6th NoRCEL HYBRID CONFERENCE

THE CHEMICAL INFORMATIONAL UNIVERSE

9, 10, 11 AUGUST, 2022

UNIVERSITY OF ST ANDREWS, UK

Preface

The Network of Research on the Chemical Evolution of Life (NoRCEL) was inaugurated in 2013 as the brainchild of Sohan Jheeta. Its aim is to provide an independent platform for airing and sharing ideas pertaining to the chemistry of the emergence and evolution of life on Earth. On the apparently reasonable assumption that this fundamental chemistry will be the same throughout the universe, it follows that any of the ideas and research shared here could be useful for the research and study life on other planets and/or their moons.

Since 2020, the pandemic has wreaked havoc on all nations; in fact, these last two years will probably go down in history for all the wrong reasons. In addition to the general debilitating Covid-19 symptoms and risk of potential death in some cases, the widespread lockdowns imposed by governments have undermined the world economy almost to the brink of recession. In addition, and in the context of military activity and ongoing concerns around climate change, the net effect of all this is an understandable focus on survival and wellbeing. Unfortunately, this comes at the expense of less immediately imperative things, such as attendance at conferences. In the light of this, NoRCEL's executive have created a hybrid conference, so as to offer the opportunity for both our international speakers and attendees from farther afield to participate in this event.

Accordingly, we are pleased to announce an eclectic mix of oral presentations from eminent scientists from all over the world. We hope that you find these proceedings both thought provoking and informative.

I would like to thank NoRCEL's international committee, in particular Martin Dominik, University of St Andrews, UK (President), Oleg Kotsyurbenko, Yugra State University, Russia (Vice President) and Elias Chatzitheodoridis, National Technical University of Athens (CEO).

Thank you.

Sohan Jheeta HND, BSc, MSc, PhD
Founder and Chairman of NoRCEL
Fellow of the Royal Society of Biology
Fellow of the Royal Microscopical Society
31st July 2022

Brief history of University of St Andrews

The town of St Andrews is located on the east coast of Fife—a historic county in Scotland. Its nearest city is Dundee; Edinburgh is some 30 miles away. As of 2011, the town has recorded permanent population of 16,800 which swells by 10,500 in university term time. The University of St Andrews was inaugurated in 1413 by a group of Augustinian clergies and at present, boasts four faculties, namely Arts, Divinity, Medicine and Science. The latter faculty comprises of eight schools: Biology, Chemistry, Computer Science, Earth and Environmental Sciences, Geography and Sustainable Development, Mathematics and Statistics, Physics and Astronomy, Psychology and Neuroscience. The infrastructure of these faculties is spread throughout a collection of buildings both ancient and modern. The oldest of which date back to the time of the university's inauguration, including St Salvator's Chapel, St Leonard's College (Figure 1a) Chapel and St Mary's College quadrangle; with modern constructions exemplified by the Gateway building, built in 2000 (Figure 1b).

(a) (b)

Figure1 (a) St Salvator's Chapel and (b) the Gateway building

Historically, the university also boasts links with the United States of America—for example James Wilson, a signatory of the Declaration of Independence, attended (but did not graduate from) the University St Andrews; other noted famous dignitaries include Andrew Carnegie, Edward Harkness and Bobby Jones. In terms of the present-day intake by the university, it draws students from 145 nations globally, including 15% from North America alone.

Famous alumni mater includes Prince William, Duke of Cambridge, the future King of the Great Britain and his wife Catherine, Duchess of Cambridge. In addition, five Nobel Laureates: three in Chemistry and two in Physiology or Medicine are among St Andrews' alumni. The list of international alumni includes Baron Narendra Patel, a Tanzanian-British obstetrician; Asha de Vos, a Sri Lankan born marine biologist; John Jonston, who was a Polish scholar and physician and Zbigniew Pełczyński who was a Polish-British political philosopher and academic.

Accommodation Address

Agnes Blackadder Hall
University of St Andrews
North Haugh
St Andrews, UK

Conference venue

Physics Theatre B
School of Physics and Astronomy
University of St Andrews
North Haugh
St Andrews, UK, KY16 9SS

Registration

It will be at 08:30 BST (07:30 UTC)

Emergency

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6th NoRCEL conference, St Andrews, 9–11 Aug 2022

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Tuesday, 9 Aug 2022	
9:00 BST 8:00 UTC	**Martin Dominik** Introduction
9:10 BST 8:10 UTC	**Prof Lorna Milne**, Master of the United College and Deputy Principal Welcome on behalf of the University of St Andrews
9:30 BST 8:30 UTC	**Sohan Jheeta** NoRCEL update
9:50 BST 8:50 UTC	**David Smith** Microbiome Studies: The Germ in the Machine
10:30 BST 9:30 UTC	**David Holmes** Constraining the Possible Evolutionary Trajectories of the Emergence of LUCA as it Colonized the Biosphere of Planet Earth
11:00 BST 10:00 UTC	*Coffee break*
11:30 BST 10:30 UTC	**Oleg Kotsyurbenko** Different scenarios for the emergence of life in the cloud layer of Venus
12:00 BST 11:00 UTC	**Dmitry Skladnev** Analytical lab-on-chip for Life detection in the Venusian clouds
12:30 BST 11:30 UTC	**Ralph Lorenz** Titan's Prebiotic Chemistry and Prospects for Dragonfly
13:00 BST 12:00 UTC	*Lunch*
14:00 BST 13:00 UTC	**Sibsankar Palit** Molecules in Interstellar Medium: their genesis and roots to Prebiotic Chemistry
14:30 BST 13:30 UTC	**Elias Chatzitheodoridis** Detection of Reactive Oxygen Species (ROS) as an indicator for areas where life or biosignatures cannot exist
15:00 BST 14:00 UTC	**Angeliki Sofrona** Biosignature detection in soils using Laser Induced Breakdown Spectroscopy (LIBS)
15:30 BST 14:30 UTC	*Coffee break*
16:00 BST 15:00 UTC	**Andrew Pohorille** What Was the Architecture of the Earliest Proteins?
16:30 BST 15:30 UTC	**David Deamer** & **Bruce Damer** 1) Urability: on what worlds and under what conditions can life begin? 2) Updates on testing and the Hot Spring Hypothesis for an Origin of Life
17:10 BST 16:10 UTC	**Helen Hansma** Potassium from micaceous clay for the origins of life
17:40 BST 16:40 UTC	*Bob Bruner's meteorite collection* presented by Elias Chatzitheodoridis
17:55 BST 16:55 UTC	*Ends*

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Wednesday, 10 Aug 2022	
9:00 BST 8:00 UTC	**Claudio Maccone** A mathematical model for the Energy of Ontogeny
9:30 BST 8:30 UTC	**Daniel Helman** Ordering Processes and Living Systems
10:00 BST 9:00 UTC	**Rowena Ball** Optimal stochasticity favours development of complex proto biochemical systems
10:30 BST 9:30 UTC	**Nick Nielsen** Toward Universal Biology: An Observational Research Program in Origins of Life
11:00 BST 10:00 UTC	*Coffee break*
11:30 BST 10:30 UTC	*The NoRCEL gap map – Moving forward…* Discussion led by Martin Dominik
13:00 BST 12:00 UTC	*Lunch*
14:00 BST 13:00 UTC	**David Lilley** The extent of RNA catalysis – are there any limits?
14:30 BST 13:30 UTC	**Giovanna Costanzo** Formamide chemistry, cyclic ribonucleotides polymerization and primitive RNA-catalysis: a unique chemical frame for the origin of life
15:00 BST 14:00 UTC	**Tue Hassenkam** RNA-like polymers produced by hot wet dry cycling
15:30 BST 14:30 UTC	*Coffee break*
16:00 BST 15:00 UTC	**Richard Gordon** On the improbability of discovering the origin of life
16:30 BST 15:30 UTC	**Miryam Palacios-Pérez** Genetic code evolution as revealed by proteins and RNA
17:00 BST 16:00 UTC	**Sávio Torres de Farias** Origin of Metabolism in a Ribonucleoprotein Scenario
17:30 BST 16:30 UTC	**Sohan Jheeta** NoRCEL and its Outreach in Sub-Saharan Africa
18:00 BST 17:00 UTC	*Ends*

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Thursday, 11 Aug 2022	
9:00 BST 8:00 UTC	**Vladimir Kompanichenko** Stages of the origin of life recorded in the sequence of a bacterial cell exit from anabiosis
9:30 BST 8:30 UTC	**Tony Jia** The Effects of Dehydration Temperature and Monomer Chirality on Primitive Polyester Synthesis and Microdroplet Assembly
10:00 BST 9:00 UTC	**Henrich Paradies** Autonomous *de-novo*-phases from lipid A-biomimicry
10:30 BST 9:30 UTC	**Dhanalakshmi Vadivel** Parity Violation Energy Difference calculation of atropisomers
11:00 BST 10:00 UTC	*Coffee break*
11:30 BST 10:30 UTC	**Amy Riches** Building habitable worlds
12:00 BST 11:00 UTC	**Eva Stueeken** Revisiting Earth's oldest biosignatures
12:30 BST 11:30 UTC	**Valentina Erastova** **Computational chemistry - space & time travellers' tool**
13:00 BST 12:00 UTC	*Lunch*
14:00 BST 13:00 UTC	**Oliver Herbort** Chemical state of CHNOPS elements in atmospheres of rocky exoplanets
14:30 BST 13:30 UTC	**Patrick Barth** Follow the Nitrogen – Using isotopes to trace nitrogen fixation by lightning on the early Earth
15:00 BST 14:00 UTC	**Paul Savage** Zinc isotopes in meteorites indicate a low-mass core-collapse supernova source to our Solar System
15:30 BST 14:30 UTC	*Coffee break*
16:00 BST 15:00 UTC	**Andjelka Kovacevic** Large Interferometer For Exoplanets (LIFE): Initial statistical simulations of possible life transmission within a Galactic patch
16:30 BST 15:30 UTC	**Hitesh Changela** Unravelling Prebiotic Evolution in the Early Solar System by Sample Return
17:00 BST 16:00 UTC	**Duncan Mifsud** Exploring Radiation Ice Astrochemistry in the Laboratory – The Production of Ozone from Irradiated Carbon Dioxide Ices
17:30 BST 16:30 UTC	*Closing remarks*
17:45 BST 16:45 UTC	*Ends*

