The second Italian National Congress of (Proto-)planetary Astrochemistry (CNAP II)

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Foreword

The early phases of stellar and planetary formation are very much important for the chemical evolution of gas, ice and dust that will eventually build up the bulk and atmospheric composition of planets. A key question in modern astrophysics is whether the chemical composition of planets, asteroids and comets is inherited from the pre-stellar phase or whether there is a chemical reset during the formation and evolution of the protoplanetary disk. A synergic approach is needed to answer this question.

The Italian National Congress of (Proto-)planetary Astrochemistry (CNAP) is aimed to gather researchers working in different areas of astrochemistry to join and discuss together recent developments and future perspectives. The main objective of the congress is to investigate and promote synergic strategies among the different communities working on the early evolutionary phases of star and planet formation, planetary atmospheres, Solar System exploration and laboratory and computational astrochemistry, with the ultimate goal of preparing the community to future observations with e.g. SKA, ELT and ARIEL.

The second edition of the congress, CNAP II, was held at the University of Trieste, Aula Baciocchi, on September 11-14 2023, gathering together about 70 researchers working in the field of Astrochemistry. The list of SOC members, scientific sessions, invited speakers, and participants can be found in the conference website: https://indico.ict.inaf.it/event/2344/

The aim of this volume is to give an overview of the plethora of topics that have been covered during the meeting, and to strengthen the ties between the groups working on complementary fields through collective chapters, with the final aim to keep boosting the collaborations in the field of Astrochemistry in Italy and abroad.

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The Editors: Linda Podio, Davide Fedele, and Stavro Ivanovski

When chemists and astrophysicists meet together: Interview with Nadia Balucani

Q: ***Why is astrochemistry key in the study of star and planet formation?***

A: Planets, stars, and small celestial bodies are made of matter. Chemistry, together with physics, is one of the disciplines that deal with matter. Chemistry, in particular, deals with the transformation of matter. Every time that, for example, hydrogen and oxygen combine to form a water molecule, a chemical transformation takes place. And, since ours is a universe of molecules (and compounds), the chemistry behind their formation is fundamental to understanding the universe and its evolution. Obviously, here I am referring to ordinary matter. But it would be really cool to be able to study the chemistry of dark matter one day! Astrochemistry is a young discipline exploiting physical chemistry tools to study the composition and reactions of atoms, ions and molecules in space. This discipline includes the gathering of spectroscopic information from ground- and space-based observatories, laboratory-based studies that replicate the harsh environments of space and astrochemical modeling. The detection of > 300 molecules in interstellar regions in extreme temperature and pressure conditions is a great challenge to our comprehension of chemical reactivity. How are complex molecules, up to cyanonaphthalene, formed in regions with number densities of 10 000 particles/cm^{-3} and temperatures of 10 K? Obviously, if we unveil the secrets of astrochemistry, we are bound to understand common chemistry better. Also, the relation of some of those species (e.g. formamide, glycolaldehyde) to the bricks of life (amino acids, sugars, nucleobases) suggests that interstellar objects are the chemical factories from which massive deliveries of organic compounds (via comets/asteroids/meteorites) to newly formed planets occur, possibly triggering the emergence of life. The connection with astrobiology and the origin of life is one of the most exciting aspects of astrochemistry.

Q: ***As a chemist, how did you become interested in astronomy?***

A: As often happens, I approached astronomy and astrochemistry totally by chance. During my PhD at the University of Perugia (supervisor Prof. P. Casavecchia), I dealt with the study of elementary chemical reactions in extremely rarefied conditions with the aim of studying the fundamental aspects of chemical reactivity (Alagia et al. 1996; Volpi et al. 1995). Indeed, to characterize the forces that come into play during the transformation between reactants and products, it is necessary to work under high-vacuum conditions to avoid secondary collisions, that is, collisions other than the reactive ones and that will alter the real reaction outcome, such as the nature of the primary products (which are often very reactive radicals) and their characteristics at the moment of their formation (such as the spatial and the energy distributions – the differential cross section - from which it is possible to reconstruct the forces that come into play in the reactive event) (Casavecchia et al. 1999). The experimental conditions necessary to undertake that kind of investigation nicely reproduce the conditions of reactive collisions in the interstellar medium, as well as upper planetary atmospheres or cometary comae. During my postdoc at UC Berkeley, I approached astrochemistry working with Prof. R.J. Saykally on PAHs IR emission spectroscopy (Cook et al. 1996). On my return to Perugia with a permanent position, after some years working on elementary reactions of interest in the chemistry of terrestrial atmosphere, it was natural to extend the crossed molecular beam method (first developed by the Nobel Laurates D.R. Herschbach and Y.T. Lee, Lee 1987) also to the study of neutral-neutral bimolecular reactions of interest in the chemistry of the interstellar medium (e.g. OH+CO, C + C_2H_2 , C_2 + C_2H_2, Caracciolo et al. 2018; Costes et al. 2006; Leonori et al. 2008) or in the upper atmosphere of Titan (e.g. $N(^2D)$ + CH_4, C_2H_6, C_6H_6, etc, Balucani et al. 2009, 2010; Balucani

