t) + 2 n_{H2}(t)} = \frac{2 n_{H2}(t)}{n}$ $\frac{df(t)}{dt} = K n^2 (1 - f(t))^3 \quad f(t) = 0.5 \text{ for which time } ?$

EXAMPLE

f(t)=**0.5**

The three body mechanisms is only efficient for densities larger than 10¹⁰ cm⁻³. Even in this case, the density is not enough taken into account the dynamical time scale of evolution of the object.

For a density of 10^{14} cm⁻³, i.e., the photosphere of an AGB star, the time necessary to transform H into H₂ is 6 10⁻⁴ yr = 5.3 hours !!!!

Interstellar and Circumstellar chemistry require very different Chemical reactions to produce significant molecular abundances !

Dust grains

Formation Evolution Processing Carbon material (PAHs) Chemistry on their surfaces



The role of C/O ratio on the gas

O-rich or C-rich, that is the question

O-rich star [C]/[O] < 1

C-rich star [C]/[O] > 1



O-bearing molecules: CO, H₂O, SiO, OH, ... C-bearing molecules: CO, C₂H₂, HCN, CS, ...

NANOCOSMOS The role of C/O on the nucleation seeds

Dartois et al. adapted from Ebel et al. (2000)



A dust grain of 0.1µm contains ~ billion atoms Several billion chemical reactions to form it from H, C, N, S, Si, Ti, Fe, Al, Mg,

NANOCOSMOS The challenge of dust growth modelling





Impossible to study all the reactions individually : making circumstellar grains analogs in the laboratory

The Aromatic Infrared Bands (AIBs)



Infrared Space Observatory ESA; 1995-1998



AKARI JAXA; 2006-2011



The PAH model



3.3 μm (3050 cm⁻¹); 6.2 μm (1610 cm⁻¹); '' 7.7 '' μm (1300 cm⁻¹); 8.6 μm (1160 cm⁻¹); 11.3 μm (890 cm⁻¹); 12.7 μm (785 cm⁻¹)

CH and CC aromatic modes

Stochastic heating – absorption of a single UV photon
N~50 ; T~1000 K
Sellgren 1984, ApJ 277, 623

• Candidates: PAH molecules Léger & Puget 1984, A&A 137, L5 Allamandola, Tielens & Barker 1985, ApJ 290, L25

Energetic budget: 10 to 20% of total carbon in PAHs
 Joblin et al. 1992, ApJ 393, L79
 Li & Draine 2001, ApJ, 554, 778
 Draine & Li 2007, ApJ 657, 810
 X_{PAH}~ 10⁻⁷ (N_C~50)

The AIBs in the galactic dust cycle



Adapted from http://www.nrao.edu/pr/2006/gbtmolecules/ Bill Saxton, NRAO/AUI/NSF

The AIBs in the galactic dust cycle



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AGBs → IRC +10216:

Chemical study of the envelope

¿Why is so interesting the study of chemical composition of IRC +10216?

λ=10 mm; ESO/La Silla B. Stecklum & H.-U. Kaüfl

- IRC+10216 is a prototype of C-rich stars
- 50% of the molecules known in space have been detected in its CSE





 10^{2}

 10^{1}

CO J=2-1



METHODS : Astronomical observations at all frequencies Radiative transfer modelling, Dynamical Evolution, Chemical modelling,....



Dust grain formation is an out of equilibrium process Three zones can be defined

I) Dust seeds formed in the photosphere?

 T_{K} =2500 K, n(H)=10¹⁴ -10¹⁵ cm⁻³, p=0.03-0.3 mbar Gas phase thermodynamical equilibrium applies for H₂, CO, HCN, H₂O, etc. Time to reach equilibrium from a few minutes (p=0.3 mbar) to a few hours (p=0.03 mbar). H₂/H~10⁴ at T_K ~ 1000 K

II) Seeds are accelerated by radiation pressure, density decreases as r⁻², temperature also decreases very fast. Dust nucleation
 Region 1-5 R_{*} (T_K=2500-1000 K, density decreases by a factor 25 at r=5R_{*}).
 Pressure decreases from 0.03-0.3 mbar down to <0.001-0.01 mbar

III) Dust grain growth in the region 5-20 R_* (3 10¹⁴-1.5 10¹⁵ cm)

- * Seeds formed in the region 1-5 R_* travel through a region ~10¹⁵ cm in size during ~ 50- 100 yr. At the end of this region gas and dust are decoupled.
- * Dust-dust collisions are very rare and "chemical vapor deposition" is the main growth process. Pressures are very low, accreation rates are also low.
- * In this zone most abundant (observed) gas species are H₂, CO, C₂H₂, CH₄, HCN, H₂O, SiC₂, SiO, SiS, CS, OH,... but H still an abundant species





Guélin & Coworkers PdBI data 3" resolution Radicals C_nH

and C_nN are found in the molecular ring at 14" from CW Leo

The chemical composition of the dust formation zone of IRC+10216

ALMA

CO (2-1) 30m IRAM



Leao et al., 2006, (B-V)



Astrochemistry:

