INTERNATIONAL SYMPOSIUM AND WORKSHOP ON ASTROCHEMISTRY

Understanding extraterrestrial molecular complexity through experiments, observations and models

JULY 3rd – 8th, 2016
CAMPINAS, SP, BRAZIL

www1.univap.br/gaa/iswa

Scientific Committee

Sergio Pilling (UNIVAP/Brazil), *Chair*
Edgar Mendoza (IAG-USP/Brazil), *Co-Chair*
Bertrand Lefloch (IPAG/France)
Cecilia Ceccarelli (IPAG/France)
Ewine van Dishoeck (Leiden Univ./NL)
Farid Salama (NASA Ames/USA)
Guillermo Muñoz Caro (CAB-INTA/ Spain)
Harold Linnartz (Leiden Univ./NL)
Heloisa Boechat-Roberty (OV-UFRJ, Brazil)
Jacques Lepine (IAG-USP, Brazil)
Kinsuk Acharyya (Univ Virginia/ USA)
Michel Nuevo (NASA Ames/USA)
Nigel Mason (Open Univ./UK)
Peter Woitke (St. Andrews Univ./UK)
Philippe Boduch (GANIL-CIMAP/ France)
Sun Kwok (HK Univ./China)
Yi-Jehng Kuan (Nat. Taiwan Norm. Univ./Taiwan)

Local Committee

Sergio Pilling, *Chair*
Edgar Mendoza, *Co-chair*
Sarita P. de Carvalho
Will Robson M. Rocha
Douglas Galante
Diana Gama
Maria Fernanda Cerini

Sponsors

Dear colleagues,
Welcome to the "INTERNATIONAL SYMPOSIUM AND WORKSHOP ON ASTROCHEMISTRY - ISWA: Understanding the extraterrestrial molecular complexity through experiments, observations and models". The main goal of this event is to promote discussion and collaboration among experimentalists, observers and theoreticians interested to contribute to the progress of Astrochemistry. This is the first international conference in this category at Brazil and we hope that the participants in different fields can find the words to exchange their knowledge, trigger future collaborations and can arise very good synergetic scientific projects.

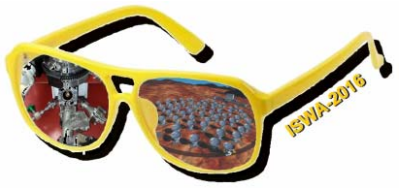
The scientific topics of this meeting are:
- Astrophysical ices - Spectroscopy, Energetic Processing (UV, X-rays, Electrons, Ions)
- Formation of complex species in ices - Astrobiology
- Surface Chemistry, Thermal programed desorption
- Gas phase experiments on Astrochemistry
- Detection of molecules in Astrophysical environments (radio, infrared)
- Astrochemical models, abundances, chemical evolution.

During the symposium, we will also have two hands-on workshops: one focused on experimental Astrochemistry and other focused on astronomical observations. The hands-on workshops will have activities on the intrumentation for astrochemistry, proposal submissions to the Brazilian Synchrotron Light Laboratory (LNLS/CNPEM), data reduction and to the Large Latin American Millimeter Array (LLAMA) and the Atacama Large Millimeter Array (ALMA) radio observatories and other subjects.

It was prepared for you a guided tour to the Brazilian Synchrotron Light Laboratory (LNLS/CNPEM), one of the most impressive project of the Brazilian science community. There, we will see different type of experiments running, learn about its characteristics and its possibilities for new measurments, and visit the construction site of the next generation Synchrotron Light Source - Sirius, even more powerful than LNLS. The Symposium will be held at the Historic Farm-Hotel "Solar das Andorinhas" located in Campinas, SP, Brazil (near the Brazilian Synchrotron lab). The participants of the meeting will have a thematic conference dinner with a typical Brazilian winter party called "Festa Julina" with includes bonfire and typical drinks and foods.

Finally, we would like to add that since the conference websinte was lunched 18 months ago we had more than 6500 visitor on line indicating how attractive and important this field is in the scientific scenario. Half of the 78 registered participants in this meeting are Brazilians, which also indicates the increasing interest of Braziliam scientific community in this field. We hope this number become even larger after the synergetic processes triggered by this meeting.

Sergio Pilling (ISWA Chairman)



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Phillipe Boduch (GANIL-CIMAP/France); Sun Kwok (HK Univ./China)
Yi-Jehng Kuan (Taiwan Univ./Taiwan)

Opening talk: A.G.G. M. Tielens (Leiden Observatory): *The Molecular Universe*

The Local Organizing Committee:
Sergio Pilling (Chair); Edgar Mendoza (Co-Chair);
Sarita Pereira; Will Robson M. Rocha; Douglas Galante;
Diana R. G. Gama, Maria Fernanda Cerini

Sponsors:
UNIVAP, LASA, IAG-USP, FAPESP, SAB, HOTEL SOLAR DAS ANDORINHAS;
THORLABS; LNLS/CNPEM

Official conference website:
http://www1.univap.br/gaa/iswa/

Time table

	3/jul (sun)	4/jul (mon)	5/jul (tue)	6/jul (wed)	7/jul (thu)	8/jul(fri)
8:30 - 9:20		Conference 2 (**Nuevo**)	Talk 16 (**Pilling**)	Conference #6 (**Lepine**)	Talk 33 (**Mendoza**)	Conference #9 (**Inostroza**)
9:20: 9:40		Talk 1 (**Rocha**)	WORKSHOP EXPERIMENTAL [Equipments, research proposals LNLS, software, techniques, data reduction, ...] (**Pilling; Rocha; Galante**)	Talk18 (**Arias**)	WORKSHOP OBSERVATIONAL [Proposal to ALMA, LLAMA, data reduction, software, techniques, ...] (**Mendoza; Gama**)	Talk34 (**Magalhães**)
9:40-10:00		Talk 2 (**Ortiz**)		Talk19 (**Pinotti**)		Talk35 (**Aleman**)
10:00-10:20		Talk 3 (**Baptista**)		Talk20 (**Canelo**)		Talk36 (**Arapiraca**)
10:20-11:00		***Coffee with Posters***	***Coffee with Posters***	***Coffee with Posters***	***Coffee with Posters***	***Coffee with Posters***
11:00-11:20		Talk4 (**Andrade**)	WORKSHOP EXP.	Talk21 (**Woitke**)	WORKSHOP OBSERV.	Talk37 (**Cerini**)
11:20-11:40		Talk 5 (**Barreto**)		Talk22 (**de la Rezza**)		Talk38 (**Parikka**)
11:40-12:00		Talk 6 (**Arumainayagam**)		Talk23 (**Monfredini**)		Talk39 (**Esmaili**)
12:00-12:20		Talk 7 (**Vinogradoff**)		Talk24 (**Jinhua He**)		Talk40 (**Bonfim**)
						Closing
12:20-14:00		***Lunch***	***Lunch***	***Lunch***	***Lunch***	***Lunch***
14:00-14:20		Talk 8 (**Kuan**)	Official conference photo VISIT TO LNLS/CNPEM Bus to LNLS	Talk25 (**Marshall**)	Free afternoon for Scientific discussions and working groups.	Check-out
14:20-14:40		Talk 9 (**Fornazier**)	Talk 17 (**Galante**)	Talk26 (**Ribeiro**)		
14:40-15:00	Registration and check-in	Talk 10 (**Vignoli Muniz**)	Guided visit to LNLS/CNPEM	Talk27 (**Gama**)		
15:00-15:20		Talk11 (**Chang**)		Talk28 (**Quénard**)		
15:20:16:10		Conference 3 (**Janot-Pacheco**)		Conference #7 (**Lefloch**)		
16:10-16:40		***Coffee with Posters***	***Coffee Break at LNLS***	***Coffee with Posters***		
16:40-17:00		Talk 12 (**Micelotta**)	Guided visit to SIRIUS/CNPEM	Talk29 (**Machaieie**)	**Social Activities (optional):** 1) Train trip to Jaguariuna*; 2) PaintBall1 at hotel*; 3) Ballon at hotel*; 4) Rafting at hotel*; 5) Trip to Campinas city center / Taquaral Lagoon; 6) Trip to Parque Dão Pedro (Largest shopping center of South America); 7) Arvorismo - Tree walking at the hotel* *reservation needed	
17:00-17:20		Talk13 (**de Barros**)		Talk30 (**Almeida**)		
17:20-17:40		Talk 14 (**Blasberger**)		Talk31 (**Boice**)		
17:40-18:00	Welcome and brief overview of Brazilian Astrochemistry (**Pilling**)	Talk 15 (**Bosco**)	Bus to hotel	Talk32 (**Brouillet**)		
18:00-19:00	Open conference (**Tielens**)	Conference 4 (**Boduch**)	Conference 5 (**Mason**)	Conference #8 (**da Silveira**)		
19:00-21:00	***Dinner***	***Conference Dinner (Festa Julina)***	***Dinner***	***Dinner***	***Dinner***	
21:00-22:00						

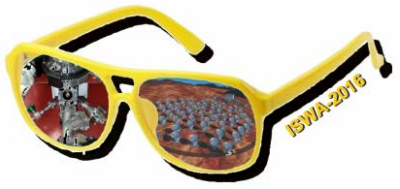
Program

July, 3rd (Sun)

14:00 - 17:40	Registration and Check-in
17:40 - 18:00	**Welcome and brief overview of Brazilian Astrochemistry: S. Pilling (LASA/Univap - BR)**
18:00 - 19:00	**Opening conference #1: A. G.G.M.Tielens (Leiden Univ.) - OBS/MOD** -The Molecular Universe
19:00 - 21:00	**Dinner**

July, 4th (Mon)

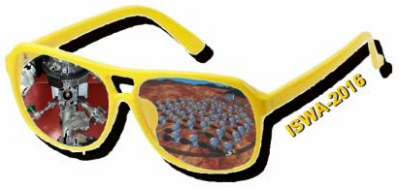
Morning chair: Sergio Pilling	
8:30 - 9:20	**Conference #2: Michel Nuevo (NASA, CA, USA) - EXP** - Sugars and Sugar Derivatives in Residues Produced from the UV Irradiation of Astrophysical Ice Analogs
9:20 - 9:40	**Talk #1: Will Robson M Rocha (Univap, Brazil) - EXP/MOD** - Effects of the X-rays from stellar source and UV from external radiation field on the Astrophysical ices survival in protostellars environments
9:40 - 10:00	**Talk #2: Pedro Ruben R. Ortiz (Instituto de Ciencias Nucleares, UNAM - Mexico)** - Astrochemistry in the Orion BN-KL region



10:00 - 10:20	**Talk #3: Leonardo Baptista (UERJ, Brazil) - THEO/EXP** - Theoretical/Experimental Investigations of the Effects of Irradiation of Astrochemical Ices
10:20 - 11:00	Coffee break w/ posters
11:00 - 11:20	**Talk #4: Diana Andrade (UNIVAP/UFRJ, Brazil) - EXP** - Cosmic Ray effects in Different Allotropic Water ices
11:20 - 11:40	**Talk #5: Patricia Barreto (INPE, Brazil) - THEO** - Theoretical Studies of HS+HX=H2S+X, with X = H, F, Cl, Br and I
11:40 - 12:00	**Talk #6: Chris R. Arumainayagam (Wellesley College, USA) - MOD/OBS** - The Role of Low-Energy Electrons in Astrochemistry: A Tale of Two Molecules
12:00 - 12:20	**Talk #7: Vassilissa Vinogradoff (IMPMC-MNHN, Paris Franca) – EXP** - Formation and evolution of a complex organic molecule, from ices to asteroids
12:20 - 14:00	Lunch
Afternoon chair: Ana de Barros	
14:00 - 14:20	**Talk #8: Yi-Jehng Kuan (National Taiwan Normal University, Taiwan) - OBS** - Interstellar Prebiotically Important Molecules
14:20 - 14:40	**Talk #9: Karin Fornazier (IAG/USP, Brazil) - MOD** - From Earth to the universe: considering alternative chemistries in the search for life elsewhere
14:40 - 15:00	**Talk #10: Gabriel Vignoli Muniz (CIMAP Caen – France) - EXP** - Radioresistance of Adenine to Cosmic Rays
15:00 - 15:20	**Talk #11: Qiang Chang (Xinjiang Astronomical Observatory, Urumqi, China) - MOD** - Complex Organic Molecules Formation in Cold Cores
15:20 - 16:10	**Conference #3: Eduardo Janot Pacheco (IAG/USP, Brazil) - OBS/MOD** - Habitable Zones Induced by Tidal Heating
16:10 - 16:40	Coffee break w/ posters
16:40 - 17:00	**Talk #12: Elisabetta Micelotta (University of Helsinki, Finland) - THEO/MOD** - Energetic processing of complex carbonaceous compounds
17:00 - 17:20	**Talk #13: A. de Barros (CEFET-RJ) - EXP** - IR Spectroscopy and physicochemical effects on astrophysical ices produced by energetic heavy ion collisions
17:20 - 17:40	**Talk #14: Avi Blasberger (Dpt of Physics, Israel) - MOD/OBS** - An Observational Link Between the 2175Å UV extinction feature and IR emission of Polycyclic Aromatic Hydrocarbons
17:40 - 18:00	**Talk #15: João Bosco P. da Silva (Univ Federal Pernambuco, Brazil) MOD/THEO** - Guanine formation mechanism from observed interstellar chemical species
18:00 - 19:00	**Conference #4: Philippe Boduch (GANIL-CIMAP, France) - EXP** - Swift heavy ions, ices and astrophysics
19:00 - 22:00	Conference Dinner (Festa Julina)

July, 5th (Tue)

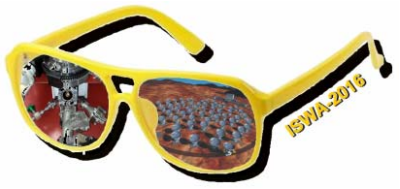
9:00 - 9:20	**Talk #16: Sergio Pilling (UNIVAP, Brazil) - EXP** - Triggering photochemical processes in frozen extraterrestrial worlds by soft X-rays
9:20 - 10:20	**WORKSHOP ON EXPERIMENTAL ASTROCHEMISTRY (chair S. Pilling):** **A: Preparing research proposal for the LNLS (Douglas Galante - LNLS; 30 min)** **B: Introduction to Vacuum Technology (Rafael Seraphim - LNLS; 30 min)**
10:20 - 11:00	Coffee break w/ posters
11:00 - 12:20	**WORKSHOP ON EXPERIMENTAL ASTROCHEMISTRY (chair W. Rocha):** **C: Ionization sources and Detectors (photons, electrons and ions) (Guilherme C. Almeida - Puc-Rio; 25min)** **D: Introduction to Mass spectrometry and IR spectroscopy (Diana P. P. Andrade - OV/UFRJ; 30min)** **E: Examples on data treatment applied to astrochemistry (origin, ominic, gas phase, ice phase). (Sergio Pilling - LASA/UNIVAP; 25min)**
12:20 - 14:00	Lunch
14:00	*Official Event Photo*
14:05	Bus to the LNLS/CNPEM



14:00- 17:40	GUIDED VISIT TO THE BRAZILIAN SYNCHROTRON LIGHT SOURCE (LNLS/CNPEM)
14:20 - 14:40	**Talk #17: Douglas Galante (Brazilian Synchrotron Light Laboratory – LNLS/CNPEM) - EXP** - Present status and future perspectives for astrochemistry at LNLS
17:45	Bust to the hotel.
18:00 - 19:00	**Conference #5: Nigel Mason (Open Univ, United Kingdom) - EXP** - Understanding molecular complexity in the ISM. Laboratory synthesis of prebiotic species
19:00 - 21:00	**Dinner**

July, 6th (Wed)

Morning chair: Sarita P. de Carvalho	
8:30 - 9:20	**Conference #6: J. Lepine (USP) - OBS -** The LLAMA project of a 12 m radiotelescope in Argentina and the USP-NOVA and other collaborations
9:20 - 9:40	**Talk #18: David Arias (Universidad Andrés Bello, Chile) - MOD/THEO** - Reaction Pathway through Classical Molecular Dynamics (MD) of Methanol and Hydroxyl cation on Interstellar Water ice surfaces
9:40 - 10:00	**Talk #19: Rafael Pinotti (UFRJ-Brazil) - MOD** - Simulations of molecular formation along the mass loss of HD 209458b and simlilar Hot Jupiters
10:00 - 10:20	**Talk #20: Carla M. Canelo (IAG/USP-Brazil) - OBS** - The 6.2 μm PAH profile as a tracer of nitrogen in the Universe
10:20 - 11:00	**Coffee break w/ posters**
11:00 - 11:20	**Talk #21: Peter Woitke (St. Andrews Univ., United Kingdom) - MOD** - Astrochemistry in protoplanetary disks – disk shape and dust properties setting the stage
11:20 - 11:40	**Talk #22: Ramiro de la Reza (ON/MCT, RJ,Brazil) - OBS/MOD** - Lithium rich K-type Giant Stars as a New Source of Organic Compounds in the Galaxy
11:40 - 12:00	**Talk #23: Thiago Monfredini (OV/UFR, Brazil) - EXP/THEO** - Photoionization and Photodissociation of Methyl benzene in a Circumstellar Environment
12:00 - 12:20	**Talk #24: Jinhua He (CASSACA, Chile) - MOD** - Modeling the effects of grain motion, charging and size distribution to interstellar chemistry
12:20 - 14:00	**Lunch**
Afternoon chair: Victor Bonfim	
14:00 - 14:20	**Talk #25: Charlotte C M Marshall (University of Nottingham, UK) - OBS** - Probing the nature of small-scale structure towards ρ Oph stars: A new avenue in diffuse interstellar band research
14:20 - 14:40	**Talk #26: Fabio de Almeida Ribeiro (IFRJ/ IQ-UFRJ, Brazil) - EXP** - Non-thermal ion desorption from nitrile-bearing astrophysical ice analogues studied by electron and heavy ion bombardment
14:40 - 15:00	**Talk #27: Diana Gama (IAG/USP, Brazil) - OBS/MOD** - Ionization-driven star formation: the case of IR bubble N10
15:00 - 15:20	**Talk #28: David Quenard (IRAP/UPS-CNRS, France) - MOD** - 3D modelling of HCO+ in the low-mass proto-star IRAS16293-2422
15:20 - 16:10	**Conference #7: Bertrand Lefloch (IPAG, France) - OBS** - The ASAI View on the Evolution of Molecular Complexity along the Formation of Sun-Like stars.
16:10 - 16:40	***Coffee break w/ posters***
16:40 - 17:00	**Talk #29: Dinelsa Machaieie (INPE/MCT, Brazil) - OBS** - Properties of dense condensations embedded in Musca derived from C13O, C18O and NH3 emission lines
17:00 - 17:20	**Talk #30: Guilherme C. Almeida (PUC/Rio, Brazil) - EXP** - Ion irradiation of NO2 Simulated Astrophysical Ice (SAI): Relevance to the Interstellar Medium and trans-Neptunian Objects.
17:20 - 17:40	**Talk #31: Daniel Boice (SC&C-USA; IAG/USP-BR) - MOD/OBS** - Understanding phosphorous chemistry in cometary comae
17:40 - 18:00	**Talk #32: Nathalie Brouillet (Univ. Bordeaux, LAB, France) - OBS** - Molecular complexity in Orion-KL: IRAM and ALMA observations of O-bearing molecules
18:00 - 19:00	**Conference #8: Enio Frota da Silveira (PUC-Rio) - EXP** - Sputtering analysis of astrophysical solids by Plasma Desorption Mass Spectrometry - PDMS
19:00 - 21:00	**Dinner**

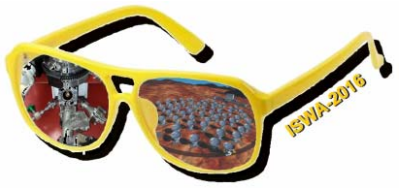


July, 7th (Thu)

9:00 - 9:20	**Talk #33: Edgar Mendoza (IAG/USP, Brazil) - OBS** - Detection of cyanopolyynes in the protostellar shock L1157-B1
9:20 - 10:20	**WORKSHOP ON OBSERVATIONAL ASTROCHEMISTRY (chair E. Mendoza):** **A: Observational facilities in the time of LLAMA (Bertrand Lefloch - IPAG; 30 min)** **B: How to observe molecular lines with LLAMA (Jacques Lepine - IAG/USP; 30 min)**
10:20 - 11:00	**Coffee break w/ posters**
11:00 - 12:20	**WORKSHOP ON OBSERVATIONAL ASTROCHEMISTRY (chair D. Gama):** **C: Line analysis and chemical modelling (Edgar Mendoza - IAG/USP; 30 min)** **D: An overview of radio astronomy analysis software (Victor de Souza Magalhaes - IPAG; 30 min)** **E: Introduction to interferometry and the ALMA telescope (to be defined ; 20 min)**
12:20 - 14:00	**Lunch**
14:00 - 19:00	Free afternoon for scientific discussions and working groups. Social activities (optional).
19:00 - 21:00	**Dinner**

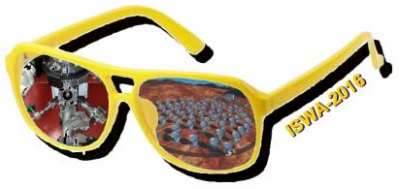
July, 8th (Fri)

Morning chair: Diana P. P. Andrade	
8:30 - 9:20	**Conference #9: Natalia Inostroza (Universidad Autónoma de Chile) - MOD** - Interstellars Molecules: The Value of Quantum Chemistry
9:20 - 9:40	**Talk #34: Vitor de Souza Magalhes (IPAG/UGA - France) - OBS** - Tracing the protosolar nebula heritage: the nitrogen isotopic ratio
9:40 - 10:00	**Talk #35: Isabel Aleman (Leiden Univ. & IAG-USP, Brazil) - MOD** - Molecules in Planetary Nebulae – Results from the Herschel Planetary Nebula Survey (HerPlaNS)
10:00 - 10:20	**Talk #36: Antonio F. C. Arapiraca (CEFET/MG, Brazil) - THEO/MOD** - Theoretical Rotational Spectra of Deuterated Benzene Isotopologues: Improvements on the Benzene' s quantification at Interstellar Medium
10:20 - 11:00	**Coffee break w/ posters**
11:00 - 11:20	**Talk #37: Maria Fernanda Cerini (LNLS/CNPEM, Brazil) - EXP** - Investigation of the molecular biosignatures' alteration under simulated space environments in support of space-based astrobiology experiments
11:20 - 11:40	**Talk #38: Anna Parikka (University of Cologne, Germany) - OBS** - Origin and excitation mechanisms of the warm CO, OH and CH^+ in PDRs
11:40 - 12:00	**Talk #39: Sasan Esmaili (University of Sherbrooke, Canada) - EXP** - Astrochemistry simulated in electron-irradiated CO2/NH3 ices
12:00 - 12:20	**Talk #40: Vícton S. Bonfim (Univap, Brazil) -THEO** - The effect of molecular environment on infrared properties of embedded species in astrophysical ices
12:20	Closing
12:20 - 14:00	**Lunch**
14:00 - 15:00	Check out