2012; Balucani et al. 2023). My interest in these topics increased by collaborating with Prof. R. I. Kaiser (now at the University of Hawaii at Manoa) (Balucani et al. 2000; Kaiser & Balucani 2001), Dr. Michel Costes, Dr. Astrid Bergeat, and Dr. K. Hickson (University of Bordeaux) (Costes et al. 2006; Leonori et al. 2008; Balucani et al. 2009; Shannon et al. 2014), Prof. I. Sims, S. Le Picard and Dr. A. Canosa (University of Rennes) (Berteloite et al. 2010a,b, 2011). But the real twist in my career and in my interest in astrochemistry came with the collaboration first with Prof. Serena Viti (UCL, now Leiden University) (Occhiogrosso et al. 2013; Holdship et al. 2019) and, especially, with Dr. Cecilia Ceccarelli (IPAG) (Balucani et al. 2015; Skouteris et al. 2018; Ceccarelli et al. 2023; Giani et al. 2023; Tinacci et al. 2023). It was through working with Cecilia that my order of priority was reversed, and I went from studying the reactions that I was able to study with my experimental technique to studying reactions of interest for astronomers with any technique, including the theoretical approach. This has greatly expanded the types of reactive systems to be studied and, consequently, the fun! But I have never become a theoretical chemist. For me, an experiment continues to be more solid than a thousand simulations. Unfortunately, the nature of most interstellar species (radicals, ions or other strange transient species, very difficult to produce in laboratory experiments) make the theoretical approach the only one viable in many cases of interest.

Q: ***What are the main challenges in astrochemistry?***

A: From a fundamental point of view, the most exciting challenge is to understand the relationship between the organic molecules we see in space and the origin of life. To those unfamiliar with the topic, the juxtaposition of chemistry in space and the origin of life may seem bizarre, but it is not. It is not, because we do not yet know how a phenomenon that relies on the chemistry of carbon in a reduced state could have occurred in an oxidizing context such as primordial Earth. It is commonly believed that life emerged spontaneously on Earth from organic compounds that are assumed to have been very abundant given the very small probability of a spontaneous emergence of the first processes underlying life. But the conditions of primordial Earth were not favorable to the necessary massive organic synthesis. In star-forming regions, many organic molecules are present, even of a certain complexity and with all the functional groups typical of biological molecules. Interstellar clouds are factories of organic compounds and, even if hydrogen remains the most abundant species, the mass of species with a strong prebiotic potential like formamide or glycolaldehyde is enormous by our standards. If we assume that even a small fraction of these chemicals was preserved on the outskirts of the newly formed Solar System, becoming part of comets, asteroids, and meteorites that then fell to Earth and fertilized it, at least the mystery of organic synthesis that preceded life on Earth (and perhaps elsewhere) would be solved (Ceccarelli et al. 2023). From a practical point of view, the greatest challenge in astrochemistry is to reproduce in the laboratory the real conditions in which the chemical reactions of interest take place. If we consider the interstellar medium, the number density can be as low as 10^2 particles/cm^{-3}, and the temperature as low as 10 K. There are no versatile experimental techniques that can easily reproduce both these characteristics. In the case of gas-phase reactions, the most diffuse techniques are based on the CRESU approach (where the low T conditions are reproduced) (Potapov et al. 2017; Heard 2018; Cooke & Sims 2019) or on free collisions experiments (like the one I use in my laboratory, in which the reactions are investigated under single collision conditions). There is one apparatus in Bordeaux, developed by M. Costes and C. Naulin, where both low number density and temperature can be achieved (Costes & Naulin 2010), but it is not very versatile and, at the moment, a limited number of processes have been investigated. The situation is even more complex in the case of laboratory experiments simulating the chemistry occurring in the icy mantles of interstellar grains. There are no experiments that can reproduce the low flux of hydrogen atoms (or other particles) (Cuppen et al. 2024) as well as UV photons impinging on the surface of the ice. Scaling the flux with time does not compensate for possible cooperative effects occurring in the lab experiments that will never occur in real space conditions. The physicochemical community is called upon to respond to this challenge. Many promising techniques are emerging (Amarasinghe et al. 2020; Meijer 2021), and new aspects of chemical reactivity, long unexplored because they only occur under the extreme conditions of interest to astrochemistry, are finally being explored (Potapov et al. 2017; Heard 2018; Recio et al. 2022).

Q: ***What would you suggest to a young chemist or astronomer that wants to approach astrochemistry?***

A: Perhaps the most difficult task for those who want to successfully undertake this line of research is to learn the fundamentals of the other discipline. I mean, for a chemist to learn the fundamentals of astronomy or for an astronomer to learn the fundamentals of chemical reactivity. It is not as trivial as it may seem, it is not enough to study a book. You really have to learn to see problems with the mentality of the other. In my entire career, I have only been able to do this through a daily exchange with Cecilia who with great patience explained to me what is really important from an astronomical perspective and what is just a side problem. At the same time, I explained to her with great patience why a certain process is plausible while another is not or not enough. So, find a colleague with whom you can share an interdisciplinary journey together, also trying to have fun and stimulate each other's curiosity.

To boldly go where no one has gone before.

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