6th Workshop
of the Italian Astrobiology Society

Cosmos within us: life on Earth as a way to study its origin and distribution in the universe

29th – 31st October, 2018

Real Museo Mineralogico
Napoli, Italy

ABSTRACT
SIAW

Organic environments in the Solar System:
The heritage of the Rosetta, Dawn and Cassini missions.

F. Capaccioni

INAF- Istituto di Astrofisica e Planetologia Spaziali

In the last 20 years several primitive objects of the Solar System have been visited by a number of international space probes. In particular, **Cassini-Huygens** (NASA-ASI-ESA, launch: 1997), **Rosetta** (ESA cornerstone, launch: 2004) and **Dawn** (NASA, launch: 2007) have carried onboard a relevant hardware contribution by the Italian community and have generated a wealth of information and scientific results, which have changed the way we look at comets, asteroids, and satellites of the giant planets.

In the Solar System we found that most diverse environments constitute suitable places for the evolution of organic molecules and complex chemistry. Primitive bodies carry memory of the first phases of evolution of the Solar System. Comets are believed to be the most primitive bodies of the Solar System and one of them, the comet **67P/Churyumov-Gerasimenko**, has been the target of the ESA's cornerstone mission **Rosetta**. The instruments onboard Rosetta observed a nucleus poorer in water than previously thought (an estimate of 18-25% was derived, Fulle et al, 2016), a very uniformly dark surface with large abundance of darkening agents, such as iron oxide and polyaromatic macromolecular compounds of similar origin to the IOM found in carbonaceous chondrites (Capaccioni et al, 2015; Fray et al, 2016); we found that the comet has been assembled in a very cold environment (20-25K, Rubin et al, 2016) mixing minerals, whose formation required conditions found in the inner part of the nebula, and organic compounds formed in the outer reaches of the nebula and possibly of pre-solar origin.

The **Dawn** mission started its activity at the dwarf planet Ceres in 2015 and observed geomorphological evidence of a dry crust and of a water rich interior (about 20% water abundance by mass, Russell et al, 2016); Ceres experienced extensive water-related processes and chemical differentiation. The surface is mainly composed of a dark component (carbon, magnetite?), Mg-phyllosilicates, ammoniated clays, carbonates, and salts (De Sanctis, 2016). The observed species suggest endogenous, global-scale aqueous alteration. Few local exposures of water ice are seen, especially at higher latitudes (Raponi et al, 2017). Sodium carbonates have been identified in several areas on the surface, notably in Occator bright faculae. Organic matter has also been discovered in several places, most conspicuously in a large area close to the Ernutet crater (De Sanctis et al, 2017). The combined presence on Ceres of ammonia-bearing hydrated minerals, water ice, carbonates, salts, and organic material indicates a very complex chemical environment, suggesting favourable environments for prebiotic chemistry.

The **Cassini-Huygens** mission contributed hugely to the knowledge of the Saturnian system and its organic environments: from the complex chemistry active on the surface and atmosphere of its largest satellite Titan, to the complex chemistry active in Enceladus interior, to the presence of organic material of endogenous origin in the Saturnian rings (Ciarniello et al, 2019), to the primitive bodies, Phoebe, trapped by Saturn gravitational field (Castillo-Rogez et al, 2012, Cruickshank et al, 2008).

The presentation will provide a summary of the most relevant finding of the mentioned missions.

Nitrogen incorporation into aromatic rings in extraterrestrial environments: toward the formation of pyridine and nucleobases

Nadia Balucani,[1] Dimitrios Skouteris,[2] Adriana Caracciolo,[1]
Piergiorgio Casavecchia[1] and Marzio Rosi[3]

[1]DCBB - Università degli Studi di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy, [2]Master-up srl, Via Elce di Sotto 8, 06123 Perugia, Italy, [3]DICA - Università degli Studi di Perugia, Via G. Duranti 93, 06125 Perugia, Italy
E-mail: nadia.balucani@unipg.it

Gas-phase reactions involving atomic nitrogen in the ground ^{4}S and first excited ^{2}D electronic states with simple hydrocarbons or hydrocarbon radicals lead to the formation of prebiotic N-containing organic molecules. These reactions are now active in the upper atmosphere of Titan (a massive moon of Saturn) and might have played an important role in nitrogen fixation in the primitive upper terrestrial atmosphere. Their products (nitriles, imines and N-containing organic radicals) are the precursors of larger N-containing molecules, which form the dense haze aerosols that completely cover Titan. If anything similar to Titan's haze has ever existed on primitive Earth, it is reasonable to imagine that, once deposited on the surface of the oceans, further chemical evolution might have transformed these molecules into aminoacids and nucleobases, the molecular building blocks of living entities.[1]

In our laboratory, we have investigated the reactions of N(^{2}D) with several aliphatic hydrocarbons common in the atmosphere of Titan[2-4] and we have verified that products containing a novel C-N bond are formed, thus corroborating the suggestion that these gas-phase reactions allow for nitrogen fixation in organic compounds. More recently, we have turned our attention to N(^{2}D) reactions with aromatic hydrocarbons, namely benzene and toluene (both present in the upper atmosphere of Titan). The main results will be illustrated in this contribution, but we anticipate here that the most striking result is the formation of an aromatic compound, pyridine, where N is directly incorporated into the aromatic ring.[5]

References

1. N. Balucani (2012). *Chem. Soc. Rev.*, **41**, 5473–5483.
2. N. Balucani, A. Bergeat, L. Cartechini, G. G. Volpi, P. Casavecchia, D. Skouteris, M. Rosi (2009). J. Phys. Chem. A, **113**, 11138.
3. N. Balucani, F. Leonori, R. Petrucci, M. Stazi, D. Skouteris, M. Rosi, P. Casavecchia (2010). Faraday Discuss., **147**, 189.
4. N. Balucani, D. Skouteris, F. Leonori, R. Petrucci, M. Hamberg, W.D. Geppert, P. Casavecchia, M. Rosi (2012). J. Phys. Chem. A, **116**, 10467.
5. N. Balucani, D. Skouteris, A. Caracciolo, P. Casavecchia, M. Rosi (2018). Astrobiology, in preparation.

Role of Meteorites in the Prebiotic Chemistry of Nucleic Acids

R. Saladino,[1] B.M. Bizzarri,[1] L. Botta,[1] J. Šponer,[2] J.E. Šponer,[2] T. Georgelin,[3] M. Jaber,[3] B. Rigaud,[3] M. Kapralov,[4] G.N. Timoshenko,[4] A. Rozanov,[4] E. Krasavin [4]and E. Di Mauro.[1]

[1]*Department of Ecological and Biological Sciences, University of Tuscia, Viterbo, Italy*
[2]*Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno, Czech Republic.*
[3]*Sorbonne Universités, UPMC Paris 06, CNRS UMR 7197, Paris, France.*
[4]*Joint Institute for Nuclear Research, JINR's Laboratory of Radiation Biology, Dubna, Russia.*

E-mail: lorenzo.botta@unitus.it

In the consensus "RNA world" scenario framing the Origin of Life, the generation of nucleosides in abiotic conditions remains the major initial hurdle. The one-pot formation of nucleosides from formamide was reported[1] but without a detailed mechanistic insight into the sequence of contributing chemical events. The experimental set-up consisted of formamide, of meteorites as catalysts, and of a 170 MeV proton beam as energy source simulating the Solar Wind radiation. In these conditions the formation of cytidine, uridine, adenosine, and thymidine was observed without isolation and/or purification of specific intermediates, along with a variety of organic compounds including nucleobases (cytosine, uracil, adenine, guanine, and thymine), carbohydrates (noticeably, ribose and 2-deoxy-ribose), aminoacids and carboxylic acids. Formamide is among others the most intensively studied chemical precursor for prebiotic syntheses[2–5]. It has been detected in dense diffuse clouds, in interstellar space, in the galactic habitable zone[6], in comets[7] and satellites[8].The formation of nucleosides in abiotic conditions is a major hurdle in origin-of-life studies. We have determined the pathway of a general reaction leading to the one-pot synthesis of ribo- and 2′-deoxy-ribonucleosides from sugars and purine nucleobases under proton irradiation in the presence of a chondrite meteorite. These conditions simulate the presumptive conditions in space or on an early Earth fluxed by slow protons from the solar wind, potentially mimicking a plausible prebiotic scenario. The reaction requires neither pre-activated precursors nor intermediate purification/concentration steps, it is based on a defined radical mechanism, and it is characterized by stereo- and regio- selectivity.

References

1. R. Saladino, *et al.* (2015) *Proc. Natl. Acad. Sci. USA*, **112**, E2746–E2755.
2. R. Saladino, *et al.* (2012) *Phys. Life Rev.*, **9**, 84–104.
3. R. Saladino, *et al.* (2012) *Chem. Soc. Rev.*, **41**, 5526–5565.
4. M. Ferus, *et al.* (2014) *Proc. Natl. Acad. Sci. USA*, **112**, 15030–15035.
5. M. Saitta, *et al.* (2014) *Proc. Natl. Acad. Sci. USA*, **111**, 13768–13773.
6. G. R. Adande, *et al.* (2013) *Astrobiology*, **13**, 439–453.
7. D. Bockelee-Morvan, *et al.* (2000) *Astron. Astrophys.*, **353**, 1101–1114.
8. S. A. Benner, *et al.* (2012) *Acc. Chem. Res.*, **45**, 2025–2034.

Ion chemistry of complex organic molecules (COMs): from interstellar space to planetary atmospheres

Daniela Ascenzi

Department of Physics, University of Trento, Via Sommarive 14, Trento, ITALY
e-mail: daniela.ascenzi@unitn.it

Organic species containing carbon, nitrogen, and oxygen atoms with six or more atoms are denoted, in astrochemical jargon, as complex organic molecules (COMs). With the advent of unprecedented high resolution and sensitivity telescopes (*e.g.* ALMA, NOEMA) and challenging exploratory missions (*e.g.* Rosetta, New Horizons, Juice) the inventory of COMs detected in star-formation areas, proto-stars, proto-planetary discs as well as in comets and in the atmospheres of planets and satellites is becoming richer and richer. COMs are considered to be the missing link in the formation of prebiotic molecules, eventually leading to the synthesis of amino acids and other bio molecules. Hence, grasping their formation mechanisms is a step forward to unravel how matter evolved from an interstellar cloud into a planetary system and how life eventually developed on our planet.

Reactions involving ions have been frequently invoked as formation (and destruction) pathways for COMs both in the interstellar medium and in planetary atmospheres, but laboratory experiment on key reactions are still sparse. The contribution of the Molecular Astrophysics group at Trento University is in the laboratory measurements of kinetic parameters (cross sections, branching ratios and their dependences on collision energy) for the reaction of charged molecules with neutrals. The experimental set-up uses tandem mass spectrometric techniques and RF octupolar trapping of parent and product ions, in some cases coupled with VUV photoionization of appropriate neutral precursors to ensure the production of state-selected ions and/or isomer selectivity. A review of the recent activity on the reactions of He^+ with dimethyl ether and methylformate[1, 2] and on the isomer selected reactivity of $C_2H_2N^+$ cations with small hydrocarbons[3, 4, 5] will be presented.