6th NoRCEL HYBRID CONFERENCE: ABSTRACTS

DAY 1

(1) Dave Smith (in-person)

Microbiome Studies: The Germ in the Machine

Network of Researchers on the Chemical Evolution of Life, NoRCEL, Leeds, UK

Abstract
The world first noticed a problem of non-communicable disease in the late 1940s, when significant numbers of people, initially mostly American, started to suffer from sudden heart attack or stroke. As the medical community began to understand this puzzling new phenomenon, an influential researcher, Ancel Keys (see below and ref. 1), threw his weight behind saturated fat as the cause. Later, an equally influential British nutritionist, John Yudkin, began to demonise sugar. Whatever the cause, such disease is clearly associated with increased obesity, and subsequent researchers split into two irreconcilable camps: those that said we eat too much (too greedy), and those that said that we rely too much on mechanical aids (too lazy). Unfortunately, neither of these adequately explain the concomitant rise of immune system problems and of poor mental health. By the year 2000 the concept of the ***microbiome*** was firmly in the hands of social media influencers, with scientists refusing to engage seriously. More recently, however, both science and industry are beginning to take note of the related expression ***microbiota-gut-brain axis***. Sadly, however, modern scientific endeavour is best characterised as a Darwinian struggle for funding, with little real opportunity to take a look at the bigger picture, and the old dietary assumptions have not been seriously challenged. Interestingly, Keys' earlier "Minnesota Starvation Experiment" described a standard food intake for a young, active, male American that averaged 3,500 kcal/day in 1944, which was reduced to 1,800 in a semi-starvation regime with significant consequences [1]. Compare this with the modern reference intake of 2,000 kcal/day – with many people safely limiting themselves to 1,500 or fewer – and it can be inferred that calorie intake has indeed decreased significantly in recent decades. Alongside this, a definitive study has shown that physical activity energy expenditure has not declined between the 1980s and 2008 [2]. This dilemma can be understood by the fact that faecal weight, and therefore faecal energy excretion, has dropped by a staggering two thirds during the move from a traditional to a modern lifestyle [3], presumably a natural consequence of the lack of microbial growth within the intestine. The primary industry response has been to generate a series of probiotic products, enthusiastically received by the general public but, as Brüssow has recently described, with little validated science [4]. The aim of this talk is to provide an evolutionary and ecological rationale for the existence of the intestinal microbiome, and for its widespread failure under the influence of anti-microbial agents in the industrialised environment of the modern age. One notable point is the necessity for a double inheritance – the standard ***parental genetic*** inheritance supplemented with a ***maternal microbial*** inheritance. Both need to be working well together for the avoidance of non-communicable disease.

References

1. Kalm, L.M.; Semba, R.D. (2005). They starved so that others be better fed: Remembering Ancel Keys and the Minnesota Experiment. *J. Nutr*. **135**(6), 1347-1352. https://academic.oup.com/jn/article/135/6/1347/4663828
2. Westerterp, K.R.; Speakman, J.R. (2008). Physical activity energy expenditure has not declined since the 1980s and matches energy expenditures of wild mammals. *Int. J. Obes.*, **32**, 1256-1263. https://cris.maastrichtuniversity.nl/ws/portalfiles/portal/73050462/westerterp_2008_physical_activity_energy_expenditure.pd
3. Burkitt, D.P. (1973). Some diseases characteristic of modern western civilization. *BMJ*, **1**, 274-278. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1588096/pdf/brmedj01541-0038.pdf
4. Brussow, H. (2020). Problems with the concept of gut microbiota dysbiosis. *Microb. Biotechnol*. **13**(2), 423-434. https://sfamjournals.onlinelibrary.wiley.com/doi/10.1111/1751-7915.13479

(2) David S. Holmes (online)

Constraining the Possible Evolutionary Trajectories of the Emergence of LUCA as it Colonized the Biosphere of Planet Earth

Center for Bioinformatics and Genome Biology, Fundacion Ciencia & Vida and University San Sebastian, Santiago, Chile

Abstract

Two roads diverged in a wood (Robert Frost, 1916). To the memory of Dennis Searcy. There is widespread agreement that the last common ancestor of life (LUCA, Last Universal Common Ancestor) gave rise to the Archaeal and Bacterial Domains and ultimately to the Eukarya about 4 billion years ago. However, there is no consensus as to where LUCA evolved, although front runner theories for a LUCA hatchery include deep oceans vent or volcanic hot spring environments. Geochemical parameters, such as salt concentration, pH and temperature, together with the type of energy and electron donors and acceptors available would have shaped not only the biochemistry of LUCA but might also have influenced the subsequent evolutionary pathways taken as it emerged from its hatchery to populate the biosphere of planet Earth. Deep phylogenomic inferences, coupled with ancestral sequence reconstruction, landscape fitness modeling and insights from protein evolution of extant polyextremophiles suggest that competing evolutionary demands of geochemical feedbacks helped microbial populations to traverse otherwise difficult or even inaccessible trajectories to high-fitness genotypes. On the other hand, certain combinations of environmental stresses induce collateral sensitivity and impede the evolution of some trajectories. It also appears that autotrophic metabolisms, perhaps rooted in prebiotic chemistry, provide greater flexibility in traversing fitness landscapes than does heterotrophy, tightly entwining metabolism and the etiology of resistance mechanisms. This study allows us to suggest plausible evolutionary trajectories of cellular life on early Earth and helps us define the envelope for the search for life on exoplanets and moons.

Work supported by Fondecyt 1181717.

(3) **Kotsyurbenko O[1,2].**, Skladnev D., Kompanichenko V., Brushkov A., Khrunyk J. (online)

Different scenarios for the emergence of life in the cloud layer of Venus

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[2]Network of Researchers on the Chemical Evolution of Life, NoRCEL, Leeds, UK
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[5]Lomonosow Moscow State University, Moscow, Russia
[6]Ural Federal University, Ekaterinburg, Russia;
[7]M.N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia

Abstract
For a long time, Venus attracted much less attention compared to Mars in the concepts of the existence of extraterrestrial life because its modern surface is heated to very high temperatures, which are unsuitable for the terrestrial living organisms. However, a recent sharp increase in interest in this planet for astrobiologists has occurred due to the active discussion of the hypothesis of habitability of its cloud layer. In such an extraterrestrial ecosystem, the existence of the so-called aerochemo(photo)lithotrophic microbial community is supposed to exist, using sulfur and iron compounds as the main elements for energy production.

An important difference between the cloud layer of Venus and the Earth's cloud system is its absolute spatial isolation as a possible habitat for organisms. If the microbial biomass in clouds on Earth is constantly replenished as a result of the entry of microorganisms from the surface with air convection flows, then such a mechanism is impossible on Venus due to the apparent absence of any terrestrial-type organisms on its super-hot surface.

Despite the extremely low concentration of water vapor in the modern clouds of Venus, it is assumed that living organisms can exist in aerosols, in which the water phase can be concentrated in a small volume and contain a certain number of microorganisms capable of active life.

To date, there are various concepts of the geological past of Venus, within which the question of the existence of water on its ancient surface is discussed. This fact determines which of the hypotheses of the possible origin of life on Venus may be dominant. Moreover, the clouds themselves can also be considered as a system that meets the requirements for the emergence and further evolution of living organisms.

In general, several different scenarios for the appearance of living organisms can be considered on Venus. These include a surface or subsurface scenario in which life emerges as molecular systems become more complex, as well as a new scenario for the origin of life in clouds.

Presently, various compounds such as CO_2, CO, N, SO_2, $FeCl_2$ have been found in the atmosphere of Venus. Under certain conditions it could be the basis for the synthesis of various bioorganic macromolecules. Moreover, it is assumed that iron and sulfur compounds may play an important role in lithotrophic metabolism as the main source of energy. The cloud layer is characterized by large temperature fluctuations, the presence of all the main biogenic elements, as well as energy sources for photo- and chemosynthetic life, and is a kind of macro-scale fermenter for various biosynthesis reactions.
An alternative direction regarding the emergence of life on Venus is the concept of panspermia, which transforms the question of the origin of life into the question of its delivery to Venus from outside and its adaptation to conditions in the Venusian clouds and subsequent evolution.

In general, Venus is a unique cosmic body, on the example of which various concepts of the origin of life and scenarios for its further evolution can be presented.

(4) **Dmitry Skladnev** [1, 2], Vladimir Sorokin [1], Sergei Karlov [3], Oleg Kotsyurbenko [2, 4] (online)

Analytical lab-on-chip for Life detection in the Venusian clouds.

[1]Research Center of Biotechnology of the Russian Academy of Sciences, Winogradsky Institute of Microbiology, Moscow, Russia
[2]Network of Researchers on the Chemical Evolution of Life, Leeds, UK
[3]Moscow Polytechnic University, Russia
[4]Yugra State University, Khanty-Mansiysk, Moscow, Russia

Abstract
To detect evidence of Life in the clouds of Venus - microbial cells - we propose to use specially designed highly sensitive chips that can quickly, selectively and reliably detect the only reliable evidence of the presence of Life. Single used acid resistant analytical lab-on-chip devices are simple and weightless tools and biosensors well established that rival conventional cells detection methods. Among them, gravimetry in combination with spectrometry methods is the most promising, since the results can be interpreted at the time of testing.

Our is concept based on the fact that a living thing is something that can be turned into inanimate by deliberately biocidal treatment. For terrestrial type of organisms such treatment could be simply destroying cell membranes. Treatment with lysing solutions or ultrasonic have the similar effects. The use of proposed biosensors makes it possible to analyze liquid samples before and after the destruction of cells presumably present in it. In particular, it is possible to distribute insoluble particles by size with subsequent spectral analysis of the corresponding chemical products of destruction.

