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From Interstellar Ice Grains to Evolved Planetary Systems: The Role of Laboratory Studies

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 Stars and Stellar Evolution Resolved Stellar Populations and their Environments
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Principal Author:

Name: Murthy S. Gudipati

Institution: Jet Propulsion Laboratory, California Institute of Technology

Email: Murthy.Gudipati@jpl.nasa.gov

Phone: 818.354.2637

Co-authors: Stefanie N. Milam (NASA GSFC), stefanie.n.milam@nasa.gov , Amanda R. Hendrix (Planetary Science Institute), arh@psi.edu, Bryana L. Henderson (Jet Propulsion Laboratory) bryana.l.henderson@jpl.nasa.gov, Harold V. J. Linnartz (Leiden Observatory, Leiden University, the Netherlands), linnartz@strw.leidenuniv.nl, Liton Majumdar (Jet Propulsion Laboratory), liton.majumdar@jpl.nasa.gov, Michel Nuevo (Bay Area Environmental Research Institute/NASA Ames Research Center), michel.nuevo-1@nasa.gov, Daniel M. Paardekooper (Jet Propulsion Laboratory), daniel.m.paardekooper@jpl.nasa.gov, Ella M. Sciamma-O'Brien (NASA Ames Research Center), ella.m.sciammaobrien@nasa.gov, Rachel L. Smith (North Carolina Museum of Natural Sciences; Appalachian State University), rachel.smith@naturalsciences.org, Neal Turner (Jet Propulsion Laboratory), neal.j.turner@jpl.nasa.gov, Karen Willacy (Jet Propulsion Laboratory, California Institute of Technology), Karen.Willacy@jpl.nasa.gov

Abstract:

Laboratory experiments and quantum calculations simulating astrophysical conditions generate data (spectra, optical constants, opacity, line lists, photochemical pathways, thermal desorption, chemical desorption, photodesorption, etc.) that are used to interpret the observational data returned by past and current missions, can provide a “path through the noise” to produce testable predictions to advance knowledge and guide future observation campaigns, and can be used as incubators for new instruments in preparation for future missions, thus enhancing the science return of NASA missions. In return, increasingly acute astronomical data provide direction for the laboratory astrophysics to carry out new

measurements and calculations. Hence, confronting observations with experimental data can be a driver of new mission proposals and development of new technologies/mission instruments. Astrophysical models also need input parameters like optical constants, opacities, branching ratios, rate constants, and kinetics that are provided by laboratory measurements and calculations, adapting them to real astrophysical conditions. Like for the observations, these models are also used to define the type of data that needs to be produced with laboratory techniques. Even though laboratory experiments are sometimes limited by their ability to reproduce space environments accurately, laboratory studies are as widely distributed as the astrophysical conditions and can transcend the boundaries of astrophysics and planetary sciences, including exoplanets.

Investment into “Laboratory Studies” for astrophysical applications by NASA needs to be step-up, with a minimum of 10% NASA budget to be allocated for the Research and Analysis (R&A Programs), including early-stage low-Technology Readiness Level (TRL) instrumentation.

Introduction

Connecting present observational data from the interstellar medium (ISM), the circumstellar medium (CSM), molecular clouds, protoplanetary disks, cometesimals, planetesimals, to evolved solar systems like our own is the vision of astrophysical and planetary science research. Laboratory studies predict the future discoveries as well as help ongoing and past observational data to be interpreted to construct a bigger picture of the evolution of matter. The area of research focused on laboratory experimental studies conducted with astrophysical and planetary analogs is generally known as “Laboratory Astrophysics”.

Laboratory experiments and quantum calculations simulating astrophysical conditions generate data (spectra, optical constants, opacity, line lists, photochemical pathways, thermal desorption, chemical desorption, photodesorption, etc.) that are used to interpret the observational data returned by missions, can provide a “path through the noise” to produce testable predictions to advance knowledge and guide future observation campaigns, and can be used as incubators for new instruments in preparation for future missions, thus enhancing the science return of NASA missions. In return, increasingly acute astronomical data provide direction for the laboratory astrophysics to carry out new measurements and calculations. Astrophysical models also need input parameters (e.g. optical constants, opacities, branching ratios, rate constants, and kinetics) that are provided by laboratory measurements and calculations, adapting them to real astrophysical conditions, and vice versa.

Here we focus on laboratory studies that are directed towards understanding how simple astrophysical molecules evolve and how complex molecules are produced, preserved, and transported from interstellar conditions through the protoplanetary phase to an evolved planetary system. We discuss these stages and emphasize the status of current laboratory research and future needs.