References

1. A. Cernuto, F. Pirani, L.M. Martini, P. Tosi, D. Ascenzi (2018) *ChemPhysChem,* **19**, 51
2. A. Cernuto, P. Tosi, L.M. Martini, F. Pirani, D. Ascenzi (2017) *Phys. Chem. Chem. Phys.* **217**, 1463.
3. P. Fathi, W.D. Geppert, F. Lindén, A. Cernuto, D. Ascenzi (2016) *Molecular Astrophysics* **5**, 9-22.
4. P. Fathi, W.D. Geppert, A. Kaiser, D. Ascenzi (2016) *Molecular Astrophysics* **2**, 1-11.
5. P. Fathi, W.D. Geppert, D. Ascenzi (2016) *Int. J. Mass Spectrom.* **411**, 1-13.

A universal geochemical scenario for formamide condensation and prebiotic chemistry

Bruno Mattia Bizzarri[1], Lorenzo Botta[1], Juan Manuel Garcia-Ruiz[2], Ernesto Di Mauro[3] and Raffaele Saladino[1]

[1]Dipartimento di Scienze Ecologiche e Biologiche, Università della Tuscia, Via San Camillo De Lellis, 01100 Viterbo, Italy.

[2]Laboratorio de Estudios Crystalográficos, Instituto Andauz de Ciencias de la Tierra, CSIC-Universidad de Granada, Avenida de lasPalmeras 4, E-18100 Armilla, Granada, Spain.

[3]Istituto Pasteur-Fondazione Cenci Bolognetti c/o Dipartimento di Biologia e Biotecnologie "Charles Darwin", University "Sapienza",Piazzale Aldo Moro 5, Rome 00185, Italy.

E-mail: bruno004@hotmail.it

The condensation of formamide has been shown to be a robust chemical pathway affording molecules necessary for the origin of life. It has been experimentally demonstrated that condensation reactions of formamide are catalyzed by a number of minerals, including silicates, phosphates, sulfides, zirconia and borates, and by cosmic dusts and meteorites. In this scenario we have investigated the catalytic effect of the mineral self-assembled structures derived from serpentinization, a geological process widespread in the early stages of Earth-like planets, in the formamide condensation.[1] We found that these bilayer membranes, made of amorphous silica and metal oxide/hydroxide nanocrystals, catalyze the condensation of formamide, yielding the four nucleobases of RNA, different amino acids and, several carboxylic acids in a single-pot thermal experiment.[2] In addiction to the selective catalysis in the synthesis of prebiotic-relevant compounds the mineral structures create at the same time space compartmentalization, suggesting a geologically plausible scenario in the prebiotic chemistry.

References

1. Bruno Mattia Bizzarri, Lorenzo Botta, Maritza Iveth Perez-Valverde, RaffaeleSaladino, Ernesto Di Mauro, and Juan Manuel Garcia-Ruiz. (*2018*). *Chem. Eur. J.*, ***24**, 1 – 8*.

2. Raffaele Saladino, Giorgia Botta, Bruno Mattia Bizzarri, Ernesto Di Mauro and Juan Manuel Garcia-Ruiz (2016). *Biochem.*, ***55**, 2806−2811.*

SOLID-STATE FORMATION OF LIPID PRESURSORS UNDER DENSE MOLECULAR CLOUD CONDITIONS

Gleb Fedoseev[1], Ko-Ju Chuang[2,3], Carlotta Scirè[1], Danna Qasim[2], Giuseppe Baratta[1], Sergio Ioppolo[4], Ewine F. van Dishoeck[3], Maria Elisabetta Palumbo[1] and Harold Linnartz[2]

[1]INAF – Osservatorio Astrofisico di Catania, Catania, Italy
[2]Sackler Laboratory for Astrophysics, Leiden Observatory, Leiden University, Leiden, The Netherlands
[3]Leiden Observatory, Leiden University, Leiden, The Netherlands
[4]School of Electronic Engineering and Computer Science, Queen Mary University of London, London, UK
E-mail: gleb.fedoseev@inaf.it

Formation of star systems similar to the Solar System start with the gravitational collapse of an interstellar cloud comprised of gas and dust. In the densest regions of this cloud the temperature drops to as low as ~10 K, while the lifetime of the cloud is long enough to accrete most of the gas-phase material (with except of He and H_2) onto dust grain surface. This depletion of gas-phase species on the grain surface results in a rich chemistry triggered by atom- and radical-addition reactions between accreting species, UV-induced reactions, and interactions with cosmic rays. We present the results of a laboratory based research that aims to investigate how lipid precursors can be formed at this early stage of star formation [1, 2, 3]. We demonstrate that hydrogenation of CO-rich interstellar ice analogues results in the formation of molecules as complex as a three-carbon bearing sugar alcohol glycerol - a backbone of all lipids known as glycerophospholipid or triglycerides, a necessary component for the formation of membranes of modern living cells and organelles [4]. The proposed reaction mechanism holds much potential to form even more complex sugar alcohols or their corresponding simple sugars. The presentation is completed by the demonstration of two possible ways to form amphiphilic molecules with a long aliphatic chain under same conditions. Such amphiphilic molecules can either themselves participate in the formation of micelles in aqueous solutions, or form ether bonds with glycerol. Thus, the presence of these simplest lipid precursors on young planets is possible under the assumption that at least a fraction of the original icy-dust material survives upon transfer to the early planet surface or, alternatively, is delivered by comets or other celestial bodies during the late bombardment stage of the early Earth.

References

1. Caselli, P. & Ceccarelli, C. (2012). A&ARv, **20**, 56.
2. Linnartz, H., Ioppolo S., Fedoseev, G. (2015). Int. Rev. Phys. Chem., **34**, 205.
3. Sabri, T., Baratta, G., Jäger, C., *et al.* (2015). A&A, **575**, A76.
4. Rothard, H., Domaracka, A., Boduch, P. *et al.* (2017). J. Phys. B: At. Mol. Opt. Phys., **50**, 062001.
5. Fedoseev, G., Chuang, K.-J., Ioppolo, S., *et al.*, (2017), ApJ, **842**, 52.

Prebiotic chemistry – from structural and energetic perspectives

Judit E. Šponer,[1]

[1]Institute of Biophysics, Academy of Sciences of the Czech Republic,
Královopolská 135, CZ-61265 Brno, Czech Republic
E-mail: judit@ncbr.muni.cz

The formamide-based synthesis of nucleic acid components offers a new alternative for the origin of informational polymers.[1,2] This chemistry represents so far the only known prebiotic scenario, which outlines a continuous transition from a simple prebiotic feedstock molecule, formamide, up to the simplest catalytic oligonucleotides.[2] Since this multistep synthesis proceeds in a very complex reaction mixture, it is very difficult to study its mechanism using purely experimental methods. The presentation is aimed to illustrate that in such complicated cases computational chemistry might be instrumental to provide an atomic-level insight into the mechanistic details of the reactions. We show that the applicability of theoretical chemistry tools is not restricted to a simple verification of experimentally suggested reaction mechanisms, and, when properly done, computational methods can be used to propose mechanistic models on their own. This is especially important when experimental methods do not allow for obtaining accurate structural information on the reaction complexes under investigation.

I will illustrate how the energy-driven chemistry characterizing the earliest stages of abiogenesis could translate into a structure-driven chemistry with increasing molecular complexity. Whereas prebiotic synthesis of the building blocks of the first genetic molecules involves a less selective high-energy chemistry,[3,4] at higher levels of molecular evolution other aspects, like structural compatibility, become decisive.[5]

References

1. R. Saladino, G. Botta, S. Pino, G. Costanzo, E. Di Mauro (2012), *Chem. Soc. Rev.*, **41**, 5526-5565.
2. J. E. Šponer, J. Šponer, O. Nováková, V. Brabec, O. Šedo, Z. Zdráhal, G. Costanzo, S. Pino, R. Saladino, E. Di Mauro (2016), *Chem. Eur. J.* **22**, 3572-3586.
3. R. Saladino, B. M. Bizzarri, L. Botta, J. Šponer, J. E. Šponer, T. Georgelin, M. Jaber, B. Rigaud, M. Kapralov, G. N. Timoshenko, A. Rozanov, E. Krasavin, A. M. Timperio, E. D. Mauro (2017), *Sci. Rep.* **7**, 14709.
4. M. Ferus, D. Nesvorný, J. Šponer, P. Kubelík, R. Michalčiková, V. Shestivská, J. E. Šponer, S. Civiš (2015), *Proc. Natl. Acad. Sci. USA*, **112**, 657-662.
5. J. E. Šponer, J. Šponer, E. Di Mauro (2017), *WIREs RNA,* **8***,* e1400.

Climate bistability of rocky exoplanets

G. Murante, E. Palazzi, L. Silva, G. Vladilo, A. Provenzale

E-mail: antonello.provenzale@cnr.it

Earth System Models indicate potential bistability in the climate of our planet, with the set-up of a icehouse state or of a moderate temperature climate depending on initial conditions, for the same level of incoming solar radiation, orbital parameters and greenhouse gas concentration. This behavior was revealed for the first time, using simple Energy Balance Models, more than forty years ago. In such models, the main mechanism responsible for bistability is the so-called temperature-ice-albedo feedback.

In the past few years, our working group developed an ESTM (Earth-like planet Surface Temperature Model), a simple climate numerical model based on an Energy-Balance Model (EBM) for the meridional heat transport coupled with a radiative-convective atmospheric column model. Using ESTM, we performed a fast exploration of known and unknown exoplanet parameters, obtaining the surface temperature as a function of the period of the year and of latitude. In this way, we have determined for what planetary parameters climate bistability such as that of Earth is potentially present.

Here we discuss the preliminary results of this study when a set of four parameters, namely obliquity, eccentricity, semi-mayor axis and atmospheric pressure are varied in the ESTM, all the other parameters being kept fixed to the Earth's values. Some general comments on the role of bistability in planetary habitability are offered as well.

ACCURATE LABORATORY ROTATIONAL SPECTROSCOPY FOR THE DETECTION OF ORGANIC MOLECULES IN SPACE

Sonia Melandri,[1] Assimo Maris,[1] Camilla Calabrese,[2] Luca Evangelisti,[1] Wolf Geppert,[3] Sergio Mariotti,[4]

[1]Dip. di Chimica Giacomo Ciamician, Università di Bologna, Italy

[2] Dpto. Química Física, Universidad del País Vasco (UPV/EHU), Bilbao, Spain

[3] INAF - Osservatorio di Radioastronomia, via P. Gobetti, 101, I-40129 Bologna, Italy

[4] Dep. of Physics, Stockholm University, Albanova University Center, SE-106 91 Stockholm, Sweden

E-mail: sonia.melandri@unibo.it

The investigation of phenomena related to the chemistry of the Cosmos is strongly based on the identification and quantification of molecules by spectroscopic methods (in particular rotational spectroscopy), thus laboratory work is essential to provide the community with the spectral features needed to analyze the cosmological surveys.

