Laboratory Astrophysics: from Observations to Interpretation
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Laboratory astrophysics: key to understanding the Universe

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Abstract. This brief overview stresses the importance of laboratory data and theory in analyzing astronomical observations and understanding the physical and chemical processes that drive the astrophysical phenomena in our Universe. This includes basic atomic and molecular data such as spectroscopy and collisional rate coefficients, but also an improved understanding of nuclear, plasma and particle physics, as well as reactions and photoprocesses in the gaseous and solid state that lead to chemical complexity and building blocks for life. Systematic laboratory collision experiments have provided detailed insight into the steps that produce pebbles, bricks and ultimately planetesimals starting from sub-μ-sized grains. Sample return missions and meteoritic studies benefit from increasingly sophisticated laboratory machines to analyze materials and provide compositional images on nanometer scales. Prioritization of future data requirements will be needed to cope with the increasing data streams from a diverse range of future astronomical facilities within a constrained laboratory astrophysics budget.

Keywords. atomic and molecular data, astronomical databases, methods: laboratory, ISM: techniques: spectrocopic

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1. Introduction

Modern astrophysics is blessed with an increasing amount of high quality observational data on astronomical sources, ranging from our own Solar System to the edge of the Universe and from the lowest temperature clouds to the highest energy cosmic rays. Spectra containing thousands of features of atoms, molecules, ice and dust are routinely obtained for stars, planets, comets, the interstellar medium (ISM) and star-forming regions, and now even for the most distant galaxies. Realistic models of exo-planetary atmospheres require information on billions of lines. Theories of jets from young stars benefit from plasma experiments to benchmark them. Stellar evolution theories and cosmology rely heavily on accurate rates for nuclear fusion reactions. The first stars could not have formed without the simplest chemical reactions producing H_2 and HD in primordial clouds. Particle physics is at the heart of finding candidates for the mysterious dark matter.

Taken together, there is no doubt that laboratory astrophysics, with ‘laboratory’ defined to include theoretical calculations, remains at the foundation of the interpretation of observations and truly ‘makes astronomy tick’. It also provides an important bridge between astronomy and physics, chemistry and other sciences, appropriately represented in Fig. 1 with laboratory astrophysics providing the ‘sigh of relief’. It is important to recognize that this is not a one-way ‘bridge’, but that astronomy and physics, chemistry can mutually stimulate and enrich each other (Dalgarno 2008).

This paper will provide some general thoughts about the field, and then briefly describe a number of recent examples of observational developments where the availability

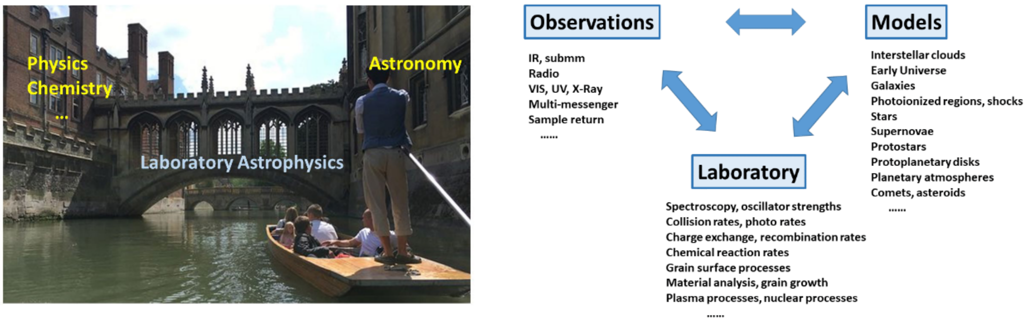

Figure 1. Left: The Bridge of Sighs in Cambridge (UK), symbolizing laboratory astrophysics as a bridge between astronomy and physics, chemistry and other sciences. Credit: Tripadvisor.co.uk. Right: the triangle of observations, models and laboratory astrophysics, with the latter underpinning both.