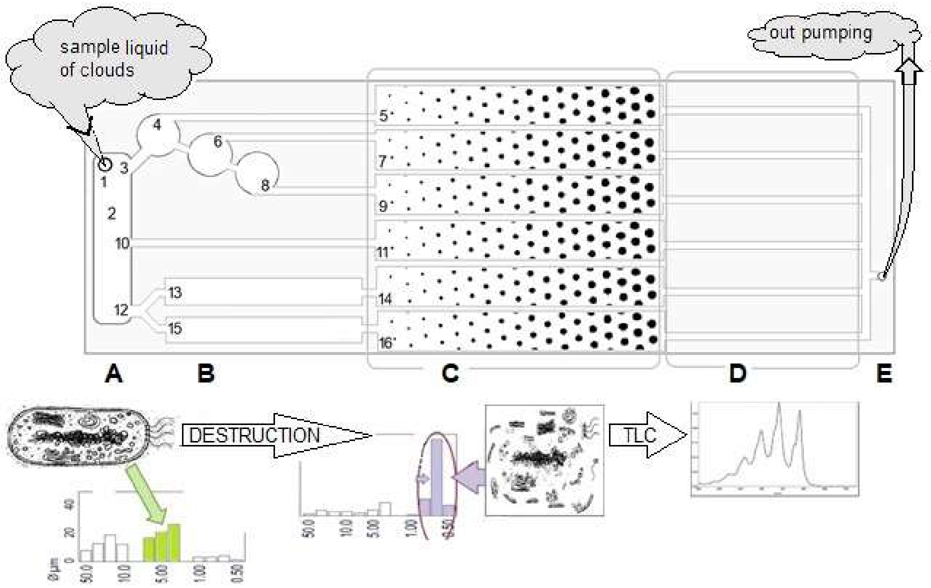


Figure. Automated multistep assay in an analytical chip format and cells changes. Life lab-on- possible

The microfluidic chip includes (A) a reservoir (2) for the sampled liquid and distribution dividing channels (3, 10, 12); (B) a zone of cell destruction by ultrasound in various modes (4, 6, 8), two type of chemical lysis (13, 15) and a control untreated sample (11); (C) a zone of particle size distribution; (D) spectrometry zone; (E) out pumping channel.

(5) Ralph Lorenz (in-person)

Titan's Prebiotic Chemistry and Prospects for Dragonfly

Johns Hopkins Applied Physics Laboratory, Laurel, MD 20723, USA

Abstract
As an organic-rich Ocean World environment, Titan attracts particular astrobiological interest. Beyond the (in this author's view, unlikely) possibility of living chemical processes in nonpolar liquid methane, the formation of amino acids, pyrimidine bases and other building blocks of life as we know it (LAWKI) from the hydrolysis of photochemical products in impact melt on Titan's surface provides a promising setting for rich prebiotic synthesis. The long freezing time (>kyr) of such environments raises possibilities that are difficult to replicate in the laboratory, and thus in-situ investigation is the logical approach to investigating how much chemical complexity may have been achieved.

The likelihood that a spacecraft happens to land at the exact spot where such organics are exposed is small: mobility is key to finding targets of interest. Titan's low gravity and dense atmosphere, fortunately, enable transformative mobility by rotor flight. NASA's next New Frontiers mission, Dragonfly, will explore Titan in the mid-2030s. This vehicle has eight rotors to make multi-km flights every couple of Titan days. It will initially land in the safe dune/interdune terrain (itself organically rich, but probably unmodified by hydrolysis) and make its way towards the Selk impact structure where material more abundant in water ice may be exposed). Dragonfly incorporates a pneumatic sampling system, and a powerful mass spectrometer with the ability to measure high-molecular weight materials and to investigate chirality.

This talk will report on Dragonfly's current development, its operations plans, and what we might hope to find on Titan.

(6) Sibsankar Palit[1,2], Bruno Curjuric[1,2], Vijaishree Sivaswamy[1], Gouripriya S Menon[1], Abhishek Sarbhukan[1], Niharika Rath[1,3] (online)

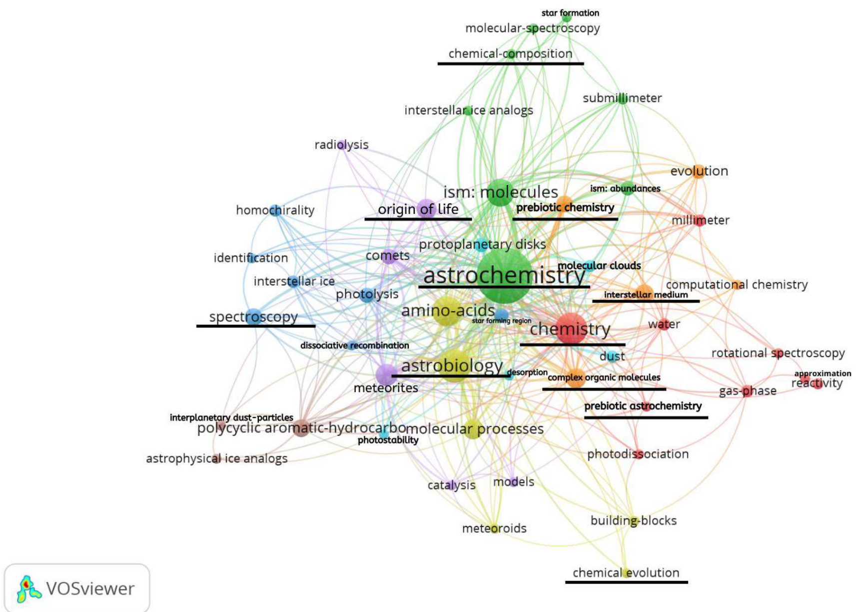
Molecules in Interstellar Medium: their genesis and roots to Prebiotic Chemistry

[1]LIFE- To & Beyond
[2]Network of Researchers on the Chemical Evolution of Life, NoRCEL, Leeds, UK
[3]InnovaSpace, UK.

Abstract

From synthesizing the first atoms in the universe to stellar nucleosynthesis and the formation of complex celestial and living systems, it can be said that chemistry originated in space. Though atoms and molecules constitute only less <5% of the total cosmic composition, they strikingly contribute to all of the chemical complexity in the universe. Perhaps it wouldn't be an exaggeration to refer to a small fraction of the universe as 'The Molecular Universe' as defined in the IAU Symposium. Thus, studying the molecules in space demands a multidisciplinary approach that would focus on the mechanism of the formation of molecules in space along with its detection and destruction. Moreover, the limitations of the Top-down approach to the study of the Origin of Life on Earth have complementarily added to the study of Astrochemistry and Prebiotic Chemistry via the Bottom-up approach. This aims to link the organic molecules in space to the basis of 'Life as we know it.' In the star-forming region, the dense interstellar clouds and proto-stellar disks help initiate the chemical pathways that form organic compounds essential for life.

Interestingly, some of these chemical species are often delivered to the surfaces of newly forming planets, where they play an important part in the origin of life. Furthermore, considering the universality of the chemical reactions (in similar environments), life may have also originated in other parts of the universe. To date, scientists have detected around 250 molecules in space. Further, observation and detection of more complex molecules will help us understand the relation between the origin of life and molecules in space. Recent works in the same direction include research into whether homochirality is generated in space, the interstellar synthesis of glycerol phosphates, and so on. Therefore, this review aims to give an overview of the rich chemical information spread throughout space, with a special focus on the genesis of the molecules in the interstellar medium, while trying to draw a link between the origin of life on Earth and other worlds.



❖ **Bibliometric outlook based on the topic, 'Molecules in Interstellar Medium: their genesis and roots to Prebiotic Chemistry' generated using VOSviewer from the indexed journals on the Web of Science database.**

** Authors would like to thank Chandigarh University for providing access to the Web of Science Database and we are also grateful to Mr. Subhajit Hazra (Ph.D. Scholar, UIPS, Chandigarh University) for generating this bibliometric outlook and for valuable suggestions.

(7) Georgiou Christos[1*,] **Chatzitheodoridis Elias[2,3**,]** Kalaitzopoulou Electra[1], Papadea Polyxeni[1], Skipitari Marianna[1], Varemmenou Athina[1], Thoma Aikaterini[2], Stavrakakis Hector-Andreas[2], Kapagiannidis Andreas[2], Markopoulos Ioannis[4], Platanou Diamanto4, Alexandrou Aggelos[4], Holynska Malgorzata[5] (in-person)

[1]*Department of Biology, School of Natural Sciences, University of Patras*
[2]*Department of Geological Sciences, School of Mining and Metallurgical Engineering, National Technical University of Athens*
[3]*Network of Researchers on the Chemical Evolution of Life (NoRCEL), Leeds, UK*
[4]*ZEROONE LTD, Athens, Greece*
[5]*Materials' Physics & Chemistry Section (TEC-QEE), Technical Reliability and Quality Division (TEC-QE), ESTEC, ESA*

Abstract

Intense irradiation of planetary surfaces from the Sun's UV rays and from cosmic rays, as well as from the fine fracturing of minerals when bombarded by micrometeorites or during dust winds, is a continuous process that induces the formation of Reactive Oxygen Species (ROS). Mineral ROS can be present as metal combinations of superoxides and peroxides. All release H2O2 upon H2O-wetting combined with certain metal catalysis. Hydroxyl radicals (•OH) also belong to this group of ROS chemicals, and can be released upon H2O-wetting of the planetary soils or regoliths.

The oxygen release has been firstly observed to exist in the Martian soils during the Viking Label release biological experiment and it is now attributed to an abiotic process that is caused by the presence of ROS in the regolith materials, and not from microorganisms.