The spectroscopic strategies for recording and analyzing the rotational spectra of larger organic molecules include the use of the cold and isolated conditions of a free jet expansion and heated sources for the non-volatile systems, coupled to absorption or Fourier Transform spectrometers which show an extremely high accuracy, resolution and sensitivity.

The experimental work is strongly supported and complemented by quantum chemical modeling and calculations with the aim of assigning the observed spectra and to obtain information on the molecular dynamics which involve, for example, conformational rearrangements, tautomeric equilibria, large amplitude motions, vibro-rotational coupling. We will explore the high resolution spectroscopic facilities in the microwave and millimeter ranges (6-18 and 52-74.4 GHz) at the University of Bologna and highlight possible future developments. With the use of some examples of published and unpublished results we will show the capabilities and the challenges that must be faced by theoretical and experimental methods in obtaining reliable results.

The data obtained from these kind of instruments are relevant for astronomical searches of complex molecules that represent excellent probes of the physical and chemical environments and history of the sources where they are detected.

Hydrogen bond networks and life in the Universe: a case study for molecular dynamic simulations

Giovanni Vladilo [1] and Ali Hassanali[2]

[1]INAF – Osservatorio Astronomico di Trieste, Via G.B. Tiepolo 11, Trieste, Italy,
[2]International Centre for Theoretical Physics, Strada Costiera 11, Trieste, Italy
E-mail: giovanni.vladilo@inaf.it

In order to cast light on the conditions that may lead to the emergence and mainteinance of life in the Universe, we consider terrestrial life as a special case of a universal chemical phenomenon driven by genetic and catalytic molecules. In a previous work we have shown that hydrogen bonding must be pervasive in any biochemistry driven by genetic and catalytic molecules, owing to its unique capabilities for molecular folding and intermolecular recognition[1]. Hydrogen bonding is also essential in the molecular medium that is required to support the structure, activity and mobility of genetic and catalytic molecules. If the medium forms a network of hydrogen bonds, genetic and catalytic processes can benefit of many important advantages, such as specific interactions, proton transfers, cooperative effects, support to hydrophobic effect, and collective reactivity to electric fields. In this perspective, water molecules are special due to their excellent capability of creating a network of hydrogen bonds. In general, other molecules can generate a network of hydrogen bonds that could support prebiotic chemical pathways or hypothetical biochemistries alternative to the terrestrial one. To investigate this possibility we are starting to perform dynamic symulations[2] of molecules known to play an important role in studies of prebiotic chemistry. Preliminary results of a case study of formamide will be briefly presented.

References

1. Vladilo G., Hassanali A. (2018) *Life*, **8**, 1-22
2. Jong K., Hassanali A. (2018). *J. Phys. Chem. B*, **122**, 7895-7906

The resistance of the thermophilic species *Parageobacillus thermantarcticus* in space simulated conditions

Paola Di Donato,[1,2] Ida Romano[1], Annarita Poli[1] and Barbara Nicolaus[1]

[1]*Consiglio Nazionale delle Ricerche (C.N.R.), Institute of Biomolecular Chemistry (I.C.B.), Via Campi Flegrei 34, 80078, Pozzuoli, Naples, Italy*

[2]*Department of Science and Technology, University of Naples "Parthenope", Centro Direzionale, Isola C4, 80143 Naples, Italy*

E-mail: paola.didonato@uniparthenope.it, paola.didonato@icb.cnr.it

The bacterial species belonging to the group of Extremophiles, i.e. those microorganisms that are able to resist extreme environmental conditions, are an interesting biological model for Astrobiology.

The relevance of assessing the resistance of bacterial species in spatial conditions has recently been highlighted also by the "AstRoMap European Astrobiology Roadmap"[1]. Indeed, according to the AstRoMap one main research issue in Astrobiology is represented by "life and habitability" i.e. the search for conditions limiting or sustaining life in the universe beyond the Earth. In this frame, the laboratory simulation of spatial conditions is one main approach to the identification of those microbial species that could potentially adapt to live in space on other planets.

Here we present the results of our studies concerning the resistance of cells and spores of the thermophilic species *Parageobacillus thermantarcticus* in laboratory conditions simulating some space parameters. *P. thermantarcticus* was subjected to several stressors mimicking the space environment including: desiccation[2,3], UV radiations[2,3], X-rays[2,3] and γ-rays[4]. Some preliminary results of the analysis, at a molecular level, of cells' response to stressing conditions are also reported[2,3,4].

References

1. Horneck et al. (2016) *Astrobiology*, **16**: 201-43.
2. Mastascusa et al.(2014) *O.L.E.B.*, **44**: 231-7.
3. Di Donato et al. (2018) *O.L.E.B.*, **48**(1): 141-58.
4. Romano et al. (2018) *Extremophiles*, **10.1007/s00792-018-1049-0**.

MICROGRAVITY-INDUCED OSTEOPOROSIS: A CHALLENGE FOR THE FUTURE OF SPACE PROGRAMS

Prisco Piscitelli[1], Cosimo Neglia[1], Emanuele Rizzo[1], Alessandro Distante[1], Antonio Scala[2], Vittorio Cotronei[3]

[1] Euro Mediterranean Scientific Biomedical Institute - ISBEM, Mesagne (Italy)
[2] National Research Council - CNR, Rome (Italy)
[3] Italian Space Agency - ASI, Rome (Italy)

Correspondence: priscofreedom@hotmail.com

Objectives Assess the impact of microgravity-induced osteoporosis and its implications on the future of space programs.

Background Osteoporosis consists in unbalanced bone resorption and formation. Microgravity-induced osteoporosis has been observed in astronauts since first human missions.

Methods We performed a narrative review of the available studies about this topic.

Results During a 4.5 to 6 month stay in space most of the astronauts develop a reduction in bone mineral density (BMD) in spine, femoral neck, trochanter, and pelvis between 1% and 14% measured by Dual Energy X-ray Absorption (DEXA). The same BMD reduction up to -2.6% has been documented in a recent RCT on 36-week bed rest, as well as increasing calciuria by the 4th week (200 mg/day lost per month) despite calcium/vitamin-D supplementations, and loss in calcaneal BMD of 5% per each month. High calcium intake (>1000 mg/d) and vitamin D supplementation (650 IU/d) has been shown to not efficiently counteract the development of space osteoporosis during several European missions. Attempts to prevent disuse osteoporosis with mechanical/biochemical means, including exercise, skeletal compression, increased hydrostatic pressure to the lower body, supplemental calcium and/or phosphorus/calcitonin/etidronate were not successful. More powerful treatments have been tested in animal models (i.e. residronate) with the same negative results, suggesting that bisphosphonates can impair the ability of mature osteoclasts to resorb bone, but cannot overcome the strong stimulus for osteoclast recruitment caused by long-term disuse. Microgravity has been shown to induce changes in genes encoding prolactins, apoptosis/survival molecules, bone metabolism and extra-cellular matrix composition proteins, chemokines, insulin-like growth factor and other molecules, thus suggesting an epigenetic framework of interactions between human genes and external environment. Diminished bone formation was shown in rats on Soviet Cosmos biosatellites with post-flight normalization of cortical bone, but persistent decline in trabecular bone mass with indications of involvement of mechanical unloading and/or hypersecretion of corticosteroids. In other studies, Gemini, Apollo and Skylab astronauts exhibited a negative calcium balance due primarily to hypercalciuria. Calcaneal BMD in Skylab crew-members declined by 4% after 84 days of orbital flight. In the International Space Station (ISS) astronauts a 4% decrease in tibial cortical thickness and a 15% increase in cortical porosity at landing was observed. Remodeling marker returned to preflight values within 6 months but tibial cortical porosity or trabecular bone failed to recover, resulting in compromised strength.

Conclusions Microgravity-induced osteoporosis still represents a major challenge for the future of space programs with human crew.

NON- ENZYMATIC OLIGOMERIZATION OF 3'-5' CYCLIC RIBONUCLEOTIDES IN PREBIOTIC CONDITIONS

G. Costanzo[1], J. E. Sponer[2,3], J. Sponer[2,3], S. Pino[4], E. Di Mauro[4]

[1] Istituto di Biologia e Patologia Molecolari, CNR, Rome, 00185, Italy.
[2] Institute of Biophysics, Academy of Sciences of the Czech Republic, Kralovopolska 135, CZ-61265 Brno, Czech Republic.
[3] CEITEC – Central European Institute of Technology, Masaryk University, campus Bohunice, Kamenice 5, CZ-62500 Brno, Czech Republic.
[4] Biological and Ecological Department, University of Tuscia, Viterbo, 01100, Italy.
giovanna.costanzo@uniroma1.it

E-mail: giovanna.costanzo@uniroma1.it

Extant biological DNA and RNA syntheses are based on template copying by highly evolved polymerases and high levels of adaptation and refinement have been achieved in studies on the *in vitro* evolution of polymerizing enzymes. Complex chemistries involved in the non-enzymatic polymerization of high-energy monomers to nucleic acids are also well described in the literature. However, these are all compounds whose likelihood of prebiotic availability and accumulation is inversely proportional to their intrinsic stability and the elaborate chemistry necessary for their synthesis. In brief, the prebiotic ur-generation of RNA remains undeciphered.

We explored in prebiotic conditions the non-enzymatic polymerization of cyclic nucleotides. Such a template-free polymerization reaction is preceded by the self-assembling of the cyclic precursors utilizing stacking interactions, which mediate the trans-phosphorylations among the pillared monomer units, resulting in covalently bound oligonucleotides. The conditions allowing this chemistry necessarily differ among the different nucleotides and depend on the propensity of the monomers to participate in various intermolecular interactions. Thus, in order to reconstruct the series of chemical events that eventually led to the prebiotic non-enzymatic synthesis of mixed-sequence RNA, the polymerization of each cyclic nucleotide requires a dedicated specific analysis. Starting by our observation of abiotic phosphorylation of nucleosides using phosphate minerals as source of phosphate and the spontaneous formation of cyclic nucleotides, the non-enzymatic polymerization of 3',5'cGMP, 3',5' cAMP, and 3',5'cCMP has been obtained and characterized.

