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Astrobiology beyond the Solar System

Challenges and Perspectives

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Abstract. For many years the search for prebiotic material and life outside Earth has been focussed on the astronomical bodies of the Solar System. In the last few decades the arena of astrobiological research has remarkably expanded with the inclusions of extrasolar planets, protoplanetary disks, and interstellar organic molecules. As a result of these advancements, we are now in a position to cast light on the chemical pathways that originate prebiotic molecules in space, to improve our understanding of the origin and evolution of habitable planets, and to search for new worlds potentially able to host life. The numerous results already obtained in these new fields of astrobiology are extremely promising. However, the full exploitation of the new observational data is challenging and requires a fresh approach to define critical concepts, such habitability and biosignatures, in remote environments where sample measurements are not feasible. Facing these challenges will pave the road to tracing the potential distribution of life in our Galaxy and beyond.

Key words. Extrasolar planets — protoplanetary disks— astrochemistry — habitability — biosignatures

1. Introduction

In mid twentieth century, at the dawn of the space era, the multidisciplinary science that we now call astrobiology was gradually built up by scientists working in widely different areas, such as the origin of life, exploration of the Solar System, and extremophilic organisms. Since these areas of research already have a long history, and a strong overlap with space-born activities, it is not surprising that their contributions to this ASI Workshop are numerous, showing that the communities working on life sciences and Solar System have well-established synergies.

The history of astrobiology beyond the Solar System is quite different. In this case, the ability to obtain high-quality experimental data appeared in later times. Even though the first exoplanets were detected in the mid nineties, their physical characterisation is still underway, and the detection of biological signatures in remote worlds has to await the deployment of the next generation astronomical facilities. The first direct images of spatially resolved proto-planetary systems, obtained in more recent years with millimiter and sub-millimiter telescopes, have opened a new window on the formation of organic material and new worlds around different stars. The same instrumentation has dramatically increased our ability to detect organic molecules in interstellar space, disclosing new possibilities to track chemical pathways of prebiotic interest. In this contribution I will briefly introduce the present status and future perspectives of these new areas of astrobiological research, highlighting the challenges that need to be faced to search for inhabited worlds in remote astronomical environments.

2. Prebiotic chemistry in space

Starting from the Miller experiment, the earliest studies of the origin of life were aimed at finding plausible chemical pathways for the production of prebiotic material in the primitive Earth. In subsequent years, the discovery of amino acids in chondritic meteorites showed that prebiotic material is present in minor bodies of the Solar System and can be delivered to our planet. Later on, with the advancements of far-infrared, submillimetric and millimetric astronomical spectroscopy, it became clear that relatively complex organic molecules can be synthesized in interstellar molecular clouds. Since molecular clouds are the cradle of planetary systems, minor bodies formed in protoplanetary disks may deliver on planets part of the prebiotic material synthesized in space. Understanding whether this material can contribute or not to the most advanced stages of prebiotic chemistry is one of the open questions in astrobiology.

The number of molecular species detected in the interstellar medium (ISM) is quite large (almost 200) and all those containing a relatively large number of atoms ($\gtrsim 6$) are carbon-based. The organic chemistry occurring in the ISM leads to the formation of interstellar complex organic molecules (iCOMs), some of which are of prebiotic interest. Because of the astronomical distances involved, detection via interaction of molecules with radiation is the only viable route of investigation. However, identifying complex molecules in astronomical spectra and determining their abundances are challenging tasks. Molecular spectroscopy plays a central role and, in particular, the rotational spectrum is a molecular fingerprint, sensitive to very small changes in the structure (conformations, internal motions) or in mass (isotopologues). Disentangling these effects requires a large amount of laboratory data, including different isotopic species and excitational and vibrational states. Therefore a strong interaction between astronomers and laboratory spectroscopists is essential to maximize the science return from space missions and ground-based observations. Laboratory research is less expensive than space missions and should receive more support for upgrading existing infrastructure. This will pave the road to developing spectroscopic databases for gases and solids over a wide range of wavelengths. Besides gas-phase molecules, also interstellar solids (e.g. ice mantles on dust grains) should be considered since they can catalyse molecule formation in space.