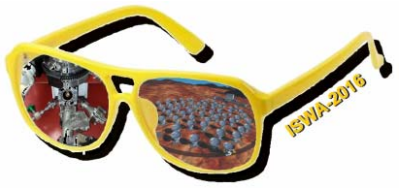
POSTER SECTION

Poster #1:	**Emmanuel E. Etim (Indian Inst.Science Bangalore, India**) - Spectroscopy of Linear Interstellar Carbon Chains and their Isotopologues: Archiving Experimental Uncertainty
Poster #2:	**Fabio A. Cardona (Univ.de Antioquia- Colombia)** - Where are the Galactic radionuclides? Toward a dynamical approach of r-process elements distribution
Poster #3:	**Oscar A. Restrepo Gaitán (IDEAM - Colombia)** - Looking for an Optimal Place in Colombia to Locate an Astronomical Observatory for Milimetric and Subllimetric Wavekengths
Poster #4:	**Anayelly López-Islas (UNAM-Mexico)** - Decomposition of formaldehyde and its relevance in chemical evolution
Poster #5:	**Sarita P. Carvalho (LASA/ UNIVAP, Brasil)** - The X-ray effects in Astrophysics Ices containing Formic Acid: Implications in the Chemistry of Star Forming Regions
Poster #6:	**Fredson de A. Vasconcelos (LASA/ UNIVAP , Brazil)** - CH_4 ice laboratory studies relevant to Titan and icy bodies in the Solar System
Poster #7:	**Heidy M. Quitián-Lara (OV/UFRJ - Brazil)** - The stability of hydrogenated PAHs in circumstellar environments
Poster #8:	**Sergio A. Paron (CONICET-UBA, Argentina) -** Molecules in the Large Magellanic Cloud
Poster #9:	**Luciene da Silva Coelho (IAG/USP - Brazil) -** A Study of Organic Molecules Formation in the Interstellar Medium
Poster #10:	**Dilia Ingrid González Quecán (Universidad de Antioquia, Colombia) -** From Galaxies to Nanoscale
Poster #11:	**Rodrigo C. Pereira (CEFET/RJ - Brazil) -** Water ices mixture in the outer Solar System: Spectroscopy and Physicochemical Effects
Poster #12:	**Henrique O. Euclides (UNIFESP/INPE-MCT)** - APUAMA: A Software Tool for Reaction Rate Calculations
Poster #13:	**Ana Claudia P. Cruz (INPE/MCT - Brazil) -** Potential Energy Surfaces for Interactions of H_2O…HX Systems, with X = H, F Cl or Br, using a Hyperspherical Harmonics Representation.
Poster #14:	**Mariana Geronés (CONICET-UNLP, Argentina**) - Evidence for the Formation of Interstellar Ions in the Dissociative Photoionization Process of Carbonylsulfenyl Compounds in the 100-1000 eV Region.
Poster #15:	**Leonardo C. Ribeiro (UFBA - Brazil)** - Photofragmentation Study of the Acetaldehyde (CH_3CHO) at the Carbon and Oxygen K Edges
Poster #16:	**Cintia A. Costa (PUC-Rio, Brazil)** - L-Valine decomposition by H+, He+ and N+ MeV ions
Poster #17:	**S. Neupane (Universidad de Chile)** - SuperMALT: Study of the Morphology and Kinematics of Dense Clumps
Poster #18:	**Lia C. Corazza (INPE, Brazil)** - The role of Population III stars in the cosmic chemical evolution
Poster #19:	**Patricia Barreto (INPE, Brazil)** - Construction and Surfaces and Potencial Energy of Diatomic Concern Ambiental, Astrophysiscist and atmospheric
Poster #20:	**Nicolas Douroena (Instituto Argentino de Radioastronomía IAR)** - Molecules and dust in the star forming region Sh2-39
Poster #21:	**Lisa Benamati (IRAP/CNRS-UPS, France)** - HIFI Automatic Line Identification Tool
Poster #22:	**Rafael Martinez Rodriguez (Univ. Fed. Amapá, Brazil)** - Sodium and Potassium sputtering analysis from astrophysical silicates analogues
Poster #23:	**Heloisa M. Boechat-Roberty (OV/UFRJ, Brazil)** - Molecular ionization, dissociation and desorption processes induced by photons and electrons in circumstellar environments
Poster #24:	**Fabricio M Freitas (LASA/UNIVAP, Brazil)** - Processing of methanol ices by ionizing agents in simulation of astrophysical environments inside laboratory
Poster #25:	**Thays Pontes Bentes (LASA/UNIVAP, Brazil)** - Study of degradation of Glycine in collisions with fast electrons and their applications in Astrobiology.



Abstracts of Conferences and Oral Talks

(in presentation order)



The Molecular Universe

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Key Words: *Interstellar molecules, Astrobiology, Astrochemistry*

Astrobiology, the study of emergence of life and the its distribution in the Universe, addresses the most fundamental questions in science: "How does life begin ?" and "Are we alone ?" Over the last 20 years, we have discovered that planets are bountiful in the galaxy and that one in every five solar-type stars has a planet in the habitable zone. We have learned that extremophiles have spread to essential every niche – even the seemingly most inhospitable ones – on our planet. And we have learned that life started essentially as soon as conditions permitted, within some 200 million of the late heavy bombardment, or perhaps even earlier. This has resulted in a paradigm shift from "Life on Earth is unique" to the premise "life is widespread". As a result, searching for biosignatures in space has taken on a life by itself. In this talk, I will summarize this shift in our thinking and the global processes that may have influenced the first steps towards life.

The focus in this talk will be on astrochemistry – the starting point of astrobiology – the chemical evolution that takes place in space where simple molecules are transformed into complex molecules and complex molecules are broken down to simple ones. This chemical dance of the elements produces a wide variety of organic compounds. I will review the processes that drive this chemical evolution in space, particularly in regions of star and planet formation. The focus will be on understanding the raw materials that are delivered to newly formed planets and their relationship to the building blocks from which prebiotic material was formed and biological systems evolve.

Sugars and Sugar Derivatives in Residues Produced from the UV Irradiation of Astrophysical Ice Analogs

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Key Words: *sugars; sugar alcohols*; *sugar acids; ice photochemistry*; *meteorites*.

A large variety of organic compounds of prebiotic interest are known to be present in carbonaceous chondrites. Among them, one sugar (dihydroxyacetone) as well as several sugar acids, sugar alcohols, and other sugar derivatives have been reported in the Murchison and Murray meteorites [1]. Their presence, along with amino acids, amphiphiles, and nucleobases [2–6] strongly suggests that molecules essential to life can form abiotically under astrophysical conditions. This hypothesis is supported by laboratory studies on the formation of complex organic molecules from the ultraviolet (UV) irradiation of simulated astrophysical ice mixtures consisting of H_2O, CO, CO_2, CH_3OH, CH_4, NH_3, etc., at low temperature. In the past 15 years, these studies have shown that the organic residues recovered at room temperature contain amino acids [7–9], amphiphiles [4], nucleobases [10–13], as well as other complex organics [14–16].

However, no systematic search for the presence of sugars and sugar derivatives in laboratory residues have been reported to date, despite the fact that those compounds are of primary prebiotic significance. Only small (up to 3 carbon atoms) sugar derivatives including glycerol and glyceric acid have been detected in residues so far [14–16]. In this work, we carried out a systematic search for sugars and sugar-related compounds in organic residues produced from the UV irradiation of simple H_2O:CH_3OH ices, and show that they contain several sugar alcohols up to 5 carbon atoms long, as well as sugars and sugar acids up to 4 carbon atoms long [17]. Results are compared with meteoritic data [1].

Acknowledgments:
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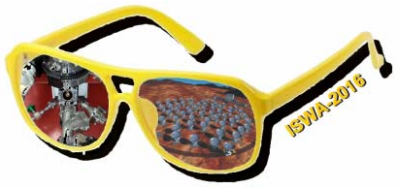

Effects of the X-rays from stellar source and UV from external radiation field on the astrophysical ices survival in protostellars environments

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Key Words: *astrophysical ices; energetic processing*; *protostars*.

Introduction

The astrophysical ices survival is directly related with the temperature and ionizing radiation field in protostellars environments such as disks and envelopes. However, besides the stellar radiation field, the external radiation field should be taking into account when the abundance of the ices is being estimated. In addition such methodology helps to answer the question where are the ices along the sight line from the observer.

Results and Discussion

To address this topic it was employed the radiative transfer code RADMC-3D based on the Monte Carlo method. The code was used to model the spectrum and the near-infrared image of Elias 29. The initial parameters of the disk and envelope were taken from our previous paper [1]. The opacities of the ices were calculated from the complex refractive index obtained at laboratory experiments performed at Grand Accélerateur National d'Íons Lourds (GANIL), by using the NKABS code from [2]. X-ray stellar radiation and UV radiation from external field is an improvement in our methodology. We expect determine in a more realistic approximation where are the ices along the sight of line, by considering different inclination of the protostellar disk. X-ray is important its cross section is small enough to interact in densest regions of the disk and UV external field to warm the outer radius of the envelope. Employing these two conditions the abundance of the ices should be better determined.

Conclusion

The partial conclusions that we have obtained shows that pure CO volatile molecule cannot be placed at disk or envelope of the many protostars, although observation of protostars indicate its presence. In this case, CO should be placed in foreground molecular clouds or trapped in the water ice matrix. The next calculations will be able to show where are placed the ices such as CH_3OH and CH_3CHO once they have been observed in several spectrum of young stars.

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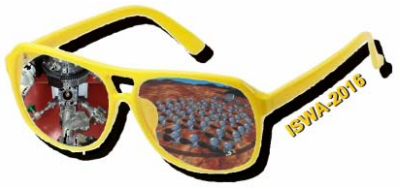

Astrochemistry in the Orion BN-KL region

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Key Words: Orion BN-KL; ISM: jets and outflows; astrochemistry; molecular processes.

Introduction

Massive and young stars inside populated clusters can suffer close dynamical encounters leading to energetic and explosive events. Evidence suggests that Orion BN-KL, at 414 pc, suffered a dynamical decay 500 years ago. This region shows one of the highest diversity of molecular abundances and a filamentary structure known as Orion fingers. In this work we present a Newton-Rhapson method to solve the kinetic chemical reactions of 31 chemical species using the reaction coefficients in the UMIST database [3].

Results and Discussion

We have tested this method using a dark cloud with homogeneous density and 10 K temperature and the relative abundances are compared to the UMIST database results. Following Bally´s [1] work we have implemented the solution to the chemical network on an over-dense spherical clump moving inside an ambient medium using the adaptive mesh code Walicxe 2D [2].

The initial relative abundances are the same as the ones used in the dark cloud model. The inclusion of cooling in the post-shock regions will tend to lower the transverse expansion of the shock-heated plasma to produce a narrower wake and a lower sideways splashing velocity. Cooling of the shock-heated layer produced by the slower, reverse shock moving back into the bullet will also tend to result in extensive fragmentation as portions of the cloud rapidly cool and condense.

Conclusion

Preliminary numerical simulations reproduce the observed morphology and kinematics of the fingers and also the spreading of the post-shock material orthogonal to the propagation of the bullets, the fragmentation of the leading edge of the high-velocity debris, the fingers internal structure and a density distribution for the chemical species involved.

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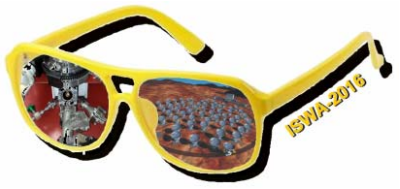

Theoretical/Experimental Investigations of the Effects of Irradiation of Astrochemical Ices

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Key Words: *solar wind; astrophysical ices*; *clusters; quantum-chemical methods*; *reaction mechanism*.

Introduction

Ice bodies are frequently bombarded by heavy ions and radiation in the interstellar medium and these phenomena originate new species and molecular transformations[1]. Experiments associated to theoretical studies can access and analyze what occurs in the solid after irradiation and identify the species ejected to the gas phase[2]. The present work shows how quantum chemical methods are useful to help the interpretation of experiments of heavy ion impact over solids.

Results and Discussion

The species formed after impact may sorted into two classes: 1) Fragments and clusters sputtered to the gas phase; 2) Molecules synthesized in the bulk of solid. Molecular clusters ejected in the gas phase may be analyzed through a thermodynamical point of view; DFT studies are capable to reproduce the expected experimental behavior obtained after irradiation of solid hydrocarbons. Indeed, it is proposed that the most stable C_nH^- clusters are linear and present a terminal hydrogen. Born-Oppenheimer Molecular Dynamics already proved to be very useful as time independent method in the analysis of cluster stability and structure. The studies of acid formic clusters formed in plasma desorption experiments showed that $(HCOOH)_nH^+$ and $(HCOOH)_nOH^-$ are stable due to hydrogen atom migration between formic acid unities[2b].

The formation of molecules in the bulk of solids is more complex to access due to chemical environment effects. In a first approach, a gas mechanism is proposed and used to give insights about the reaction in solid phase. This approach is used to study the molecules formed after the heavy ion impact in solid methane. The reactions producing $CH4^+$ and $CH4^-$ have been studied and it is proposed that $CH3$ radical is pivotal to carbon chain growth after irradiation.

Conclusion

The laboratory techniques used to reproduce processes that occurs in the interstellar medium produce a large amount of data, which are commonly complex to evaluate. Quantum-chemical methods are an important tool to asses molecular information and to give insights about experimental results.

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Cosmic ray effects in Different Allotropic Water ices

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Key Words: *astrochemistry, water ice, cluster series, comsmic rays.*

Introduction

In several environments, such as protoplanetary disks, molecular clouds and icy bodies in our planetary system, the ices are an important reservoir of more complex molecular species, which contain information about the composition and can provide details of formation of our solar system.Water ice is the dominant constituent of interstellar ices in most lines of sight and is about 70 % of the composition in comets, being a key molecule in astrochemical models. It is believed that one of the reactive species possibly evaporated from the water ices is the hydronium ion, H_3O^+, which plays an important role in the oxygen chemistry network. This ion has been detected in the lunar surface of Enceladus and Titan, and toward the Sagittarius B2 molecular Clouds (Goicoechea & Cernicharo, 2001), where H_2O and OH were also identified.

Results and Discussion

In this work, we simutated the cosmic ray effects in water ice using ^{252}Cf Fission Fragments with medium energy around 65 MeV. The measurements have been performed inside a high vacuum chamber at Van de Graaff ion accelerator located at PUC-Rio, Rio de Janeiro, Brazil. In this way, it was possible to study the ion desorption due to radiolysis in ices constituted by water at four different temperatures (30, 40, 70, 125 K), to investigate the different allotropic water ices. A discussion on the rate of H_3O^+ and water delivered to gas phase, as well as the half-life of water ice grains, inside dense molecular clouds considering a constants cosmic ray flux is given. From the Time Of Flight (TOF) spectrum of the positive desorbed ions from H_2O condensed at T = 30 and 40 K (high density) it is possible see that the main observed desorbed ions are H^+, OH^+, H_2O^+, H_3O^+ and clusters formed by $(H_2O)_nR^+$, where R^+ is H^+ or H_3O^+. For H_2O condensed at T = 125 K, temperature close of the sublimation (~145 K), other species arise trapped in the ice. Condensed at 30 K, the ice is formed by a high density amorphous structure, with a density ~1,1 g/cm^3. At 70 K, the ice is yet amorphous, but its density is lower, ~ 0,94 g/cm^3. These two different temperatures have the same (amorphous) phase and their yields are close. Therefore, the yield distribution of the high density ice (30 K) is different than those of low density ice (125 K).

Conclusion

Since the cluster distribution changes according with the ice structure, we propose that the yield distribution shape could be used as a fingerprint of the ice density. To n > 14, the yields are approximately the same for all ice structures showing that for large clusters - which are formed in a region away from the impact - the yield is not very sensitive to the sample temperature.

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Theoretical Studies of HS+HX=H_2S+X, with X = H, F, Cl, Br and I

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Key Words: *Reaction Rate, HS, H_2S, Transition State Theory.*

Introduction

Chemical models are an important tool in helping us understand various physical and chemical processes in space, the full understanding of the physics and chemistry in molecular sources requires a detailed understanding of chemical kinetics and, in particular, reaction rate coefficients over a wide range of temperatures involving the chemical species in space. In the following year of the discovery of interstellar CH, others additional neutral diatomic hydrides have been discovered in the interstellar gas, such as: OH, H_2, HCl, NH, HF, and SiH, in addition to these neutral molecules, hydride molecular ions have, also, been discovered: CH+, OH+, SH+, and HCl+. These diatomic hydrides represent the simplest of interstellar molecules, and may provide key information about the interstellar environment.

Results and Discussion

In this work, we will discuss the theoretical studies of HS+HX=H_2X+X and HS^++HS=H_2S^++X, with X = H, F, Cl, Br and I reaction. The theoretical reaction rate will be compared with the experimental data, for the neutral cases, and also, the difference among the neutral with the charged cases. The geometries are optimized at MP2/aug-cc-pVTZ using the GAUSSIAN09 program and the energies are obtained at CCSD(T)/aug-cc-pVQZ.

Table 1 present the optimized geometries of the transition state of HSHX systems,with X=H, F,Cl, Br, and I neutral or charged ones. It is possible to observe the increase of the HS distance in all cases and the decreases of the HX distances when compared the neutral and charged cases. For the HSH, SHX and dihedral angle there is not a patterned when compared the neutral and charged cases.

Neutral	H	F	Cl	Br	I
r_HS	1.3383	1.3376	1.3393	1.3400	1.3458
r_HS	1.4516	1.4022	1.4502	1.5542	1.7418
r_HX	1.0535	1.4392	1.6566	1.6235	1.7672
a_HSH	90.2730	92.6545	91.0108	90.2222	92.9803
a_SHX	172.9911	91.7260	121.2832	136.6422	172.4968
D	0.0000	80.4356	80.9575	78.1404	0.0241
Charged	H	F	Cl	Br	I
r_HS	1.3533	1.3530	1.3506	1.3495	1.3505
r_HS	1.4805	1.5694	1.6888	1.7719	1.8773
r_HX	0.8032	1.1923	1.4497	1.5465	1.7866
a_HSH	86.5789	93.9464	92.4080	91.7248	94.0477
a_SHX	175.2395	78.5141	85.5134	86.4232	87.4607
D	180.0000	89.2254	91.7040	92.3386	-92.2673

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The Role of Low-Energy Electrons in Astrochemistry: A Tale of Two Molecules

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Key Words: *cosmic ice; low-energy electrons*; methanol*; ammonia*; *radiolysis*.

Introduction

In the interstellar medium, UV photolysis of ice mantles encasing dust grains is thought to be the mechanism that drives the synthesis of "complex" molecules. The source of this reaction- initiating UV light is assumed to be local because externally sourced UV radiation cannot penetrate the ice-containing dark, dense molecular clouds. Specifically, high-energy cosmic rays penetrate and ionize the molecular clouds, generating secondary electrons. Hydrogen molecules, present within these dense molecular clouds, are excited in collisions with these secondary electrons. The UV light emitted by these electronically excited hydrogen molecules is generally thought to photoprocess interstellar ice mantles to generate "complex" molecules. In addition to producing UV light, the large numbers of low-energy (< 20 eV) secondary electrons, produced by cosmic rays, can also directly initiate radiolysis reactions in the condensed phase.

Results and Discussion

The goal of our studies is to understand the low-energy electron-induced processes that occur when high-energy cosmic rays interact with interstellar ices. Using post-irradiation temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS), we have investigated the radiolysis initiated by electrons in condensed methanol and ammonia at ~ 90 K under ultrahigh vacuum (1×10^{-9} Torr) conditions. We have identified fifteen low-energy ($\leqslant$ 20 eV) electron-induced methanol radiolysis products, many of which have been previously identified as being formed by methanol UV photolysis in the interstellar medium. We have also found evidence for the electron-induced formation from ammonia of hydrazine (N_2H_4), diazene (N_2H_2), cyclotriazane/triazene (N_3H_3) and triazane (N_3H_5). We have investigated the reaction yield dependence on film thickness, irradiation time, incident current, electron energy, and metal substrate.

Conclusion

These results provide a basis from which we can begin to understand the mechanisms by which methanol and ammonia can form more complex species in cosmic ices. Studies such as ours may ultimately help us better understand the initial stages of the genesis of life.

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Formation and evolution of a complex organic molecule, from ices to asteroids

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Key Words: *interstellar ices, organic molecules, thermal process, hydrothermal alteration, carbonaceous chondrites.*

Introduction

The complex organic molecules (including amino acids, nucleobases and insoluble macromolecules) detected in primitive carbonaceous chondrites (CC) are different from the simple molecules detected in the interstellar medium (ISM). Whether or not the ISM and meteoritic organics are genetically related is still a matter of debate [1]. In this project, we experimentally investigate the fate of simple organic molecules that may evolved during the warming of interstellar ices, may be accreted on asteroids and may experience hydrothermal alteration. In this purpose, we performed ice analog experiments to determine the formation of hexamethylenetetramine (HMT) in ices, and used this molecule as an interstellar precursor for hydrothermal experiments.

Results and Discussion We showed the formation of HMT from ice composed of water, formaldehyde, ammonia and formic acid, submitted only to thermal process between 20 K and 300 K. Products were characterized by infrared spectroscopy (IR) and mass spectrometry (MS). HMT is a simple molecule (22 atoms), which forms at elevated temperature (290 K) after a succession of intermediates and remains stable in the solid phase until 400 K [2,3]. Even though HMT represents about 50 wt% of the organic residues from interstellar ice analogs [4], it has never been detected in the ISM so far, neither in CC.

Then, to simulate the reactions that might have occurred on primitive asteroids, we submitted HMT to hydrothermal alteration (150 °C, alkaline pH, various duration). Under such conditions, HMT totally decomposes in less than 20 days (which may explain why HMT has never been detected in meteorites) into (1) a suite of soluble compounds made of aromatic nitrogen compounds and amides (m/z 73 to 250), likely precursors of nucleobases, and (2) a complex insoluble organic matter (1wt%). Products were identified by gas-chromatography (GC) coupled to MS, IR, and synchrotron-based X-ray absorption near edge structure (XANES) spectroscopy.