SPACE HARDWARE FOR ASTRO AND EXO BIOLOGY EXPERIMENTS

Michele Balsamo[1], Carlo Del Vecchio Blanco[1], Gianluca Neri[1], Luca Pieroni[1], Valfredo Zolesi[1], Alessandro Donati[1]

[1]*Kayser Italia S.r.L., Via di Popogna 501, 57128 Livorno, Italy E-mail: m.balsamo@kayser.it*

Research in astrobiology and exobiology are, since the beginning of space exploration, at the forefront of the space research. Biological and chemical experiments are performed on the International Space Station (ISS), satellites, or on landers by using small autonomous or semi-autonomous bioreactors supporting different models under biological, chemical, and physical investigation. Kayser Italia develops space hardware systems and provides mission support for investigations on biological systems in space. In particular, several types of bioreactors, have been developed. The space bioreactors reduce a laboratory into a hand-sized device dedicated to life science research experiments on space platforms, such ISS. They allow the autonomous execution of a scientific protocol, being designed to contain the cell culture and all the chemicals (culture medium, wash buffers, fixatives, etc) required by the experiment. To maintain a desired temperature during the experiment execution an incubator, such as the KUBIK or Biolab (ESA), is employed. Together with the more classical approaches to perform space experiment, and driven by current commercial space utilization programs, Kayser Italia has established a commercial service called BIOREACTOR EXPRESS, aiming to establish an "express" way to perform scientific and/or technological experiments on board the ISS. It exploits the KUBIK incubator facility of ESA which is permanently installed on the ISS Columbus module. With this approach several categories of experiments can be performed using available miniaturized "bioreactors" dedicated to biological, biotechnological and biochemistry experiments. Beyond the biology experiments performed inside the ISS, Kayser Italia is developing for ESA an EXOBIOLOGY facility to be installed on an external platform outside the ISS Columbus module. As outcome of the ILSRA 2014 ESA call, seven astrobiology experiments namely Biosign, MEXEM, IceCold, Rotifer, GENESISS, Exocube and OREOcube, have been selected for implementation and performance on board the ISS. These experiments, currently under development, will evaluate the impact of space environment (radiation, UV, vacuum, temperature variations) on different chemical and biological samples. Hence, details regarding Kayser Italia activities and future research opportunities for astro-exobiological investigations will be presented.

Hypersaline habitats: strategies and diversity of halophilic archaea and bacteria

Antonio Ventosa, Blanca Vera-Gargallo, Ana Durán-Viseras, Rafael R. de la Haba and Cristina Sánchez-Porro

Department of Microbiology and Parasitology, University of Sevilla, 41012 Sevilla, Spain.
ventosa@us.es

Hypersaline environments are represented by saline lakes, solar salterns and saline soils, as well as other habitats such as salt mines, salted foods, etc. They are divided on thalassohaline or athalassohaline depending on the percentages of the different salts present in the habitat. With a few exceptions belonging to the eukaryotic domain, such as the crustacean *Artemia salina*, the algae *Dunaliella*, some fungi and the larvae of the brine fly *Ephydra*, most organisms living in such extreme habitats are prokaryotes, belonging to the domains Archaea and Bacteria. These habitats are extreme not only because they have a high salt concentration (in some cases up to saturated NaCl), and other extreme environmental features such as the temperature, pH, radiation, pressure, etc., may influence the growth of living organisms that are thus defined as poly-extremophiles. The major challenge that these microorganisms must solve is the high salinity and two alternative strategies to balance the external ionic content are the “salt-in”, that has traditionally been considered as unique for the extremely halophilic archaea (also known as haloarchaea), consisting on the internal accumulation of ions (Na^+ and mainly K^+), and the “salt-out” strategy which is mainly carried out by the halophilic and halotolerant bacteria, consisting on the accumulation of compatible solutes. However, current studies supported that both strategies are not exclusive for each microbial group.

Hypersaline habitats have traditionally been considered as harsh environments with a very limited diversity and in which only a few microbial groups were present. In fact, most current physiological, biochemical or genetic studies have been based on a few halophiles that are easily available and grow well under laboratory conditions, even considering that maybe they are not the most abundant extremophiles in hypersaline habitats. The use of culture-independent molecular techniques, including recent metagenomic approaches have permitted to determine in detail the major microbial taxa and their metabolic activities, and also have enable the discovery of new, never described before, archaea and bacteria that may offer a new set of genes that could be of biotechnological and applied importance. Besides, these studies have permitted to determine the most abundant prokaryotic groups, which are probably better adapted to the extreme conditions and thus, could be the best candidates as model organisms for further studies in order to determine their survival mechanisms and the presence of microbial life in other planets.

Interrupted genes in extremophilic Archaea

Rosa Giglio[1], Luisa Maurelli[1], Federcia De Lise[2], Nicola Curci[1,2], Marco Moracci[1,2], and Beatrice Cobucci-Ponzano[1]

[1]Institute of Biosciences and Bioresources, National Research Council of Italy, Via Castellino 111, 80131 Naples, Italy
[2]Department of Biology, University of Naples Federico II, Via Cinthia, 80126 Naples, Italy.

E-mail: beatrice.cobucciponzano@ibbr.cnr.it

Classifications based on nucleic acids show that Archaea, together with Eukarya and Bacteria, represent the third domain of living organisms. Their basal position in phylogenetic trees suggests that Archaea might be the living organisms closest to the Last Universal Common Ancestor. The study of the molecular genetics of extremophilic Archaea makes it possible to understand fundamental aspects on the origin of life, such as the evolution of the genome and the transmission of genetic information. Sequenced genomes often reveal interrupted coding sequences and, in the past, genes interrupted by +/-1 frameshifting, stop codons, and large insertions were generally considered to be the result of sequencing errors or non-functional pseudogene. However it is now clear that a minority of these coding sequences are functionally expressed either independently or by programmed deviations from the standard decoding rules, globally named recoding. Evidence of recoding has been provided in Eukarya and Bacteria, and, more recently from our group, also in Archaea [1-3], demonstrating that the phenomenon is universally conserved. Known cases of translational recoding in Archaea were limited to termination codon readthrough [1]. However, our group found that the gene *fucA1,* encoding for a α-L-fucosidase in the archaeon *Sulfolobus solfataricus,* is expressed by programmed -1 frameshifting [2]; more recently, we demonstrated by functional highthroughput proteomic approaches and expression in *E. coli*, that disrupted genes leading to functional products can be frequently found in archaeal genomes [3]. These results will be described here and discussed with particular focus on the relevance of translational recoding in Archaea and the correlation between the flexibility of the genetic code and the limits of life

This work was supported by the projects MoMa 1/014/06/0 and ECMB 2014-026-R.0 of the Agenzia Spaziale Italiana.

References

1. Cobucci-Ponzano B, et al. (2005) *Mol Microbiol*. 2, 339-348.
2. Cobucci-Ponzano B, et al. (2003) *J Biol Chem*. 278, 14622-14631.
3. Cobucci-Ponzano, B., et al. (2010) J Proteome Res., 9, 2496-2507.

ENDURANCE LIMIT OF A DESERT CYANOBACTERIUM UNDER SPACE AND MARS-LIKE CONDITIONS

Daniela Billi[1]

[1]*University of Rome "Tor Vergata", Department of Biology, Via della Ricerca Scientifica snc, Rome, Italy*
E-mail: billi@uniroma2.it

Desert members of the genus *Chroococcidiopsis* are characterized by a remarkable capability to withstand environmental stressors that are lethal to the majority of the organisms. In nature they dominate hot and cold deserts [1] and cope with laboratory conditions of prolonged desiccation [2], high and low LET radiations [3], space and Mars-like simulations [4,5]. Recently their exposure under space and Mars-like conditions in low Earth, performed in the contest of the BIOMEX (BIOlogy and Mars EXperiment) and BOSS (Biofilm Organisms Surfing Space) experiments, has pushed the limits of life at several extremes. When the exposure to such conditions did not exceed the repair capabilities more data were available on the physico-chemical limits of life. When the accumulated damage exceeded the survival potential, the persistence of biomarkers contributed to a database needed to search for life elsewhere [6]. The survival of dried cells was ascribed to a synergic action between permanence in dried cells of proteins protected against oxidative damage [7] and up-regulation of DA repair genes upon rewetting.

References

1. Smith HD, Baqué M, Duncan AG, Lloyd CR, McKay CP, Billi D. (2014). *International Journal of Astrobiology*, **13**, 271-277.
2. Billi D (2009). *Extremophiles*, **13**, 49-57.
3. Verseux C, Baqué M, Cifariello R, Fagliarone C, Raguse M, Moeller R, Billi D. (2017). *Astrobiology,* **17**,118-125.
4. Baqué M, Verseux C, Böttger U, Rabbow E, de Vera J-P, Billi D. (2016). *Origin of Life and Evolution of Biospheres,* **46**, 289-310.
5. Baqué M, Verseux C, Rabbow E, de Vera J-P, Billi D. (2014). *Origin of Life and Evolution of Biospheres* **44**, 209–22.
6. Billi D (2018). *International Journal of Astrobiology* (in press).
7. Fagliarone C, Mosca C, Ubaldi I, Verseux C, Baqué M, Wilmotte A, Billi D. (2017). *Extremophiles,* **21**, 981-991.

We will BioRock you: experiments on biofilm formation of *Sphingomonas desiccabilis* in preparation for the International Space Station (ISS).

Rosa Santomartino[1], Natasha Nicholson[1], Claire Loudon[1], Charles Cockell[1]

[1]UK Centre for Astrobiology, School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK
E-mail: rosa.santomartino@ed.ac.uk

Microgravity has been demonstrated to induce several morphologic and phenotypic changes on bacterial cultures. Recent experiments conducted on the International Space Station (ISS) showed that cells size were incremented during the Space flights, as well as cell concentration and antibiotic resistance[1,2]. Moreover, microgravity had an effect on biofilm formation and altered biofilm architecture [3].

In this work we describe the results of the preliminary experiments on the bacterium *Sphingomonas desiccabilis* in preparation to the ESA BioRock experiment (ILSRA-2009-0952). This latter has the aim to investigate how bacteria interact with basalt rock in microgravity and simulated Mars (0.38 g) and Earth (1 g) gravities. The experiment will be performed on the ISS in May 2019 and will take advantages of the BMR hardware (Kayser Italia), specifically designed for the experiment. Two main features of bacterial growth will be assessed: biofilm formation and bioleaching extent[4].

Biofilm is an intricated matrix of biopolymers produced by bacterial cells after attachment to several surfaces (biotic or abiotic)[5]. During the BioRock experiment, biofilm formed by the bacteria on a basalt rock surface after the flight will be analyzed by several microscopic techniques. The results obtained from our preliminary tests showed interesting features of biofilm formation on basalt slides, and gave clues on what would be interesting to focus on after the flight in the ISS.

The BioRock experiment will give important information regarding the changing occurring on bacterial bioleaching capacity and biofilm formation in different gravities. Moreover, the preliminary analysis in preparation to the flight could provide useful data on what will be the main features we expect to be modified when gravity changes.

References

1. Taylor Peter William (2015), Infection and Drug Resistance 2015:8 249-262
2. Zea L, Larsen M, Estante F, Qvortrup K, Moeller R, Dias de Oliveira S, Stodieck L and Klaus D (2017), Front. Microbiol. 8:1598.
3. Kim W, Tengra FK, Young Z, Shong J, Marchand N, et al. (2013), PLoS ONE 8(4).
4. Loudon, CM, Nicholson, N, Finster, K, Leys, N, Byloos, B, Van Houdt, R, Rettberg, P, Moeller, R, Fuchs, FM, Demets, R, Krause, J, Vukich, M, Mariani, A & Cockell, C (2017), International Journal of Astrobiology, pp. 1-11.
5. Balcázar JL, Subirats J and Borrego CM (2015), Front. Microbiol. 6:1216.