1. Interstellar Molecular Evolution

There has been significant laboratory work conducted both in the gas-phase and in the solid-phase (condensed ice and dust grains) and the interplay between gas- and solid-phase to understand the composition and molecular evolution of interstellar matter. Quantification of desorption mechanisms, condensation mechanisms, sintering mechanisms, and overall formation and destruction of grains and their organics at a variety of temperatures and under a variety of irradiation conditions are still needed. Dissociation channels and branching ratios are not well quantified for many species, and kinetics of key reactions under relevant conditions are needed. While sputtering of water ice is relatively well understood, experiments involving sputtering and shock effects of different non-ice materials and of organics are less common. These could provide valuable input into dust and ice grain formation and destruction models.

In dense interstellar clouds, nanometer-sized dust grains are present and have temperatures of 10–30 K therefore accreting ice mantles from the surrounding gas. Molecular ices can be produced in the laboratory at astrophysically-relevant temperatures and characterized with spectroscopy providing experimental data directly comparable to observational data. Combined observation and laboratory efforts have demonstrated that ices are ubiquitous in the Universe’s cold environments, and dominated by very simple molecules (H_2O , CH_3OH , NH_3 , CO , CO_2 , and

CH₄), but can also contain other small molecules and more complex species that condense or are formed via various processes on the surface of cold, silicate or carbonaceous grains.

Laboratory studies investigating the irradiation processes (UV, protons, electrons) of interstellar ice mixtures have resulted in the production of organic residues that are stable at room temperature (Bernstein et al. 1997; Gerakines et al. 2001; Muñoz Caro & Schutte 2003; Dworkin et al. 2004; Nuevo et al. 2011). These residues consist of a wide range of complex organics, including compounds of astrobiological interest (e.g. Bernstein et al. 2002; Muñoz Caro et al. 2002; Nuevo et al. 2008, Meinert et al. 2016; Nuevo et al. 2018; Dworkin et al. 2001). By introducing small cyclic aromatic hydrocarbons and nitrogenated compounds to such ice mixtures before irradiation, it has been demonstrated that functionalized aromatic compounds can be formed (e.g. Bernstein et al. 1999; Elsila et al. 2006; Ashbourn et al. 2007; Materese et al. 2015 & 2018; Nuevo et al. 2014). Interestingly, all these compounds have been routinely found in several carbonaceous meteorites including Murchison and shown to be of extraterrestrial origin (Deamer 1985; Cooper et al. 2001; Martins et al. 2008, 2015; Martins & Sephton 2009; Callahan et al. 2011; Cooper & Rios 2016), which indicates that ice photochemistry is an important formation process for organics from the interstellar medium to meteorites and their parent bodies (asteroids and comets).

More recent studies have focused on how to determine the interstellar ice composition at a given temperature without having to warm up the sample to ~300 K. This work includes in-situ laser ablation and laser-ionization or electron ionization mass spectrometry [Bossa et al. 2015; Gudipati and Yang 2012; Henderson and Gudipati 2014; Henderson and Gudipati 2015; Paardekooper et al. 2014; Paardekooper et al. 2016; Yang and Gudipati 2014]. Advantages of IR laser ablation over UV laser ablation are clear in terms of least damage to the organic composition and dmp: this is only the case in specific situations, consider removing? high desorption yields. In the future, these in-situ methods, that complement the conventional IR and UV spectroscopy and TPD mass spectrometry approaches, should be supported to mature becoming mainstream analytical tools. Recently, single photon ionization with a tunable VUV laser has been used in combination with Temperature Programmed Desorption to assess the molecules moving to the gas phase with minimal fragmentation Jones et al. 2013; Abplanalp et al. 2015; Abplanalp et al. 2016; Abplanalp et al. 2018. This is a promising ionization approach and should be considered to be combined with a laser desorption scheme to provide insights in the composition of ice at any given temperature.

2. Evolution of Molecules, Ice, and Grains in Protoplanetary Systems

The evolution of molecules and ices in the interstellar medium has been extensively studied. However, far less is known, both observationally and in the laboratory, about the chemical and physical evolution of molecules, ices, and grains in protoplanetary environments. Advances in (sub)millimeter interferometry in the last two decades have provided observational data on dust in protoplanetary disks with the SubMillimeter Array (SMA) and the Atacama Large Millimeter Array (ALMA) (Andrews & Williams 2007, Williams & Cieza 2011, van der Marel et al. 2013) as well as on the gas-phase molecular distribution in protoplanetary disks with ALMA (Casassus et al. 2013). Since the commissioning of ALMA, observational data on the gas-phase molecular spatial distribution in protoplanetary disks is becoming available, leading to unprecedented views