The existence of ROS species in planetary soils and regoliths is proposed to be used as an indication of the absence of biosignatures in the surface soils of planets and that is because ROS are highly reactive with organics, resulting to their disintegrating. The construction of a miniaturised oxygen release detection device (OxR) which can indirectly detect ROS in planetary soils and regoliths, as well as in ices, is necessary to detect soils with ROS which are not appropriate samples to search for life or its traces, or to collect it during sample return missions.

Furthermore, the scaling up of such an OxR device can be used to scavage the oxygen gas released from regoliths that are rich in ROS or repeatedly after allowing certain time between operations to reactivate from the sun's UV radiation. The whole process is of very low energy consumption while parallel process of large areas might cover all the oxygen requirements of a small community of astronaut workers.

(8) Angeliki Sofrona[1,2,4], Elias Chatzitheodoridis[1,2,3] (in-person)

Biosignature detection in soils using Laser Indused Breakdown Spectroscopy (LIBS)

[1]National Technical University of Athens, School of Mining and Metallurgical Engineering, Department of Geological Sciences
[2.]STELLAR DISCOVERIES Scientific Association, Athens, Greece
[3]Network of Researchers on the Chemical Evolution of Life (NoRCEL), Leeds, UK
[4]Agricultural University of Athens, Faculty of Biotechnology, Athens, Greece

Abstract
Preliminary work involved the study of biosignature detection from LIBS spectra acquired from the mineral montmorillonite, mixed with the fungus *Ulocladium Chartarum*. However, the presence of atmospheric air during the analysis was misleading in the interpretation of the spectra, because the air consists of the same major volatile elements as *U. Chartarum* does (i.e., H, O, N). Additional to these elements, other chemical elements are also detected (i.e., K, Na, and possible P) which constitute the montmorillonite clay mineral. The comparison of the spectra acquired from the mixed sample, the mineral itself, and the fungus alone could not provide any secure evidence.

In the present work, we are going to remove the atmospheric air background, by performing the analyses in Helium, and eventually magnify any possible differences.

With LIBS we will analyse three different samples: (a) pellet of pressed Montmorillonite powder; (b) pellet of pressed powder of Montmorillonite mixed with *U. Chartarum*; and, (c) the fungus alone. Specific care will be taken to sample the fugus alone and not the nutrient substrate, so that contamination from the nutrient constituents is precluded.

The experiment will run in a specially made vacuum chamber with the sample inside it. The chamber will be filled with He gas of purity 99.999 vol.%, thus the atmospheric air will be removed or highly reduced in volume proportions. Helium is a noble gas, chemically inert under all normal conditions [1]. Prior to any analyses, we will perform background measurements, i.e., with no samples.

The samples will be placed on a moving table, inside the Plexiglas cubic chamber. A tightly attached objective lens will be located on the front side of the chamber. Gas inlets will serve the purpose of vacuum generation and gas venting, in a sequential way, so that atmospheric gases from the chamber are removed. Another inlet will allow close proximity of the optical fiber that is connected to a spectrometer.

Reference
[1] Lide, D. R., ed. (2005). *CRC Handbook of Chemistry and Physics* (86th ed.). Boca Raton (FL):CRC Press. ISBN 0-8493-0486-5.

(9) Andrew Pohorille (online)

What Was the Architecture of the Earliest Proteins?

NASA Ames Research Center, Moffett Federal Airfield, USA

Abstract
Most modern, water-soluble proteins share a common architecture. They all have hydrophobic core surrounded by a mostly hydrophilic exterior exposed to the aqueous medium. Even with a minimal core, this requires a length of at least 40 residues. This requirement creates “the protein problem”. The earliest proteins must have been shorter. If so, what was their structure? In combination with in vitro experiments, atomic-level computer simulations by way of molecular dynamics reveal an answer to the puzzle. Small, protein that contain a flexible, hydrophilic core stabilized by a metal and a catalytic loop have been evolved and are functional. The core has been found to be quite robust to mutations, which is a considerable advantage in the early evolution. A possible evolutionary path from the early to the modern architecture can be outlined.

(10) David Deamer & Bruce Damer (online)

Updates on Origin of Life Research

Urability: on what worlds and under what conditions can life begin?
Testing and the Hot Spring Hypothesis for an Origin of Life and new directions

University of California at Santa Cruz, USA

Abstract

Two decades of field testing prebiotic chemistry at volcanic hydrothermal settings, results from early Earth geology, and the search for life on Mars and other worlds have provided a foundation for a current article in Astrobiology: Urability: A Property of Planetary Bodies That Can Support an Origin of Life. Presenters David Deamer and Bruce Damer will introduce the proposed term and an associated chemical, geological and combinatorial framework conducive to key prebiotic processes. An update on the latest tests of the "Hot Spring Hypothesis" scenario for an origin of life will then be provided including recent field work at Fly Geyser in Nevada, USA. This work offers a glimpse of future field testing of protocell synthesis "in the wild" with the polymerization and encapsulation of RNA and DNA in hot spring conditions at a differing range of pH and temperatures. The addition of peptides, also polymerized in these same conditions, will provide protocells a richer starting set of potentially emergent functions through selection. Another line of research involves wet-dry cycling of the monomers of RNA and direct visual confirmation of long chains and rings of RNA by Atomic Force Microscopy featured recently in Scientific Reports in a recent article with Tue Hassenkam. A final research direction will propose applying the concept of a "progenitor" to origin of life scenarios. A progenitor is a substrate within which combinatorial chemistry and selection can be supported and pathways to the first biological functions and forms discovered. A progenitor for the hot spring scenario would consist of multilamellar lipid complexes and populations of cycling vesicles containing sets of polymers, some colocalized and mobilized on membrane surfaces, thereby enabling interaction in a 2D planar interface overcoming entropic and combinatorial barriers.

(11) Helen Greenwood Hansma (online)

Potassium from micaceous clay for the origins of life

Department of Physics, University of California at Santa Barbara, CA 93106

Abstract

This hypothesis for the origins of life includes recent research results in areas such as Liquid-Liquid Phase Separation by Brangwynne and many others, mechanochemistry in biological systems, and the polymerization of nucleotide monophosphates on mica by Hassenkam, Damer, Mednick, and Deamer [2020]. According to this hypothesis, mica in micaceous clay provided an ideal environment for emerging life (1-4). Life also imitates mica in many ways. One similarity between life and mica is the presence of high concentrations of potassium ions, K^+. Potassium ions are present at concentrations of ~0.1 M in living cells of all types. Mica's negatively charged mineral sheets are held together by 6 potassium ions per square nanometer between the mica sheets. This gives a K^+ concentration of 10 M, when the mica sheets are separated by 1 nm, or 0.1 M when the mica sheets are separated by 100 nm. Biotite is a black mica rich in Mg^{++} and Fe. Fe is useful for the redox reactions used at life's origins to produce reduced organic molecules, and Mg^{++} interacts with DNA in living cells.

Please visit this link to view the following recorded event:
When and where did intracellular potassium arrive at the origins of life? - a Biophysical Society virtual event - the recording is available here:
https://www.biophysics.org/upcoming-networking-events/when-and-where-did-intracellularpotassium-arrive-at-the-origins-of-life

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(12)Bob Bruner's Martian Meteorites Exhibition collection

Mars Society member and Volunteer, Denver Museum of Nature and Science, USA

presented by **Elias Chatzitheodoridis** (in-person)

DAY 2

(13) Claudio Maccone (online)

A mathematical model for the Energy of Ontogeny

SETI, Italy

Abstract

Ontogeny (previously called Ontogenesis) is the amount of time between birth and puberty. In this paper we present a mathematical model to compute the Energy of Ontogeny. In other words, we have discovered some simple mathematical equations telling us how much energy is necessary to build a new Human, or a new animal, or plant, or (perhaps) even a new cell. The idea is that the part of one's life in between birth and peak is a LOGNORMAL probability density IN THE TIME, rather than in another independent variable, and that the time of puberty is the ascending inflexion point of such b-lognormal (a lognormal starting at time b=birth, rather than at time t=0). Now about the ENERGY of Ontogeny. If we regard this b-lognormal as a POWER curve (measured in Watts), the relevant ENERGY of Ontogeny is of course the INTEGRAL of that Power Curve in between birth and ascending inflexion. We were able to find an exact formula for this integral, and so, potentially, to find how much ENERGY is needed by all Species to create new offspring.

(14) Daniel Helman (online)

Ordering Processes and Living Systems

College of Micronesia - FSM

Abstract

Chirality arises from a threshold. Molecules with only two or three atoms, for example, cannot be chiral because the required elements of form are not present. The threshold from non-living to living systems involves implicit ordering processes for systems functions, without which a system will not be able to maintain its functions. By analogy with chirality, there is likely some mathematical structure to the required elements for ordering. This talk gives a brief overview of the subject, and includes thermodynamic entropy, information entropy and species entropy in its descriptions.

(15) Rowena Ball (in-person)

Optimal stochasticity favours development of complex proto biochemical systems

Australian National University, Canberra

Abstract

A primordial environment that hosted molecular pre- or proto-biochemical activity would have been subject to random fluctuations. What might be the optimum variance of such fluctuations, such that net progress could be made towards a living system? We investigated using a dynamical model for the competitive formation of simple micelles and peptide-stabilized micelles, as a proxy for a ‘simple’ complex prebiotic molecular system. The aim was to develop a picture of the behaviour of the system subject to Gaussian fluctuations of differing variance between simulations. We find that outcomes are highly dependent on the fluctuation variance and locate an optimum range of the variance that favours production and retention of the more complex system of peptide-stabilized micelles over unstable simple micelles. Such an environment may be self-selecting for a complex, evolving chemical system to outcompete simple or parasitic molecular structures. These results suggest that a 'messy’ or fluctuating environment was essential for the emergence of life, and that some

(16) Nick Nielsen (in-person)

Toward Universal Biology: An Observational Research Program in Origins of Life

Network of Researchers on the Chemical Evolution of Life, NoRCEL, Leeds, UK

Abstract

Technology for exoplanet search has come into use only in the past thirty years, and we are now on the cusp of exoplanet atmospheric spectroscopy, which will reveal the atmospheric composition of some exoplanets. If life is not a cosmological imperative, if its appearance is not inevitable once the necessary prerequisites are in place, then there will be geologically complex planets that also develop chemical complexity without the particular form of chemical complexity that we identify as life. Differentiation of non-biological chemospheres from biospheres based on atmospheric spectroscopy may be possible through following the model of reconstructing stellar evolution. A taxonomy of planetary types surveyed at different periods of time in their development in different planetary systems may allow for the reconstruction of chemospheric evolution, in turn revealing a taxonomy of typical forms of chemospheric development for given planetary types. The more comprehensive our observational research program in reconstructing the history of chemospheres across diverse types of planets, the more likely we are to be able to reconstruct the typical developmental pathway of a living biosphere, allowing us to distinguish between non-living chemospheres and living biospheres, and to focus on the turning point at which the transition is made from chemosphere to biosphere.