Conclusion

Our study reveals that chemical transformations encountered by simple organic molecules in the ISM (heating) and in asteroids (hydrothermal alteration) may lead to the formation of prebiotic molecules very similar to those observed in CC. A genetic relationship seems to exist between simple molecules observed in ISM and the complex molecules in CC, throught unobservable molecules such as HMT, yet crucial in the organic evolution.

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Interstellar Prebiotically Important Molecules

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Key Words: *prebiotically important molecules; COMs; glycine; pyrimidine.*

Many interstellar, complex organic molecules (COMs) are known to have essential functions in terrestrial biochemistry. Observations of COMs thus enable us to better understand the origin of primitive organic materials found in our Solar System. Pyrimidine and glycine, respectively, the building block of nucleic acid and the simplest amino acid, are key molecules for astrobiology and were both detected in meteorites and comets. Although the formation of prebiotic molecules in extraterrestrial environments and their contribution to prebiotic chemistry hence the origin of life remains unsettled, the connection between interstellar organic chemistry, meteoritic pyrimidines and amino acids, and the emergence of life on the early Earth would be strengthened with the discovery of interstellar pyrimidine and glycine. We therefore used ALMA to observe these two interstellar molecular species.

We will present some of our encouraging results; in particular, we will address the seeming issue of the alleged “missing” key line for glycine confirmation.

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From Earth to the universe: considering alternative chemistries in the search for life elsewhere

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Key Words: Astrobiology*; Astrochemistry*; Prebiotic molecules*; Astrobiology*.

Introduction

One fundamental concern in the search for life in the Universe is to avoid narrow concepts about how life should be like in extraterrestrial environments otherwise a number of biosignatures could be missed. In particular, it is essential to examine if Earth-centered assumptions would lead to the non-detection of life, even when it is present (1; 2).

An universal definition for life is extremely difficult and rather unattainable on the basis of the present knowledge. Regardless of this constraint, a living system can be characterized through some required essential elements, if occurring simultaneously: the capability of reacting to external stimulation; the possibility of permanence in an out-of-equilibrium thermodynamical state; the control of a self-contained mechanism to store and decode information; and the capability of self-replication and evolution (3; 4; 5)

In the field of searching for life outside Earth, any concept should be subject to careful thought to help define strategies among a large number of possibilities. We raise here some arguments on why keep some Earth-centeredness when searching for life in the cosmic neighborhood. Additionally, we propose an emphasis on tracking informational molecules.

Results and Discussion

In the present work, we adopt this approach when considering many aspects of the problem. We first discuss the abundances of the main chemical constituents of terrestrial living matter and show that they can be considered as being ubiquitous in the Universe. The logical consequence is that they may have been incorporated in any putative alien life. A broader physico-chemical discussion on the roles of solvents other than water and gases other than oxygen in terms of affording feasible metabolic pathways is also framed. A survey on the prebiotic compounds ever detected in extraterrestrial sources and targets is analyzed, in the sense that all life building blocks should form and, in the near future, will be detected by the high-resolution observational instruments and satellites. The quest for DNA as the informational molecule is sketched as a terrestrial matter, and the role of other complex aromatic compounds as "alien informational molecules" is also envisaged.

Conclusion

We outline the main precautions to be taken in the search for life outside Earth in order to avoid reduced concepts about alien life. They could result in the non-detection of life, even when it is present.

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Radioresistance of adenine to cosmic rays

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Key Words: *Adenine; nucleobases; infrared spectroscopy; astrochemistry; cosmic rays; heavy ions.*

Introduction

Adenine, $C_5H_5N_5$, is a purine nucleobase and part of important biomolecules such as DNA and RNA. Several theories claim that organic complex molecules possibly have reached the early Earth via comets and meteorites[1]. Indeed, the recent space missions identified nucleobase's precursors, but not yet nucleobases[2]. However, analysis of carbonaceous meteorites on Earth shows presence of nucleobases, including adenine[3]. A strong indication of its existence in outer space. Nonetheless, space is permeated by ionizing radiation which can have damage these molecules. The aim of the present study is to evaluate the resistance of adenine exposed to cosmic rays analogues (swift heavy ions). The destruction or resistance of adenine in the condensed phase have been studied with different projectiles such as UV photons [4], X-rays[5] and electrons [6]. However, there is no such data about the effects of heavy ions at high energy. In this work, we will focus on the effects caused upon adenine from exposure to galactic cosmic ray analogues. By using different swift heavy ions, we determined the destruction cross section of adenine as a function of the electronic stopping power.

Results and Discussion

We studied the radioresistance of adenine in solid phase at low temperature under bombardment by heavy ions. The experiments were performed in high vacuum ($\approx 10^{-8}$ mbar) at GANIL (Caen, FR) and GSI (Darmstadt, DE). Adenine films were irradiated by 820 MeV Kr^{33+}, 190 MeV Ca^{10+}, 92 MeV Xe^{23+} and 12 MeV C^{4+} ion beams. The evolution of adenine molecules under heavy ion irradiation was studied by infrared absorption spectroscopy as a function of projectile fluence. New infrared absorption bands arise under the irradiation and can be attributed to HCN, CN^-, $C_2H_4N_4$,, nitrile groups (R-C≡N) and isocyanide groups (R-N≡C) . Half lifetime of adenine exposed to cosmic rays in the interstellar medium was estimated to be (10±8) Myears.

Conclusion

The destruction cross section was determined as a function of electronic stopping power: A S_e^n, where n = (1.17±0.06). The present results exhibit an adenine destruction cross section about 10^9, 10^5 and 10^3 times higher than for UV photons, X-rays and 5 keV electrons, respectively. Our results show that destruction of adenine exposed to cosmic rays is dominated by iron nuclei and protons. These results may help understating the survival of nucleobases in outer space.

Acknowledgments:

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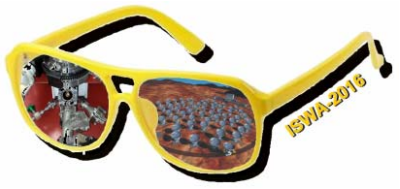

Complex Organic Molecules Formation in Cold Cores

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Key Words: ISM: clouds; ISM: molecules, molecular processes

Introduction

Methyl formate and dimethyl ether were recetly discovered in the gas phase of cold cores such as L1689b with temperatures as cold as 10 K[1]. The new discovery challenges our previous astrochemical models concerning the formation of complex organic molecules. Moreover, there is strong correlation between the abundances and distributions of methyl formate and dimethyl ether , which shows that current astrochemical models may be missing important chemical processes in cold astronomical sources.We investigate a scenario in which complex organic molecules and the methoxy radical can be formed on dust grains via a so-called ``chain reaction'' mechanism, in a similar manner to CO_2. A unified gas-grain microscopic-macroscopic Monte Carlo approach with both normal and interstitial sites for icy grain mantles is used to perform the chemical simulations[2]. We also introduce reactive desorption with varying degrees of efficiency to enhance the non-thermal desorption of species formed on cold dust grains.

Results and Discussion

The observed abundances of a variety of organic molecules in cold cores can be reproduced in our models. Especially, the abundance of methyl formate in L1689b, which was severely underproduced in other astrochemical models can also be reprocued in our models. The correlation between the abundances of methyl formate and dimethyl ether in cold cores can also be explained in that the formation of both molecules requires a common primary precursor, atomic carbon in gas phase.

Conclusion

Non-diffusive chemical reactions on dust grain surfaces may play a key role in the formation of some complex organic molecules. Reactive desorption is important to desorb large molecules from grain surface.

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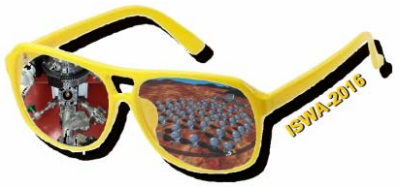

Habitable Zones Induced by Tidal Heating

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Key Words: *astrobiologia, Zona Habitável, extremófilos*

Introduction

Natural satellites of planets in eccentric orbits are heated internally by gravitational tide, resulting from the variation of the planet-moon distance. This heating essentially depends on the internal structure of the moons, of their orbital characteristics and on the masses of the bodies involved. In the Solar System, extreme examples occur in the large satellites of Jupiter and Saturn. Extremophiles are terrestrial microorganisms that resist to extreme physical or geochemical conditions such as temperature, pressure, pH, radiation, salinity, humidity, etc... They are found with relative ease on our planet in regions such as deserts, Antarctica, the bottom of the sea, inside rocks, craters of volcanoes and geysers, and have been the subject of special scientific attention in recent years.

Results and Discussion

Physical and chemical conditions of the giant moons of Jupiter and Saturn have been studied by space probes Galileo and Cassini/Huyghens. The fact that these living beings withstand extreme conditions, makes them natural candidates to exist in the roughest extraterrestrial habitats.
In this work, a survey was done of the physical and chemical conditions of these extraterrestrial habitats, and cross-checked them with the survival characteristics of terrestrial extremophiles in order to verify the possibility for some of them to live in these environments.

Conclusion

We show that some terrestrial extremophiles can dwell in subsurface oceans of Titan, Europa and Encelladus.

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Energetic processing of complex carbonaceous compounds

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Key Words: *molecules; nanoparticles*; *interstellar medium; shocks*.

Introduction

In the context considered here, energetic processing in space indicates the interaction of astrophysically relevant species with energetic photons, typically UV and X-rays, and ions and electrons, these latter arising from interstellar shocks, hot gas and cosmic rays. Energetic processing has a profound impact on complex carbonaceous structures like Polycyclic Aromatic Hydrocarbons (PAHs), fullerene molecules and hydrocarbon nanoparticles. These species represent a major component of interstellar dust and their emission features dominate the mid-infrared spectrum of almost any astronomical object.

Results and Discussion

I will present recent theoretical and experimental results from studies of the energetic processing of complex carbonaceous compounds occurring under astrophysical conditions. My presentation will focus on the bombardment of PAHs and fullerenes C_{60} and C_{70} by energetic ions and electrons (the so-called collisional processing), and on the role of UV photons in modifying the structure of PAHs and hydrocarbon nanoparticles, leading to the formation of different molecular species [e. g., 1, 2]. I will highlight the physics underpinning the theoretical models and the laboratory experiment, and discuss the implications on the observable characteristics of the population of interstellar carbonaceous compounds in different environments and under different conditions. I will show in particular how the non-trivial determination of the stability of PAHs, fullerenes and nanoparticles under the harsh conditions of the interstellar medium is necessary for the proper interpretation of infrared observations.

Conclusion

Energetic processing occurs throughout the universe, but its importance has not been recognized until very recently, especially in terms of the interaction with ions and electrons. It is a complex phenomenon which has to be investigated jointly by theorists, experimentalists and observers. Theoretical developments and new experimental and observational facilities are already making this possible.

Acknowledgments:
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IR Spectroscopy and physicochemical effects on astrophysical ices produced by energetic ions collisions

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Key Words: *Astrochemistry – circumstellar matter – clouds – molecules*

Introduction

Understanding the nitrogen and oxygen chemistry in space is an important step to link the formation of interstellar grain mantles, comets, and frozen surfaces of outer solar system bodies to the origin of life. Nitrogen-containing molecules are essential for life on Earth, and nitrogen oxides are considered to be important astrochemical precursors of complex species and prebiotics, one such molecule is N_2O, nitrous oxide [1].

Results and Discussion

The current laboratory experiments performed at PUC-Rio, simulates the energy transfer processes that occur when protons and helium bombarded por example the nitrous oxide ice at 10 K. Those results will help to understand the effect of those ions in the radiolysis of ices in ISM. Infrared spectroscopy (FTIR) was performed before and during irradiation of icy targets with 1.5 MeV H+ and He+ beams, permitting absorbance analysis of the main bands.

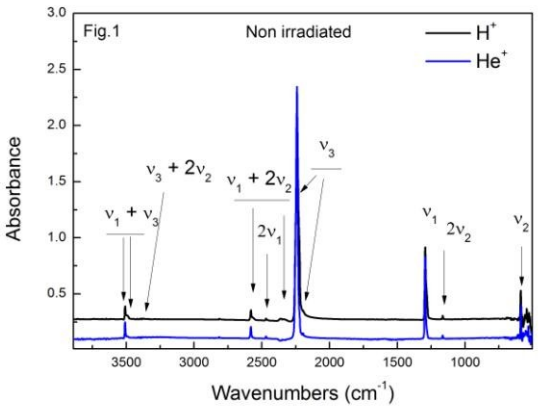

Fig. 1 shows the most important rotational and vibrational transitions correspond to the more intense absorption bands of N_2O for different ions. In the experiment was observed, that the destruction of the solid ice N_2O leads to the formation of a series of nitrogen oxides such as NO, NO_2, N_2O_2, N_2O_3, N_2O_4, N_2O_5; azide - N_3 and ozone - O_3. The formation and destructions cross sections of each observed molecular species were obtained and the atomic nitrogen and oxygen budgets are determined and used to verify the process stoichiometry

Conclusion

As an astrophysical application, the dissociation cross-sections due to these projectiles and other ion beam projectiles at different energies are determined, assuming validity of the $\sigma_d \propto S_e^{3/2}$ power law. As a consequence, the predicted values of the integrated dissociation rates confirm the importance of lighter ions as a constituents of cosmic rays in astrochemistry.

Acknowledgments: The agencies CAPES, CNPq (INEspaço) and FAPERJ (E-110.087/2014).

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An Observational Link Between the 2175Å UV extinction feature and IR emission of Polycyclic Aromatic Hydrocarbons

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Key Words: *UV extinction feature, Polycyclic Aromatic Hydrocarbons*

Introduction

The 2175Å UV extinction feature was discovered in 1965 (Stecher 1965) with sounding rocket observations. Since then several satellite observatories helped to characterize this feature (Savage et al 1985, Fitzpatrick & Massa 1986, 1988, 1990, 2005, 2007, Cardelli, Clayton & Mathis 1989), yet it remains poorly understood, and its physical origin is still being debated. One suggested origin is absorption by Polycyclic Aromatic Hydrocarbons (PAH) molecules, which is supported by theoretical molecular structure computations (Leger et al 1989, Li & Draine 2001 and Zubko et al. 2004), and lately by laboratory experiments (Steglich et al. 2010, 2011). PAHs are detected by their 3.3, 6.2, 7.7 8.6, 11.3 & 12.7 μm emission bands, and are specified by their modes of vibration (Allamandola et al. 1989). Mid IR observations with the ISO and Spitzer space telescopes helped the analysis of the PAH emission band profiles, and their relative intensities (Van Diedenhoven et al. 2004, Hony et al 2001, Galliano et al. 2008, Mori et al. 2012). Observations showed also a correlation between the illuminating star temperature and the central wavelength of the 6.2, 7.7, and 8.6 μm bands (Sloan et al. 2007, Acke et al 2010), which has been attributed to the size and charge of the PAH molecules (Pino et al 2008, Ricca et al 2012). A conclusive empirical link between the 2175Å UV extinction feature and the PAH IR emission bands, however, is still missing.

Results and Discussion

We assembled a new sample of sightlines, which have both PAH IR emission as well as 2175Å absorption. The IR spectra were taken from ISO and Spitzer, while the UV spectra are from IUE observations. We used the customary drude function superimposed on stellar atmosphere models (Castelli & Kurucz 2004) to fit the UV spectra, and to measure the feature properties. We used Gaussian functions to characterize the IR emission bands. Consequently, we find new interesting results that show a possible observational connection between the IR emission and UV absorption. Our results show that the central wavelength of the PAH emission in the range of 7.6μm and 7.95μm depends linearly on the stellar temperature up to ~14000K, while at higher temperatures it remains constant at 7.65 ± 0.05 μm. This is a significant extension of the relation found by Sloan et al. (2007) and by Acke et al (2011). We also find a dependence of the central wavelength of the 2175 Å feature (ranging between 2150 Å to 2350 Å) on the stellar temperature with a similar behavior to the PAH emission central band that has never before been reported. We argue that these similar dependences of both the UV and IR features on stellar temperatures hint to a common origin of the two in PAH molecules. We also found a direct correlation between The UV feature central wavelength and the PAH central wavelength around 7.7μm.

Conclusion

The new stellar sample selection, the analyses method and the resulting correlations may contribute to link the theory, and the laboratory measurements of the 2175Å UV extinction feature with the observed PAH IR emission bands.

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Guanine formation mechanism from observed interstellar chemical species

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Key Words: *Guanine; formation model; interstellar medium*; *quantum chemistry calculations*; *energy barrier*.

Introduction

Guanine, adenine and the related structures 2,6-diaminepurine and 6,8-diaminepurine were inequivocaly identified in carbonaceous chondrites[1]. Although adenine is, in general, considered a HCN pentamerization product[2], recently our group proposed a new mechanism of adenine formation using only the previously observed interstellar molecules C_3NH, HNCNH and its isomer H_2NCN[3].

As part of our continuated research to understand how fundamental molecules for life in Earth can be formed in the space, in the present work a mechanism for guanine formation is investigated considering the previously observed interstellar species HNCNH, CCO and CNH. For that purpose, *ab initio* calculations were performed at MP2/6-311++G(2d,2p) level for characterization of reactants, products and transition state. All calculations were performed at 1 bar and 10 K, using the default interal convergence criteria of Gaussian 09 program.

Results and Discussion

The Gibbs free energy calculations predict that CCO and CNH form HNCCCO throught a essentialy barrierless reaction. Next, HNCCCO is predict to react HNCNH to form first a six-member heterocycle ring with an energy barrier *ca*. 9 kcal mol^{-1}. Following, a second HNCNH molecule form the five-member ring with an energy barrier *ca*. 7 kcal mol^{-1}. To achieve the final structure of guanine proton transfer processes are necessary. The ability of HNCNH to make hydrogen-bond interactions and therefore to promote proton transfer shows the potential of this molecule to form purine bases in space.

Conclusion

An simple mechanism for guanine formation starting from three observed interstellar molecules HNCNH, CCO and CNH is proposed. The rate determinant step is predicted to involve a moderate energy barrier of *ca.* 9 kcal mol^{-1}. The whose mechanism is predicted to be exergonic which suggests that the formation of guanine starting from these three molecules is a spontaneous process.

Acknowledgments:

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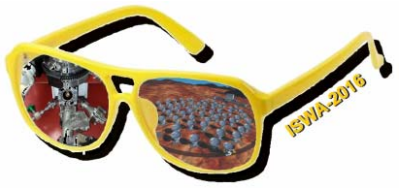

Swift heavy ions, ices and astrophysics

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The main objective of this research program is to simulate the effects of heavy ion irradiation on astrophysical ices. Heavy ions (C, O, S, Fe, Ni) are present in the solar wind, in cosmic rays and in the magnetosphere of giant planets. Ices, found e.g. on comets and dust grains (dense clouds) in space are mainly formed by simple molecules (like H_2O, CO, CO_2, NH_3 ...). In the laboratory, the icy samples are deposited at low temperature (typically 15K-150K) and are irradiated with swift heavy ions delivered by GANIL (Grand Accélérateur National d'Ions Lourds, Caen, France). In situ infrared absorption spectroscopy allows to observe the disappearance of molecules (fragmentation or sputtering), and the appearance of new molecular species as a function of the projectile fluence. Two examples will be presented:

- High energy ion irradiation of H_2O ices. In this domain (simulation of cosmic rays), the projectile deposits a large amount of energy on the electrons of the icy target. This leads to the structure modification (compaction or amorphization), the destruction of the mother molecule, to sputtering and to the production of newly formed (daughter) molecules.
- At low energy (solar wind and magnetospheres), the incoming ion is implanted in the icy mantle. The aim of this study is to know if the contribution of the implantation process can explained the abundance of e.g. sulphuric acid, or SO_2 and CO_2 molecules on the Jovian moons.

Triggering photochemical processes in frozen extraterrestrial worlds by soft X-rays

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Key Words: *Astrophysical Ices; X-ray; FTIR; Molecular processes*

Introduction

In this work, we investigate the effects produced mainly by broad band soft X-rays (and X-ray-induced secondary electrons) in ice mixtures that simulates the surface of three moons of giant planets: Europa, Titan and Enceladus. Such environments are constantly exposed to space ionizing agents (UV and soft X-rays photons, electrons and ions) allowing photodissociation processes, surface photochemistry and prebiotic chemistry. The experiments have been performed using a high vacuum portable chamber from the Laboratório de Astroquímica e Astrobiologia (LASA/UNIVAP) coupled to the SGM beamline in the Brazilian Synchrotron Light Source (LNLS) at Campinas, Brazil. The beamline was operated in off-focus and white beam mode, which produces a wide band spectral range of photons, mainly from 6 eV up to 2000 eV, with the total average flux at the sample of about 10^{14} photons cm^{-2} s^{-1}.

Results and Discussion

Briefly, the samples were produced by the adsorption of a gaseous mixture at 12 K and following by slowly heating to the temperatures in which the irradiation occur, simulating this way the frozen surface of an specific moon of a given giant planet: a) H_2O:CO_2:NH_3:SO_2 (10:1:1:1) at 90 K for Europa, moon of Jupiter; b) N_2:CH_4 (19:1) at 12 K for Titan, moon of Saturn, and c) (H_2O:CO_2:CH_4:NH_3) (10:1:1:1) at 80 K for Enceladus, another moon of Saturn. For experiment b, we simulate the effect of incoming radiation in the aerosols in the upper atmosphere of Titan. *In-situ* sample analyses were performed by Fourier transform infrared (FTIR) spectrometer. Complete experimental description is given elsewhere [1]. The spectral analysis of the processed samples shows several new bands associated with the formation of organic molecules, including nitriles, hydrocarbons, acids and other organic compounds. The dissociation cross sections of parental species were in the order of 10^{-18}-10^{-19} cm^2. Half-lives of the parental species extrapolated to the astrophysical scenario was determined.

Conclusion

In case of Europa´s experiment, we observe the presence of H_2O_2, H_3O^+, SO_3, CO, and OCN^- among the new species produced. For the experiment simulation aerosols in Titan, we identify the formation of HCN, HNC, CCCN, NH_3 and C_2H_2. Such molecules possibly will be deposited into the ground and increase the chemical complexity of the surface with time. The irradiation of Enceladus like surface shows as daughter species, OCN^-, H_2CO and CO among others. Such environments are constantly exposed to space ionizing agents (UV and soft X-rays photons, electrons and ions) allowing photodissociation processes, surface photochemistry and prebiotic chemistry. The processing of such spatial ices have promoted an enhancement in the chemical complexity, similar what may have happened in the early earth triggering the arising of life.

Acknowledgments:

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Understanding molecular complexity in the ISM: Laboratory synthesis of prebiotic species.

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Key Words: electron chemistry; synchrotron radiation; prebiotic synthesis; chirality; origins of life.