In addition to laboratory data, spectral models are needed to correctly assign the recorded spectra and obtain quantitative abundances of the species of interest. Thanks to the growth of computational power and the advancements of computational approaches, nowadays it is possible to simulate the conditions of interstellar matter, which are difficult to reproduce in the laboratory. Quantum chemistry calculations are especially important to reconstruct the reactions that may lead to the formation of organic molecules (Enrique-Romero et al. 2016). Ab initio methods are necessary to track processes in which quantum effects are not negligible and that are impossible to describe by means of classical physics. In this context an important tool is provided by molecular simulations, which may span a wide range of resolutions and time scales. More detailed simulations describe complex phenomena and offer higher accuracy. Less detailed modes allow for simulation of larger systems and/or longer time scales.

A few examples highlighting the prebiotic relevance of astrochemistry are: studies on the origin of water, the formation of iCOMs and the production of formamide. Understanding the origin of water in astronomical environments is fundamental in astrobiology and is a subject of theoretical interstellar studies (Molpeceres et al. 2019). Concerning iCOMs, it is becoming clear that quantum mechanical effects and interstellar ice mantles play an important role in their formation (Zamirri et al. 2019). Of special interest for astrobiology is the production of formamide in interstellar space (López et al. 2019) since this molecule is a key ingredient of succesfsul prebiotic chemical experiments (Saladino et al. 2019). Quantum chemical computations of formamide deuteration support gas-phase formation of this prebiotic molecule (Skouteris et al. 2017).

This Session of the Workshop features: a paper on the importance of the interplay between laboratory spectroscopy and observational surveys (Melandri et al.); a presentation on amino acetonitrile as an example of prebiotic species (Dore et al.); and results from quantum-based simulations of shock-wave-driven chemistry leading to the formation of glycine and the building blocks of other amino acids (Cassone and Saija).

3. Protoplanetary disks

Protoplanetary disks are the most recent contribution of astronomy to astrobiology. This area of research is particularly important in this context for two reasons: (1) protoplanetary disks are the factories of the planets that may develop conditions suitable for the emergence of life; (2) they process the dust, gas, and ice inherited from the parent molecular cloud and incorporate the processed prebiotic material in planetesimals (e.g. comets) and planets. Understanding the physics and chemistry of disks provides much needed insight into the conditions under which planets form. Determining their molecular content reveals the raw ingredients that contribute to the composition of planetary atmospheres.

As for interstellar complex molecules, the advancements of (sub)millimetric astronomy, and in particular the deployment of ALMA (the Atacama Large Millimeter/submillimeter Array), have been particularly important for protoplanetary disks. In particular, the observations have revealed the composition of the planet building zone and have provided detections of prebiotic molecules. By mapping the spatial distribution of simple organics the observations cast light on the location of the "ice line" for different types of volatile compounds. The location of the ice line is important to understand which type of material can be inherited by planets forming at different distances from the star. Combining this type of information with studies of the architecture of planetary systems (Covino et al. 2013) will provide insight into the planetary composition as a function of semi-major axis for host stars of different types.

Examples of recent studies of prebiotic chemistry include the first detection of formic acid (HCOOH), the simplest organic acid, in the TW Hydrae protoplanetary disk (Favre et al. 2018) and the formation of formaldehyde and methanol in the DG Tauri disk (Podio et al. 2019). Given the strong potential for synergies, an effort should be made to foster interactions between the community working on protoplanetary disks and those working on interstellar chemistry and exoplanets.

4. Exoplanets

Since the first detections of planets outside the Solar System a quarter century ago, more than 4000 exoplanets have been discovered. Many of them belong to a multiple planetary system, the number of systems identified exceeding 3000. The wealth of high-quality data collected has provided fundamental insights into the complex processes of planet formation and structural and atmospheric evolution (Winn & Fabrycki 2015; Madhusudhan et al. 2016). These findings have unveiled a spectrum of planetary physical properties (masses, radii) and architectural characteristics (orbital shapes, separations, multiplicity) vastly exceeding the variety found in the Solar System. The largest number of results has been obtained using the planetary transity and radial-velocity methods. Among future challenges of this type of research is the retrieving of planetary signals in the presence of quasi-periodic stellar activity (Damasso et al. 2019).