Observation of molecules and dust in space

1) Molecular Astrophysics:

Interpretation of the observations involving emission/absorption of molecules

2) Laboratory Astrophysics:

Gathering data from laboratory to help in the interpretation of Astrophysical data

Using theoretical methods in quantum chemistry to get properties Of molecules observed by astrophysicists

What kind of laboratory experiments are of interest for astrophysics? NANOCOSMOS: A synergy project of the European Research Council

NANOCOSMOS

José Cernicharo ICMM, CSIC, Spain Christine Joblin, IRAP, CNRS, France José A. Martin-Gago, ICMM, CSIC, Spain





Astronomers, Chemists, Physicists, and Engineers working together at the frontiers of knowledge. *Understanding the formation of cosmic dust and chemical complexity in Space and on Earth*

NANOCOSMOS A complementary and multidisciplinary team

Ultra-high vacuum Technologies NanoSciences



Laboratory Astrophysics Carbonaceous macromolecules & nanograins Photodissociation regions

> Radioastronomy Molecular spectroscopy Evolved Stars

Nanocosmos Yebes – 06/2/2014

erc

European Research Council

Established by the European Commission

+15 MEuros



OBSERVATIONS

ICMM-Madrid

Beyond the current frontiers





Stars, as factories of molecular complexity and dust Understanding formation of dust in space Impact on our vision of the origin of planets and life

EXPERIMENTS



Technical and scientific innovation through synergy

nanocosmos



Dust formation in evolved stars:

- Investigating chemical and physical conditions in the dust formation zone

- Characterizing dust properties

Dust formation: laboratory approach

- Producing analogues of circumstellar dust
- Investigating formation mechanims

Dust properties in cosmic (circumstellar and interstellar) conditions

- Spectroscopy from 10 to ~1000 K
- Processing (UV, thermal, electrons, high-energy ions, H,....)
- Gas-grain interactions: Atomistic view and grain size effects. Reactivity of dust analogues



Nanocosmos: The StarDust chamber in Madrid (design v3)



MICS Chamber: to produce nanoparticles from atoms

The Stardust molecular analyzer in Toulouse





Working activities and Goals

Determine gas





June 2016

Tests with two mangetrons M1 + M2

 Φ total = 100 sccm ϕ 1 = ϕ 2 =50 sccm L1 = L2 = 192mm (also L1=242mm) L3 = 242mm Lbb = fully extended P1 = P2 = 30W

Rates (ng*s/cm2): M1 = 120 ng*s/cm2 M2 = 2 ng*s/cm2 M1+M2 = 204 ng*s/cm2 (L1=L2) M1+M2 = 221 ng*s/cm2 (L1=242mm)



The Stardust molecular analyzer in Toulouse



The Gas Cell Simulator Chamber

- A gas cell equipped with HEMT receivers covering 30-50 & 70-116 GHz. Instantaneous bandwidth 20x3 GHz with FFTs and spectral resolution of 0.19 MHz for broadband spectroscopy. 24 x 1.5 GHz bands with 20 KHz spectral resolution for high spectral resolution spectroscopy. Observing thermal emission
- A molecular cloud with 10²² cm⁻² molecules of H₂ in the line of sight will contain 10¹⁸ cm⁻² molecules of CO and 10¹⁴ molecules of HCN, HCO⁺, HNC, CCH, CN, CS,



The prototype installed in the electrical path of a 40 m radiotelescope



The Stardust machine from scratch

nanocosmos



Main institutes involved in Spain

PIs: J. Cernicharo, J. A. Martín-Gago

- Instituto de Ciencia de Materiales de Madrid (CSIC)
- OAN and Centro Tecnológico de Yebes (IGN)
- Universidad de Castilla la Mancha (chemistry)
- Instituto de Estructura de la Materia (CSIC)
- Universidad de Valladolid (microwave, millimeter and submillimeter spectroscopy)

Involved teams at CNRS/ Univ. Toulouse PI: C. Joblin

- Milieu Interstellaire, Cycle de la Matière, Astro-Chimie at IRAP
- Matériaux et Procédés Plasmas at LAPLACE
- Interactions Ions-Matière at LCAR-IRSAMC
- *Modélisation, agrégats, dynamique* at LCPQ-IRSAMC



SUMMARY

NANOCOSMOS

- Laboratory experiments are mandatory to understand the growth processes (coagulation, molecular condensation)
- Observations at all lambdas are needed to fully characterize the chemistry of dust formation
- A good, close and fruitfull collaboration with teams of many areas are needed to address this fundamental problem
- NANOCOSMOS project is open to collaborate with other teams interested in the physical and chemical studies we are going to perform

NANOCOSMOS Nanocosmos puts stardust into your hands

A synergetic multidisciplinary project at the frontiers of technology and knowledge



Astronomers, chemists, physicists, and engineers working together to understand the formation of cosmic dust and chemical complexity in Space and on Earth



CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS





We know that human beings are made from stardust NANOCOSMOS will show us how cosmic dust is made

MUCHAS GRACIAS POR SUATENCIÓN