Introduction. Throughout the last four decades the complexity of the chemistry prevalent in astronomical environments has become clear. Rich and unexpected chemistry has been observed in many solar system bodies whilst the exotic chemistry of exoplanet atmospheres is now being revealed. The commissioning of ALMA and its advances in both spatial and spectroscopic resolution is providing new insights into the composition of the ISM and how it evolves in the stellar cycle from stellar synthesis from the dust cloud through the creation of solar systems to the star's death and reseeding of chemical material in the ISM. The next challenge will be to not only explain the mechanisms that produce the observed chemical species but to understand how they may lead to the synthesis (and assembly) of more complex species which in turn may provide the building blocks of life, hence merging astochemistry with astrobiology. At present we do not know whether larger (prebiotic molecules) such as the larger amino acids, nucleobases and sugars are present in the ISM but increasingly laboratory studies suggest routes by which they may be formed under ISM conditions. Is there a limit to the complexity of such molecular formation? And if there is, what is it? and what does this tell us about how and where life may develop in the universe?

Results and Discussion. Laboratory simulations provide a method for exploring chemical complexity of astrochemistry. In this presentation I will discuss a range of laboratory experiments that are currently being undertaken to explore the synthesis of prebiotic molecules in the ISM (and often on planetary/lunar surfaces). These experiments primarily explore the synthesis of molecules in ice films which replicate ice mantle on dust grains in the ISM, with the chemistry being induced by irradiation using stellar UV and cosmic ray mimics. It is shown that much of the synthesis can be attributed to the primary incident radiation but the secondary species (mainly electrons) induced by the primary radiation. Complex chemistry is readily produced and a rich ensemble of products results from relatively simple ice mixtures. This suggests that the 'building blocks of life' may be readily formed in the stellar/planet formation process but how they are assembled to create the molecular complexity needed for emergent life remains largely unknown and must be the target of future laboratory work, coupled with observations and development of astrochemical models.

Conclusion. We are on the threshold of unparalleled advances in our understanding of the astrochemistry (astrobiology) that may (will) provide answer to one of the greatest remaining scientific questions - our origins and the ubiquity of life throughout the universe.

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The LLAMA project of a 12 m radiotelescope in Argentina and the USP-NOVA and other collaborations

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LLAMA (Large Latin American Millimetric Array) is a joint Argentinean-Brazilian project of a 12m mm/sub-mm radio telescope similar to the APEX antenna, to be installed at a site at 4830 m altitude near San Antonio de Los Cobres in the Salta Province in Argentine, at 150 km from ALMA.
The scientific cases for single dish and VLBI observations include black holes and accretion disks, the molecular evolution of interstellar clouds, the structure of the Galaxy, the formation of galaxies, and much more.

The antenna was ordered to the company Vertex Antennentechnik in June 2014, and will be installed at the site in 2016. The radio telescope will be equipped with up to six receivers covering bands similar to those of ALMA. At the very beginning of the operation, we will have 2 receivers, at band 5 (162-200 GHz) constructed by NOVA (Groningen, Netherlands) and band 9 (600 720 GHz) constructed by Chalmers University (Sweden).

About 2 years after start of operation, the lowest frequency (ALMA band 1 at 45 GHz) will allow it to be part of a VLBI network that will include the Chinese-Argentine Radio-Telescope (CART) and possibly the Itapetinga radio telescope near São Paulo. At higher frequencies, VLBI observations could be made with ALMA, APEX and ASTE, and Northern radiotelescopes. In this way, LLAMA will be a seed for a Latin-American VLBI network.

Reaction Pathway through Classical Molecular Dynamics (MD) of Methanol and Hydroxyl cation on Interstellar Water ice surfaces

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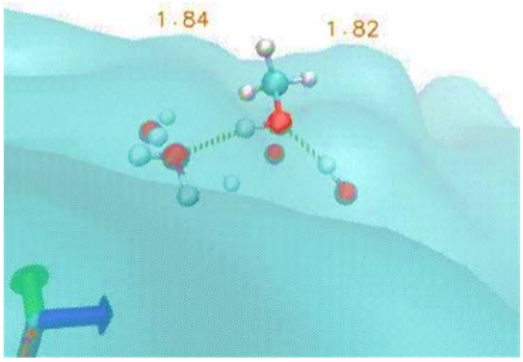
Key Words: *astrochemistry; interstellar molecules*; *dust grain ; Molecular dynamic*

Introduction

Dust grains are constituted by carbon and silicate and are then released into the interstellar medium. After this, due to the low temperatures in the interstellar medium, dust grains are covered by ice mantles. These ice mantles have several components; water ice is the dominant one. We also found carbon-bearing molecules as CO, CO_2, and CH_3OH . These mantles provide a surface where species can react. CO and CO_2 relative abundances are quite stable, in comparison to H_2O. However, the mobilities of C and O atoms over the grain surface are not widely known. [1]. Generally, these molecules suffer accretion over the grain surface. After accretion, the hydrogenation reaction can convert CO into formaldehyde and methanol. Energetic processes (through UV photons or cosmic rays) convert these molecules into complexes species. In addition, these energetic processes (e.g., UV Photolysis) produce radicals, like H^+ and OH^-, which may react with other molecules [2]. In the light of facts, the reaction in the condensed phase between methanol and hydroxyl radical on water ice surface was studied.

Results and Discussion

Classical Molecular Dynamic (MD) was used to find the optimal structure conformation of a dust grain covered by water ice at 10K in an NVT ensemble running 10,000 steps to minimize the energy system. A second MD was carried out using the preceding dust grain, along with a methanol molecule. Eight equally-probable positions (four above and four below the dust grain) were tested, and the lowest energy conformation was found. The lowest energy conformation has a magnitude of -2,113.622 Kcal/mol. The molecule is stabilized by two hydrogen bonds (1.84Å and 1.82Å)



Preliminary Conclusion

The stabilized molecule of methanol exhibits its CH_3 group outward; thus, CH_3 could be used as a target in a reactive or non-reactive collision with other molecules or ions (e.g., an HO^- ion). These kinds of reactions shall be investigated using Quantum Molecular Dynamics.

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Simulations of molecular formation along the mass loss of HD 209458b and simlilar Hot Jupiters

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There are several studies dedicated to modeling the atmospheric mass loss of Hot Jupiters, particularly of HD 209458b (Bourrier and Lecavelier des Etangs 2013, Guo 2013, Guo 2011, Koskinen et al. 2013a,b, Murray-Clay et al. 2009, Penz et al. 2008, Garcia-Muñoz 2007). Nevertheless, the study of chemical reactions along the mass loss has been overlooked, supposedly because it is thought that the intense UV radiation field of the host stars would prevent molecular formation (Koskinen et al. 2013a,b, Garcia-Muñoz 2007). However, these studies are limited to a distance of five times the planet´s radius. In order to probe the region where the temperature is low (T < 2000 K) and the radiation field less intense, we developed a 1D chemical and photochemical reaction model of the atmospheric mass loss of HD 209458b, involving 56 species, including carbon chain and oxygen bearing ones, interacting through 566 reactions.

The simulation results indicate that simple molecules like OH^+, H_2O^+ and H_3O^+ are formed inside the region, considering that residual H_2 survives in the exosphere, a possibility indicated by recent observational work. The molecules are formed and destroyed within a radial distance of less than 10^7 km, but the estimated integrated column density of OH^+, a potential tracer of H_2, is high enough to allow detection, which, once achieved, would indicate a revision of chemical models of the upper atmosphere of Hot Jupiters. For low density Hot Jupiters receiving less intense XUV radiation from their host stars than HD 209458b, molecular species could conceivably be formed with a higher total column density.

The 6.2 µm emission line as a tracer of nitrogen in the Universe

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Key Words: Astrobiology*; galaxies: starbursts*; astrochemistry; infrared: galaxies; line: identification.

Introduction

A considerable fraction of the carbon in the interstellar medium (ISM) – 20% or more – is in the form of polycyclic aromatic hydrocarbon (PAHs), and its mid infrared emission lines are dominated by bands related to this class of molecules [1]. When a PAH incorporates one or more atoms of nitrogen, that substitute the carbon atoms, it becomes a polycyclic aromatic nitrogen heterocycle (PANH). They can provide the missing link between the abundant PAHs chemistry at the ISM and the nucleobases that compose all living beings. Recent studies revealed that these molecules can be formed by ultraviolet radiation of benzene and naphthalene mixed in ices [2]. Analyses of the PAHs features profiles, especially the 6.2 µm feature, could indicate the presence of nitrogen incorporated to the rings.

Results and Discussion

Peeters et al. (2002) [3] has suggested the division of spectra into three class – A, B and C – according to the interpretation of the profile peak positions. Identification of the feature class can show the presence of PANHs. For this work, 207 starbursts and ULIRGs (Ultra-luminous Infrared Galaxies), extracted from the Spitzer/IRS ATLAS project [4], have their 6.2 µm profiles fitted and distributed into the Peeter's classes. A total of 125 galaxies were classified as class A, 44 galaxies as class B and 4 galaxies as class C. The class A, corresponding to a peak position of 6.22 µm, has only been explained by carbon replaced by nitrogen, despite other attempts of explanation [5]. Besides, class B can represent a mix between PAHs and PANHs.

Conclusion

PANHs seem to dominate these spectra, what could indicate another reservoir of nitrogen in the Universe, with density and temperature conditions different from those of gas phase and ices. The fact of just a few sources belong to class C could mean that most of PAHs have incorporated nitrogen to their rings.

Acknowledgments:
Special acknowledgments to the creators of the PAHFIT routine [6], used in this work, and to A. Hernan-Caballero and E. Hatziminaoglou for provide the sources already reduced.

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Astrochemistry in protoplanetary disks – disk shape and dust properties setting the stage

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Key Words: *protoplanetary disks, dust and PAH opacities, radiative transfer, line formation*.

Introduction

The chemistry in protoplanetary disks depends critically on how much of the FUV radiation and X-rays emitted by the central star reaches the disk. Therefore, questions about dust, PAH, and gas opacities, as well as the shape of the disk, are crucial to set up realistic astrochemical models for protoplanetary disks.

Results and Discussion

Based on detailed 2D radiative transfer models (MCFOST, MCMax), we run ProDiMo models for protoplanetary disks which include chemistry and heating/cooling balance. We carefully select 100 gas phase and ice species based on the UMIST 2012 database with individual UV photo cross-sections from the Leiden Lamda database and 145 detailed X-ray reactions. We systematically vary all disk shape, dust and PAH parameters in the model to study their impact on continuum and line observables, like SED, mm-slope, continuum visibilities, and emission lines including [OI] 63 μm, high-J CO lines, (sub-)mm CO isotopologue lines, and CO fundamental ro-vibrational lines. We find that evolved dust properties, i.e. large grains, often necessary to fit the SED, have important consequences for disk chemistry and heating/cooling balance, leading to stronger near to far-IR emission lines in general. Strong dust settling and missing disk flaring have similar effects on continuum observations, but opposite effects on far-IR gas emission lines. PAH molecules can efficiently shield the gas from stellar UV radiation because they do not settle and do not scatter, but have strong UV absorption opacities in comparison to evolved dust.

Conclusion

Astochemical models for disks require a careful setup of the stellar properties, disk shape, PAHs, and dust properties, which varies from disk to disk. In the large European FP7 project *DIANA*, we have fitted these properties for 12 individual disks (AB Aur, MWC 480, HD 163296, GM Aur, TW Hya, DM Tau, CY Tau ...) to all available multi-wavelength and multi-kind observations (SED, images, line fluxes, line profiles). We offer our data collection and all modelling results in a public database, see http://www.diana-project.com/data-results-downloads, to provide a more realistic setup for Herbig Ae, T Tauri and transitional disks for future astrochemical models.

Acknowledgments:
The research leading to these results has received funding from the European Union Seventh Framework Programme FP7-2011 under grant agreement no 284405.

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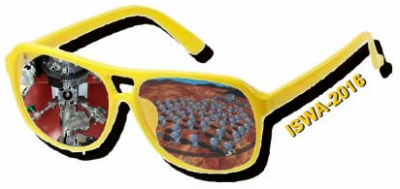

Lithium rich K-type giant stars as a new source of organic compounds in the Galaxy

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Key Words: complex organic and inorganic compounds, comet, Giant stars

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We have recently found [1] the presence of complex organic and inorganic compounds by means of emission features in the Mid-IR spectra of Li rich K giant stars. These are located at the Luminosity Bump in the initial ascending giant branch. We proposed that the Li enrichment phenomenon could result as a consequence of the outward transfer of angular momentum of a rapidly rotating stellar core. This way, the internal mass will be transported up to the stellar surface producing the ejection of a circumstellar shell. This mechanism acts continuously and can have peaks of rapid short episodes transporting internal 7Be to the surface and transforming it into 7Li. before 7 Be could be destroyed. The organic material is formed in the expanding shell with mass losses thousand times larger than normal values of K giants and lasting less than 2000 yr. The inorganic material would be the result of the interaction of this shell with the debris disk remaining of the MS evolution. It is interesting to notice that the lifetimes of these emerging shells of recently Li enriched giants stars, is the same as that of pre-planetary nebulae winds considered to be the first main sources of organic compounds.

We propose here, that the winds of these recently Li rich stars could be considered as a second source of organic material in the Galaxy. Also, these Li rich giants have shown the presence of an anomalous strong dusty continuum emission characterising the shell giving support to Sun Kwok's suggestion that these organic compounds are solid nano particles. It is in fact very impressive to find today that the surface of the Churyumov–Gerasimenko comet or the large dunes of Titan are covered and formed by solid organic compounds.

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Photoionization and Photodissociation of Methyl benzene in a Circumstellar Environment

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Key Words: *PAHs; methylated*; *dicátions; AGB*; *X-ray*.

Introduction

The formation of PAHs and their methyl derivatives occurs mainly in the dust shells of AGB stars. Toluene ($C_6H_5CH_3$) is a precursor of methylated PAHs, as the simplest alkyl-substituted benzene derivative. Ziegler et al. (2005) proposed a formation process of a methylated benzene in the gas-phase that could take place in the warm layers of the circumstellar envelope of AGB stars [2]. The object T Dra is a carbon-rich AGB star associated with FUV and X-ray emission [3]. The photochemistry of toluene was experimentally studied in order to apply the findings at this scenario.

Results and Discussion

The absolute single and double photoionization and photodissociation cross sections were determined. The ionization and destruction of toluene induced by X-rays examined in the T Dra conditions suggest a minimum photodissociation radius of 21 AU of toluene from the AGB star, where the molecule is subjected to the incidence of the soft X-ray flux emitted from a companion white dwarf star. Partial ion yields of a large number of ionic fragments were extracted from single and 2D-spectra, where electron-ion coincidences have revealed the doubly charged parent-molecule and several doubly charged fragments containing seven carbon atoms with considerable abundance. *Ab initio* calculations based on density functional theory were performed to elucidate the chemical structure of these stable dicationic species.

Conclusion

The relatively high photoabsorption cross section of toluene at the C1s edge increases the photoionization and photodissociation cross sections of the molecule, when compared to benzene. Eventually, this could be responsible for the higher detection of doubly charged species of toluene. About the dication species, it was found a previously non-reported methyl-biscyclopropenyl structure as the global minimum for $C_7H_6^{++}$, and the loss of structural integrity of $C_7H_8^{++}$ when compared to neutral toluene. The results also suggest that the ion production on the side of the envelope that faces the companion white dwarf could affect other regions. If magnetic activity is present, the chemical network reactions could be highly affected, triggering ion-molecule reactions through ambipolar diffusion.

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Modeling the effects of grain motion, charging and size distribution to interstellar chemistry.

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Key Words: *gas grain chemistry; grain motion*; *grain charging; grain size distribution*.

Introduction

Interstellar gas-grain chemical system is complex. Some key physics could be missing in the traditional gas-grain chemical models which could be at least partially responsible for the inability to achieve higher levels of agreement with observations. In order to explain our peculiar observed abundance patterns of complex organic molecules (COMs) in high mass star forming regions, we have tried to introduce turbulent gain motions, grain charging and grain size distribution into our rate equation code. We will report obvious chemical effects of grain motions and show how the surface abundances on grains differentiate over grain sizes when grain charging is included.

Results and Discussion

We find that, because the dust grains are drifting through gas with km/s-scale velocities, the accretion of heavier species will be greatly enhanced by the grain motion, which results in the change of both gaseous and surface abundances up to orders of magnitude in typical interstellar environments. We also find that, when grain charging is considered, the surface abundances can be very different on grains of different sizes. When a realistic grain size distribution is adopted, some surface species can have their abundances 2-4 orders of magnitude different from that in corresponding single grain-size models, even if the total grain surface areas are kept the identical.

Conclusion

Grain motion in the turbulent interstellar clouds and a realistic treatment of both grain charging and grain size distribution may bring new chances to improve the agreement between chemical models and observations.

Acknowledgments:
We are in great debt to many nice colleagues in doing these studies, including Dr. T.I Hasegawa, and Dr. D. Semenov., among others.

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Probing the nature of small-scale structure towards ρ Oph stars: A new avenue in diffuse interstellar band research

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Key Words: *ISM; DIBs; rho oph stars; dust; modeling*.

Introduction

The longest standing challenge in astronomical spectroscopy is identifying the carriers of the diffuse interstellar bands (DIBs) [1]; absorption features seen in optical and near-IR spectra towards stars with significant foreground material. The band carriers are thought to be carbonaceous molecules such as PAHs, carbon chains and fullerenes. Hence, the DIB carriers represent a large fraction of the cosmic carbon quota, and once identified, will make them a unique tool to probe the interstellar medium. We present the results from a high resolution UV Hubble Space Telescope investigation of small scale structure (SSS) towards a selection of ρ Oph stars. Previous ρ Oph observations show DIB strength variations of up to 9% over distances as small as ~350 AU, and larger still for those further apart. [2] We examine the factors that control DIB strength in this relatively small system, and examine the properties of the gas responsible for SSS.

Results and Discussion

We have compiled an inventory of different atomic and molecular species seen towards ρ Oph A, B and D - the three sightlines investigated. We have modeled 17 C(I) multiplets in the 115-135 nm range in order to compute the interstellar gas pressure through collision/radiative excitation analysis. Our preliminary results suggest there is a notable difference in the abundance of atomic carbon in 3 different levels (ground state and two excited levels) towards each line-of-sight. We have begun preparing models for the C_2 D-X band at 231 nm, in which we will obtain gas temperatures and densities that are accurate to ~10% [3]. With the measurements of both atomic and molecular carbon, we will derive the most accurate temperature and density measurements possible of the diffuse gas towards the ρ Oph system. We will present these results at the meeting.

Conclusion

We will present conclusions on the gas pressures, temperatures and ionizations to yield insights into the nature of the SSS in the diffuse molecular gas of this star-forming region, helping constrain theories of molecular cloud formation.

Acknowledgments:
Don Lindler, Ed Jenkins, EPSRC

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Non-thermal ion desorption from nitrile-bearing astrophysical ice analogues studied by electron and heavy ion bombardment

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Key Words: *Astrophysical ices; nitriles; non-thermal desorption; Time-of-Flight Mass Spectrometry (TOF-MS); Electron Stimulated Ion Desorption (ESID)*; *Plasma desorption Mass Spectrometry (PDMS)*.

Nitriles (molecules bearing the C≡N functional group) represent a quite abundant class of molecules in the gas-phase of a variety of astrophysical environments. The organic nitriles methyl cyanide (CH_3CN), ethyl cyanide (CH_3CH_2CN), vinyl cyanide (CH_2CHCN) and isopropyl cyanide ($(CH_3)_2CHCN$) have been detected towards star-forming regions in the interstellar medium (ISM), and some of them are also present in Solar System bodies, like cometary comae and on Titan's atmosphere. Despite their relevance, little is known about their formation and processing under astrophysical conditions. In the ISM, these molecules are expected to condense onto the ice mantles of cold dust grains, which are constantly bombarded by cosmic rays. At the Solar System, nitriles may be incorporated in the ice matrix of cold objects, like comets and on Titan's organic haze particles, being exposed to the solar wind and to energetic charged particles trapped in planetary magnetospheres. The incidence of high-energy radiation onto icy surfaces triggers a radiation induced surface chemistry, which constitutes an important route for leading new neutral or ionized molecular species back to the gas phase in interstellar/circumstellar and planetary environments, enhancing the molecular complexity. In this work, we have studied the ion desorption of cations from pure CH_3CN, CH_3CH_2CN, CH_2CHCN and $(CH_3)_2CHCN$ ices due to the impact of high energy electrons and energetic heavy ions, from the ^{252}Cf fission, simulating the incidence of cosmic rays and/or solar wind particles onto icy surfaces. The desorbed cations from each sample were identified by time-of-flight mass spectrometry (TOF-MS), by means of the Electron Stimulated Ion Desorption (ESID) and Plasma Desorption Mass Spectrometry (PDMS) techniques. Several ionic species were identified, indicating strong fragmentation on surface. Proton-transfer processes are suggested to play an important role in ion desorption, as evidenced by the abundant desorbed protonated parent molecules CH_3CNH^+, $CH_3CH_2CNH^+$, CH_2CHCNH^+ and $(CH_3)_2CHCNH^+$ and ion clusters such as $(CH_3CN)_2H^+$, $(CH_3CH_2CN)_2H^+$, $(CH_2CHCN)_2H^+$ and $((CH_3)_2CHCN)_2H^+$. The energy dependence on the positive ion desorption yield indicates that ion desorption is initiated by Coulomb explosion following Auger electronic decay [1]. Ion desorption induced by electrons or heavy ions onto nitrile-bearing ices is suggested to constitute an important non-thermal route by which new neutral or ionized molecular species may be delivered to the gas-phase, contributing to the production of more complex molecules. The derived desorption yields per projectile impact may contribute to chemical evolution models in different cold astrophysical objects, especially where the abundance of nitriles is expected to be high.

Acknowledgments:
CAPES, CNPq, FAPERJ.