(17) David M.J. Lilley (in-person)

The extent of RNA catalysis – are there any limits?

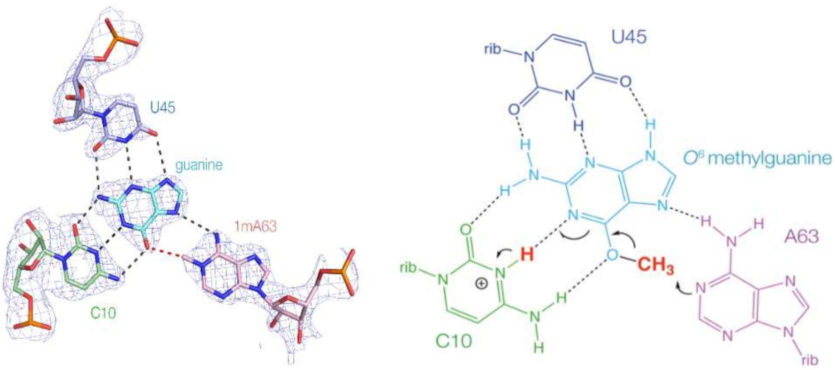
School of Life Sciences, University of Dundee, United Kingdom

Abstract

The RNA world hypothesis for the early development of life on the planet requires that RNA molecules (ribozymes) could have catalysed a wide variety of chemical reactions. Known ribozymes in contemporary biology carry out a limited range of chemical catalysis, mostly involving phosphoryl transfer, but *in vitro* selection has generated species catalysing a broader range of chemistry. To gauge the feasibility of an RNA world it is useful to explore if ribozymes can exploit sophisticated catalytic strategies.

A ribozyme has recently been selected that can catalyse a methyl transfer reaction using O6-methylguanine as donor. We have solved the crystal structure of this ribozyme at a resolution of 2.3 Å, showing how the RNA folds to generate a very specific binding site for the methyl donor substrate. The structure immediately suggests a catalytic mechanism, involving a combination of proximity and orientation, and nucleobase-mediated general acid catalysis. The mechanism is supported by the pH dependence of the rate of catalysis. This small chemical machine employs a relatively sophisticated catalytic mechanism, broadening the range of known RNA-catalysed chemistry. This lends new support to the RNA world hypothesis

Going still further, how could RNA overcome its relative chemical simplicity and expand its catalytic repertoire ? The RNA world would have required a much broader range of RNA catalyzed chemistry, including “difficult” reactions like making C-C bonds. Modern protein enzymes achieve this by using co-enzymes, and perhaps RNA could do the same. RNA is a superb receptor for small molecules, as exemplified by the riboswitches. A significant number of these bind coenzymes, including SAM, TPP, NAD+ and FMN, and it’s not a big leap to imagine that the riboswitch might have evolved from an ancient ribozyme, or might be converted into a novel ribozyme.



Deng *et al* Structure and mechanism of a methyl transferase ribozyme *Nature Chem Biol* **18**, 556–564 (2022)

(18) Giovanna Costanzo[1], Angela Cirigliano[1], Judit E. Šponer[2], [2]Ernesto Di Mauro (in-person)

Formamide chemistry, cyclic ribonucleotides polymerization and primitive RNA-catalysis: a unique chemical frame for the origin of life

[1]*Institute of Molecular Biology and Pathology (IBPM), CNR, Rome, Italy*
[2]*Institute of Biophysics of the Czech Academy of Sciences, Brno, Czech Republic*

Abstract
Life is made of the intimate interaction of metabolism and genetics, both built around the chemistry of the most common elements of the Universe (hydrogen, oxygen, nitrogen, carbon).

The origin-of-life quest has long been split in several attitudes exemplified by the aphorisms "genetics-first" or "metabolism-first". Overstepping the opposition between these approaches by a unitary theoretical and experimental frame and taking into account energetic, evolutionary, protometabolic and ur-environmental aspects, we propose a simple pathway leading to a complete prebiotic reactive system. Specifically, we analyze the synthetic reactions leading from the onecarbon atom compounds HCN and its hydrolyzed form NH2COH formamide to prebiotically relevant compounds in the presence of catalysts. We observe the formation of all the extant biological nucleic bases, of carboxylic acids, of aminoacids and of condensing agents in the presence of tens of catalysts of terrestrial origin and of 12 meteorites. We also observe in the same chemical frame: the formation of cyclic nucleotides and their spontaneous polymerization to oligonucleotides; their terminal ligation yielding longer polymers; a ribozyme activity causing the terminal transfer of nucleotides between *in vitro* generated oligomers and, more recently, short oligonucleotide sequences with a higher propensity to fold into functional biomolecules.

This path to the spontaneous generation of chemical complexity highlights the ability of RNA to potentially solve the problem of the origin of genetic materials, based on its intrinsic catalytic properties and on the attainment of increasingly higher levels of molecular stability and complexity.

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https://doi.org/10.1101/2020.05.04.075614
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(19) Tue Hassenkam (in-person)

RNA-like polymers produced by hot wet dry cycling

University of Copenhagen, Denmark

Abstract
It has been suggested that the earliest forms of life relied on RNA-like polymers, an era now referred to as the RNA world. Although previous investigations (see references) reported that wet–dry cycles simulating prebiotic hot springs provide sufficient energy to drive condensation reactions of mononucleotides to form oligomers, so far there has been no plausible process that can produce polymers long enough to fold into catalytic structures and store genetic information. Here we visualize the products of wet-dry cycles by atomic force microscopy. Particles consistent with globular oligomers were often observed, but when nucleotide mixtures capable of base pairing were used we often observed ring-like structures with an average diameter of 30-40 nm. The thickness of fibers forming the rings was consistent with single stranded products, but some had thicknesses indicating possible base pair stacking. In other cases we observed very long continuous polymers stretching for several micrometers. Control experiments confirmed that these were not contaminants from biological sources. The dimensions of the polymers were consistent with long, single stranded polymers that in some stretches bundled up into multi-stranded segments. We conclude that RNA-like rings and polymer structures could have been synthesized nonenzymatically on the prebiotic Earth with lengths sufficient to fold into ribozymes and carry genetic information.

(20) Richard Gordon[1], Deb Mainak[2] (online)

On the improbability of discovering the origin of life

[1]Gulf Specimen Marine Laboratory & Aquarium, 222 Clark Drive, Panacea, FL 32346 USA (Retired (from the University of Manitoba,)
[2]Amrita Vishwa Vidyapeetham, Kolkata, India,

Abstract
Let us suppose there were *N* steps to the origin of life. Lacking a time machine, while we will never know *N* nor the order of the steps, the best we can do for now is to carry out those steps we reason happened, and try to create life from scratch. Suppose that for each step *i*, there are T_i theories we have communally thought of. If only one theory was right, then the probability of choosing the right theory for that step is $p_i = 1/ T_i$. The probability P of choosing the correct sequence of theories is then the product of the p_is. The vast literature of tens of thousands of papers purporting to bear on the origin of life sometimes argue for some step being "First". If we think we know *N*, there could be up to *N!* ways of ordering the steps. We thus arrive at a worst-case analysis that:

$$P = (1/N!)\prod_{1}^{N}\frac{1}{T_i}$$

which could be a very small number. I will try to estimate some of the T_i and *N* to guesstimate *P*. Constraints that we deduce on which theories are more likely, and which steps might have come before other steps, could increase *P*.

(21) Miryam Palacios-Pérez[1,2], Marco V. José[1,2] (online)

Genetic code evolution as revealed by proteins and RNA

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[2]Network of Researchers on the Chemical Evolution of Life, NoRCEL, Leeds, UK

Keywords: RNA; peptides; proteins; amino acids; primeval code; extended codes 1 and 2; evolution of genetic code; FUCA; LUCA

Abstract
There are several models on the evolution of the genetic code. One of them starts with Eigen's proposal on the primeval genetic code (PGC), that later evolved by two different pathways dubbed Extended Genetic Code 1 and 2 (ExGC1 and ExGC2), which finally conformed the current standard genetic code (SGC). Herein, we describe the evolutionary path of the encoded molecules based on such route.

The aa encoded by the PGC form a collection of peptides capable of binding the various molecules formed prebiotically on the early Earth, mainly nucleotide-type cofactors, or not-complex molecules (Palacios-Pérez et al. 2018). While it was revealed that some portions of the main RNA molecules of the translation process were the first to be encoded, and they configured as hairpins.

The fragments encoded by one or the other type of ExGC belong to distinct and complementary portions of the corresponding modern molecules, either proteins or RNAs. However, while the portions of proteins encoded by the ExGC1 are shorter and more numerous than the less numerous and longer portions encoded by the ExGC2, in RNA molecules we only see the complementary behaviour of the portions encoded by one or the other ExGC.

The proteins already formed encoded by ExGCs, probably performed functions related to the modern ones (Palacios-Pérez & José 2019). On the other side, the complete rRNAs and tRNAs, as well as the RNA moiety of other molecules were encoded almost completely by triplets pertaining to both ExGCs.