In the context of astrobiology, the main driver of exoplanetary studies is the quest for inhabited worlds. The best candidates of this search are rocky planets (earths or super-earths) with temperate surface conditions. Two main goals can be distinguished: finding habitable worlds and detecting signatures of life. The second goal is more ambitious and challenging than the first one, since the only possibility to detect life is tied to the identification of spectral features of biological origin in exoplanetary atmospheres (Schwieterman et al. 2018). Even if improvements in spectroscopic techniques will soon revolutionise our ability to characterise the exoplanetary atmospheres, the remote dectection of biosignatures in thin atmospheres is an extremely challenging task. The atmospheres of rocky planets are expected to be thin because the mass-radius relationship of exoplanets suggests that there is a sudden transition between rocky planets poor in volatiles, in principle suitable for life, and atmosphere-dominated planets, which are not considered to be habitable.

Transiting exoplanets are particularly important for astrobiology because they offer the possibility of performing transmission spectroscopy of their atmospheres to search for biosignatures. After the huge number of transits discovered with the Kepler mission, the Transiting Exoplanet Survey Satellite (TESS) has been performing the census of close-in transiting planets orbiting the nearest stars (Ricker et al. 2015). The TESS results provide the astronomical community targets suitable for atmospheric characterisation (Kempton et al. 2018).

The actual search for atmospheric biosignatures will require the use of the most powerful spectroscopical facilities on ground and in space. Among ground-based facilities, the Echelle Spectrograph for Rocky Exoplanets and Stable Spectroscopic Observations (ESPRESSO) is able to discover habitable planets around solar-type stars and obtain high-resolution atmospheric spectra of giant planets and super-Earths (Pepe 2010). In the future, these capabilities will be expanded by extremely large telescopes equipped with state of the art spectrographs, such as HIRES at E-ELT. Among current space born facilities, the CHaracterising ExOPlanet Satellite (CHEOPS) mission, due to its ultra-high precision photometry, is collecting accurate radii measurements, in particular for those planets for which the mass has already been estimated from ground-based spectroscopic surveys (Benz et al. 2020). In the near future of space-born facilities, the James Webb Space Telescope (JWST) will allow a rapid identification, confirmation, and mass measurement of the top atmospheric characterization targets discovered in previous surveys. Beyond JWST, future dedicated missions for atmospheric studies such as the Atmospheric Remote-sensing Infrared Exoplanet Large-survey (ARIEL) will provide a representative picture of the chemical nature of the exoplanetary atmospheres and will relate this directly to the type and chemical environment of the host star (Tinetti et al. 2018). With the above-mentioned facilities and more advanced future projects, the search for atmospheric biosignatures in habitable planets with relatively thin atmospheres will eventually become a reality.

The identification of atmospheric biomarkers requires a considerable effort of modelization of the relatively thin atmospheres of habitable planets. Only with accurate models will it be possible to infer accurate molecular abundances from the best quality atmospheric spectra. In turn, the modelization of the atmospheres in a broad range of chemical and physical conditions requires large databases of molecular cross-sections; physical effects which can be more critical in atmospheres different from that of the Earth, such as pressure broadening, must be taken into account (Gandhi et al. 2020).

The data collected by exoplanet surveys keeps growing at an impressive rate. An effort should be made to integrate these data and maximize their scientific return. In this Workshop a dedicated tool is presented, designed and optimized for the study of exoplanetary systems as a whole, rather than single exoplanets (Zinzi et al.). The study of the impact of the activity of the host stars on planetary atmospheres is relevant to astrobiology. The possible consequences of huge magnetic flaring episodes emitted by the host stars on the exoplanetary space weather and habitability are discussed in this Workshop (Longo et al.).

5. Outlook of habitability studies

Planetary habitability is a precondition for the existence of biosignatures in planetary atmospheres. However, the definition of exoplanetary habitability is challenging. Here I summarize some perspectives in this field.

5.1. Habitability criteria

In principle, habitable environments may exist in different locations of planets or minor bodies (surface, underground, atmosphere, oceans, etc.). While in the Solar System we must be open to any these possibilities, in exoplanets it is convenient to restrict our attention to the surface habitability, because surface life has the best chance of generating atmospheric biosignatures detectable via remote spectroscopy.

5.2. Steps towards a multi-dimensional definition of habitability

In the past decades the search for habitable exoplanets has largely relied on the concept of habitable zone (HZ). The classic HZ defines an interval of stellar insolation that allows the persistence of liquid water on the planetary surface for a host star of given spectral type (Kasting et al. 1993; Kopparapu et al. 2013). The maximum and minimum insolations are calculated with climate models that simulate extreme atmospheric conditions: hot, H_2O-rich atmospheres for the inner edge, and cold, CO_2-rich atmospheres for the outer edge.