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Ionization-driven star formation: the case of IR bubble N10

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Key Words: *Interestelar Medium (ISM); Molecular Clouds; Star Formation; Infrared Bubbles; Molecules.*

Infrared bubbles are ideal regions to investigate the impact of the ionizing radiation and strong UV field on the conditions of star formation at the border of HII regions. The infrared bubble N10, first detected by Churchwell et al. (2006), is especially interesting as it undergoes a burst of star formation. Infrared studies of the young stellar content suggest a sequential star formation scenario, possibly triggered, at the border of the HII region. The interaction of young massive stars with the surrounding molecular gas of the parent cloud – and the possibility of triggering star formation – have stimulated lot of work both observationally and theoretically. The "collect and collapse" scenario was first proposed by Elmegreen & Lada (1977). In this scenario, the radiation of the massive stars of an HII region creates an ionization front at the interface with the molecular cloud, which drives the propagation of a shock front into the neutral material, which accumulates mass and eventually becomes gravitationally unstable (see Deharveng & Zavagno (2008) for a review). This scenario has been revisited since (Whitworth & Francis, 2002) and other scenarii of triggered star formation have been proposed, like e.g. the "Radiatively-Driven Implosion" model, though still based on the overpressure exerted by the ionized gas (Lefloch & Lazareff, 1994). Deharveng et al. (2010) studied the triggered star formation on the border of a number of HII regions enclosed by infrared bubbles. They discussed the possible link between bubbles and HII regions that they enclosed, looking for clues about triggered star formation. Detailed multi-wavelength studies have been published for a number of these bubbles. Although these works point to the presence of Class I YSOs associated with clumps in the PDR region, the question of the existence of triggered star formation associated with the expansion of the HII region is not closed. We have studied the distribution of YSOs in the vicinity of N10 (Gama et al. 2016). A spatial stratification is observed between Class I and Class II sources, the latter being located closer to the central region. Such a stellar age distribution is suggestive of a sequential star formation process. The star formation process in the bubble N10 is possibly induced by the HII region, as a result of the interaction between the expanding ionizing gas and the interstellar medium that surrounds it.

In order to constrain the star formation scenario, we used IRAM 30-m telescope to examine the physical properties and the kinematics of the molecular gas, by mapping the emission of the specific molecular tracers to characterize the properties of the prestellar and protostellar condensations, as well as the properties of the photon dominated region at the interface between the HII region and the molecular condensations. We have detected species like HCO+(1-0), HCN(1-0), SiO(2-1), N_2H+(1-0), CS(2-1) and CS(3-2). Putting all the results together, we will be able to obtain a detailed view of the interaction between the high-energy radiation and the molecular gas, its possible role as a trigger of star formation, and its influence of the chemical evolution of the molecular gas.

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3D modelling of HCO^+ in the low-mass proto-star IRAS16293-2422

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Key Words: *3D modelling; radiative transfer codes; star-forming regions; astrochemistry.*

Introduction

The ionisation processes play an important role in star formation. Ions and electrons, following the magnetic field, interact with neutral species, slowing down the gravitational collapse towards the central proto-star. Ionisation can also help to create and destroy big molecules as Complex Organic Molecules (COMs), thus it is involved in the chemistry that takes place in the source. This ionisation can be traced with molecules such as HCO^+.

Results and Discussion

HCO^+ is an abundant species in IRAS16293-2422 in which 11 transitions of the main isotope and 20 transitions of its isotopologues ($H^{13}CO^+$, $HC^{18}O^+$, DCO^+ and $D^{13}CO^+$) have been observed with the TIMASSS (IRAM and JCMT, plus APEX data) and CHESS (*Herschel*/HIFI) spectral surveys. This allows us to determine accurate constraints on the physical conditions that occur in the source. We have modelled the 3D physical structure of the source (envelope and outflow) and we predict the lines spectra with the 3D radiative transfer code LIME [1].

The observed lines shapes and intensities cannot be explained only with the contribution of the envelope of the source, particularly for high upper energy level transitions. Recent studies [2] have shown that young outflows can lead to an enhancement of the HCO^+ abundance in a short period of time. Such a young outflow (~400 yrs) has been traced by $H^{13}CO^+$ in IRAS16293-2422 [3]. We have included this outflow in our 3D model together with the physical properties of the envelope (H_2 density, gas and dust temperature) that have already been determined [4]. We derive the radial HCO^+ abundance profile using the gas-grain astrochemical code Nautilus [5]. We varied several parameters (age of the proto-star, cosmic ionisation rate, C/O ratio, etc.) to test their influence on the resulting abundance profile. We also considered fractionation and deuteration reactions to estimate correctly the abundances of the different isotopologues.

Conclusion

The resulting line emission predicted by LIME for all transitions fits correctly the observations. Both the envelope and the outflow are needed to explain the HCO^+ line emission. We have successfully coupled 3D radiative transfer and astrochemical modellings to constrain the abundance of the formyl ion in IRAS16293-2422.

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The ASAI View on the Evolution of Molecular Complexity along the Formation of Sun-Like stars

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Key Words: *radioastronomy; spectroscopy; star formation*; *protostars; jets and shocks*.

Introduction

The Large Program ASAI carried out at the IRAM 30m telescope joins the efforts of several groups in Astrochemistry, in Spain and France to address the question of our "chemical origins"[1]. Its goal is to obtain a complete census of the gas chemical composition, the chemical evolution along the main stages of the star formation process, from prestellar cores to protostars in order to understand the processes which govern the emergence of molecular complexity and the formation of pre-biotic molecules. This is achieved through highly sensitive, unbiased spectral line surveys of a sample of sources illustrative of the various stages of protostellar evolution. The resulting data set is aimed to serve as a reference database for the astrochemical community: astronomers, chemists, and theoreticians.

Results and Discussion

ASAI is an extremely fruitful project. New molecular species have been discovered [2]. Many molecular species have been discovered at all stages of the evolution of sun-like protostars [3,4,5]. ASAI has revealed the importance of feedback processes on the chemical evolution of protostellar cores, and their potential as astrochemical laboratories. I will review the major results obtained by ASAI. I will pay special attention to Formamide (NH_2CHO), one of the simplest molecules of pre-biotic interest. Recently, Formamide has been proposed as a precursor of both metabolic and genetic material, suggesting it could have played an important role in the emergence of life [6]. ASAI has permitted the first comprehensive study of formamide towards solar-type environments, revealing new discoveries [7,8], including its detection for the first time in outflow shock spots[5]. The presence of NH_2CHO in such a variety of star-forming environments, as well as on a Solar System comet, suggests that it could have been exogenously delivered onto Earth in the past. I will present the results of this study and will discuss their implication for the formation route of this molecule and other related pre-biotic species in solar-type protostellar environments [9].

Conclusion

ASAI has shown spectral line surveys in the (sub)millimeter range to be extremely powerful diagnostic tools to investigate the chemical evolution of star-forming regions. I will show how LLAMA can play an important role in the legacy of ASAI, in parallel to the high-angular resolution studies which will be carried out with the large millimeter arrays ALMA and NOEMA.

Acknowledgments:
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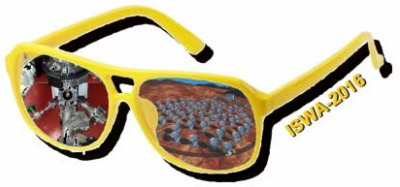

Properties of dense condensations embedded in Musca derived from $C^{13}O$, $C^{18}O$ and NH_3 emission lines

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Key Words: *molecular hydrogen*; emission lines; thermodynamic equilibrium.

Abstract

The structure and physical conditions of dark clouds must be derived from H_2 tracers such as CO, NH_3, CS (Myers et al., 1983; Myers et al., 1991). We studied the kinematic and dynamics properties of 8 dense condensations (Mu4, Mu5, Mu6, Mu8, Mu9, Mu10, Mu11 e Mu13) embedded in Musca with J=1-0 transition of ^{13}CO and $C^{18}O$ and J=K=1 transition of NH_3. Mu13 has associated the IRAS 12322-7023 source and the remaining are starless cores. From ^{13}CO and $C^{18}O$ we found a systematic increasing of the radial velocity of about 0.2 km s^{-1} pc^{-1} from Mu4 to Mu13. The ^{13}CO and $C^{18}O$ radial velocity dispersion is greater in Mu13 but the observed line widths do not vary significantly between the condensations. The emission of NH_3 was detected in Mu9 and Mu13, being most intense toward Mu13. The intensity ratio lines of the satellite to main hyperfine component in Mu13 is ~0.3, suggesting that this condensation is in thermal equilibrium. Almost all emission lines of ^{13}CO and $C^{18}O$ are single-peaked and symmetric, with Gaussian-like shapes, except in those positions with splitted lines, shifted by ~1.0 km s^{-1}, such as in Mu13 and in Mu10. The integrated intensity maps of ^{13}CO and $C^{18}O$ toward Mu13, suggest that the double-peaked lines are due to the superposition of clouds with different radial velocities seen in the line of sight as suggested by Vilas-Boas (1994). In general, the observed line widths of ^{13}CO are 5-9 times larger than the expected thermal broadening, which suggest that the nonthermal pressure is the primary source of suport against gravity. The kinetic temperature ranges between 8 and 15 K. Assuming spheric geometry, we estimated the mean volumetric density of ~10^3 cm^{-3} from ^{13}CO and $C^{18}O$ lines and ~10^4 cm^{-3} from NH_3 lines. This last value is similar to that estimated from visual extinction maps derived from near-infrared data.

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Ion irradiation of N_2O Simulated Astrophysical Ice (SAI): Relevance to the Interstellar Medium and trans-Neptunian Objects.

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Keywords: Ion Irradiation, Nitrous Oxide, Cosmic Rays, FTIR, Simulated Astrophysical Ice (SAI)

Introduction

Nitrous Oxide, N_2O, was the first N-bearing molecule found in the interstellar medium (ISM). The discovery of N_2 ice on the surfaces of Triton (Neptune's largest moon) and Pluto [1], the last one recently confirmed by the NASA New Horizons probe [2], shed light on a new ice phase mechanism for the formation of N_2O based on non-equilibrium chemistry, where an electronically excited oxygen atom adds to a frozen nitrogen molecule in a no barrier reaction [3]. This pathway could explain the formation of N_2O in the ice mantles of interstellar grains and on the surfaces of the trans-Neptunian objects where N_2 ice are present. That makes of N_2O a key molecule for the comprehension of the nitrogen chemistry in extraterrestrial environments.

Regarding to better understand the N_2O ice phase chemistry, the aim of this work is to investigate the effects of cosmic ray impact on a N_2O astrophysical ice analog. We employed a 1.5 MeV N^+ (Z=14) beam from a Van de Graaff accelerator as the irradiation source.

Results and Discussion

The N_2O astrophysical ice analog was condensed in an ultra-high vacuum chamber at 10K which is the typical temperature of an interstellar grain and is also a good model temperature for a trans-Neptunian object as well. Chemical modifications within the ice due to the irradiation were monitored by Fourier Transform Infrared Spectroscopy (FTIR). The unknown integrated band strengths of mid-infrared features of solid N_2O were determined and the new compounds produced by chemical reactions induced by irradiation of the ice matrix were identified and characterized.

Conclusions

Our experiment simulated the effect of cosmic rays impacting on a N_2O astrophysical ice analog. The N_xO_y (x = 1-2 and y = 1-5) oxides and ozone (O_3) produced by the chemical reactions induced in the ice matrix were identified by FTIR. The most abundant oxide produced was NO_2. Some band strengths for the vibration modes of N_2O in ice phase were also determined. The obtained spectroscopic data could be helpful for future astronomical investigations beyond Neptune's orbit and also for a better understanding of interstellar nitrogen chemistry.

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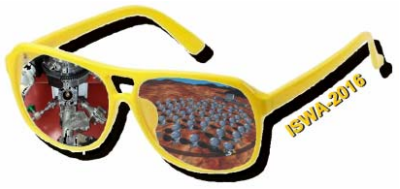

Understanding phosphorous chemistry in cometary comae

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Key Words: *phosphorous chemistry; comets*; *reactive gas dynamics; prebiotic chemistry*; *origins of life*.

Introduction

Phosphorous is a key element in all known forms of life. P-bearing compounds have been observed in space. They are ubiquitous in meteorites, have been detected in the dust component in comets 1P/Halley and 81P/Wild 2, but searches of the gas phase in comets have been unsuccessful [1], including the Rosetta Mission to date. We present results from the first quantitative study of P- bearing molecules in comets [2,3,4] to aid in future searches for this important element in comets, shedding light on issues of comet formation and prebiotic to biotic evolution of life.

Results and Discussion

Our gas dynamics model of cometary comae with chemical kinetics [5], has been adapted to study this problem. We used phosphine (PH_3) as a native molecule with a cosmic abundance mixing ratio. Over 100 photo and gas-phase reactions and 30 P-bearing species were added to the chemical network. The chemistry of PH_3 in the inner coma shows the major destruction channels are photo-dissociation and protonation with water-group ions, leading to the recycling of PH_3 in this region.

Conclusion

The model identifies the relevant phosphine chemistry in cometary coma. Protonation reactions of PH_3 with water-group ions are important due to its high proton affinity. Abundances are found to be on the order of 10^{-4} relative to water, about the same as isotopic species. The scale length of PH_3 in the coma is about 13,000–16,000 km. Collaborations with observers using modern telescopic facilities (e.g., Keck 2 and Subaru) are underway to search for phosphorus in comets.

Acknowledgments:

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Molecular complexity in Orion-KL: IRAM and ALMA observations of O-bearing molecules

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Key Words: *astrochemistry; radio lines; molecules; Orion-KL.*

Introduction

The Orion-KL region is one of the two richest interstellar molecular sources, with SgrB2, known in our Galaxy. A better knowledge of the physical and chemical conditions in this region will help us to constrain the molecular formation pathways and to investigate the limit of molecular complexity in the interstellar medium.

Results and Discussion

Several complex O-bearing molecular species and continuum emission clumps have been identified and mapped toward the Orion-KL nebula at high spatial resolution (below 1.9") in the 213 to 247 GHz range using the IRAM Plateau de Bure interferometer and ALMA Science Verification data. Our IRAM maps show the presence of several methyl formate clumps with major peaks toward the Compact Ridge and the Hot Core [1] and a close relationship between methyl formate and dimethyl ether distributions [2]. In contrast, our acetone maps exhibit a spatial distribution distinct from other complex O-bearing molecules and similar to that of N-bearing molecules [3]. These results do not provide a single formation/destruction model of complex molecules but rather suggest that the formation of some of the organic species is probably related to the presence of shocks. In addition, the $^{12}C/^{13}C$ ratio derived from our recent detection of both ^{13}C-methyl formate isopotologues suggests that grain surface chemistry is at work in both the Compact Ridge and the Hot Core and that complex molecules are released from ice mantles [4]. Another O-bearing molecule, ethylene glycol, the di-alcohol related to ethanol, was firmly identified for the first time in Orion, whereas it is relatively abundant in comets [5]. This was achieved with the Orion ALMA Science Verification data thanks to both high resolution imaging and identification of tens of lines in the instantaneous broad bandwidth of the ALMA array. Finally the distribution of species containing methyl and ethyl groups could also be compared thanks to the ALMA data [6].

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Sputtering analysis of astrophysical solids by Plasma Desorption Mass Spectrometry – PDMS

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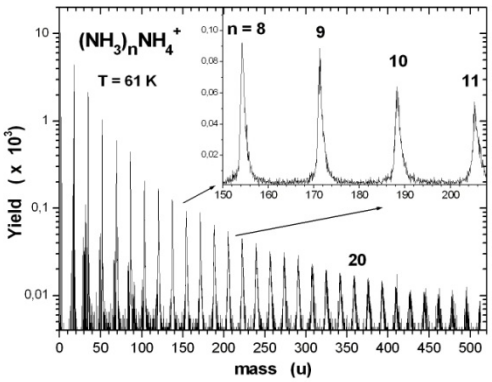
Key Words: *mass spectrometry; meteorites; astrophysical ices; PDMS*

Introduction

Sputtering is a process in which atoms, molecules or clusters (ionized or neutrals) are ejected from the surface of solid materials as a result of a projectile impact (energy >> eV). In astrophysical environmemts, sputtering occurs when atmosphere-less bodies (e.g., interplanetary grains, asteroids or moons) are exposed to stellar winds or to galactic cosmic rays. The induced particle emission is accompanied by mini-crater formation, surface erosion, chemical reactions and material phase modifications, phenomena that contribute to the space weathering.

Results and Discussion



^{252}Cf- Plasma Desorption Mass Spectrometry (^{252}Cf- PDMS) is a convenient method to study the emission of ions induced by ~100 MeV projectiles (^{252}Cf fission fragments - FF) [1,2]. Unpublished results obtained with this technique for the Isna, Allende and Zagami meteorites are discussed [3]. Moreover, a review on sputtered ions from astrophysical ice surfaces exposed to ^{252}Cf- FF impacts is also presented. The analyzed ices are: H_2O, CO, CO_2, NH_3, N_2, O_2, CH_4 and C_2H_6 [4]. The figure illustrates a typical PDMS mass spectrum of NH_3, in which a long series of positive cluster ions is represented.

Conclusion

^{252}Cf- PDMS is indeed a very suitable technique for analyzing the ion desorption process induced by cosmic rays. The main effects observed in this electronic sputtering are: i) the sputtering yields of low mass secondary ions are of the order of 10^4 ions/ impact; ii) new chemical species are produced and identified; iii) large series of positive and negative cluster ions are emitted.

Acknowledgments:
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Detection of cyanopolyynes in the protostellar shock L1157-B1

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Key Words: *molecular abundances*; *methods: observational*; *protostellar shocks, outflows;*

Introduction

The carbon-chain molecules known as cyanopolyynes ($HC_{2n+1}N$, n = 1, 2, 3) are present during the different phases of the evolution of Sun-type protostars [1,2], their spectral analysis offer a powerful diagnostic to understand the molecular complexity in protostellar objects [3,4]. Through the Large Program ASAI [5] (Astrochemical Surveys At IRAM) a full search for $HC_{2n+1}N$ molecules is being carried out in the protostellar shock L1157-B1, whose copious chemistry is triggered by the compression of the interstellar material caused by the passage of the shock [6]. The observations were performed with the IRAM-30m antenna covering all its millimeter windows at 3 mm (80 – 115 GHz), 2 mm (130 – 170 GHz), 1.3 mm (200 – 320 GHz) and 0.8 mm (330 – 350 GHz).

Preliminary results and discussion

We detected bright lines of HC_3N from J=9-8 to J=32-31, HC_5N from J=31-30 to J=43-42, as well as the transitions with J_{up} = 9, 10, 11 and 12 of the rare isotopologues $H^{13}CCCN$, $HC^{13}CCN$ and $HCC^{13}CN$. Their emissions have been analysed in the Large Velocity Gradient approximation and under Local Thermodynamic Equilibrium. As a preliminary result, the analysis of the HC_3N and HC_5N lines yielded three different excitation temperatures around 15, 55 and 110 K. Likewise, the analysis of the line profiles unveils the origin of the emission from different physical components of L1157-B1, as reported in previous works [7,8]. The derived column densities indicate a ratio $N(HC_3N)/N(HC_5N) \geq 10$, with a low precision we also estimated $N(H^{13}CCCN):N(HC^{13}CCN):N(HCC^{13}CN) \approx 2:2:1$. Despite the absence of an accurate evidence of ^{13}C fractionation, preliminary analysis show that the reactions with low energy barriers $C_2H_2 + CN \rightarrow HC_3N + H$ and $C_2H + HNC \rightarrow HC_3N + H$ [9,10] might explain the formation of HC_3N in the gas phase of L1157-B1.

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Interstellars Molecules: The Value of Quantum Chemistry

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Key Words: quantum chemistry, interstellar molecules, astrochemistry.

Introduction

More than 200 organic and inorganic molecular species consisting of up to 13 atoms have been identified in space, of which about 10% are molecular ions. The rich variety of the observed molecules implies that much more relevant yet undiscovered species must participate in the formation and destruction processes of theirs. However, the formation of these molecules it has not been yet fully understood. Also, the number of isomeric form increases as the number of atoms in molecules is increased. Knowing which molecules are in the interstellar medium will allow a better understanding of what types of chemical reactions are possible in space. However, to make a reliable interpretation of observations it necessary to know properties as structure, frequency and intensity. From this point of view, properties such as transitions and spectroscopic constants sections collision and intensity of the lines through ab initio calculations are relevant and useful. For this reason, ab initio calculations are an essential tool for astrochemistry. Thus, in this work, we would want to present a part of our work applying different methods of quantum chemistry. The main goal has been to predict properties of astrophysical relevant molecules as CF^+, HCCN, SiC_3, SiC_3H^+, SiC_3H, HCO^+ and CH_2OH.

Our calculations allow us determined with reasonable accuracy stable structures and vibrational frequencies of the most relevant isomers and cations. Anharmonic spectroscopic parameters for the ground electronic state of the most stable structures were also obtained from anharmonic force fields using second-order perturbation theory. In all cases, we are available to reproduce and interpret experimental data, and even conduct experimental research. In the case of unstable systems or difficult system to reproduce at the laboratory, the theoretical data are the only sources of information that is available. In many of these systems, ab initio methods are able to explain, predict, confirm or disapprove harshly assignments. Thus, our data are helpful for understanding structures and properties of CF^+, HCCN, SiC_3, SiC_3H^+, SiC_3H, HCO^+ and CH_2OH families, being valuable data for their detections in the interstellar space and laboratory.

Acknowledgments:
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Tracing the protosolar nebula heritage: the nitrogen isotopic ratio

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Key Words: *Nitrogen; Isotopic Ratio*; *Fractionation; Protosolar Heritage*; *star formation*.

Introduction

The extent to which the chemical reservoirs in interstellar molecular clouds are preserved during the formation of stars and planetary systems is a central question with implications from astrophysical, chemical, and biological perspectives. However, the degree to which the original cloud composition may be altered or even reset during the star and planet formation process is unknown. Isotopic ratios are powerful tools to trace the chemical heritage of planetary systems in general [1]. For nitrogen, the $^{14}N/^{15}N$ isotopic ratio indicates that comets have preserved, to some extent, the Sun's original interstellar chemical reservoir [3]. However, the mean cometary isotopic ratio of 150 is in sharp disagreement with the protosun value of 441 [2]. The reasons are not clear and represent a challenge for astrochemical models.

Results and Discussion

In this talk, I will present an overview of the nitrogen isotopic ratio from cosmochemical and astrophysical perspectives. Particular emphasis will be put on the various reservoirs of nitrogen and isotopic ratios in the prestellar phase prior to the protostellar phase. I will also present on-going research performed with the IRAM/NOEMA interferometer to uncover a possible prestellar icy reservoir of fractionated nitrogen [4]. Perspectives for astrochemical modelling, shall also be proposed.

Conclusion

Understanding the protosolar heritage is an undertaking of paramount importance. The recent advances in astrochemistry, cosmochemistry (Rosetta) and chemistry are leading to a more complete scenario of the protosolar heritage and the convergence of cometary values points towards an icy reservoir of nitrogen that may be preserved during star formation.

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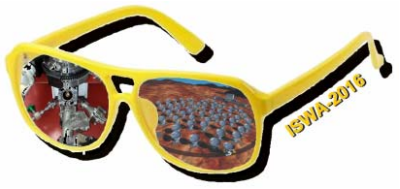

Molecules in Planetary Nebulae – Results from the Herschel Planetary Nebula Survey (HerPlaNS)

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The Herschel Planetary Nebula Survey (HerPlaNS) obtained far-infrared broadband images and spectra of eleven well-known planetary nebulae (PNe) using the PACS and SPIRE instruments aboard the Herschel Space Observatory. In this talk I will discuss the results of the spectroscopy data analysis of the molecular component in these data. Among our results is the first detection of OH+ in a PNe (Aleman et al. 2014, Etxaluze et al. 2014). Line emission of this molecule has only been detected in a few objects, all of them showing hard ionizing sources (the Orion Bar and Ridge, a supernova remnant, and an AGN). We detected OH+, CO, and CH+ rotational line emission in three out of the eleven objects searched.