All these molecular constituents finally assembled cooperatively, and eventually resulted into the modern cellular molecules when LUCA appeared and beyond until today.

(22) Sávio Torres de Farias (in-person)

Origin of Metabolism in a Ribonucleoprotein Scenario

1) Lab. Evolutionary Genetics - Paulo Leminski, Department of Molecular Biology, Federal University of Paraíba
2) Network of Researchers on the Chemical Evolution of Life, NoRCEL, Leeds, UK

Abstract
The occurrence of organized chemical transformations defined as metabolism is one of the most important characteristics of life. Surprisingly though, there is not a consensus about how those transformations were originated in the origin of life. RNA world advocates suggest that biochemical pathways started with ribozymes that were further substituted by enzymes. However, most of the biosynthetic routes of ribozymes described do not overlap with the enzymatic routes, and there is not a clear theory about how this transition happened. An important step to solve this dilemma has been elucidated in the last decade when researchers found that some complex routes of chemical transformations, such as the glycolytic and the citric acid pathways, already existed in prebiotic Earth due to physicochemical forces alone. Defined here as protobiotic pathways, we propose that those metabolic exchanges working without the aiding of any biological catalysts were the ones that guided the origin of metabolism. Under this scenario, some quasi-randomly encoded peptides at the origins of translation systems would be capable to bind metabolites in protobiotic routes. When those bounds facilitated or accelerated the conversion of metabolites along the protobiotic path and the products were beneficial, then natural molecular selection acted to preserve the system. Thus, we propose that the origin of metabolism happened when peptides started to bind metabolites in protobiotic routes without disturbing (and possibly aiding) their chemical transformation paths.

(23) Sohan Jheeta (in-person)

NoRCEL and its Outreach in Sub Saharan Africa

Network of Researchers on the Chemical Evolution of Life, Leeds, UK

Abstract
Currently there are low levels of access to high quality education and learning facilities in certain developing nations, especially in sub-Saharan Africa. For example, at best, some university facilities there are barely comparable to western high school levels and, at worse, they don't even have modern laboratory equipment; the basics that they do have being relics from the 1960's and 70's. In addition, I know of at least one secondary school in Malawi where there are two "sittings" —a morning session for one set of pupils and an afternoon for the second. Both with the same teachers. That is to say, there is both the lack of qualified teachers and they cannot afford to expand the school. During the last six years I myself have been promoting science throughout parts of the developing world, principally through astronomy because this is one science which is common to humanity.

I have given numerous oral presentations on space in general, astrochemistry, astrobiology and astrophysics as well as helping to promote an interest in these subjects by holding specific workshops. Until now, I have been operating as a "one-man band" and the challenge is to encourage students to become involved and active in astronomy, astrophysics, astrochemistry and astrobiology (the astroscience) and then to support them should they wish to progress further and take up a career in these fields. There are many difficulties to overcome, including lack of awareness and inclusion with the wider world, as well as a severe lack of funding. The many talented and able students who could become assets in the field of astronomy are missing out and if only they had the opportunity, they could really develop their capabilities and become excellent researchers and astronomers. In order to even stand a chance of making this happen, we need liaison with European established organisations that can deliver both expertise, funding and definitive, quantifiable schemes which will raise the expectations of these students as well as the universities. The ultimate goal is to put astronomy on the curriculum. The interest I have so far been able to generate amongst students is intense and I have been inspired by their enthusiasm, so the time is now right to develop and widen these activities in a more organised and proactive manner and this is where NoRCEL comes into force.

We are now developing and have thus launched NoRCEL's innovative initiative, the Astro Science Exploration Network (ASEN) which had its inaugural online conference in April 2022. The aims and objectives of this venture centre around establishing a hub for creating the opportunity to deliver more education in the fields of astrobiology, astrochemistry and astrophysics in the sub-Saharan regions of Africa.

Day 3

(24) Vladimir N. Kompanichenko (online)

Stages of the origin of life recorded in the sequence of a bacterial cell exit from anabiosis

Institute for Complex Analysis of Regional Problems RAS, Birobidzhan, Russia

Abstract

According to the concept of thermodynamic inversion (the TI concept) of the origin of life, the intermediate position of a prebiotic system between non-living and living states maintains in the oscillating mode. Thermodynamically, such a position corresponds to the approximate equality of the total contributions of entropy and free energy in the system [1]. In framework of the theory of anabiosis in microbiology, a resting (dormant) bacterial cell takes similar intermediate position between non-life and life: on the one hand, it is no longer able to counteract the increase in entropy, but, on the other hand, it retains structural memory of the previous living state. The sequence of metabolism origin in primary living cells has not been reliably stated by researchers yet, while the sequence of changes in metabolic processes of a cell entering the state of anabiosis and coming out of it (usually proceeding in reverse order), has been well studied both theoretically and experimentally. In this presentation, I attempt to outline a general sequence of the metabolism formation in the process of life emergence, based on the correlation of these two intermediate states between non-life and life (pre-biotic and bacterial). According to the TI concept, life originated in a pulsating updraft of hydrothermal fluid. It included four stages. 1) Self-assembly of a cluster of organic microsystems (complex liposomes). 2) Activation (formation of protocells): appearance in the microsystems a weak energy-giving process of respiration due to redox reactions; local watering in the membrane. 3) Initiation (formation of living subcells): formation of a non-enzymatic antioxidant system; dawning of the protein-synthesizing apparatus. 4) Growth (formation of living cells - progenotes): arising of the growth cell cycle; formation of the genetic apparatus [2]. Life

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(25) Tony Jia (online)

The Effects of Dehydration Temperature and Monomer Chirality on Primitive Polyester Synthesis and Microdroplet Assembly

1) *Earth-Life Science Institute, Tokyo Institute of Technology, Japan*
2) *Blue Marble Space Institute of Science, USA*

Abstract

Synthesis of polyester gels via dehydration of α-hydroxy acid (αHA) solutions through mild heating is a plausible route to form primitive functional polymers for the origins of life. These gels can then assemble into membraneless droplets upon rehydration in aqueous media through phase separation. Such droplets are believed to be plausible primitive compartments that can segregate and compartmentalize early biomolecules and biopolymers. However, the conditions for polyester synthesis and microdroplet assembly have yet to be explored broadly. We investigated here the effects of heat and monomer chirality on simple dehydration synthesis and assembly of homopolyester microdroplets from several αHA types using microscopy and mass spectrometry. We observed that lower dehydration temperature (≤ 80°C) resulted in shorter polyesters than higher temperatures (up to 150°C). After rehydration of polyester products, droplet assembly propensity correlated with longer polymer length. Low temperature (40°C) dehydration yielded only short polyesters and nearly no droplet formation. Finally, polyesters derived from dehydration/rehydration synthesis of homochiral lactic acid and phenyllactic acid monomers were of equal length and propensity for droplet assembly as those derived from racemic starting materials. These results suggest that polyesters and membraneless microdroplets derived from polyesters can form under a wide variety of temperatures and from different monomer chiralities, thus enabling many possibilities for such varied systems to have played a role in systemic self-organization during the origins of life.

(26) Henrich Paradies[1,2], Chester A. Faunce[1(†)] and Hendrik Reichelt[1]
(online)

Autonomous *de-novo*-phases from lipid A-biomimicry

[1] *The University of Salford, Joule Physics Laboratory, Manchester M5 4WT, UK*
[2] *University of Paderborn, Natural Sciences, Warburger Strasse 100, Germany*

Abstract

Biological structures are important material feasts and are capable of self-organizing, self-replication and repair and low interfacial tension. These biomaterials act as building blocks in multiple autonomous ways depending on their functionality only in unique surrounding parameters: charge, thermal fluctuations creating undulations, or roughness of the order of $\sim\sqrt{k_B T/\gamma}$ and particle number density. A density mismatch between the solvent and colloid can create thermal capillary waves at the interface with a characteristic capillary length $\xi \sim \sqrt{\gamma}$ /g, which is within the µm regime, and the time scale associated with the decay of interfacial fluctuations $\tau \sim \xi\eta/\gamma$ is of the order of seconds. Spatial arrangements occur in membranes by forming rafts engaged in series of processes noticed for lipopolysaccharides (LPS), where the biological activities rest only on a small portion known as lipid A. Therefore, it has been also an intense target to construct specific antagonistic molecules in order to compete with the lipid A-receptor site to eliminate endotoxic events. The interactions between the lipid A are electrostatic, hydrophobic, conformational and van der Waals by nature, and is related to nm-scaled ordered assemblies in aqueous distinct dispersions, uniquely as quasicrystals where these ordered materials exhibited noncrystallographic packing of non-identical lipid A spheres. It was noted that the observed (3.3.4.3.4) was a crystalline analogue of the icosahedral quasicrystal with a tiling of triangles (N_3) and squares (N_4) resemble a p4gm plane group. Another coded lipid A-diphosphate approximant shows an 8/3 ratio, with 6-fold symmetry and plane group p6mm. Both dodecagonal phases revealed a N_3/N_4 ratio of approximately 2.34, within the different observed phases the various lipid A-particles are randomly positioned and the system is both orientationally and positionally isotropic, when examined as a function of ø, T. Lipid A-phosphate clusters reveal an intermediate degree of order in which the clusters are randomly distributed, as observed in fluids, glasses but forming discrete colloidal crystals revealing shapes of spheres, squares, pentagons and hexagons, which are elements of close sphere packing processes except for the pentagons. Nevertheless, this system change upon confinement and behaves now orientationally anisotropic and will appear differently in different spatial directions resembling discrete time crystals in equilibrium, but they are not. This influence can be both direct and indirect, to control the size, shape, structure, properties of the crystals formed. A transition of lipid A-diphosphates is observed between phase-separated-fatty acid chains and a mixed honeycomb phase. The corresponding monophosphates form complex structures and colloidal crystals from stoichiometric mixtures of lipid A-diphosphate and their approximants. Quasicrystals exhibited noncrystallographic packing of non-identical lipid A-phosphate spheres. The spatial packing of these spheres was in either a cuboctahedron or an icosahedron. For lipid A-monophosphate, rhombodo-decadecahedra (*Fd3m*) packing was suppressed because of instability in the mean curvature between the tetrahedral & the octahedral nodes. Tetrakaidodecahedra packing showed only tetrahedral nodes; the tetrahedral angle could not be retained between all edges if the hexagonal faces of the truncated octahedron were changed. The tiling pattern of triangles (N_3) and squares (N_3) possessed a p4gm plane group. Another coded lipid A-diphosphate approximant showed an 8/3 ratio, with 6-fold symmetry and plane group p6mm. Both dodecagonal phases revealed a N_3/N_4 ratio of ~2.34.