A LIVELY LIFE AT HIGH TEMPERATURE: MICROBIAL COMMUNITY DYNAMICS DURING GEOCHEMICAL AND SEASONAL EVENTS.

Roberta Iacono[1,2], Andrea Strazzulli[1,3], Beatrice Cobucci-Ponzano[2], Luisa Maurelli[2], Rosario Avino[4], Antonio Carandente[4], Stefano Caliro[4], and Marco Moracci[1,2,3]

[1]Department of Biology, University of Naples Federico II, Via Cinthia, 80126 Naples, Italy.
[2]Institute of Biosciences and Bioresources, National Research Council of Italy, Via P. Castellino 111, 80131 Naples, Italy.[3] Task Force on Microbiome Studies, University of Naples Federico II, Naples, Italy,
[4]Istituto Nazionale di Geofisica e Vulcanologia, sezione di Napoli, Osservatorio Vesuviano, 80124 Naples, Italy
E-mail: roberta.iacono@unina.it

The study of the microbial dynamics in the extreme environments such as fumaroles, hot springs, and geysers, in relation to geothermal variations allows providing important information on the microbiome inhabiting extreme environments. Microbial survey applied to specialized environments which might resemble those of primitive Earth, offers the possibility to understand the evolution of complex biotypes and their correlation with the environmental parameters playing a key role in the study of the origin, evolution, distribution and adaptation of extremophiles (organisms thriving at these conditions) as primitive forms of life populating our planet and, in an astrobiological perspective, other bodies in the Universe.

Here, we report the temporal survey of the hyperthermophilic microbial community in response to seasonal and geochemical variations, by using microbial and geochemical data of 54 environmental samples collected between February 2015 and April 2016, of a mud pool (pH 2.3 – 6.5; temp 82 – 101 °C) of the Pisciarelli solfatara in the volcanic area of the Phelgrean Fields (Naples, Italy). Currently, Pisciarelli hotsprings showed an evident increase of the geothermal activity being affected by a continuous increasing temperature of the existing fumaroles, local seismicity, and occurrence of novel fumaroles mixed with jets of gas and boiling water [1]. Our analysis revealed severe changes in the Genera ratio within the microbial population, due to seasonal modifications, and dramatic drops of the whole microbial community triggered by geochemical events.

References

1. Fedele A, Di Giuseppe MG, Troiano A, *et al*. (2014), Geophysical Research Abstracts Vol. 16 EGU2014-858-1

Preservation of molecular biomarkers on Mars and their detectability

J. R. Brucato[1], T. Fornaro[2], I. L. ten Kate[3], S. Siljeström[4], A. Steele[1], and R. M. Hazen[1]

[1]INAF-Astrophysical Observatory of Arcetri, L.go. E. Fermi 5, 50125 Firenze, Italy – john.brucato@inaf.it
[1]Geophysical Laboratory, Carnegie Institution for Science, 5251 Broad Branch Rd NW, Washington, DC 20015, USA - tfornaro@carnegiescience.edu, asteele@carnegiescience.edu, gcody@carnegiescience.edu, rhazen@carnegiescience.edu
[3]Earth Sciences Department, Utrecht University, Budapestlaan 4, 3584 CD Utrecht, The Netherlands - I.L.tenKate@uu.nl
[4]RISE Research Institutes of Sweden, Drotting Kristinas väg 45, 114 28 Stock-holm, Sweden - sandra.siljestrom@ri.se

Mineral surfaces may have a central role in the enrichment of chemical complexity assisting prebiotic self-organization, selectively adsorbing molecules and allowing their concentration. Nowadays we know that in space environments minerals can act as catalysts promoting selective synthesis of biomolecules and influencing the photostability of biomolecules catalysing important chemical reactions or protecting molecules against degradation. Studies about the stability of molecular biomarkers in a Martian-like environment allow us to explore the conditions for the preservation of biomarkers and develop models for their degradation in the Martian geological record. In particular, ultraviolet (UV) radiation and perchlorates are among the main degradation agents on Mars. Therefore, a systematic study of the effects of UV radiation and the presence of perchlorates on a variety of molecule-mineral complexes mimicking Martian soil can be key for choosing the landing sites for future space missions, as well as the selection of the most interesting samples to analyze *in situ* or collect for sample return.

In this regard, we present laboratory activities pertaining to the UV-irradiation processing of the Mars soil analogues under Martian-like conditions and the characterization of the Mars soil analogues through various techniques such as Fourier Transform Infrared (FTIR) and Raman vibrational spectroscopies, powder X-Ray diffraction (XRD), Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS).

CHEMICAL COMPLEXITY FROM PROTOSTELLAR DISKS TO PLANETS

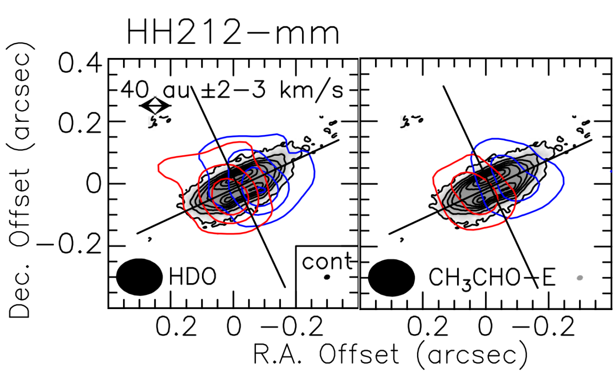
L. Podio,[1] C. Codella,[1] N. Balucani,[2] C. Ceccarelli,[3] and the FAUST & ACO teams

[1]INAF - Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, 50125 Firenze, [2]Dip. di Chimica, Biologia e Biotecnologie, Università di Perugia, I-06123 Perugia, Italy, [3]Université Grenoble Alpes, 38401 Grenoble, France

A key open question in astrochemistry is how chemical complexity builds up along the formation process of Sun-like stars from prestellar cores to protoplanetary disks and ultimately to planets. Is the chemical composition of planets inherited from the prestellar and protostellar stages? Or reflects chemical processes occurring in the disk? Are organics efficiently formed in disks and through what mechanism(s)?

The chemistry of disks is difficult to probe observationally due to their small sizes (<100 au) and to the low gas-phase abundance of (complex) organic molecules (iCOMs). It is only with the advent of millimetre interferometers such as ALMA that we started to unveil the disks molecular content at unprecedented angular resolution and sensitivity.

I will show the first detections of organics in planet-forming disks from the protostellar (~10^4 yrs) to the protoplanetary (~10^6 yrs) stage and I will discuss how these observations are revolutionising our comprehension of the distribution and formation of volatile organics in disks. Building on these results we are now ready to perform the first astrochemical survey of disks around young Solar analogs in the context of the recently approved Large Programme ALMA-FAUST (Europe, Japan, and USA), and EU ITN project ACO, both based on a strong synergy between astrophysicists, chemists, and laboratory experts.



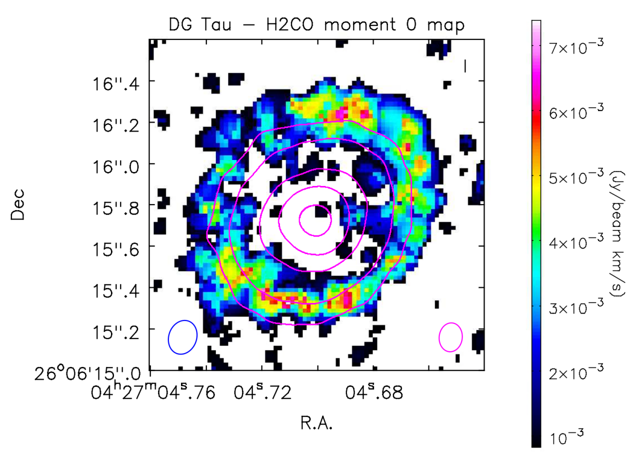


Figure: ALMA observations of simple organics in the disk of the HH 212 protostar (*left;* from Codella et al. 2018, A&A, 617, A10), and in the protoplanetary disk of the T Tauri star DG Tau (*right;* from Podio et al. 2018, submitted to A&A).

Primitive small bodies: a sneak peek to the origin of life

Simone Ieva[1], Elisabetta Dotto[1], Elena Mazzotta Epifani[1], M. Micheli[2], Davide Perna[1,3], Ettore Perozzi[4], John Robert Brucato[5], Giovanni Poggiali[5,6]

[1]INAF – Osservatorio Astronomico di Roma, Via Frascati 33, 00078 Monte Porzio Catone, Rome, Italy, [2]ESA SSA-NEO Coordination Centre, Frascati, Rome, Italy, [3]LESIA – Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universités, UPMC Univ. Paris06, Univ, Paris Diderot, Sorbonne Paris Cité, 5 Place J. Janssen, 92125 Meudon, France, [4]ASI – Agenzia Spaziale Italiana, Rome, Italy, [5]INAF – Arcetri Astrophysical Observatory, Largo Enrico Fermi 5, 50125 Firenze, Italy, [6]University of Firenze, Department of Physics and Astronomy Via Sansone 1, 50019 Sesto Fiorentino, Italy
E-mail: simone.ieva@inaf.it

Primitive small bodies, such as carbonaceous Near-Earth Objects (NEOs) and Centaurs, formed in the water- and organic-rich outer regions of the proto-planetary disk, very likely containing primordial material from the proto-solar cloud, as well as elements issued from alteration processes. Their current physical and orbital properties provide information about the earliest processes that governed the formation and evolution of the proto-nebula at different solar distances[1],[2]. Moreover, recent exobiological scenarios for the origin of life on Earth[3] invoke the exogenous delivery of organic matter to the early Earth due to an intense influx of organic-rich material after its formation, for which the most likely source is the impact of many small bodies formed in the outer SS[4].

We will present the latest results we have obtained during our observational campaign to investigate the surface composition of several primitive bodies through photometric and spectroscopic observations in the visible and near-infrared range. We found NEOs with dynamical and physical connection with outer Solar System bodies, which make them particularly interesting for a future rendez-vous or sample-return mission. Moreover, we characterized the peculiar surface colours and the activity for an interesting Centaur, flagged before as inactive.