Our results showed that the emission is produced in the photoionization region of these objects, which are illuminated by the hottest central stars in the sample (T ~100000K), that is the objects with the highest fraction of high-energy photons.

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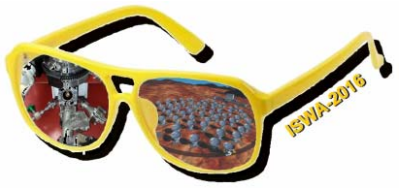

Theoretical Rotational Spectra of Deuterated Benzene Isotopologues: Improvements on the Benzene' s quantification at Interstellar Medium.

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Key Words: *Rotational spectroscopy; Deuterated isotopologues; Interstellar medium; PAD; Radio astronomy* .

Introduction:

Ground based measurements of molecular rotational spectra can be improved with theoretical predictions and the search for deuterated isotopologues of otherwise apolar molecules can be amplified using radio-telescopes if we have good synthetic spectra for these ones. This work show a theoretical and computational approach for building a highly accurate ab initio pure rotational spectra of deuterated isotopologues with the aim of using these spectra to assist possible detections of polyatomic isotopologues of astrophysical interest. This methodology was applied to build spectra to benzene isotopologues in order to support in the future the search for this one andDeuterated Polycyclic Aromatic Hydrocarbons (PAD) in interstellar media (ISM) by radio astronomy.

Results and Discussion:

An adiabatic variational correction called Finite Nuclear Mass Correction (FNMC) [1] was used to calculate the isotopic dipole moments of benzene isotopologues, which have the ability to compute the effects of finite nuclear mass, together with a perturbation method which takes into account the effects of anharmonic force field, and vibrational averaging [2]. The FNMC was implemented in the The Dalton quantum chemistry program [3]. Then, the Gaussian 09 [4] was used to evaluate the vibrationally averaged rotational and centrifugal constants for these systems and techniques were employed to simulate the pure rotational spectra for some typical ISM temperatures using the PGOPHER [5] program.

Conclusion:

It was verified that the pure rotational spectra of benzene deuterated isotopologues obtained presented good accuracy relative to experimental data, showing that the methodology was appropriate. Beyond the general capacity to build spectra, a line survey of some ISM's unidentified lines was done and compared with our results for benzene, which indicated that lines can correspond to spectra of these molecules.

Acknowledgments:

The authors acknowledges the CNPq, FAPEMIG, FAPESP for the financial support.

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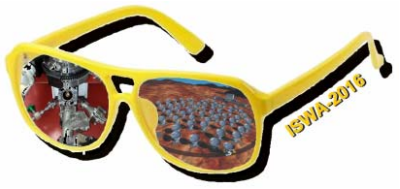

Investigation of the molecular biosignatures' alteration under simulated space environments in support of space-based astrobiology experiments

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Key Words: *Astrobiology; Biomolecules; Space and Planetary Simulation*; *Synchrotron Light; CubeSat.*

Introduction

Life as we know it is based on complex organic compounds interacting in aqueous media, forming compartmentalized autopoietic systems, the cells. Ground and space-based astronomical observations have identified many different types of carbon based molecules in our own as well as distant galaxies [1]. Some of these material was concentrated on the early Earth by the planetary formation process, and later carried to its surface by asteroids, comets, and their fragments [2]. Hence, knowledge of the stability and degradation pathways of these compounds in the outer space environment, and the effect of their interaction with inorganic substrates, are key to our understanding of life's origin, evolution, distribution and future.

Results and Discussion

The main goal of this work is to investigate the detectability, photostability and resilience of astrobiologically important biomolecules in simulated space and planetary environments. The results will be used as preliminary studies for small and low cost astrobiology experiments, that will be sent in space missions with stratospheric balloons and CubeSats, both in preparation by the research group. The selected biomolecules, both in pure form and mixed with inorganic substrates, will be exposed to: (1) the photon flux of the TGM beamline at LNLS (Campinas-SP/Brazil), which works at the VUV region (3-310 eV), to simulate the conditions of the space environment, measuring the biomolecules changes by *in-situ* UV-Vis reflectance spectroscopy; and to (2) the Space and Planetary Simulation Chamber (AstroCam), which is a multiparametric chamber that can simulate a number of environments by setting different irradiation conditions, pressure, gas composition, and temperature, in addition to vacuum, measuring the changes *in-situ* by spectroscopic analysis and conventional laboratory procedures.

Conclusion

The expected results are different degrees of photodegradation for each biomolecule on each of the inorganic surfaces (due to their potential catalytic and/or photolysis-inhibiting effect). Also, we expect to validate laboratory-based exposure experiments in comparison with space experiments, building a database of spectra and other parameters for further studies on prebiotic molecules.

Acknowledgments:
Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), for the scholarship of the student. NAP/Astrobio for the access to the simulation facilities for planetary surfaces.

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Origin and excitation mechanisms of the warm CO, OH and CH^+ in PDRs

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Key Words: *ISM; PDRs*; *Orion Bar; molecular lines*.

Introduction

Photon Dominated Regions (PDRs), where physics and chemistry are driven by FUV photons, show an extremely rich and warm photochemistry that is closely related to that of protoplanetary disks and starburst galaxies. The rotationally excited lines of CO, 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 and high-J CO emission lines have been associated with the presence of unresolved dense structures and high pressure gas [e.g., 1, 2, 3]. For CH^+, highly reactive, excitation is driven by collisions and by chemical pumping after reaction of C^+ with vibrationally excited H_2 [4, 5].

Results and Discussion

For the first time we present fully sampled PACS maps (110" x 110") of the CO J=19-18, 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 high-J CO, OH, and CH+ to the dense clumps. Excitation mostly occurs at the PDR edge, where the UV flux is at maximum in the PDR. Photoelectric effect on small particles is the dominant heating source of the observed high excited molecular gas and the effect of cosmic rays is excluded. Using the spectral and spatial distribution of several CO lines and its isotopes, we present temperature and column density maps over this area covering the entire Orion Bar.

Conclusion

It is clear that the vibrationally excited H2 is the key in the formation and excitation of CH^+. To a lesser extent, excited H2 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. We estimate the thermal pressure and the size of the small irradiated dense structures from the CO and ^{13}CO data. This study strongly supports the high pressure PDR model of Joblin et al. (in prep.).

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Astrochemistry simulated in electron-irradiated CO_2/NH_3 ices

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Key Words: *radiation processing; low energy electrons; X-ray photoelectron spectroscopy.*

Introduction

Abundant low energy secondary electrons are produced in astrophysical or planetary ices b y the various ionizing radiation fields encountered in space environments, and may thus play a role in the radiation processing of such ices [1]. One approach to simulate their astrochemical effect is to irradiate nanometer thick molecular solids of simple molecular constituents in ultra-high vacuum (UHV) with energy selected electron beams, and to monitor changes in film chemistry with surface analytical techniques [2]. Of particular interest is the formation of HCN, which is a signature of dense gases in interstellar clouds, and is ubiquitous in the ISM. Moreover, the chemistry of HCN radiolysis products such as CN− may be essential to understand of the formation of amino acids [3] and purine DNA bases.

Results and Discussion

Here we present new results on the UHV irradiation of cryogenic (22 K) multilayer films of CO2 and NH3 with 70 eV electrons, leading to CN, and other new bond formations. Mass resolved electron stimulated desorption yields of cations and anions are recorded as a function of electron fluence. The prompt desorption of cationic reaction/scattering products [4] is observed at low fluence. Detected ions that suggest formation of new chemical species include C2+, C2O2+, C2O+, CO3+, C2O3+ or CO4+ from pure CO2, and N+, NH+, NH2+, NH3+, NH4+, N2+, N2H+ from pure NH3, and NO+, NOH+ from CO2/NH3 mixtures. Most saliently, increasing signals of new negative ion products desorbing during prolonged irradiation of CO2/NH3 films included C2-, C2H-, C2H2-, as well as CN-, HCN- and H2CN-. The identification of product ions was aided by using 13CO2 and 15NH3 isotopes.

Conclusion

The chemistry induced by electrons in pure films of CO2 and NH3, as well as mixtures with composition ratios (3:1), (1:1), and (1:3), were studied by X-ray photoelectron spectroscopy (XPS). The XPS results show that electron irradiation of CO2/NH3 mixed films produces new chemical species containing C=O, O-H, C-O, C=N and N=O bonds.

Acknowledgments: Work funded by NSERC

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The effect of molecular environment on infrared properties of embedded species in astrophysical ices

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Key Words: dielectric constant; interstellar ices; PCM; theoretical chemistry; vibrational spectroscopy.

Introduction

In interstellar medium, the astrophysical ice mantles over dust grains surface can vastly vary in composition. For some cases, species of interest are extremely diluted in the icy matrix containing them. Besides solid water, the most constituent of such matrices are also CO_2, CO, CH_3OH, CH_4 or even SO_2 [1], among others, and a combination of them. As a first approximation, the net effect of the solvent medium (solid matrix) in a given chemical species which is there embedded can be accounted by simply considering the presence of an average electric field surrounding this species, this field being parameterized by the dielectric constant (ε) of the medium. This level of description can be achieved employing Polarized Continuum Model (PCM) approach [2], which is commonly implemented in Computational Chemistry packages. In this work one evaluates through vibrational analysis how the chemical environment influences some features of molecular infrared (IR) spectrum profiles, specifically, the peak positions and their respective intensities, of some trial molecules, such as CO, NH_3 and SO_2. All Calculations are performed at Second-order Møller-Plesset perturbation theory (MP2) level, with cc-pVTZ basis set. The different matrices (ice bulk) of astrophysical ices are simulated using different dielectric constant values representing different ice compositions at PCM approach. The ice temperature is also taken in account implicitly, since it is known it affects the dielectric constant of the ice bulk.

Results and Discussion

Preliminary results show that a gradual variation of ε leads to significant changes in the IR spectrum, for both frequencies and intensities, which are sign and magnitude dependent on the vibrational modes. An interesting feature of intensity variation is to be proportional to the change on band strength, which in turn plays an important role in the calculation of the absorption cross section, molecular property of major astrophysical interest.

Conclusion

This study will probably help us to achieve a better understanding of some astrophysical ices properties and their interaction with radiation, since from the IR spectral profile of diluted species it is expected to one to infer physical and chemical properties of the surrounding medium.

Acknowledgments:
The authors would like to thank the Brazilian agencies FAPESP (JP2009 / 18304-0) and CAPES.

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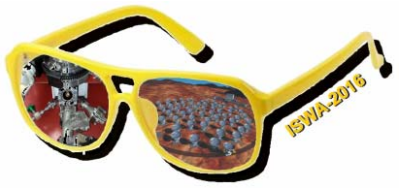

Abstracts of Posters

(in presentation order)

Spectroscopy of Linear Interstellar Carbon Chains and their Isotopologues: Archiving Experimental Uncertainty

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Key Words: *spectroscopy; astrochemistry; carbon chains; isotopologues; "U" lines.*

Introduction

Linear carbon chains remain the dominant theme in interstellar chemistry among the different classes of interstellar molecules. These set of molecules [C_n, H_2C_n, HC_nN, HC_nNC, HC_nO, HC_nS, $CH_3(C{\equiv}C)_nCN$, $CH_3(C{\equiv}C)_nH$, and C_nX (X=N, O, Si, S, H, P, H^-, N^-)] account for more than 20% of all the known interstellar molecules. Their continuous astronomical observation depends on the availability of accurate spectroscopic parameters. Providing these parameters has been the research interest of many groups. However, the unstable nature of some of these linear carbon chains, radicals and ions makes it difficult for the laboratory measurement of their rotational spectra needed for their astronomical observation. Theoretical predictions of spectroscopic parameters have been instrumental for probing molecules both in the terrestrial laboratory and in interstellar medium (ISM). But accurate predictions are not easily archived by most of the commonly used methods.

Results and Discussion

Theoretically calculated moments of inertia coupled with reported experimental rotational constants have been employed to predict accurate spectroscopic constants for these systems within experimental uncertainty. With three to four experimental data, accurate rotational constants within the experimental uncertainty of few KHz are obtained for the chains of interest. The observed correlation between the rotational constants of the linear carbon chains and their corresponding isotopologues is utilized for estimating accurate spectroscopic parameters for the isotopologues of the different linear carbon chains examined.

Chain	B_{exp} (MHz)	B_{cal} (MHz)	ΔB (MHz)
$HC_{15}N$	71.950133	71.939598	0.010535
$HC_{17}N$	50.703230	50.695964	0.007266
C_9O	222.72006	222.725727	0.005667
$CH_3(CC)_5H$	210.23883	210.243464	0.004634
$CH_3(CC)_6H$	129.07609	129.082687	0.006597
$CH_3(CC)_7H$	84.8622	84.866072	0.003872
HC_8N	398.547430	398.537714	0.009716
$CH_3(C{\equiv}C)_4CN$	208.736990	208.745338	0.008348
$CH_3(C{\equiv}C)_5CN$	128.072300	128.079621	0.007321

$(B_{exp}/B_{cal})_{carbon\ chain} = (B_{exp}/B_{cal})_{isotopologue}$

Conclusion

These accurate spectroscopic paramters obtained via this inexpensive appraoch could guide successful observation of some the linear carbon chains with no experimental paramters and could also be used in reducing the "U" lines some of which could be corrsponding to the isotopologues of the known carbon chains. These results will be highlighted in the poster.

Acknowledgments:

EEE acknowledges a research fellowship from the Indian Institute of Science, Bangalore.

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Where are the Galactic radionuclides? Toward a dynamical approach of r-process elements distribution

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Key Words: *Galactic chemical evolution; r-process elements*; *binary neutron stars*.

Introduction

Short- and long-lived radionuclides are required to sustain geodynamical processes in rocky planets and probably exomoons. The existence and persistence of life in those bodies critically depend on those processes. In Earth ~60% of the total energy emerging from the interior of the planet comes from the decay of Potassium, Thorium and Uranium (Fiorentini et al. 2005, Murthy et al. 2003, Gando et al. 2011). This energy maintains plate tectonics and critical geochemical cycles. When assesing the question of how many ”habitable” or even ”inhabited” planets are in the Galaxy, we need to also ask for how many radionuclides and how they are distributed across the Galaxy. Planetary critical radionuclides, are produced via neutron capture processes, especially rapid processes, r-processes (Hillebrandt 1976). Those processes happens in neutron-rich and energetic environments that seem to be uncommon in core collapse supernovae. It has been calculated that important amounts of those elements are created in the relatively uncommon neutron-star mergers (Just et al. 2014, Shen et al. 2015, Mateucci et al. 2013, Argast et al. 2004). Starting with this hypothesis the of r-process elements distirbution have been estimated using different theoretical approaches, from semi analytical cosmological simulations (Shen et al. 2015) to inhomogeneous chemical evolutionary models (Whemeyer et al. 2015). In this work we asses the problem through a Monte Carlo and dynamical simulations.

At testing Galactic chemical evolution models, comparisons with observations play a key role. The r-process elements are commonly detected through measurements of Europium (Eu) abundances.This detection is due to the characteristic absorption lines of Eu near 4130 Å (Barklem et al. 2005). In our case,we compare the amounts of r-process elements produced by neutron star mergers with the Eu solar abundances and other objects in the Solar System. Our model must explain the abundances in the Solar System and in stars around the solar neighborhood (Aoki et al. 2003). We note that the meteorites abundances help us in refining the measurements made on the Sun (Lodders 2008)

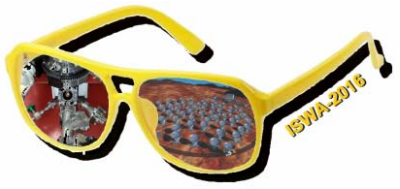
Results and Discussion

We generated synthetic population of neutron star binaries with gravitational waves emision decay timescales smaller than the age of the Galaxy. We integrated the orbits of those binaries in the static potential of the Milky Way taking into account the effect of kicks during the supernova explosions. The distribution of Neutron-star mergers in the Galaxy has been computed and used to seed an SPH simulation intended to calculate the density of r-process elements across the galactic disk. We found that the resulting distribution does not match that of normal supernova progenitors which synthetizes most of the metals and other s-process elements required for the formation and evolution of planets and life. Our results are consistent with those obtained with independent techniques and also with observations. Our method is particularly advantageous since we do not rely on assumptions of the distribution and rate of neutron star mergers, but on the contrary it applies robust models regarding the spatial distribution of high mass-stars and their expected properties and evolution (Portegies & Yungelson 1998).

Conclusion

The distribution of metals in the Galaxy is key to asses the distribution and properties of planets around the stars in the Galaxy. Although most of the heavy elements that constitute rocky planets and moons come from core collapse supernova, which follow the distribution of stars and gas in the Galaxy, key radionuclides, essential to sustain geodynamical processes and hence habitable conditions, are produced in somewhat ”exotic” processes, whose distribution is very different from that of normal heavy elements progenitors. Our results are a key ingredient to evaluate the distribution of potentially habitable planets and hence life in the Galaxy.

Acknowledgments: We want to thank Simon Portegies-Zwart for insightful discussions regarding our methods. We alsothank Brad Gibson and Marco Pignatari for useful comments



Looking for an Optimal Place in Colombia to Locate an Astronomical Observatory for Milimetric and Submilimetric Wavelengths

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Key Words: millimetric and submillimetric wavelengths*; water vapor*; *Radiation; Relative Humidity*.

Introduction

We analyze maps of incident radiation, relative humidity and cloud coverage in Colombia to evaluate the viability of locating an astronomical observatory for millimetric and submillimetric wavelengths. The data is taken from NASA (for incident radiation, cloud coverage and relative humidity) and IDEAM (for relative humidity and altitude over sea level) databases which cover 22 and 29 years respectively. The analysis is performed in four steps. First, we obtain radiation incident and cloud coverage maps each from the NASA database. Second, we validate these results by comparing them with those obtained via satellite and in situ. Third, we determine those regions showing the best conditions for astronomical observations, in the desired wavelength range, according to every single analyzed variable. And fourth, we overlap all the favorable regions to find the optimal location for a mm/sub-mm wavelength astronomical observatory, which postulates the east of the Colombian Caribbean region as a potential candidate.

Results and Discussion

Averaged normal direct radiation, relative humidity and cloud coverage along the Colombian land have been analyzed according to results reported in Refs. [1, 2]. In general, the tropics have a significant amount of atmospheric water vapor, which limits the visibility required for modern astronomical research in the optical, and probably in the mm/sub-mm wavelength ranges. For this reason we want to evaluate potential sites for a future antenna operating at millimeter or sub-millimeter wavelengths that can be used for VLBI observations. In order to do this, we want to measure the main variables that affect atmospheric absorption at these wavelengths; most importantly the water vapor column above a potential site. We propose that it is possible to correlate cloud coverage fraction, relative humidity and water vapor satellite measurements first in a coarse grid on a map of Colombia and later with a finer grid to pinpoint an ideal location, or at worst a “least bad” location for a mm/sub-mm observatory.

Conclusion

The Caribbean Colombian region, especially the department of La Guajira, is postulated as the candidate zone for astronomical applications for three reasons:

1. High levels of incident radiation.
2. The clearest day sky along Colombia.
3. Lowest relative humidity.

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Decomposition of formaldehyde and its relevance in chemical evolution

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Key Words: *comets, formaldehyde, high-energy radiation*

Introduction

Comets have been studied due to the large contain of organic molecules with biological importance, like formaldehyde. There is also evidence that formaldehyde is a precursor of sugars. The sugars are important in all forms of life that we know because, they are part of DNA and RNA and other molecules to storage energy.

This work is focused in evaluating some space conditions (low temperature, high-energy radiation and mineral composition) in ice analogous, regarding the formation and stability of formaldehyde and its conversion to organic molecules with biological importance.

Results and Discussion

To this end, formaldehyde solutions (1.1%) were exposed to different irradiation doses (8.29 to 159.58 kGy), the unreacted formaldehyde and the formation of other molecules by the irradiation were analyzed by GC and HPLC-MS.

Our results demonstrated that gamma radiation promotes decomposition of formaldehyde. The destruction of formaldehyde is dose-dependent, for example, 23% was destroyed with doses of 80 kGy). The pH of the solution changed abruptly, from 6 in unirradiated solutions to pH 2.5 with an irradiation doses of 80 kGy. This change suggests the formation of formic acid.

Conclusion

The analysis by HPLC-MS confirmed the apparition of formic acid after of expose to radiation and other molecules also were detected. Further studies will be performed at low temperature and in the presence of mineral surfaces.

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The X-ray effects in Astrophysics Ices containing Formic Acid: Implications in the Chemistry of Star Forming Regions

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Key Words: astrochemistry; molecular data ; methods: laboratory: molecular ; spectroscopic – ISM: molecules

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Since it was detected toward SgrB2 [1], formic acid (HCOOH) has been studied in laboratory experiments simulating star formation environments. This is one of the few molecules that can occur in star formation environments in the solid and gaseous phases. The formic acid was observed in several astronomical sources, such as comets, ice protostellar, chondrite meteorites, dark molecular clouds and some massive star-forming regions (Sgr B2, Orion KL and W 51) [2]. In interstellar medium (gas and grains), under action of ionizing many agents, which can cause changes in its molecular structure, formic acid is a possible precursor of pre-biotic species such as Glycine (NH_2CH_2COOH) [3].

We study the physical and chemical effects produced by radiation interaction synchrotron (broadband soft X-ray combined with a small fraction of photons in the ultraviolet vacuum) in pure formic acid and a binary mixture with water (1:1). With these experiments promote a simulation of photochemical induced energy photons in ice in the vicinity of young stellar objects.

This study can become wider in order to promote a better understanding of photofragmentation processes and formation of complex biomolecules. Among the results found the formation of different daughter species (CO, CO_2, H_2O, HCO) as the cross-sections of destruction and formation of molecules were also calculated. The results show an increase in dissociation of the molecules of the cross section with the presence of water in the mixture. With the utilization of the average cross sections for destroying the positions of the vibrational modes of the molecule HCOOH, we calculated as $4.2x10^{-18}cm^2$ the value for the sample of pure ice and $1.2x10^{-17}cm^2$ for binary mixture with water.

These results were 3 to 5 orders of magnitude smaller than the measures employed using cosmic rays and similar experiments with samples [2,3], this shows that X-rays have much smaller cross-section than UV photons can penetrate and larger columns, showing to be more efficient. [4].