of young stellar systems, many with planets in their nascent phase. In addition, high-spectral-resolution observations of molecules – such as CO and CO₂ – in absorption, using large ground-based facilities (i.e., VLT-CRIRES and Keck-NIRSPEC) have opened a window into precise analyses of protoplanetary processes such as CO self-shielding (Brittain et al. 2005; Smith et al. 2009), the potential interplay between CO ice and gas reservoirs (Smith et al. 2015) in the disks and envelopes surrounding YSOs, and the role of supernova in isotopic enrichment of the early solar nebula (Young et al. 2011). Further, observations of solid-phase CO and CO₂ have yielded valuable insights into carbon chemistry in protoplanetary ices, as traced by ¹²C-¹³C fractionation (Boogert et al. 2000 & 2002). These later studies complement the suite of millimeter and submillimeter observations and understanding of carbon-bearing molecules – including CO, CN, CH⁺, and H₂CO – in the ISM, as observed toward diffuse clouds (Langer & Penzias 1993; Wilson 1999; Milam et al. 2005; Casassus et al. 2005). This work established the need to consider Galactic chemical evolution in the gas reservoirs of forming planetary systems, and paved the way for the use of high-precision instruments for comparing ice- and gas-phases along a single line-of-sight.

However, more targeted laboratory studies (both experiments and theory) that can connect equilibria among gas-phase molecules and condensed ices and grains at various temperatures and radiation environments are needed, in particular to generate data (optical constants, spectra, etc.) to be used as input parameters and constraints in physico-chemical radiative transfer models for the interpretation of astrophysical observations. Laboratory studies need to provide information on which processes could be efficient for a given molecule, for example: thermal desorption vs. photodesorption (Oberg et al., 2007) vs. photochemical desorption (Oba et al., 2018). Isotopic studies and binding energies of molecules on ice and dust will provide further insight into dynamics of desorption and accretion of molecules making gas-phase and ice-phase composition in the protoplanetary phase. These laboratory studies also provide data that is critical to evaluate how active the protoplanetary phase is in molecular chemistry - whether in the gas-phase or in the ice/dust-phase. Present models vary between no chemical evolution in the protoplanetary phase to complete evaporation of interstellar ice grains and synthesis of complex organics in the gas-phase in the protoplanetary systems. This leads to the question yet to be clearly answered: whether or not interstellar ice grains retain their primordial composition during the protoplanetary stage leading to the formation of cometesimals and planetesimals. Laboratory work conducted at relevant conditions is needed to constrain the temperature (hence radial mixing) and radiation environments of the protoplanetary disks. Molecular adsorption binding energies on ice and dust grains need to be determined accurately in order to fully understand equilibria between gas and ice in protoplanetary disks. Laboratory investigations of the chemical interaction between ice (with organic composition that is consistent with astrophysical observations) and dust (mineral or carbonaceous) are critical to understand the chemical processes occurring in disks and to determine whether astrobiologically-important organics are produced in the protoplanetary disks or before or after. Experimental and theoretical studies are also needed to investigate specific chemical pathways and reaction networks that go from small molecules to more complex molecules up to grains to provide invaluable inputs to computer simulations of protoplanetary disks. The dust density and size distribution set the temperature structure of the disk, therefore dust composition and opacity are also required to accurately model protoplanetary disks. Laboratory experiments producing

circumstellar grain analogs and providing optical constants in the NIR-FIR range as well as size distribution are therefore needed as well.

3. Models of Protoplanetary Disks vs. Lab Data

Many detailed simulation programs of PPDs exist, however input to these models such as reaction rates, photodesorption rates, thermal desorption rates, molecular binding energies, coagulation efficiencies, etc., are not fully exhausted by laboratory data for a wide range of potential molecular species. Similarly, the spectroscopic data for minor molecular species is far from complete. Laboratories dedicated to derive these experimental data and parameters should be supported to continue their work.

The transition from ice to gas or so-called snowlines in protoplanetary disks are critical ingredients for the physical and chemical evolution of planets. Many models predict that these snowlines are the locations where planetesimal formation begins. Providing observational/theoretical constraints on the locations of the major snowlines (N_2 , CO, CO_2 , NH_3 , and H_2O) is, therefore, crucial for fully connecting planet compositions to their formation mechanism. To do that, experimental binding energies of these molecules (both in multi- and mono-layer regime) to the ice-phase determined from the Temperature Programmed Desorption (TPD) mass-spectrometry and infrared spectroscopy techniques are the most critical parameters needed in order to improve existing models of PPDs.