(27) Dhanalakshmi Vadivel,[1,2] Stefano Crespi,[3] and Daniele Dondi[1,2] (online)

Parity Violation Energy Difference calculation of atropisomers

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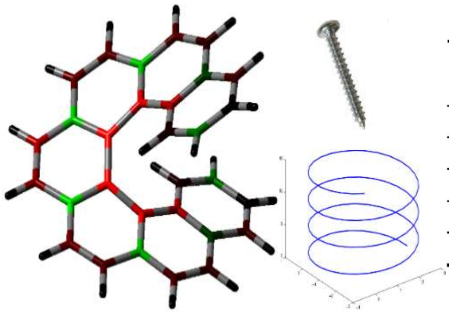
[2]*Istituto Nazionale Di Fisica Nucleare (INFN), Via Bassi 6, 27100 Pavia, Italy*
[3]*Stratingh Institute for Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands*

Abstract
The emergence and evolution of life on the Earth is the result of many interacting smaller chemicals; however, the important aspect of some of these smaller chemicals is the relevance of their structural properties, especially for those pertaining to chirality. The debate relating to chirality is not new as it has been around for nearly a century. Life, in essence, is composed of macromolecules such as DNAs, RNAs and peptides; such molecules are composed of monomers. The monomers of DNAs and RNAs are nucleotides, which in turn are composed of nitrogenous bases (GCAT/U), pentose sugars (ribose or deoxyribose) and a phosphate group; and peptides are made up of chains of twenty α-amino acids. Both the mentioned sugars and α-amino acids display chiral properties, with the exception of glycine which is achiral—all life forms on the Earth use right-handed (D)-sugars and left-handed (L)-amino acids, meaning that DNA, RNA and peptides can form alpha-helix supramolecular structures.

Since chiral molecules can have two different geometric arrangements of atoms (ie enantiomers) around the central alpha-carbon atom, this means the two enantiomers have small discernible energy level[1] difference. This small discernible energy difference between enantiomers is caused by the weak neutral current mediated by the Z boson known as Parity Violation Energy Difference (PVED).

The aim of this work is to formulate the basis for a theoretical PVED calculation (**Fig. 1**) of atropisomers, elucidating whether the small energy difference is additive or not. Compounds studied are already known in literature and thus their practical synthesis is feasible and the theoretically investigated properties can be experimentally verified. Calculations were performed by using a customized version of the Dirac08 program (http://wiki.chem.vu.nl/dirac/index.php/Dirac_Program) running at the CINECA Supercomputer Center, with computer time granted by ISCRA ARCAT project (HP10CXJWQY).



	Basis set		
	STO-6G	6-31G*	cc-pVDZ
Hexahelicene **1**	-4.542E-20		
Heptahelicene **2**	-6.387E-20	-4.241E-20	-4.789E-20
Diazahelicene **3**	2.586E-20	1.560E-20	1.738E-20
Twistedpentacene **4**	-2.404E-19		-2.182E-19
Paracyclophane **5**			-9.069E-21

Figure 1. Helicene (left) with atoms coloured with respect to the sign of PVED.

Reference

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(28) Amy J. V. Riches (in-person)

Building Habitable Worlds

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SETI (Search for Extraterrestrial Intelligence) Institute, Carl Sagan Centre, Mountain View, California, USA.

Abstract
Earth remains the only planet for which a multitude of complex biota is a certainty. Thus, our home world is a critical reference for understanding the conditions and complicated series of events that could result in habitable bodies and sentient life elsewhere in the cosmos.

Knowledge of the birth and evolution of Earth and other planets in our Solar System is a major and fundamental challenge. The infant stages of the earliest phases of planetary growth specific to Earth's formation can only be probed by studying rocks from space. This is because the earliest records on Earth are obscured by the hypothesised violent Moon-forming giant impact roughly 4.51 billion years ago, and the intense geologic processing of ancient rocks.

My work targets extraterrestrial rocks that are stony and collectively termed 'achondrites'; chosen due to having formed on planets and their precursors that were sufficiently large and hot to have recrystallised or melted their original materials. This research explores the utility of textural evaluations in combination with broad-based diagnostic chemical tools considered to enhance our understanding of the chronologies and narrative of planet formation and the workings of our Solar System. Among these, unique insights can be gleaned from the highly siderophile elements (HSEs; osmium, iridium, ruthenium, platinum, palladium, rhodium, rhenium, gold) and other elemental and isotopic tracers. Resultant data inform advanced computational modelling of planetary melts, extraterrestrial volcanic processes, and the movement of materials of the Solar System to shed new light on how Earth arose. Yet, how robust are the chemical findings from current study approaches? What are the implications for models of celestial mechanics / the history of the asteroid belt / migration of giant planets if existing understanding is flawed?

(29) Eva Stueeken (in-person)

Revisiting Earth's oldest biosignatures

University of St Andrews, UK

Abstract
The antiquity of life on Earth and the conditions under which the first ecosystems thrived are important parameters for constraining the likelihood of an independent origin of life on other worlds. This talk will revisit some of the oldest evidence of life on Earth from 3.7 billion years ago and present further indications of biogenicity in the form of nitrogen distributions within the host rock. The nitrogen isotopic record of these samples are unusual and may reflect input of lightning-derived nitrogen species. Collectively, these observations reveal that life was able to colonize the Earth's surface soon after the late heavy bombardment and may have relied on lightning as an important nutrient source, which important implications for the habitability of other planets.

(30) Valentina Erastova (in-person)

Computational chemistry - space & time travellers' tool

School of Chemistry, University of Edinburgh, UK

Abstract
'Where to land the next Mars rover?', and 'I found a peptide on a rocky planet - is it a sign of extraterrestrial life?'

Within this talk, I will discuss the role of minerals in the emergence of proto-biomolecules, in the preservation of biosignatures and their lookalikes. I will show how computational chemistry can be a handy tool to explore experimentally unattainable systems; to develop, test and refine our hypothesis of the Origin of Life. My aim is to showcase the methodology while fostering discussion, and developing new and exciting ideas together.

(31) Oliver Herbort (in-person)

Chemical state of CHNOPS elements in atmospheres of rocky exoplanets

University of St Andrews, UK

Abstract
Understanding the origin of life is a fundamental question in astrobiology. From the (exo)planetary perspective, this question can be targeted by investigating the conditions present on a planet in which life could potentially form. In other words: Which elements are available for the formation of pre-biotic molecules, in which chemical state are these, and how does this depend on the planetary composition and environment?

The atmospheric model used for this study is based on atmospheres in chemical and phase equilibrium with the crust for various different elemental compositions. The hydrostatic atmosphere, which takes element depletion by cloud formation into account, allows the investigation of the gas and cloud condensate phases. In order to constrain the potential likelihood of the formation of pre-biotic molecules, we introduce 'habitability' levels by taking into account the presence and chemical state of the CHNOPS elements. Not all planets showing the presence of liquid water condensates are expected to have the liquid water present at the surface, but rather at some point in the atmosphere in forms of clouds which do not have to be in contact with the surface. The used atmospheric model together with the introduced habitability levels allow the investigation of such potential 'aerial biospheres.'

Our models show that in the surrounding of liquid water condensates the presence of carbon, nitrogen, and sulphur in a reduced form is a common result for various different elemental abundances. However, phosphorus and metals are not available for the formation of life in aerial biospheres and can therefore be seen as limiting elements for the origin of life.

(32) Patrick Barth, Eva E. Stüeeken, Christiane Helling, Lukas Rossmanith, Yuqian Peng, Wendell Walters, Mark Claire (in-person)

Follow the Nitrogen—Using isotopes to trace nitrogen fixation by lightning on the early Earth

University of St Andrews, UK

Abstract

Nitrogen is an essential building block of DNA, RNA, and proteins and, subsequently, it must have been bioavailable since the origin of life. On modern Earth, biological sources are mostly responsible for making nitrogen bioavailable via N_2 fixation with only a few percent coming from abiotic sources. On early Earth, before the origin of life and the onset of biological nitrogen fixation, these abiotic sources such as lightning must have been the dominant producer of bioavailable nitrogen. Previous experiments have shown that in N_2-dominated atmospheres lightning leads to the formation of nitrate (NO_3^-) and nitrite (NO_2^-), which could not only have facilitated the origin of life but also sustained the earliest ecosystems. This hypothesis has been difficult to test with the available rock record because geochemical fingerprints of this fixed nitrogen source have not been developed. We present new results from spark discharge experiments in varying atmospheric compositions corresponding to different points of time in Earth's evolution. We find nitrogen fixation to be similarly efficient in an N_2/CO_2 atmosphere as an N_2/O_2 atmosphere suggesting that lightning provided a reliable source of fixed nitrogen on the early Earth. Furthermore, we investigate the effect of lightning on the isotopic composition of the resulting nitrogen oxides in solution. Our fixed nitrogen is depleted in heavy ^{15}N in comparison to atmospheric N_2. While most rock samples from the early Archean are less depleted or even enriched in ^{15}N, suggesting an earlier onset of biological nitrogen fixation, one sample (3.7 Ga) indicates a potential contribution by lightning. This allows us for the first time to assess to what degree lightning chemistry may have influenced the origin and early evolution of life. However, the spark in our experiment is much smaller and cooler than lightning channels in Earth's atmosphere. To extrapolate our experimental results to full-scale planetary atmospheres we plan to complement them with simulations of the atmospheric chemistry of exoplanets and Earth. This will allow us to extend our experiments to real lightning conditions and develop observable tracers for lightning chemistry in exoplanetary atmospheres. Being able to predict the bioavailability of nitrogen on other worlds will be another factor determining the potential habitability of these worlds.