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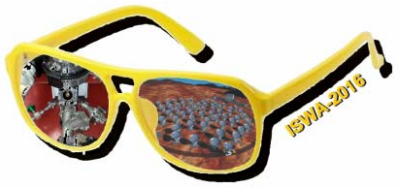

CH_4 ice laboratory studies relevant to Titan and icy bodies in the Solar System

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Key Words: Astrochemistry – molecular data – methods: laboratory – ISM: molecules - ISM: cosmic rays

Introduction

In various icy bodies in the Solar System it was observed the presence of CH_4. For example, it is a important components in the amosphere of Saturn's moon Titan, as well as of the icy surfaces of others planetary satellites as Triton, Neptune's satellite, and also present on the surface of Pluto. This compound is highly exposed to ionizing and exciting radiation such as UV photons and cosmic rays, which may cause changes in the molecular structure, thus leading to formation of new species.

Here, an experimental study of the interaction of highly energetic ions (15.7 MeV $^{16}O^{5+}$) with pure CH_4 ice, astrophysical ice analogs, at 16 K is presented. The experiment with ions was performed at Grand Accélérateur National d'Ions Lourds (GANIL) located at Caen, France. Briefly, the gaseous sample was condensed over a clean ZnSe substrate inside an ultra-high vacuum chamber and exposed to the ionizing source (energetic ions). In-situ sample analyses were performed by a Fourier transform infrared spectrometer at different fluences.

This study focuses, mainly, on the determination of the cross sections of destruction and net production of the species with astrophysical implications for the chemistry around icy bodies inside of Solar System.

Results and Discussion

Some intense peaks of CH_4 were identified in the infrared spectra (at 1304 cm^{-1} and 3018 cm^{-1}), as well as minor peaks of this molecule at 2821 cm^{-1} e 3855 cm^{-1}, which were also identified in the works of Moore and Hudson (2003), and Kaiser & Roessler (1998), for example. The infrared spectra also presented new molecular species such as C_2H_2, C_2H_4, C_2H_6, C_3H_8, and others. The destruction cross section of the parental specie CH_4 was determined, as well as the formation cross-sections of the selected daughters species: CH_3, C_2H_2, C_2H_4, C_2H_6, and C_3H_8.

Conclusion

We have performed an experimental study of the interaction of highly energetic ions (15.7 MeV $^{16}O^{5+}$) with pure CH_4 ice. The results demonstrate that irradiation of ice contending CH_4, similar to the ice astrophysics, by this projectiles leads to production of many molecules (for example C_2H_2, C_2H_4, C_2H_6, C_3H_8, and others).

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The stability of hydrogenated PAHs in circumstellar environments

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Key Words: *PAHs; Benzene; Hydrogenated*; *Planetary Nebula.*

Introduction

Polycyclic aromatic hydrocarbons, (PAHs), constituted by benzene rings, as well as hydrogenated PAHs (Hn-PAHs), compounds with excess peripherals H atoms, emit infrared bands (3-12 μm) due to the vibrational transitions. These molecules are present in different astrophysical environments. For example, the band at 3.3 μm, assigned to vibration of aromatic C-H bonds, is generally accompanied by the band at 3.4 μm, assigned to vibration of aliphatic C-H bonds. The abundances of these aromatic and aliphatic molecules in interstellar and circumstellar environments depend on the rates of formation and destruction by UV and X-rays radiation.

Methodology

We study experimentally the photoionization and photodissociation of hydrogenated Benzene, the Cyclohexane molecule (C_6H_{12}), using synchrotron radiation at UV (10-100 eV) and soft X-ray (280-310 eV) energies and the time-of-flight mass spectrometry. The measurements were performed at Brazilian National Light Synchrotron (LNLS) using the toroidal grating monochromator (TGM) beamline. From the mass spectra of ionic fragments produced by the interaction of photons with the molecule in gas phase, the production for each ion was quantified as a function of the photon energy. Moreover, the stability of the Cyclohexane and Benzene (C_6H_6) molecules was analyzed by the identifications the ions formed.

Results and Conclusion

It was observed a greater production of ions such as the ethyl group (C_2Hn^+) and propyl group (C_3Hn^+), products of the photodissociation of C_6H_{12} molecule. In addition, we also observed the formation of important ions to circumstellar chemistry, H_3^+ and methyl ion CH_3^+, possibly by molecular rearrangements. We determined the photon flux as a function of the energy in the photodissociation region (PDR) of the planetary nebula NGC 7027, taking into account the attenuation caused by the H and the dust grains. From these photon flux values and the photoionization and photodissociation cross-sections, the ionization and destruction rates of the Cyclohexane and Benzene were determined. We concluded that the aromatic structure is much more stable than the aliphatic structure against UV and X-ray radiation emitted by the central star in photodissociation region of this nebula.

Acknowledgments: CNPq, CAPES, LNLS

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Molecules in the Large Magellanic Cloud

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Key Words: *H II regions; ISM: molecules*; *galaxies: ISM; Magellanic Clouds*.

Introduction

The Large Magellanic Cloud (LMC) is a gas rich environment with reduced metallicity (Z about half of the Galactic value) that allow us to study star formation in an interstellar medium (ISM) that may be comparable, to certain degree, to those conditions of some star-forming sites in our Galaxy in the early stages (see for example Yamada et al. 2013).

We have studied the ISM towards the HII regions N113, N159-W, N166, and N132 in the LMC using molecular lines observations obtained with the Atacama Submillimeter Telescope Experiment (ASTE) with an angular and spectral resolutions of about 22" and 0.11 km s^{-1}.

This presentation is based on results presented in Paron et al. 2014 and 2015.

Results and Discussion

Several molecular lines: ^{12}CO, ^{13}CO, $C^{18}O$ J=3-2, HCO^+, HCN, HNC, C_2H J=4-3, and CS J=7-6 were successfully detected towards the molecular clouds associated with the HII regions N113 and N159-W. Additionally, centered at the peaks of the clouds, two areas of about 2.5' 2.5' were mapped in the ^{13}CO J=3-2 line. It is important to note that some of the observed lines represent the first reported detection towards these regions. In the case of the HII regions N166 and N132, only ^{12}CO and ^{13}CO J=3-2 were observed.

Based on the obtained integrated line ratios we studied the chemistry in the molecular clouds related to the HII regions. From a non-LTE analysis performed with RADEX using the results obtained from our observations and other lines from previous works, we derived some parameters for the physical conditions of the molecular gas.

Conclusion

We found that the chemistry involving the C_2H in compact and/or ultracompact HII regions in the LMC should be similar to that in Galactic ones. Concerning to the N113 and N159-W regions, we conclude that we are probing high-density and warm gas. In particular, the CO emission from N159-W arises from both, gas at 20 K with a density of about 1.5 10^4 cm^{-3}, and gas at 80 K and densities between 10^5 and 10^6 cm^{-3}. We also conclude that the molecular gas in these regions should be affected by star-forming processes. Respecting to N166 and N132, we conclude that the physical conditions should be similar in both regions, which are not so dense and warm as N113 and N159-W.

Acknowledgments:

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A Study of Organic Molecules Formation in the Interstellar Medium

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Key Words: Astrobiology; *Organic Molecules*; PAHs; *ISM*.

Introduction

This work presents the study of some molecules of the interstellar medium that could be useful for the bookkeeping of the organic content of the universe and for the assessment of prebiotic conditions on Earth and in other environments in the universe. The Horsehead Nebula was chosen as test object because it is considered as an archetype for molecular clouds[1], and due the fact that it has been extensively studied in several works.

Results and Discussion

The main tool used in the present work was the Meudon PDR code[2] due the fact that it is widely used as one of the legacy data analysis programs of current astronomy projects, e.g. the Herschel project, and it is public. The code can reliably model the Horsehead Nebula, since this object is a prototypic PDR (photodissociation region). We have updated the chemical sector of the code - at least a hundred more molecules - in order to test several scenarios of molecule production.

We derived the abundances of several molecules, including some of potential prebiotic importance and we investigated the role of PAHs. We explored production channels for astrobiologically relevant nitrogenated heterocycles, such as benzene[3], pyrrole and pyridine[4,5,6]. Moreover, we study the role of formamide in the formation of nuclesides. PAHs are important as intermediary species that favor the production of important prebiotic complex molecules, like pyridine. Furthermore, we have checked the role of the cosmic rays flux, within a scenario in which cosmic rays could raise the cation abundances, therewith increasing the abundances of complex molecules.

Conclusion

This presents simulations show us how the exploration of only a small number of possible paths of production of heterocycles already resulted in significants abundances at least one N-heterocycle species, pyridine. Systematic tours along other productions paths are expected to reveal more species with abundances high enough to be targeted in future observational surveys.

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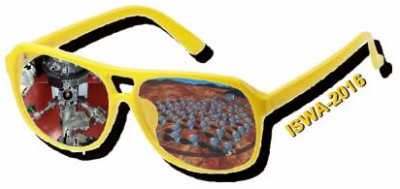

From Galaxies to Nanoscale

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Key Words: Fullerenes*; Graphenes*; Nanotechnology*; Nebulae*; *Spitzer Telescope*.

Introduction

In this article the reader will find a relation from macroscale, like the nebulae are in the Universe to nanoscale like in the real molecules. For example Fullerenes synthesized in laboratories here on Earth, were also discovered in space. We will discuss how they could be used in the future.

Results and Discussion

We believe that this environments are a special place of birth of large aromatic species like Polyclyc Aromatic Hidrocarbures (PAHS) and Fullerenes. Fullerenes have unique physical and chemical properties and their molecules detection and the identification of their formation are a priority in the interestellar organic chemistry field. With the Spitzer Telescope in August 2010 were detected Fullerenes C_{60} y C_{70} in the circumstellar media of Nebulae Tc1.

Conclusion

-Through molecules specters found in the Earth we can detect molecules in space.
-Thanks to technology we had discovered around 240 molecules in space using diferents technique like spectroscopy (IR and mass) and analysis in laboratories.
-Investigation of molecules in space will continue calling our atention like its applicability in the Earth awakening the curiosity and interest employing different technologies with purposes from astronomy, chemistry, physics, biology, geology, informatics, among others.
-Nanotechnology is nowadays important part of scienceo study that involves many sciences and confirm to do research showing we need an interdisciplinary integration.
-Use of clean energies can be applied in Telescopes or spaceships released to space using solar panels with carbon nanotubes and/or graphenes.

Acknowledgments:

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Water ices mixture in the outer Solar System: Spectroscopy and Physicochemical Effects

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Key Words: *Astrochemistry – circumstellar matter – clouds – molecules*

Introduction

The atmosphere of Titan, one of Saturn's moons, is rich in water and hydrocarbon molecules such as ethane (C_2H_6). The passage of energetic ions through the ice causes ionization which triggers chemical reactions. These reactions can be studied in laboratory by bombarding ice analogues with MeV ion beams. We carried out experiments on a C_2H_6:H_2O ice mixture radiolysis induced by fast heavy ions and monitored the chemical evolution by infrared spectroscopy (FTIR) [1]. The jet of the mixture vapor was directed towards a CsI substrate at 15 K where ~ 0.75 μm ice layer was formed. The film was bombarded by 40 MeV $^{58}Ni^{11+}$ ion beam delivered by the GANIL accelerator in Caen, France. FTIR analysis of ethane, water and molecular products was performed.

Results and Discussion

The ice thickness is thin enough that the layers are traversed by projectiles at constant velocity close to the equilibrium charge state. The induced C_2H_6 + H_2O reaction produces daughter molecular species: CH_4, C_2H_4, C_2H_2, C_3H_8, CO, CO_2, CH_2OH and CH_3OH. Their formation and dissociation cross sections are determined. The A-value used for cross section calculations is given by [1]. The value obtained for ethane is (1.9 ± 0.5) x 10^{-14} cm^2, which is close to the one obtained for Zn beam bombardment [1]. The carbon budget analysis of the mixture with its molecular products shows that the column density of carbon and oxygen atoms contained in the destroyed mixture by the ion irradiation is 30 - 50% larger than the sum of the column densities corresponding to the newly formed species.

Conclusion

As an astrophysical application, the C_2H_6 + H_2O dissociation cross-sections due to other ion beam projectiles and energies are determined, assuming validity of the $\sigma_d \propto S_e^{3/2}$ power law. As a consequence, the predicted values of the integrated dissociation rates confirm the importance of nickel and other heavy ion constituents of cosmic rays in astrochemistry.

Acknowledgments:
The agencies CAPES, CNPq (INEspaço) and FAPERJ (E-110.087/2014) for partial support.

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APUAMA: A Software Tool for Reaction Rate Calculations

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Key Words: Transition state theory; rovibrational levels; rate constant.

Introduction

This study aims to obtain the reaction rate of a reagents system, applying the tunneling correction of Wigner, Eckart and small curvature transmission coefficient, after that the rate is presented in the form of Arrhenius. In that way, we can determine the reaction rate over a wide range of temperature involving different chemical species in space, such as reaction type CO+CO in high rovibrational level, important in the Mars atmosphere, reaction type od $CN+C_2H_4$, common in the Titan atmosphere, and so on. The program developed is named APUAMA, that means "fast" in Tupi-Guarani. The code has a graphical interface for calculations of reaction rates.

Results and Discussion

Figure 1(a)

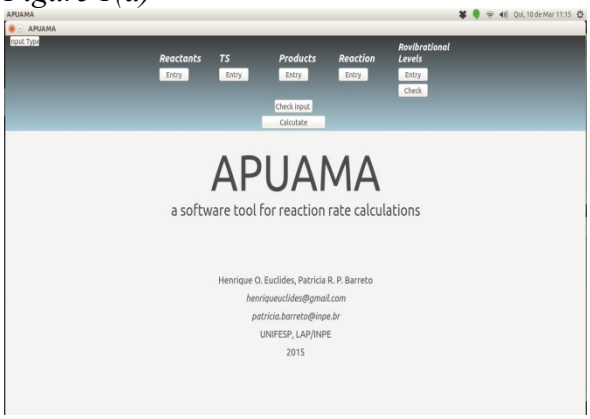

Figure 2(b)

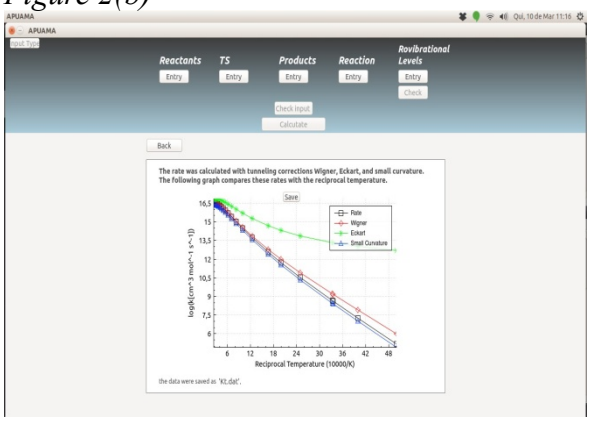

Figure 1(a) shows the initial page with the buttons for data entry and information while Figure 1(b) shows a example of the rate constant calculated as a function of the reciprocal temperature, the rate constant in the figure is plotted as Log(k).

Conclusion

Our goal was to develop a simple code of self explanatory graphical interface, easy to use and obtain quick results for determining the reaction rate for general systems. The code developed allows us to calculate the rate of bimolecular and unimolecular systems, taking into account rovibracionais levels of diatomic species. The outputs of the program are tabulated and saved as text file, and images can be saved to .bmp file.

Potential Energy Surfaces for Interactions of H_2O…HX Systems, with X = H, F Cl or Br, using a Hyperspherical Harmonics Representation.

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Key Words: *Potential Energy Surfaces; H_2O…HX Systems*; *Supermolecular Approach; vdW*; *Rydberg Function*.

Introduction

The long-standing problem in astrochemistry is to explain how molecules can form in a highly diluted environment, such as the interstellar medium. One explanation for this would be vdW clusters. In that way we propose a potential energy surface for interactions of H_2O...HX systems, with X = H, F, Cl or Br atoms, via harmonic expansion functional depending on the distance between the centers of mass of the two molecules and on four angles, assuming that the two molecules are rigid[1-3], account for two contributions: an external one depending on the three angle variables which define the mutual orientations of the two molecules and an internal one expressed by the angle which describes the positions of the oxygen atom in H_2O with respect system.

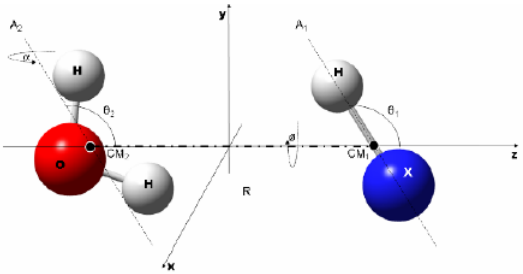

Figure 1. The mutual position of the H_2O and HX molecules is expressed by five coordinates in the Cartesian coordinate framework *xyz*.

Potential Energy Surface (PES)

$$V(R;\alpha,\theta_1,\theta_2,\varphi)=\sum_i w_i(\alpha)\sum_{L_1,L_2,L}\begin{pmatrix}L_1 & L_2 & L\\ m & -m & 0\end{pmatrix}v^L_{L_1,L_2}(R)Y^m_{L_1}(\theta_1,\varphi_1)Y^{-m}_{L_2}(\theta_2,\varphi_2) \quad \text{with } \varphi=(\varphi_2-\varphi_1) \text{ and } L_1=L_2=2$$

Methods

The surface was generated in the framework of the supermolecular approach, using the counterpoise-corrected interaction energies at the CCSD(T), aug-cc-pVQZ level with the Molpro code. Comparisons with the atoms involved are presented and their features are discussed. The analytical form of the potential energy surfaces is constructed by fitting the energies to a fifth degree generalized Rydberg function[4] into the *ab initio* points.

Conclusion

The PES was computed for about one hundred points for each of the 27 leading configurations, whose number reduces to 23 because of symmetry properties. The results for the system reducing the computational cost simplifying the fitting of the potential energy surface. The isotropic energy were compared between similar systems and demonstrated interesting behavior that provide insights for future works.

Acknowledgments: The authors are grateful for the support given from the CAPES.

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Evidence for the Formation of Interstellar Ions in the Dissociative Photoionization Process of Carbonylsulfenyl Compounds in the 100-1000 eV Region.

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Key Words: *PEPICO; PEPIPICO; SYNCHROTRON; HCS^+; H_3^+*

Introduction

In this work we present a study of the dissociative photoionization of carbonylsulfenyl derivatives, XC(O)SY (X, Y: F, Cl, CH_3), by using multicoincidence time-of-flight mass spectrometry and synchrotron radiation in the S 2p, C 1s, Cl 2p, O 1s and F 1s edges. Total and partial ion yield spectra together with PEPICO and PEPIPICO spectra were measured.

Results and Discussion

The photofragmentation processes occurring under synchrotron radiation conditions are very interesting and varied. From the many species formed during the synchrotron experiments reported in the present work at least two call our attention, HCS^+ and H_3^+.[1-3] The thioformyl ion is not only one of the more than 140 species recognized in the interstellar medium up to date but one of the key species to understand the interstellar sulfur chemistry. Its C=S bond is extremely strong and the abundance ratio HCS^+/CS^+ observed in the interstellar medium was found to be unusually higher than the theoretical predictions. This is due to its low recombination energy (charge transfer reactions are inhibited therefore) and the relatively large proton affinity of CS which inhibits proton transfer from HCS^+ to most molecular species. The high stability of the interstellar HCS^+ ion can be observed over the whole range of photon energies analyzed in our work. The formation of H_3^+ is quite remarkable since three C−H bonds of the CH_3 moiety have to be broken and three new H−H bonds have to be formed. In contrast with the first remarked HCS^+, H_3^+ presents a high acidity. Its proton donor ability serves to initiate ion−molecule reactions in the interstellar medium. In this medium its formation is clearly dependent on both abundant H_2 and H_2^+ species. The production of H_3^+ via the photodissociation of interstellar methyl compound organic molecules like methanol, methylamine, and acetonitrile was also studied at the LNLS by using photoelectron−photoion coincidence techniques employing soft X-ray photons.[4]

Conclusion

The most intense PEPICO peak for the S 2p energy range corresponds to the HCS^+ ion. The contribution of HCS^+ in the PEPIPICO spectra is also significant. A comparison of the CH_xS^+ (x = 0-3) islands, for instance, appearing in different PEPIPICO spectra confirms the high stability of the HCS^+ species, now formed under synchrotron conditions.

Acknowledgments: CONICET, UNLP, ANPCyT, LNLS.

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Photofragmentation Study of the Acetaldehyde (CH_3CHO) at the Carbon and Oxygen K Edges.

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Key Words: Acetaldehyde, Photofragmentation, Mass Spectroscopy, PEPICO, PEPIPICO.

Introduction

In recent decades, due to the progress of astronomical observations, a lot of more complex organic molecules have been discovered in the interstellar medium, located millions of light years from Earth. One of these molecules is the acetaldehyde (CH_3CHO), which has great importance in astrophysics. It is considered a prebiotic molecule. According to some theories, these molecules have been formed in space and brought by comets and meteorites, giving rise to life on Earth. It would be related with the formation of biomolecules necessary for the generation and maintenance of life, like the nucleic acids (DNA and RNA) and proteins. Acetaldehyde was one of the molecules observed in Hale-Bopp comet using radio spectroscopic observations [1]. Other prebiotic molecules had also been studied by our group (see, for example, reference [2]).

Results and Discussion

This work presents an experimental spectroscopic study of the acetaldehyde, also known as ethanal (CH_3CHO). Our main purpose was to investigate the possible ionization and dissociation routes of this molecule. Therefore, as the ionizing radiation it was used the Brazilian Synchrotron Radiation Facility (LNLS), in Campinas-SP. The experiment was performed with photons in the energy range of soft X-ray at the SGM beamline. We have used the time of flight mass spectroscopy technique to measure coincidence of electrons with one (PEPICO) or two (PEPIPICO) ions. Initially, we have obtained the Total Ion Yield (TIY) spectra to find the energy of the main electronic transitions. From the PEPICO spectra in this energy region, we identified the fragments produced according to their mass to charge ratio. We have also obtained Partial Ion Yield (PIY) spectra for each ionic fragmentation as a function of the incident radiation energy. Analyzing the PEPIPICO spectra, we have determined the relative yield of ionic fragment pairs measured in coincidence. Finally, we have found the most probable dissociation paths of the acetaldehyde for the different photon energies.

Conclusion

We observed at the TIY spectra, both at the lower energy of the C (carbonyl) edge as at the O edge, a more intense peak assigned to the transition to a π* antibonding orbital. The other structures were assigned to excitations to Rydberg series orbitals. With the analysis of PIY spectra we identified the more produced fragments in each energy region. From the PEPIPICO spectra we assigned the delayed charge separation as the main fragmentation mechanism for most of the measured pairs.