While there is no doubt that the insolation and spectral type are key factors of the planetary energy budget, the classic HZ is overly simplified (Ramirez et a. 2019) as we enter into the era of targeting exoplanets for life detection. This is because the habitability is affected by many factors that are not parametrized in the classic HZ formulation, despite their effects on the climate. Examples of planetary factors are the atmospheric mass and composition, surface gravity acceleration, radius, rotation period, axis tilt, and geography. The activity of the host star is an example of stellar factor. To take into account all these effects it is necessary to develop climate models sufficiently flexible to explore the impact of a broad range of parameters.

A hierarchy of climate models should be used to simulate different types of exoplanets and to perform cross-validation tests. Global circulation models (GCMs) are extremely time consuming and can be used to study in detail some specific planets (Suissa et al. 2020). Global models of intermediate complexity, such as PlaSim (von Hardenberg et al. 2007), may provide simulations of an atmosphere coupled with a mixed-layer slab ocean and a thermodynamical sea-ice model. Zonal models of lower complexity, validated with global models, can be used to explore the wide range of parameters that impact the climate and habitability (Vladilo et al. 2015). These tools are useful to explore the habitability of exoplanets that have a limited amount of observational data (Silva et al. 2017b).

The predictions of climate simulations can be used to calculate quantitative indices of surface habitability (Vladilo 2019). By studying the indices of habitability as a function of input parameters one can: (1) quantify the habitability at each location between the inner and outer edge of the HZ; (2) define the HZs not only as a function of spectral type, but also as a function of planetary parameters.

A parameter of special interest for the habitability is the atmospheric columnar mass, p/g, where p and g are the surface atmospheric pressure and gravity acceleration. Habitable zones calculated as a function of p/g provide a wealth of information because the atmospheric columnar mass affects both the horizontal and the vertical energy transport and, in addition, regulates the rate of secondary particles hitting the planetary surface (Silva et al. 2017a).

By calculating HZs as a function of multiple parameters, one can build a multidimensional HZ, each dimension being representative of a factor that is known to influence the climate system. With this aim in mind, one can build a database of climate simulations for a broad range of initial conditions, each simulation being associated with an index of habitability[1]. With a large number of simulations in hand, statistical properties of habitability, such as climate bistability, can be investigated (Murante et al. 2020).

5.3. Thermal limits of habitability for exoplanetary studies

Habitability criteria are based on the assumption that life can be supported only within specific intervals of physico-chemical conditions of its environment. As an example, here I discuss habitability criteria based on the temperature of the environment.

Given the importance of liquid water for terrestrial life, the liquid-water temperature interval provides a natural choice for defining a quantitative index of habitability based on the planetary surface temperature calculated by climate models (Spiegel et al. 2008). In general the surface pressure, p, will differ from the terrestrial one and the pressure dependence of the boiling and melting points must be taken into account. In this way, it is possible to define a pressure-dependent, liquid-water habitability index (Vladilo et al. 2013).

Also climatological and biological considerations can provide temperature limits of habitability. In a climatological perspective, the long-term persistence of water on the planet is limited by the onset of the Runaway Greenhouse instability which may lead to the complete evaporation of the surface water in a geologically short time scale. (Kasting et al. 1993). Predictions of this instability are uncertain due to the difficulty of modeling the climate system in conditions of high temperature and high water vapour content (Kasting et al. 1993; Leconte et al. 2013; Wolf & Toon 2014; Gómez-Leal et al. 2018). Even if a threshold for the onset of these effects is not well-defined, present-day calculations suggest that they may develop above $T \geq 50 \approx 60$ °C. In practice, this restricts the habitability to temperatures well below the water boiling point.

The fact that life processes are strongly dependent on temperature (Precht et al. 1973) may provide biological thermal limits of habitability. In exoplanets we are interested in life that is able to generate atmospheric signatures detectable with remote observations. In practice, this means life with active metabolism and capability of reproduction, because dormant life would hardly generate atmospheric signatures. The approximate thermal interval for active metabolism and reproduction of multicellular poikilotherms (plants, invertebrates and ectothermic vertebrates) is $0 \leq T(°\mathrm{C}) \leq 50$ (Clarke 2014). These limits are also relevant for more evolved multicellular life and for the biological production of atmospheric O_2 because the metabolism of the main O_2 producers (cyanobacteria and plants) drops outside such an interval (Silva et al. 2017a). Since the oxygenic metabolism is much more efficient that anaereobic metabolism, the presence of atmospheric O_2 might be a necessary condition for the emergence of multicellular life in any planet (Catling et al. 2005).