(33) Paul Savage[1,2], Moynier F[2] (in-person)

Zinc isotopes in meteorites indicate a low-mass core-collapse supernova source to our Solar System

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[2]Université Paris Cité, Institut de Physique du Globe de Paris, CNRS UMR 7154, Paris, France

Abstract
Introduction: Iron-peak (IP) isotope anomalies in primitive meteorites point to a supernova-derived com-ponent in the pre-solar grain population of our proto-solar nebula [e.g. 1-3]. The main nucleosynthetic path-way for these anomalies is thought to be through explosive nucleosynthesis (NSE or QSE [4]), as the anoma-lies are generally in isotopes that have relatively high binding energies per nucleon. The simplest explanation for the linear covariation between different IP isotope anomalies in the same meteorites is of a single hetero-geneously distributed phase in the solar nebula; however, it has been difficult to identify a unique nucleosyn-thetic model that can satisfy the different anomalies for all IP isotope systems.

One anomalous IP isotope is 48Ca [1]; explaining the (over)formation of this isotope is a long-standing problem [5]. Nevertheless, most workers agree that a low-entropy, n-rich environment is required to produce this isotope. One environment that satisfies these conditions is in Type Ia supernovae; however, such events are relatively rare. More recently, Wanajo and co-workers [6,7] suggested that electron-capture SN (ec-SN) or other low-mass (<10M☉) core-collapse supernovae (cc-SN) could also explain an overproduction of 48Ca. These low-mass cc-SN models also predict relative over-production of some Zn isotopes – specifically 66Zn, 68Zn and 70Zn. Here we apply new Zn isotope anomaly data in primitive meteorites and a paired-anomaly mix-ing model to investigate if the Zn isotope heterogeneity in the solar system can be explained by a pre-solar phase formed in a low-mass cc-SN.

Methods: The Zn isotope anomaly data used in this work is taken from [8]; briefly, these data show posi-tive ε66Zn and (smaller but still positive) ε68Zn anomalies (normalized to 67Zn/64Zn) in carbonaceous chon-drites relative to Earth, with corresponding negative anomalies in these same isotopes in ordinary/enstatite chondrites; as with other IP isotope anomalies, this appears to reflect a "NC-CC dichotomy" [e.g., 9]. There are also good positive correlations seen between Zn isotope anomalies and other IP anomalies in the same meteorites [8]. Because there are two resolvable Zn anomalies when normalizing to the same ratio (67Zn/64Zn), we can follow the approach of [2] in modelling the array in ε66Zn vs. ε68Zn space as a mixture between "solar" and a small amount of isotopically exotic material. These potential exotic end-members can be calculated from a representative selection of nucleosynthetic reaction network yield models which take into account different initial stellar masses, supernova types and nucleosynthetic pathways – we have chosen a wide varie-ty of models, including the yield data from [6-7]. In this way, our model can help to rule in or out specifical stellar progenitors for the Zn isotopes heterogeneity in primitive meteorites.

Results and discussion: The main result of our modelling is that very few extant nucleosynthetic yield models can explain the paired magnitudes of 66Zn and 68Zn anomalies in primitive meteorites. This includes the S-process, wherein these models predict an overproduction of 68Zn (and 67Zn) relative to 66Zn, leading to higher 68Zn anomalies relative to ε66Zn. Equally, no Type 1a SN model can explain the relative magnitudes of the Zn anomalies (these models typically underproduce 68Zn relative to 66Zn). Finally, all high-mass cc-SN (i.e. Type II SN) models fail to explain the solar system Zn anomalies.

The models that are most in agreement with the measured Zn anomalies are those of the electron-capture SN (8.8M☉) and low mass core-collapse SN (9.6M☉) models of Wanajo et al. [6-7]. Both models imply for-mation of Zn isotopes in a low-entropy, high-n flux environment on a low-mass SN – this is in complete agreement with potential for formation of anomalously-rich 48Ca material in the same environments. This same paper provides yields from the inner-most ejecta of larger cc-SN (11M☉, 15M☉ and 27M☉) – these mod-els predict Zn anomalies that are extremely different to those measured in solar system materials, because although these are potential low-entropy environments, their slower rate of shock radii expansion leads to different (generally more proton-enriched) nucleosynthetic yields.

To summarise, it appears that the best match for the source of solar system Zn isotope anomalies is that of a low-mass, electron-capture SN (or ec-SN-"like") stellar environment. This stellar progenitor could explain 48Ca meteorite anomalies, and we also find that the ec-SN yield data [6] can well explain measured solar sys-tem Ni isotope anomalies.
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(34) Andjelka Kovacevic (online)

Large Interferometer For Exoplanets (LIFE): Initial statistical simulations of possible life transmission within a Galactic patch

University of Belgrade, Serbia

Abstract
The most essential exoplanet science goal is to characterize the atmospheres of a statistically meaningful number of temperate terrestrial planets. This will allow investigation into whether or not there are other worlds similar to Earth that may potentially support life.

Direct detection and characterization of temperate terrestrial exoplanets in reflected light is one of the key science drivers for new space observatory missions under consideration, such as the Habitable Exoplanet Observatory (HabEx) and the Large UV/Optical/IR Surveyor (LUVOIR).

Recent years have seen the development of a novel observational strategy as well as a brand-new project with the objective of creating a space-based mid-infrared (MIR) nulling interferometer that is able to identify and characterize the thermal emission of (temperate) rocky extrasolar planets. It was just recently announced that the characterization of temperate exoplanets in the MIR could be a viable scientific focus for a future science mission that will be a part of the ESA's Voyage 2050 program.

The Large Interferometer For Exoplanets (LIFE) initiative came forth as a direct result of these interesting new breakthroughs, as well as ongoing laboratory activities linked to nulling interferometry. I will be presenting an initial statistical simulation for the possible characterization of life transmission throughout the galactic regions that are the focus of the LIFE investigation.

(35) Hitesh Changela (in-person)

Unravelling Prebiotic Evolution in the Early Solar System by Sample Return

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2) *Department of Earth & Planetary Sciences, University of New Mexico, USA*

Abstract
Sample return missions are arguably at the forefront of space exploration. The current inventory of samples returned to Earth from human and robotic missions include: lunar samples from the Apollo and Luna Missions in the 1960s-70s; samples of Comet 81P/Wild2 and interstellar grains from the National Aeronautic Space Agency (NASA's) Stardust Mission in 2006; and asteroid samples from 25143Itokawa 162173Ryugu from The Japanese Aerospace Exploration Agency's (JAXA's) Hayabusa-1 and -2 missions in 2010 and 2020, respectively. The Chinese National Space Administration (CNSA) returned samples from the Moon with the Change – 5 Mission in December 2020. NASA's Origins, Spectral Interpretation, Resource Identification, Security, Regolith Explorer OSIRIS-ReX mission will return samples from asteroid Bennu in 2023. JAXA are set to launch a Phobos sample return in the mid 2020's with the Mars Moons Exploration Mission (MMX). Mars sample return is being formulated.

The focus of this presentation is carbonaceous asteroid sample return. Hayabusa-2 is the first sample return mission to the Carbonaceous Asteroid, 162173Ryugu, providing unprecedented insight into early Solar System prebiotic evolution. The major fraction of total organic carbon from the early Solar System – insoluble organic matter – played a role in the physiochemical evolution of organic material on early planetary bodies. However, the origins of insoluble organic matter are unclear. Interstellar space, protoplanetary disks and asteroids themselves have all been interpreted as settings under which the organic phases retained in carbonaceous asteroids originated from. Alteration on Ryugu clearly evolved macromolecular organic material. By characterising the distribution of macromolecular organic particles, their functional chemical, morphological variation in situ, can constraints on the evolution of macromolecular organic material from Ryugu be made. We will demonstrate how coordinated advanced characterisation techniques in focused ion beam, electron microscopy and synchrotron-based X-ray microscopy can unravel prebiotic chemistry from the early Solar System.

(36) Duncan V. Mifsud (online)

Exploring Radiation Ice Astrochemistry in the Laboratory. The Production of Ozone from Irradiated Carbon Dioxide Ices

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2) Institute for Nuclear Research (Atomki), Debrecen H-4026, Hungary

Abstract
The presence of a rich and extensive chemistry in the ice mantles adsorbed to interstellar dust grains or on the surfaces of icy outer Solar System objects has been well-established, and has been demonstrated to produce molecules of prebiotic interest such as amino acids and nucleobases [1,2]. However, the underlying mechanistic routes towards the formation of such molecules, as well as simpler molecules of planetary or geochemical significance, are still not completely understood. We have therefore developed a new experimental set-up at the Institute for Nuclear Research (Atomki) in Debrecen, Hungary, called the Ice Chamber for Astrophysics-Astrochemistry (ICA) with which we may simulate the radiation processing of astrophysical ices by galactic cosmic rays, stellar winds, or giant planetary magnetospheric plasmas [3,4]. In this talk, an overview of the unique features of the ICA will be provided, together with a tangible example of how this set-up can help us further understand the radiation chemical formation of a simple molecule of planetary interest: ozone. Electron irradiations of pure carbon dioxide ices as well as solid mixtures with oxygen have been performed and have allowed us to constrain the formation of ozone as a result of this radiation chemistry [5,6]. Experiments were performed at different temperatures and on ices with distinct stoichiometric compositions, thus allowing us to understand the variation in ozone formation productivity under different astrophysical conditions. Furthermore, an infrared spectral analysis of the asymmetric stretching mode of ozone produced under different conditions has been carried out. Such an analysis may prove useful for the detection of ozone in various interstellar and outer Solar System environments by current and future missions, including the recently launched James Webb Space Telescope.

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