Acknowledgments:
This work is supported by CAPES, LNLS and UFBA.

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L-Valine decomposition by H^+, He^+ and N^+ MeV ions

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Key Words: *FTIR; amino acid; radiolysis; cosmic rays*

Introduction

Valine (Fig. 1) is an amino acid that has been observed in extraterrestrial environments and in the Murchison meteorite [1]. The understanding of the abundance evolution of small organic molecules under ionizing radiation is relevant for models describing the spread out of prebiotics across the solar system or the Galaxy. Effects of MeV ions impinging on prebiotic molecules have been studied by FTIR at the PUC-Rio Van de Graaff Laboratory [2].

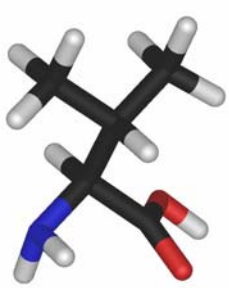

Fig. 1

Results and Discussion

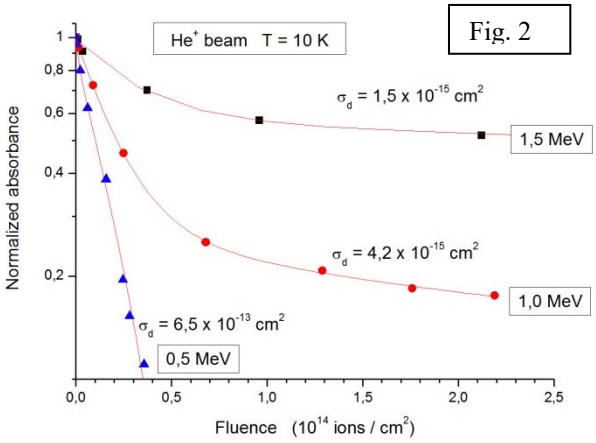

Fig. 2

Pure valine films, deposited by evaporation on KBr substrates, were irradiated by H+, He+ and N+ ion beams of 0.5, 1.0 and 1.5 MeV, up to a fluence of 10^{15} projectiles/cm^2. The sample damage was monitored by Mid-FTIR analysis. Typical results of the absorbance dependence on beam fluence are presented in Fig. 2. Solid lines represent two-exponential fittings; the indicated destruction cross sections (σ_d) correspondent to long fluence irradiation. It has been observed that higher is the beam energy, lower is the stopping power and lower is the σ_d value. The most abundant molecular daughter species is CO_2, which in turn, undergoes radiolysis into CO + O.

Conclusion

The main effects observed are: i) under irradiation, the valine column density decreases with cross sections in the 10^{-15} - 10^{-13} cm^2 range; ii) similar results were observed for all three ion beams.

Acknowledgments:
The agencies CAPES, CNPq (INEspaço) and FAPERJ are acknowledged for partial support.

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SuperMALT: Study of the Morphology and Kinematics of Dense Clumps

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Key Words: Astrochemistry – ISM: molecules - stars : formation - clumps: morphology

Introduction

We present the current status of SuperMALT which is a follow up of the MALT90 project which uses Mopra 22m telescope to observe 16 molecular lines near 90GHZ (mostly, J = 1 to 0 transitions) towards 3000 star forming clumps. SuperMALT uses APEX telescope to observe a subsample of 78 star forming clumps at different evolutionary stages (Pre stellar or Quiescent, Proto stellar and HII regions) in higher J transitions (J = 3 2 and J= 4 3) of different molecular species (e.g. N2H+, HCO+, HCN, HNC, H13CO+). Combining the low and high J transition line data, we aim to understand the physical and chemical properties of the clumps at different evolutionary stages. In this work, we present some early results on the morphology and kinematics of high mass star forming clumps of different evolutionary stages.

Results and Discussion

The clumps are mapped within a region of size 2'x2' in 8 different molecular lines using the on the fly (OTF) mapping technique. The angular resolution is ~20" and the velocity resolution ~0.1 km/sec. Contour maps of the velocity integrated line emission of different evolutionary stage clumps in 6 different molecular lines show similar morphology to that of the dust emission, with the HCO+(3-2) emission more closely matching the dust emission (870μm). The high transition lines [HCO+(4-3) & HCN(4-3)] clearly show that clumps typically exhibit substructures. We find the width of this line increases with evolutionary stage of the clump. On the other hand, the line profiles of the more evolved clumps (P & H types) are not Gaussian, but show features such as self absorption and line wings indicating they are either collapsing or expanding and presence of outflows.

Conclusion

We have studied the morphologies and line profiles of the clumps for different density tracers. We find the line width of the molecules increases towards evolved sources indicating the increase in turbulance. Combining the low transition data from MALT90 and the high transition data from SuperMALT, we will determine the physical properties of the clumps, such as temperature, density, column density and chemical abundance.

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The role of Population III stars in the chemical cosmic evolution

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Key Words: *chemical evolution; chemical abundance*

In this work we present the cosmic chemical evolution from redshift z = 20 to 0 for eight chemical elements: Oxygen (O), Iron (Fe), Zinc (Zn), Nickel (Ni), Chromium (Cr), Manganese (Mn), Cobalt (Co) and Titanium (Ti). We also present the value for the total metalicity of the Universe Z. The metodology consists in using a code that calculates the cosmic formation of structures considering the hierarchical structure formation scenario and using the Press-Schechter formalism (Pereira & Miranda 2010). The code effectively calculates the cosmic star formation rate and then considers a chemical evolution model with a formalism similar to the work first published by Tinsley (1972). In the preliminary phase of the work we considered yields of Population III stars published in the work of Heger and Woosley (2010) for masses between 140 and 260 $M_{\odot}$ and a Salpeter Initial Mass Function (IMF).

The model presented good theoretical values for cosmic enrichment of all the elements, with exception of Iron that shows a super-metalicity and Zinc that shows a sub-metalicity in comparison with data from Damped Lyman-α Systems (DLAs). Oxygen and Zinc have already been studied in this context (Vitti, 2012) showing good values for the cosmic enrichment of Oxygen in comparison with data from DLAs and sub-DLAs.

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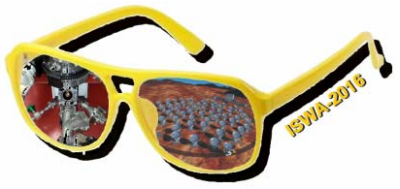

Construction and Surfaces and Potencial Energy of Diatomic Concern Ambiental, Astrophysiscist and atmospheric

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Key Words: *surfaces of potencial energy; diatomic molecules; spectroscopic*

Introduction

This work presented eight different models to describe surfaces of potential energy (SEP) of diatomic species, including the determination of spectroscopic properties using Dunham methodology [1]. These spectroscopy properties are important to determine the interstellar species detected by their microwave spectrum. The *ab initio* points were calculated via electronic structure code GAUSSIAN09 [2] and MOLPRO [3].

Results and Discussion

Sixteen diatomics neutral or charged system are studies [4]. The calculation were made in CCSD(T) using three diferents bases set, aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ. The results were adjusted for Generalized Rydberg, Bond Order, Morse, Lennard Jones, Improved Lennard Jones, Varshni, Tang and Toennies, and Tietz functions. The spectroscopic properties are compared with experimental data, when available, in order to specify the best fitting for the diatomic system.

Conclusion

This present work calculated the ab inito points using Gaussian09, determining the potential surface energy values (SEP) od diatomics species. The obtained values were accurate according to the Duham metodolody.

Acknowledgments: The authors are grateful for the support given from the CNPq.

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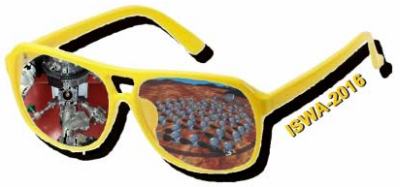

Molecules in the star formig region Sh2-39

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Key Words: molecules*; star formation* ; interstellar medium.

Introduction

Diverse studies show that massive stars are formed in dense regions (clumps and/or cores) inside giant molecular clouds (Bronfman et al. 1996)[1]. The formation process of high-mass stars is, however, still under debate (Garay & Lizano 1999)[2]. Studying and characterizing the molecular gas in star forming clumps during early stages of the formation of stars is necessary to understand the physical process that laed to the formation of massive stars.

To that end, we have analized CO(3-2) and HCO+(4-3) line data obtained with the ASTE telescope, aimed to find dense molecular clumps in the star forming region Sh2-39, and to study their physical properties. We have also used public far infrared images, aimed at studying the physical properties of the dust associated with the molecular gas.

Results and Discussion

We have identified 5 molecular clumps in the CO(3-2) and HCO+(4-3) lines, having IR counterparts, which suggests the existence of high-density molecular gas. Clumps are placed in the border of the HII region. Molecular masses of the clumps are in the range from 7300 to 1600 solar masses, and dust temperatues are in the range from 60 K to 25 K. We notice that densest (> 10^5 cm^-3) and hottest (60 K) clumps harbour a significant number of candidates to young stellar objects (YSOs).

Conclusion

Although results are very preliminary at this point, we can confirm the existence of dense and hot molecular gas in clumps near the ionization front of Sh2-39 were star formation is taking place. Further studies are necessary to go deep in this matter.

Acknowledgments:

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HIFI Automatic Line Identification Tool

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Key Words: *Herschel: HIFI*; *Line: identification*; *Astrochemistry*.

Introduction

The Herschel Space Observatory [1] was launched on May 14, 2009 equipped with 3 focal plane instruments, PACS, SPIRE and HIFI. HIFI, the Heterodyne Instrument for the Far Infrared [2,3] was designed to provide high spectral resolution spectroscopy (~$2x10^6$ to $2x10^7$) on a broad frequency range, 480-1272 GHz and 1430-1906 GHz. During the mission, hundreds of lines of sights have been observed in the 3 observing modes, pointed observations and OTF mapping modes providing 4 GHz bandwidth spectra or spectral maps around chosen frequencies, and spectral survey mode providing spectral surveys in broad ranges of frequencies.

Results and Discussion

In this work, we will present the tool used to automatically detect and identify the observed lines. This tool is a Jython task implemented in the Herschel Interactive Processing Environment (HIPE, [4]). All 69 sources available in the Herschel Science Archive (HSA), observed with the spectral survey observing mode, were analysed with this tool except the 2 very line rich ones, Orion KL and Sgr B2. We will present a statistical study of the observed species and lines as well as some considerations about the physical and chemical properties of the sources.

Conclusion

The catalog of species and identified transitions observed in all HIFI spectral survey observation will be distributed to the community along with the spectra of each observation. A general catalog of unidentified lines will also be distributed.

Acknowledgments:

These results are based on observations with *Herschel*/HIFI. *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA. CASSIS (http://cassis.irap.omp.eu) is a spectra analysis package developed at IRAP.

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Sodium and Potassium sputtering analysis from astrophysical silicates analogues

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Key Words: *Sodium & Potassium; Silicates*; *Sputtering*; *Astrophysics; Mercury.*

Introduction

Silicates are the dominant surface material of many Solar System objects (e.g. Moon, Mercury and main belt or near Earth asteroids), which are exposed to ion bombardment by solar wind and cosmic rays. Induced physico-chemical processes include sputtering which can contribute to the formation of an exosphere [1,2,3].

Results and Discussion

We measured sputtering yields and velocity spectra of secondary ions ejected from nepheline, an aluminosilicate thought to be a good analogue for Mercury's surface, as a laboratory approach to understand the evolution of silicate surfaces and the presence of Na and K vapor in the exosphere. Highly charged ion beams were delivered by the ARIBE (low-energy, keV/u) and SME (medium energy, MeV/u) beamlines of GANIL. Secondary ions emitted from thin nepheline films on Si substrates were detected using an XY-TOF-SIMS (imaging time of flight secondary ion mass spectrometry) device under ultrahigh vacuum conditions [3,4]. The projectile fluence dependence of sputtering yields gives information about the evolution of surface stoichiometry during irradiation. From the energy distributions N(E), the fraction of particles which could escape from the gravitational field of Mercury, and of those falling back and possibly contributing to populate the exosphere can be roughly estimated.

Conclusion

Energy distribution determination allowed us to analyze the emission process of Na^+ and K^+ when irradiated by swift heavy ions. Energies with maxima on the order of ~3 eV for Na and ~2 eV for K were found. From these distributions was also possible to estimate the escaping velocity of Na^+ and K^+ from Mercury's gravitational field. 85 % and 45 % of the emitted ions, respectively, may reach the exosphere. Concerning the interaction of slow heavy ions with nepheline, simulating solar wind, we observed that the composition and stoichiometry of the sample change along the irradiation: at the beginning, Na^+ is emitted more efficiently remaining almost constant until the end of the irradiation. Instead, K^+ yields increases nearly continuously. Therefore, we could say that K^+ emission varies more than Na^+ along the irradiation. This may explain the apparently non-uniform variations of Na/K ratio, which is due to several factors.

Acknowledgments:
The experiments were performed at GANIL (Caen, France). The region of "Basse-Normandie", the French-Brazilian exchange program (Capes-Cofecub) and the Brazilian agency CNPq (**INEspaço**) supported this work.

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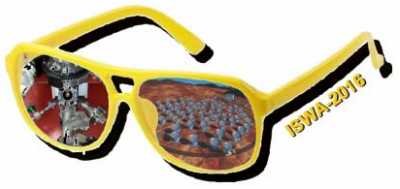

Molecular ionization, dissociation and desorption processes induced by photons and electrons in circumstellar environments.

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Key Words: *Astrochemistry; laboratory, dissociation*; *desorption.*

Introduction

The chemistry in circumstellar gas and dust particles around young stars (protoplanetary disks) or evolved stars (planetary nebulae) and in the solar system is strongly modified by the UV and X-ray photons and charged particles emitted from the central star. Molecules are ionized and dissociated leading to the formation of more complex organic compounds. Part of this processed material surrounding young stars ends up in the rotating disks where rocky and gaseous planets are formed, called protoplanetary disks. Due to the low absorption cross sections, X-ray photons coming from the central stars are able to penetrate deep inside cold and dense regions leading to ionization, dissociation and desorption of photo-products from icy molecules on grain mantles. The abundances of molecules depend on the mechanisms of their formation and destruction that can occur both in the gas phase and in the condensed phase on dust grain surfaces. In addition, non-thermal desorption from grain surface species may explain the relative high abundances of gaseous neutral or ionic species detected in cold environments.

Methods and Results

We have experimentally studied the interaction of electrons, UV and X-rays photons with organic molecules in the gas and condensed phases, analyzing the charged fragments by the time of flight mass spectrometry. The experiments using photons and electrons were carried out at the Brazilian synchrotron light source (LNLS) and at the Surface Chemistry Laboratory at Federal University of Rio de Janeiro (UFRJ), respectively. From photoionization and photodissociation cross sections (cm^2) values and the photon flux as a function of the energy (photon cm^{-2} s^{-1}) of a given object, we determined the respectively rates (molecules s^{-1}) and half--lives of molecules. For condensed molecules, the photodesorption and electron desorption yields were obtained. For example, we studied organic compounds such as benzene (C_6H_6) in the pre-planetary nebula CRL618 [1], methanol (CH_3OH) [2] and pyrimidine ($C_4H_4N_2$) [3] in the protoplanetary disk of TW Hydra and acetonitrile (CH_3CN) in solar system [4].

Conclusions

The formation, destruction of organic molecules and production of ions rates were obtained in some circumstellar regions. This study helped to understand how some molecular species are destroyed and formed qualitatively and quantitatively by determining their destruction rates, desorption ion yields, pointing out to the important role of ionic species in the evolution of molecular abundance and complexity of several astrophysics environments.

Acknowledgments: CNPq, CAPES, LNLS

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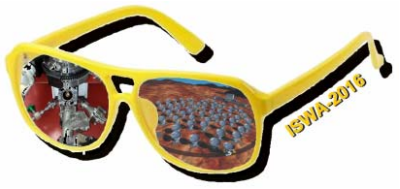

Processing of methanol ices by ionizing agents in simulation of astrophysical environments inside laboratory

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Key Words: Astrochemistry – Methanol ice – FTIR – Electron Bombardment – X-ray irradiation

Methanol CH_3OH is one of the most abundant organic molecules in various locations of the interstellar and the interplanetary medium. It was located in the solid state in comets wandering in interplanetary medium or in the solar system satellites (in smaller percentages - than 2% of the solid material of the body) like in Europe (from Jupiter), Enceladus and Titan (both of Saturn).

The present work aims to analyze the behavior of methanol molecule when subjected to ionizing radiation (electrons and X-rays)in astrophysical environments simulated in the laboratory. The experimental data were collected in two different environments: i) Bombardmnet with fast electrons carried out in methanol ice on LASA Laboratory (Laboratorio de Astroquimica e Astrobiologia da Universidade do Vale do Paraíba in São José dos Campos - SP); 2) Irradiation with X-rays realized with methanol ice at LNLS/CNPEM (Brazilian Synchrotron Light Laboratory located in Campinas - SP). In both experiments the methanol ice blocks were produced in-site inside high-vacuum chamber and exposed to radiation. The analysed was performed by infrared spectroscopy after different fluences. Details of the experiment setup is given by [1].

From the experiments, were determined the dissociation cross sections, the identification of daughters species such as H_2O and CO_2 and were estimated the half-life of solid methanol extrapolated to astrophysical environments. The experiments also helps to understand the role of secondary electrons in the processing of interstellar ice.

Acknowledgments:

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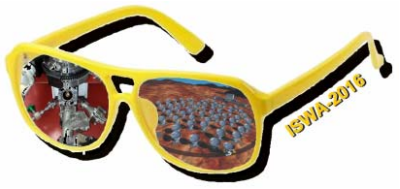

Study of degradation of Glycine in collisions with fast electrons and their applications in Astrobiology

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Key Words: Astrobiology, Astrochemistry; Prebiotic molecules; glycine; electrons.

We present here a research proposal to study the degradation of glycine molecule in condensed phase (solid) (+NH3CH2COO-) at different temperatures (12-300 K), similar to those existing in different spatial environments. The samples will be studied in two different ways (zwiterionic crystals of α- and β- type glycine), in the presence of fast electrons (100 to 1000 eV) to promote molecular degradation and formation of new species including possible peptide bonds.
The experiments will occur at the Astrochemistry Laboratory and Astrobiology LASA - UNIVAP. The sample will be deposited over clean ZnSe substrate and irradiated by electrons at diferent fluences and at different temperatures. The chemical analysis will be performed in situ by Fourier transform spectroscopy (FTIR) following the methodology described elsewhere [1]. A comparison with measurement employing other ionizing agents and at gas-phase will be also conducted [2, 3,4]. The destruction cross section and desorption yield will determined. The astrochemical and astrobiological implications on the survival of glycine in the interstellar medium and interplanetary medium will be discussed.

Acknowledgments
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HOTEL MAP

A - Hotel main entrance; B - Hotel reception; C - Restaurant;
D - Conference Hall (talks and posters); E - Conference Dinner (July 4th, Evening)

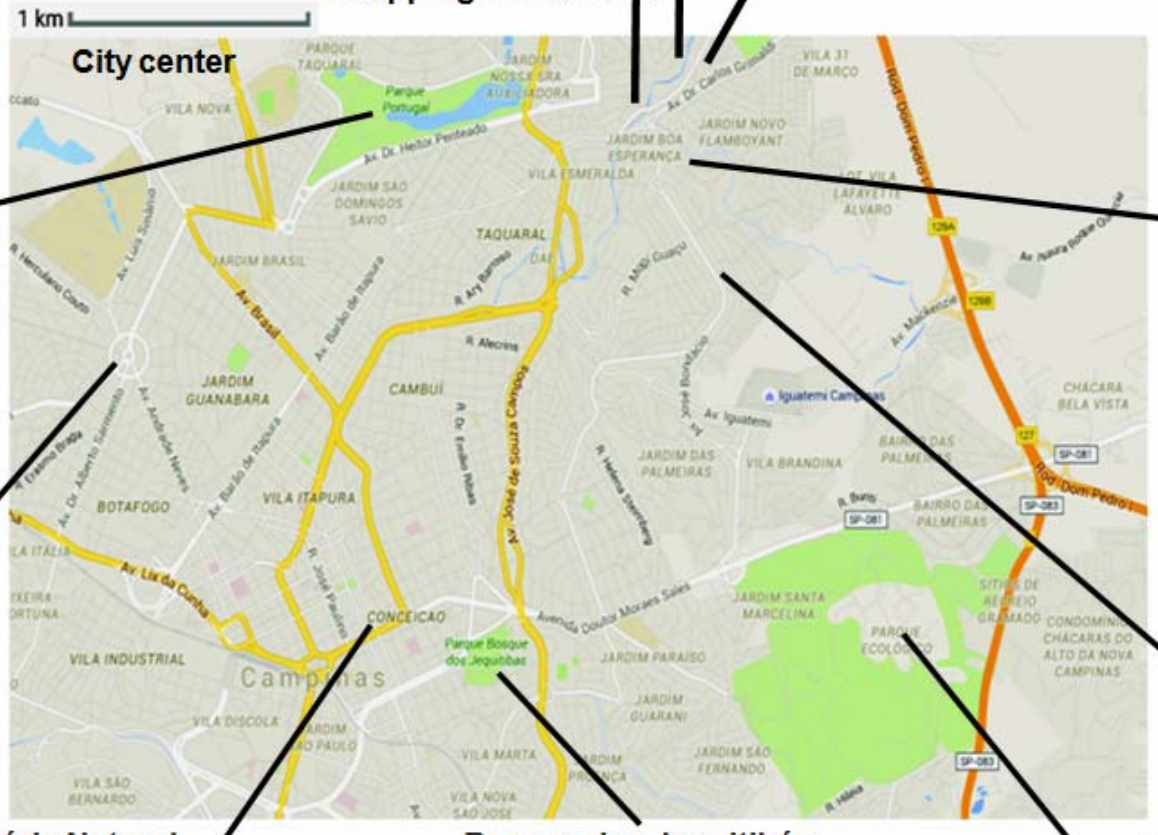
CAMPINAS Top Tourist Destinations

Parque Lagoa do Taquaral
(Lagoa do Taquaral Park)

Laboratório Nac. de Luz Sinctrotron
(Sinchroton light Source – LLS)

Shopping D. Pedro

Hotel Fazenda
Solar das Andorinhas



Jóquei Clube
(Jockey Club)

Torre do Castel
(Castle Tower)

Catedral Metropolitana
(Metropolitan Cathedral)

Museu de História Natural
(Natural History Museum)

Bosque dos Jequitibás
(Jequitibás Wood)

Parque Ecológico
(Ecological Park)