The synergy between laboratory experiments that explore chemical processing in interstellar ice analogues, and observations of key molecular reservoirs in a range of protoplanetary environments, is thus essential toward establishing a comprehensive understanding of ice-gas interactions in protoplanetary disks and systems which arise from these icy envelopes, with relevance to the formation of the solar nebula.

4. Molecular Evolution from Comets and Asteroids to Evolved Planetary Systems

While large fractionated bodies such as planets and their moons may not preserve the memory of their parent molecular composition a few billion years ago (such as ours at 4.567 Gyr), it is expected that small unfractionated bodies with very low gravity and low thermal conductivity, such as the Kuiper Belt Objects (KBOs) and Oort Cloud icy bodies (the reservoirs of comets) might preserve the primordial molecular composition to the present day. Indeed, the molecular inventory detected by the recent Rosetta Mission (ROSINA Instrument) from the comet 67P/Churyumov–Gerasimenko (67P/CG) is very similar to the molecules detected in the studies conducted on laboratory investigations of interstellar ice analogs described above [Altwegg et al. 2017]. This indicates that molecular evolution could have occurred in the interstellar ice stage and that the resulting primordial molecules could have subsequently been preserved within cometesimals and delivered to Earth since the time of early formation of our solar system.

5. Molecular Tracers of Evolution from Interstellar Medium to Early Solar Systems

Though presently laboratory studies (in combination with observational data discussed above) indicate that, interstellar ice grains essentially coagulated in the outer accretion disk regions to form cometesimals and KBO/Oort Cloud precursors -- retaining the chemical integrity of these grains throughout the evolution of our solar system -- we do not have unambiguous proof for

such a hypothesis. In order to obtain rigorous support, laboratory studies need to identify these “molecular tracers”, which would be retained throughout the evolution of interstellar ice grains to present-day KBOs and Oort Cloud icy bodies. These molecular tracers should be sensitive to ice sublimation and recondensation, UV-radiation, and temperature. Such tracers should not be produced or destroyed during the phase when the ice-coated grains accrete to form cometesimals of a few millimeters to a few centimeters in diameter. The search for such “molecular tracers” in the laboratory should be a high priority, as these tracers would shine better light on molecular evolution in the protoplanetary phase.

If the interstellar ice conditions were to be preserved, then both the primordial composition of the icy grains and the microscopic co-existence of various molecules, particularly the supervolatiles such as CO, CH₄, O₂, along with amorphous water ice and silicate dust should also be preserved in the present-day cometary nuclei. Thus, laboratory studies investigating the thermal evolution of interstellar icy grains at their molecular level of composition are critically needed to better understand the formation and evolution of matter at the edge of our solar system. As for the long-lasting question of the primordial nature of cometary interiors, in-situ spectroscopic characterization at depths beyond thermal equilibration to temperatures above 70 K of a cometary nucleus and return of cryogenic comet nucleus samples with temperatures <25 K would answer the long-unanswered question of the primordial nature of cometary interiors. Such missions will connect interstellar ice grains to evolved solar systems - bringing Astrophysics and Planetary Sciences together.

Studying the astrochemistry of various astrophysical environments requires detailed knowledge of the molecules (and their charge-state, neutral and ionic) that are present. Herschel (HiFi) has contributed significantly to our understanding here, but there are still many lines detected with HiFi that have yet to be assigned, and the EXES instrument on SOFIA will suffer from the same problem. Highly accurate rovibrational line lists that contain upwards of hundreds of millions of transitions assigned are required, and these are best obtained through a combination of high-resolution experiments together with state-of-the-art ab initio quantum chemistry methods. It is important to note that a synergy between experimental and theoretical efforts is necessary here. The line lists hence produce are also used in the analysis and understanding of (exo)planetary atmospheres.

6. Recommendations

Laboratory studies in support of Astrophysics and Planetary Sciences that are now more transcendent than ever before, particularly with the emergence of Exoplanetary Science, should be supported with healthy Reach and Analysis (R&A) Programs that take realistic investment necessary both in terms of experimental infrastructure and human resources. Investing in laboratory studies is investing in the future of NASA. Laboratory studies typically lead to concepts for new instruments, which evolve to higher Technology Readiness Levels (TRLs) in the future. Such investment both in Laboratory Studies in low-to-high-TRL instrument technologies will pay off in the long-run reducing the risks of expensive overruns of Missions due to lack of maturity of instrument technologies and lack of laboratory data to understand the observational phenomenon. A minimum of 10% budget of NASA should be dedicated to incubating Laboratory Studies and early-stage Technologies, both of which need long-term commitment to mature.

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