References

1. Morbidelli A. et al., (2008), in The Solar System beyond Neptune, Eds. M.A. Barucci et al., Univ. Ariz. Press, 275-292
2. Vernazza P. et al., (2017), *AJ* **153**, 72, 1-10
3. de Marcellus P. et al., 2011, *ApJL* **727**, L27, 1-6
4. Walsh K.J. et al., 2011, *Nature* **475**, 7355, 206-209

SUPERMASSIVE BLACK HOLES AND PLANETARY HABITABILITY

Amedeo Balbi[1], Andjelka B. Kovacevic[2], Francesco Tombesi[1,3,4], Agata M. Wislocka[5]

[1] *Dipartimento di Fisica, Università degli Studi di Roma "Tor Vergata", via della Ricerca Scientifica, 00133 Roma, Italy*

[2] *Department of Astronomy, Faculty of Mathematics, University of Belgrade, Studentski trg 16, 11000 Belgrade, Serbia*

[3] *Department of Astronomy, University of Maryland, College Park, MD 20742, USA*

[4] *NASA/Goddard Space Flight Center, Code 662, Greenbelt, MD 20771, USA*

[5] *Institute for Astro & Particle Physics, University of Innsbruck, Technikerstr. 25/8, 6020 Innsbruck, Austria*

It is generally thought that the habitability of a planet is strongly influenced by the amount of ionizing radiation incident on its atmosphere and surface. While the host star is usually the prevalent origin of such high-energy radiation, previous studies have also considered the effect on a hypothetic biosphere of other possible sources, in particular with regard to potentially catastrophic transient events such as nearby gamma ray bursts or supernova explosions. Here we consider a phenomenon whose astrobiological consequences are much less explored, i.e. the production of X-ray and extreme ultraviolet (XUV) radiation during the peak of the active phase of supermassive black holes. In particular, we investigated [1] how the activity of the supermassive black hole at the center of the Milky Way, known as Sagittarius A* (Sgr A*), may have affected the habitability of Earth-like planets in our Galaxy. Our results show for the first time that the combined effect of atmospheric loss and of the direct biological damage to surface life was probably significant during the AGN phase of Sgr A*, possibly hindering the development of complex life within a few kiloparsecs from the galactic center.

References

1. Balbi, A. & Tombesi, F. (2017) *Scientific Reports* **7**, 16626

Life in space – Origin, Presence, Persistence of life in Space, from molecules to extremophiles

Silvano Onofri and the OPPS Project Group

University of Tuscia, Viterbo, Italy

onofri@unitus.it

The origin of life and its possible existence, past or present, beyond our planet, are subjects of great scientific and general interest and one of the main objectives of space research. The Italian astrobiological scientific community has been developing these themes for long time at national and international level, actively participating in congresses and workshops, publishing many scientific papers in international journals, resulting from ground and space experiments (mainly on ISS), funded by ASI and ESA.

The researches have focused and are focusing on the origin of life, its limits on Earth and possible theoretical limits, the search for life outside the Earth, the limits of habitability, the resistance of microorganisms to space and Martian conditions, the search for exoplanets in the range of habitability. The aim of this project is to networking the best skills in our country, to carry out a wide-ranging research, with a common goal.

The study of the origin of life in the universe is the basis of this project, which investigates prebiotic chemistry in various possible scenarios, whether in polar or non-polar solvents (e.g. Titan environment): these results will link with the study of the effect of simulated space conditions on possible chemical biosignatures. The limits of life as we know will be investigated in ground-based experiments on experimental microbiological models that, for the most part, have already demonstrated their resistance to real or simulated space conditions and in extreme environments. Their potentialities will be studied also by up-to-date molecular methods. The ability of some microorganisms to produce atmospheric biosignatures, in simulated conditions, will be tested and compared with the possible existence of atmospheric biosignatures on habitable exoplanets. The search for habitable exoplanets will be carried out with theoretical models aimed at optimizing space-based observational methods.

The realization of a project, including a wide range of life studies in the Universe, but very related to each other, will set the conditions and provide tools to propose various experiments that can be realized in space, especially on the ISS; these proposals could be submitted by research teams that have been already tested for their ability, expertise and experience.

From Atoms to Biomolecules in the Space: the Fascinating World of Astrochemistry

Vincenzo Barone and Cristina Puzzarini

STAR Ineruniversity Center, Pisa

For many years, the inter-stellar medium (ISM) was considered too hostile an environment for molecules. This paradigm of thought began to deteriorate roughly forty years ago with the discovery of molecules containing carbon chains and rings. As time has gone on, the pace of molecular discovery has accelerated and the original point of view has been definitively abandoned.

Indeed, the detection of almost two hundred molecules in space suggests that the ISM is characterized by a rich chemistry. Unthinkable to astronomers a half-century ago, the presence of *prebiotic* molecules has attracted particular interest in the general scientific community. Debate on the origins of these biomolecular building blocks has been further stimulated by the discovery of nucleobases and amino acids in meteorites and other extra-terrestrial sources. This is the playground leading to the birth and development of astrochemistry, an interdisciplinary field at the interface of chemistry, physics, and astronomy on the road toward astrobiology. At least three different pieces of information, namely astronomical observations, laboratory experiments, and quantum mechanical computations are mandatory for a deeper understanding of the chemical evolution of the universe. In this contribution I'll try to sketch the present situation and to delineate some of the most promising perspectives with special reference to the spectroscopic detection and characterization of biomolecular building blocks in the ISM and to reaction mechanisms (including both thermodynamic and kinetic aspects) leading from simple molecules to the so-called astronomical complex organic molecules (ACOMS), i.e. sugars, nucleobases, aminoacids and their precursors.

Melli, M. Melosso, N. Tasinato, G. Bosi, L. Spada, J. Bloino, M. Mendolicchio, L. Dore, V. Barone, C. Puzzarini, *Rotational and Infrared Spectroscopy of Ethanimine: A Route toward Its Astrophysical and Planetary Detection*, Astrophys. J. **855**, 123 (2018).

V. Barone, M. Biczysko, C. Puzzarini, *Quantum chemistry meets spectroscopy for astrochemistry: increasing complexity toward prebiotic molecules*, Acc. Chem. Res. **48**, 1413-1422 (2015).

UNVEILING THE CHEMISTRY OF P IN STAR FORMING REGIONS

C. Mininni,[1,2] F. Fontani,[2] V. Rivilla[2], M.T. Beltrán[2], P. Caselli[3], A. Vasyunin[4]

[1]Università degli Studi di Firenze, Italy , [2]INAF – Osservatorio Astrofisico di Arcetri, Italy, [3]Centre for Astrochemical Studies MPE, Germany, [4]Ural Federal University, Russia

E-mail: mininni@arcetri.astro.it

Phosphorus is one of the crucial elements for life. It plays a central role in the structure of essential biotic molecules, such as nucleic acids (DNA and RNA), phospholipids (the skin of all cellular membranes) and the adenosine triphosphate (ATP).[1] Despite its importance for life, the chemistry of Phosphorus in the interstellar medium (ISM), and in particular in star-forming regions, the birthplaces of stars and planets, is still poorly known. In fact, until 2016 the only P-bearing molecule detected in star-forming regions was PN towards 6 sources[2,3]. From 2016, a series of studies conducted by our group led to new detections that allowed us to make a significant step forward in the comprehension of the P chemistry in star-forming regions. Our group detected PN (2-1) in 8 new massive cores, which allowed us to increase by more than a factor 2 the statistics, and detected PO, the basic bond of phosphates, for the first time in a star-forming region[4,5]. In order to investigate the main chemical route that leads to the formation of PN, we performed multi-line observations of PN towards 9 massive dense cores and compared the results (abundance, excitation temperature and line profile) obtained for PN with other molecules, tracing different chemical and physical conditions: SiO and SO (shock tracers), CH_3OH (grain surface tracer), and N_2H^+ (cold and dense gas tracer). Our results indicate sputtering of grains in shock regions as relevant release mechanism of PN, but not unique; in fact, PN can also be found in more quiescent gas.[4,6] The importance of shock regions emerges also from our observations towards sources in the Galactic Center.[7] From these observations, we infer also that intense UV/X-ray/cosmic rays radiation can destroy P-bearing molecules.

References

1. Pasek, & Lauretta (2005). *AsBio*, **5**, 515-535.
2. Ziurys (1987). *ApJ*, **312**, L81-L85.
3. Turner, & Bally (1987). *ApJ*, **321**, L75-L79.
4. Fontani et al. (2016). *ApJL*, **822**, L30-L35.
5. Rivilla et al. (2016). *ApJ*, **826**, L161-L166.
6. Mininni et al. (2018). *MNRAS*, **476**, L39-L44.
7. Rivilla et al. (2018). *MNRAS*, **475**, L30-L34.

Ultraviolet photoprocessing of glycine adsorbed on various space relevant minerals

Giovanni Poggiali,[1, 2] John Robert Brucato,[2] Teresa Fornaro,[3] Simone Potenti,[4]

[1]Università degli Studi di Firenze, Dipartimento di Fisica ed Astronomia, Via Sansone 1, 50019 Sesto Fiorentino (FI), Italy, [2]INAF - Osservatorio Astrofisico di Arcetri, Largo Enrico Fermi 5, 50125 Firenze, Italy, [3]Carnegie Institution for Science, Geophysical Laboratory (GL), 5251 Broad Branch Rd. NW, 20015 Washington DC, USA, [4]Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy

E-mail: giovanni.poggiali@inaf.it

Mineral surfaces may have a central role in the enrichment of chemical complexity assisting prebiotic self-organization, selectively adsorbing molecules and allowing their concentration[1,2]. Nowadays we know that minerals can act as catalysts promoting selective synthesis of biomolecules on their surface, mediating the effects of electromagnetic radiation and influencing the photostability of bio-molecules catalysing important chemical reactions or protecting molecules against degradation[3,4].

Such relevant interactions acquire even greater importance after the discovery of organic molecules on asteroids confirming their role as transport and delivery vehicles of building blocks of life on Earth and possibly on other bodies of the Solar System[5]. In this context, surfaces of airless bodies hit by UV photons are favourable sites for the formation of highly reactive radical species by photochemical processes and the study of this kind of process can improve our knowledge on the role of asteroids in astrobiology[6].

We report a laboratory study of UV irradiation of glycine adsorbed on various space relevant minerals, such as forsterite, antigorite, spinel and pyrite, using a calibrated enhanced UV Xenon lamp, which has shown to be a good choice for solar simulation[7].

References

1. Hazen, R.M. and Sverjensky D.A. (2010). *Cold Spring Harb. Perspect. Biol.*, **2 (5)**, a002162.
2. Brucato, J.R. and Fornaro T. (2018) “Role of Mineral Surfaces in Prebiotic Processes and Space-like Conditions” in Cavalazzi B. and Westall, F. (eds.) *Biosignatures for Astrobiology*, Springer Int. Pub.
3. Fornaro, T.; Boosman, A.; Brucato, J.R.; ten Kate, I.L.; Siljeström, S.; Poggiali, G.; Steele, A.; Hazen, R.M. (2018). *Icarus*, **313**, 38-60.
4. Potenti, S.; Manini, P.; Fornaro, T.; Poggiali, G.; Crescenzi, O.; Napolitano, A.; Brucato, J.R.; Barone, V.; d'Ischia, M. (2018) *ACS Earth Space Chem., DOI: 10.1021/acsearthspacechem.8b00060*
5. Rivkin, A.S. and Emery, J.P. (2010). *Nature*, **464 (7293)**, 1322-1323.
6. Hendrix A.R. and Vilas F. (2006). *Astron. J.*, **132**, 1396-1404
7. Fornaro, T.; Brucato, J.R.; Pace, E.; Cestelli Guidi, M.; Branciamore, S.; Pucci, A. (2013). *Icarus*, **226**, 1068-1085.