Based on the climatological and biological arguments discussed above, when we search for life in exoplanets it is advantageous to define a temperature-dependent index of habitability in the interval $0 \leq T(°\mathrm{C}) \leq 50$ (Silva et al. 2017a). Below the lower limit, an exoplanet would undergo a transition to a snow-ball state, with an extremely limited possibility to generate atmospheric biomarkers. Above the higher limit, the planet would undergo a Runaway Greenhouse instability. Outside these limits, multicellular life would hardly leave imprints on the atmosphere and, at the same time, the biological production of O_2, a fundamental atmospheric biomarker, would be hampered.

5.4. Steps towards a universal definition of habitability

The habitability criteria discussed above are based on the properties of terrestrial life. This approach is safe in the sense that the criteria are based on life that exists and can be tested in a wide range of physico-chemical conditions. On the other hand, we cannot exclude that life thriving in unexpected ranges of conditions may exist in distant worlds. To broaden our point of view, we may consider terrestrial life to be a special case of a univer-

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[1] See https://wwwuser.oats.inaf.it/exobio/climates.

sal phenomenon with the same defining properties (e.g. metabolism and reproduction), but different biochemistries. This approach may provide broader conditions of habitability that include the terrestrial conditions as a special case. In this perspective, it is advantageous to focus on the properties of life at the level of its molecular constituents. From a materialistic viewpoint, metabolism and reproduction are nothing more than a collection of processes performed by functional (i.e. catalytic and genetic) molecules. Even if functional molecules alternative to the terrestrial proteins and nucleic acids may exist, the intermolecular and intramolecular interactions of this type of polymers will need to be mediated by hydrogen bonds (Vladilo & Hassanali 2018). This requirement constrains hypothetical biochemistries alternative to the terrestrial one. For instance, due to their electronegativities, N and O atoms are best suited to form hydrogen bonds in the active sites of functional molecules, while Si atoms do not suit the same purpose. Moreover, the molecular medium of life should feature molecules with significant capabilities of hydrogen bonding, such as water, formamide or, to a less extent, ammonia, but not methane. Finally, hydrogen bonding works in a limited range of temperatures that broadly brackets the liquid-water temperature range. In summary, viable biochemistries may not deviate significantly from the biochemistry that we know. If so, the habitability criteria based on the properties of terrestrial biochemistry could be appropriate for any form of life that requires intermolecular and intramolecular interactions mediated by hydrogen bonds.

6. Broadening the arena

The search for habitable worlds and life beyond the Solar System is gradually extending to investigate Milky Way environments far from the solar vicinity and beyond our own galaxy. In this context, studies of the Galactic Habitable Zone (Lineweaver et al. 2004) should propose new approaches to define and quantify the physical processes underlying the concept of ”Galactic habitability” (Prantzos 2008). Considering a large fraction of stars in the Milky Way lies in binary, or multiple, stellar systems, an effort is required to estimate the long-term habitability in presence of dynamical interactions that characterize binary, or multiple, systems (Simonetti et al. 2020). In this broader arena it is worth mentioning that astrochemistry in space is expected to be different in environments where conditions – like temperature, metallicity, and cosmic ray flux – are different from those of the solar vicinity. These differences would affect interstellar prebiotic pathways that might take place at different epochs and locations in the Universe. Pioneering studies of interstellar grains and molecules at high redshift emphasize the role of quantum chemistry in space (Ceccarelli et al. 2018).

Progress in astrobiology requires a larger synergy between the communities working on interstellar chemistry, protoplanetary disks and exoplanets, and those working in the classic astrobiological areas of origin of life, Solar System exploration, and life in extreme environments. Dedicated projects are required to foster these forms of collaborations (Onofri et al. 2020). Given the expectations generated by the search for atmospheric biosignatures, the exoplanet community will probably become more and more involved in astrobiology-oriented research. Understanding the planetary conditions that may allow life to emerge, besides being a key aspect of astrobiology, will certainly help in addressing remote searches for atmospheric biosignatures.

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