EUROPEAN CURATION FACILITY: CORRELATING BIOSIGNATURES AND DETECTION TECHNIQUES USING THE CORRELATION MATRIX METHOD

John Robert Brucato[1], Andrea Meneghin[1], Aurore Hutzler[2], Sara Russell[3], Caroline Smith[3] and the EURO-CARES Team

[1]*INAF - Astrophysical Observatory of Arcetri, Firenze, Italy,* [2]*USRA - Lunar and Planetary Institute, Houston, USA,* [3]*Natural History Museum, London, UK*

E-mail: meneghin@arcetri.astro.it

EURO-CARES (European Curation of Astromaterials Returned from Exploration of Space) was a three year (2015-2017), multinational project, funded under the European Commission's Horizon 2020 research programme to develop a roadmap for a European Extra-terrestrial Sample Curation Facility (ESCF). The facility main purpose is to store, curate, prepare and distribute samples collected by sample return missions from comets, asteroids and Mars. For restricted missions, i.e sample returned from Mars, one goal of the project was to find the best suite of techniques to detect the presence of extinct or extant life when samples are brought back to Earth. At the state-of-art there are a wide number of proposed approaches [1-3]. All studies lead to a list of techniques suitable for life detection along with details about their field of application, efficiency and limits. What is missing is a critical approach able to make a comparison between the techniques in terms of effectiveness, to find a prioritizing ranking. In this study the correlation matrix engineering tool approach was used to support the choice of the techniques for biosignatures detection [4,5]. Our work was to analyse, evaluate and measure the efficiency of each technique in detecting life. To do it, a wide panel of experts was involved in the following scientific and technological fields: process engineering, astrobiology, biology, chemistry, and physics. We will show how, using the correlation matrix method, it was possible to identify critical issues, highlight the priorities and facilitate the design choices.

References

1. Kminek G. et al., Report of the workshop for life detection in samples from Mars, 2014.
2. Race M. et al., Assessment of Planetary Protection Requirements for Mars Sample Return Missions, National Research Council, 2009.
3. Wilson A. et al., Exobiology in the Solar System & The Search for Life on Mars, ESA, ISBN 9290925205, 1999
4. Akao Y., Development History of Quality Function Deployment - The Customer Driven Approach to Quality Planning and Deployment, Asian Productivity Organization. p. 339,1994.
5. Cohen L. et al., Quality Function Deployment and Six Sigma: A QFD Handbook, Prentice Hall, 2009.

BRIDGING THE GAP BETWEEN LIFELESS MOLECULES AND EARLY LIFE: A LABORATORY-BASED APPROACH IN AGREEMENT WITH A LAND-BASED BIRTHPLACES ON EARTH AND BEYOND

Rosanna del Gaudio

Dept of Biology Sciences, University of Naples Federico II, Italy
E-mail: rosanna.delgaudio@unina.it

In this research topic a new approach, aimed at revealing the ability of some terrestrial rocks and meteorites both containing iron to perform catalytic reactions operative in present-day life, was firstly reported and patented in 2003[1].

The aim of this work is to present and discuss the results of past[2,3], recent[4,5], and further ongoing (molecular and catalytic) mineral-organic interfacial experiments supporting the Multiple Root Genesis hypothesis (MuRoGe) already proposed[4] to approach the questions surrounding the origin of life on Earth and on Earth-like planets.

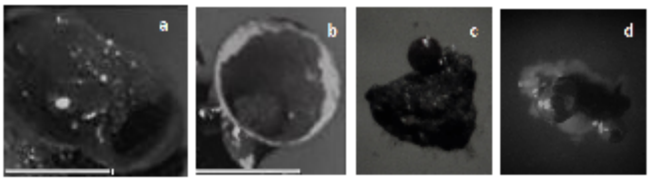


Fig1. *Examples of Micro-nano Magnetic Metallorganic Material (M4) self organizing obtained from iperstenic chondrite (a), siderites (b) olivine (c) and magnetite (d).*

Utilizing as a model for the emergence and early evolution of life on Earth, the self-organizing M4 material[6] obtained from meteorites (Fig.1a-b), and terrestrial rocks and minerals (Fig.1c-d), the results of my experiments could point a way towards understanding how Earth kick-started metabolism emerged on landmass that arose from Archean oceans rather than in the depths near a deep sea hydrothermal vent.

In conclusion, designing plausible geochemical scenarios in which abiotic, photo-geochemical reactions could become photobiological reactions, the results so far obtained do not prove or exclude the possibility that the self-organizing M4 materials, having a complex chemistry, might be examples of proto-metabolic reactions occurred in a pre-biotic hydrogel context as recently proposed[7]. Moreover, they are certainly the result of several coordinated activities and only some of them can be attributed to the meteorite or terrestrial rock components.

References

1. Geraci, G,D'Argenio, B, del Gaudio, R, (2003) *Italian Patent* RM2003A000026 (granted)
2. Geraci, G, del Gaudio, R, D'Argenio, B.(2001) *Rendiconti Lincei*, **12**: 51-68.
3. del Gaudio, R, D'Argenio, B, Geraci, G. (2009) *Orig. of Life and Evol of Biosph.*, **39**, 357- 358.
4. del Gaudio,R, D'Argenio, B, Geraci, G. (2010) 3rd Workshop of the *Italian Astrobiol Society* **Abs**, 47-48.
5. del Gaudio R, (2014) *EPSC Abstract* **9:**199-2
6. Geraci, G,D'Argenio, B, del Gaudio, R, (2016) *Patent* US9328337 B2 (granted)
7. Gorrell, B, Henderson, T.W, Albdeery, K, Savage P.M, Kee, T.P, (2017) *Life* **7:**45

Evo-SETI Scale for Exoplanets with Life

Claudio Maccone[1]

[1]*Istituto Nazionale di Astrofisica (INAF), Via Martorelli 43, 10155 Torino (TO), Italy*
E-mail: clmaccon@libero.it

Abstract. The Evo-SETI Scale (Evo-SETI stands for “Evolution and SETI”) is a scale of information measured in bits.

It ranges between zero (corresponding to the time of the origin of life on Earth, 3.5 billion years ago or a little more, like 3.8 billion years ago, or so) and 25,595 bits, that is today’s value of the scale.

The straight line between these two values is the Scale measuring the EvoEntropy, i.e. the Shannon Entropy of Information Theory for a family of lognormal probability densities constrained between the time axis and the exponential curve representing the number of Species living on Earth at each instant between 3.5 billion years ago and now. In reality, this exponential is rather the mean value of the number of living Species in the 3.5 billion years of time, since many Species went extinct in the past. Mathematically speaking, we thus have a stochastic process with this exponential mean value and this is called Geometric Brownian Motion (GBM). This GBM turns out to be a lognormal process, and not a Gaussian process.

The relevant mathematics is rather difficult, and was developed by this author in a series of some ten highly mathematical papers published in the International Journal of Astrobiology and in Acta Astronautica since 2010.

But the meaning of the Evo-Scale is quite neat: it shows “how much evolved” a certain Species is with respect to all other Species, both of the past and of the present. And if we replace “Species” with “Complexity”, the Evo-SETI scale becomes the Complexity Scale that we can extrapolate into the future in order to find how much more complex than Humans a certain ET Civilization will turn out to be when SETI, the Search for ExtraTerrestrial Intelligence, will put us in touch with Alien Civilizations.

In conclusion, our Scale really is an Evo-SETI Scale, combining both the past (Evolution) and the future (SETI) into a unique, highly mathematical scheme.

References

1. Claudio_Maccone__SETI_Evolution_and_Human_History__*Int_J_Astrobiology*_vol_12_issue_3_pages_218-245_2013.
2. Claudio_Maccone_New_Evo-SETI_Results_about_Civilizations_and_Molecular_Clock__*Int_J_Astrobiology*_vol_16_(2017)_1_40-59.

Meteorite assisted phosphorylation of nucleosides under proton irradiation conditions

Raffaele Saladino[1], Lorenzo Botta[1], Bruno Mattia Bizzarri[1], J. Šponer[2] and Ernesto Di Mauro[3]

[1]*Dipartimento di Scienze Ecologiche e Biologiche, Università della Tuscia, Via San Camillo De Lellis, 01100 Viterbo, Italy.*

[2]*Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno, Czech Republic*

[3]*Istituto Pasteur-Fondazione Cenci Bolognetti c/o Dipartimento di Biologia e Biotecnologie "Charles Darwin", University "Sapienza",Piazzale Aldo Moro 5, Rome 00185, Italy.*

E-mail: saladino@unitus.it

Phosphorylation is fundamental to cell life, supplying energy and structural stability. It controls metabolic pathways, realizes the compartmentalization process and provides reactivity[1]. Sophisticated enzymes have been selected during molecular evolution to reach this goal in the biosynthesis of nucleotides. Simpler reagents and chemical scenarios are expected to be operative in pre-biological conditions[2]. In this context our research was focused on the phosphorylation of adenosine that was performed in three different experimental conditions: 1) adenosine, NaH_2PO_4 and the meteorite NWA 2828 of the chondrite type; 2) adenosine, NaH_2PO_4 and NWA 2828 in the presence of NH_2CHO; and 3) adenosine and NaH_2PO_4 in NH_2CHO without NWA 2828. The irradiation of adenosine and NaH_2PO_4 in dry-film conditions was also performed as a reference. As shown in figure 1 alicyclic and cyclic nucleotides were detected by MALDI-TOF and HPLC-MS analyses. In particular, the irradiation of adenosine **1** and NaH_2PO_4 afforded 5'-adenosine mono-phosphate (5'-AMP) **2**, 3'-adenosine mono-phosphate (3'-AMP) **3**, 2'-adenosine mono-phosphate (2'-AMP) **4**, 2', 3'-cycloadenosine monophosphate (2',3'-cAMP) **5**, 3', 5'-cycloadenosine monophosphate (3',5'-cAMP) **6**, and 5'-adenosine diphosphate **7** (5'-ADP) (Figure 1). Moreover, a large panel of molecular ions corresponding to nucleotides poly-phosphates.

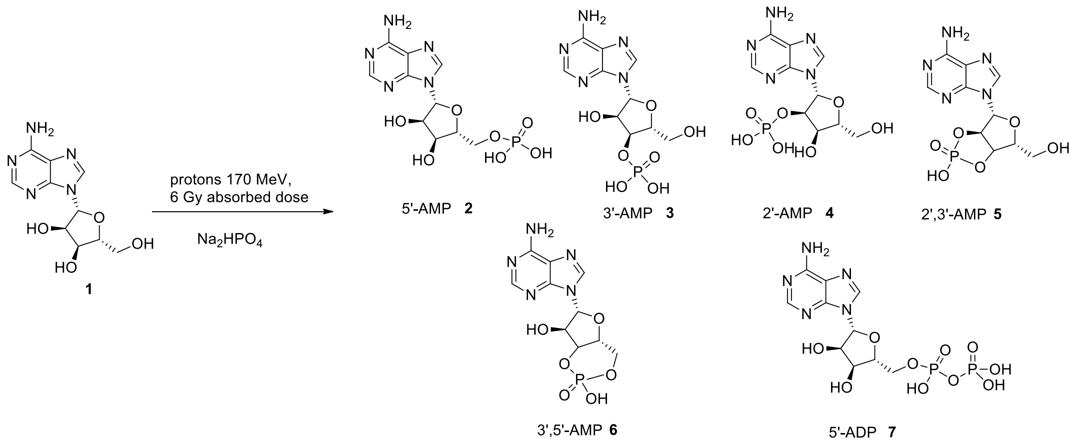


Figure 1. Irradiation of adenosine **1** and NaH_2PO_4 with a high energy proton beam (170 MeV)

References

[1] Dou, Y., Yao, B., Zhang, C. (2017). *Methods in Molecular Biology* **1484**, 265-274.

[2] Gull M. (2014) *Challenges*, **5**, 193-212.

Submillimeter-wave spectroscopy for astrochemistry

Luca Dore[1]
[1]Department of Chemistry "Giacomo Ciamician", University of Bologna
via Selmi 2, Bologna, I-40126, Italy
luca.dore@unibo.it

The origin of life may be modeled as a sequence of so-called "emergent" events, each of which added chemical complexity to the prebiotic earth. Such events include: *i*) the emergence of biomolecules, *ii*) the emergence of organized molecular systems, *iii*) the emergence of self-replicating molecular systems; *iv*) the emergence of natural selection[1]. As for the emergence of biomolecules, molecules formed in the interstellar medium (ISM) represent an important source of life's building blocks. Therefore, an important issue in astrochemistry is the observation of complex organic interstellar molecules (COM): they are probes of the physical conditions, of the history, and of the molecular complexity of their environment[2].

To support radio astronomical detection, laboratory data are needed, which can be provided by instruments such as the Bologna spectrometer, which can record spectra above 1 THz with accuracy, precision, and high resolution.

We recently observed in the millimeter- and submillimeter-wave regions the rotational spectra of two prebiotic molecules produced by pyrolysis: C-cyanomethanimine (HNCHCN)[3] and ethanimine (CH_3CHNH)[4], both in the two Z and E isomeric forms. A search of spectral features of HNCHCN in spectral surveys obtained with the IRAM 30-m antenna led to upper limits on its abundances of a few 10^{-10} and 10^{-9} for starless and hot-corinos, and shocks, respectively.

Moreover, the observation of the rotational spectrum of cyanoketene (NCHCCO), produced by pyrolysis of methylcyanoacetate (NCH_2COOCH_3), was extended up to 520 GHz. This COM is still unidentified in the ISM and we studied possible formation paths in the gas phase by a full QM approach.

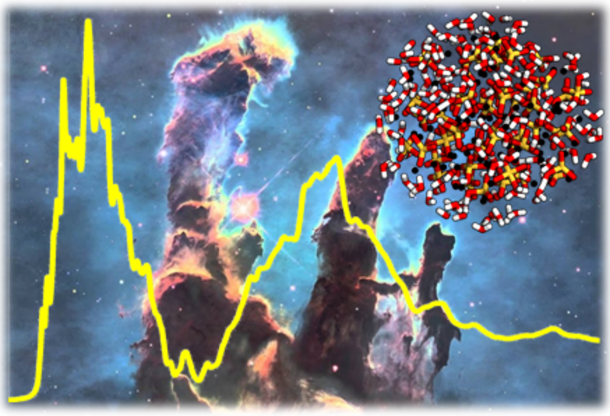
[1] R. M. Hazen "The Emergence of Chemical Complexity: An Introduction" in *Chemical Evolution: Chemical Change Across Space and Time* (L. Zaikowski and J. M. Friedrich, Eds.), ACS symposium series 981, 2008.
[2] E. Herbst and E. F. van Dishoeck "Complex organic interstellar molecules", Annu. Rev. Astron. Astrophys. 47 (2009) 427.
[3] M. Melosso, A. Melli, C. Puzzarini, C. Codella, L. Spada, et al., A&A 609 (2018) A121.
[4] A. Melli, M. Melosso, N. Tasinato, G. Bosi, L. Spada, et al. ApJ 855 (2018) 123.

Computer simulations of interstellar dust particles

Lorenzo Zamirri,[1] and Piero Ugliengo.[1]

[1]*Dipartimento di Chimica, Università degli Studi di Torino, via Pietro Giuria 7, 10125, Torino, Italy*
E-mail: lorenzo.zamirri@gmail.com

Classic (CM) and quantum (QM) mechanical computer simulations represent a powerful tool in today's astrochemical research because they can provide for atomistic details that cannot be directly obtained from experimental and astronomical observations. Solid nanoparticles (NPs) represent an important fraction of the interstellar medium (ISM). IR observations revealed that some of these NPs have a forsterite (Mg_2SiO_4, Fo) like composition,[1] and that in the dense molecular clouds (MCs), they are covered in different layers of water-dominated, *dirty ices*.[2] These NPs are expected to play a fundamental surface catalytic role, allowing the formation of the large variety of molecules usually observed in the ISM.[1] While IR observations are useful to investigate the chemical composition of solids, they cannot properly provide for structural information. However, Fo NPs are usually assumed to be highly amorphous because their IR spectra closely resemble those from amorphous *bulk* silicates.[1] On the same vein, the solid carbon monoxide (CO) IR stretching frequency is usually exploited to infer the structural features of the covering ices and the atomistic nature of the solid CO-solid H_2O interface, that may influence several chemico-physical processes occurring in MCs.[3] In order to shed some light on these two important topics, we resorted to CM and QM computer simulations on Fo NPs and CO/H_2O models. Our results clearly show that *i*) amorphous- and crystalline-like Fo NPs cannot be distinguished only from their IR spectra, and *ii*) very different atomistic environments can produce the observed features of solid CO.



References

1. Henning, T. (2010), *Annu. Rev. Astron. Astrophys.*, **48**, 21–46.
2. Boogert, A. C. A., et al. (2015), *Annu. Rev. Astron. Astrophys.*, **53**, 541–583.
3. Zamirri, L., et al. (2018), *Mon. Not. R. Astron. Soc.*, **480**, 1427–1444.

Amide and Peptide Bond Formation in Dry Conditions on Silica Surface

Marco Fabbiani,[1] Albert Rimola,[2] Mariona Sodupe,[2] Piero Ugliengo[1] and Gianmario Martra[1]

[1]Department of Chemistry and Nanostructured Interfaces and Surfaces (NIS) Inter-Departmental centre, Università degli Studi di Torino, via P. Giuria 7, 10125 Torino, Italy
[2]Departament de Química, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
E-mail: marco.fabbiani@unito.it

The fundamental interest concerning the formation of the first molecules of life is a constant challenge in the panorama of astrochemical and prebiotic studies. While the formation of the simplest molecules is assessed in many different environments ranging from the ISM to the early Earth, the linkages between them to form functional and self-assembled structures still underlies many uncertainties. In this, the comprehension of the formation of amides and peptides is a key passage among all the chainrings.[1]

The amide bond (AB) formation between non-activated carboxylic acids and amines is studied on the surface of amorphous silica in dry conditions combining spectroscopic measurements and quantum chemical simulations.[2] The results suggest a mechanism involving a hybrid catalytic site formed by both molecules and surface. The experimental careful tuning of silica surface OH groups is achieved to progressively isolate families of surface sites. The atomistic interpretation of indicates the coexistence of an ionic and a canonical pairs of reagents hosted by specific surface SiOH is of key importance in orienting and promoting the amide bond formation. In this, the canonical pair is the one that undergoes the amide bond formation, while the ionic one directly participates in the final dehydration step. A further step is considered: Glycine sublimations are carried out in a controlled atmosphere on the same materials used to study the AB formation. The results confirmed the formation of long peptides up to 16 units long.

References (Arial 10)

1. Martra G., Deiana C., Sakhno Y., Barberis I., Fabbiani M., Pazzi M., Vincenti M. (2014) *Angewandte Chemie international Edition* **53**, 4671-4674.
2. Rimola A., Fabbiani M., Sodupe M., Ugliengo P., Martra G. (2018). *ACS Catalysis*, **8**, 4558-4568.

PROTENZ: THE IBISBA 1.0 INFRASTRUCTURE WITH SPECIAL FOCUS ON PROTEINS AND ENZYMES FROM EXTREMOPHILES

Mauro Di Fenza[1], Maria Ciaramella[1], Sabato D'Auria[2], Emanuela Pedrazzini[3], Andrea Scaloni[4], Marco Moracci[1,5], Beatrice Cobucci-Ponzano[1]

[1]Institute of Biosciences and BioResources–CNR, via Castellino 111, Naples, Italy; [2] Institute of Food Sciences-CNR, via Roma 64, Avellino, Italy; [3]Institute of Agricultural Biology and Biotechnology-CNR, via Corti 12, Milan, Italy, *[4]Institute for the Animal Production System in the Mediterranean Environment-CNR, via Argine 1085, Naples, Italy [5]Department of Biology, University of Naples "Federico II", Via Cinthia 21, Naples, Italy*

E-mail: mauro.difenza@ibbr.cnr.it

Industrial biotechnology is a key enabling technology (KET) of Europe's bioeconomy, providing sustainable production and processing systems. However, to fully realise its potential, this KET requires further development, notably to bridge the gap between bioscience research and bioprocess development and accelerate innovation. To achieve this goal, 16 organisations from 9 different European member states have launched the the H2020-INFRAIA project "Industrial Biotechnology Innovation and Synthetic Biology Accelerator" (IBISBA 1.0)[1]. Coordinated by the French National Institute for Agricultural Research (INRA), this project will create a coordinated network of research infrastructure facilities organised to provide transnational research services, expert support and hands-on training to public and private sector (SMEs and multinational companies) researchers both in EU members states and other countries.

One component of the IBISBA 1.0 network is ProtEnz, a multisite infrastructure owned by the National Research Council of Italy (CNR), the Italian partner of IBISBA 1.0. ProtEnz provides transnational access to the discovery, production, characterization, and engineering of proteins and enzymes, with special focus on those from extremophiles, for applications in Green Chemistry, Synthetic Biology, Sustainable Bioenergy, and in pharmaceutical/agroindustrial processes.

For more information on IBISBA 1.0 please visit www.ibisba.eu.

References

1. Industrial Biotechnology Innovation and Synthetic Biology Accelerator (IBISBA) 1.0 - H2020-INFRAIA Grant agreement n. 730976. Contact info: Michael O'Donohue, Project Coordinator. michael.odonohue@insa-toulouse.fr