of new laboratory data has been important in the analysis. Often, a comparatively minor investment in basic studies can greatly enhance the scientific return from expensive missions. Examples are included from (i) atomic physics; (ii) nuclear physics; (iii) molecular physics; (iv) solid-state and condensed matter physics; and (v) planetary sciences, topics which are also covered at this Symposium. Not included here are (vi) plasma physics and (vii) (astro)particle physics. A comprehensive review of all of these aspects of Laboratory Astrophyscs is provided by Savin et al. (2012), with some updates in Savin et al. (2019). The molecular part is well covered in reviews by Tielens (2013); van Dishoeck et al. (2013); Cuppen et al. (2017) and the 2013 special issue of Chemical Reviews, whereas an overview of exoplanetary atmosphere cases can be found in Fortney et al. (2019). This paper also makes good use of on-line presentations from recent workshops of the AAS Laboratory Astrophysics Division. Only limited (and highly incomplete) references and examples are given throughout this paper.

In 2019, the IAU celebrates its 100 yr existence †. The exhibition highlights major discoveries over the century, many of them enabled by laboratory astrophysics. This is also the UN International Year of the Periodic Table of Chemical Elements ‡, appropriately reminding people worldwide that the elements in our body originate from nuclear reactions in stars.

2. Laboratory astrophysics as a field

Some history. Astronomy and laboratory astrophysics have gone hand in hand since the earliest spectroscopic observations. The Fraunhofer lines in the spectrum of the Sun, first seen in 1814, could not be understood without basic atomic spectroscopy. The solar spectrum also provides an excellent example of the opposite case: unidentified lines led to the discovery of Helium in a laboratory on Earth in 1868. Huggins used spectroscopy around 1864 to demonstrate that there are two different types of nebulae: those that resembled the Orion nebula which is full of (electric dipole) forbidden lines and those like the Andromeda galaxy that resemble the spectra of stars. The [O I] atom with its ^3P-^1D 6331 Å red (so-called 'nebular) and ^1D-^1S 5577 Å green ('auroral') lines is prime example of a system for which deep knowledge of its spectroscopy and excitation serves both the astronomy and aeronomy communities.

† www.iau-100.org
‡ www.iypt2019.org

Another early example is provided by the diffuse interstellar bands, first seen in optical spectra of bright early-type stars by Heger (1922). Modern instruments have recorded more than 500 different lines, the majority of which are still unidentified after a century (Cox et al. 2017).

Importance of new facilities. Major new facilities and technology drive the field. On the laboratory side, this includes large synchrotron and advanced light sources as well as the most powerful computers, often offered as national facilities across the world. At the individual institute and researcher level, there are innovative laboratory set-ups including, for example, cavity ringdown and CHIRP spectroscopy, He droplets and crossed beam experiments, and UHV surface science techniques. On the astronomical side, the field has been fortunate to have powerful 8-10m optical ground-based telescopes, UV and X-ray spectroscopy from space with $HST, XMM, Chandra$ and soon $XRISM$, and (far-)infrared and submillimeter with *Spitzer*, *Herschel*, SOFIA and ALMA. With $JWST$, ELTs and many other missions on the horizon providing increasingly sharp and sensitive data, the need for further laboratory data will surely increase.

Funding challenges. In spite of the enormous opportunities, there are some worrying signs. Budgets for laboratory astrophysics are under stress. Several decades ago, most of the funding for experiments or theory came from physics or chemistry because the astronomical questions were driving fundamental new insights in those fields. However, hot topics in physics and chemistry have now moved to other areas that have little connection with astronomy. While these fields occasionally still provide funding for new equipment or sophisticated computer codes and packages that can subsequently also be used to address astrophysical questions, the manpower to carry out these 'routine' experiments or calculations has to come from other sources, most notably astronomy itself.

This then runs into another problem, namely that the current generation of astronomers is used to large turn-key software packages and hardly appreciates the importance of the basic data that goes into them, as well as their uncertainties. Huge amounts of computer time are spent on MCMC or Bayesian fits to observational data using a 'black box' program to infer physical and chemical parameters such as abundances, temperature, density, radiation field, filling factor etc., but the answer is only as good as the basic data that go into the model.

Citation pyramid. Take as an example the CLOUDY model and package for photoionized regions (Ferland et al. 2017). Many thousands of manyears and decades of work have gone into computing and compiling all the atomic data (line positions, oscillator strengths, collisional and photoionization cross sections, recombination rate coefficients) that enter the program. Each of these thousands of papers has a few tens of citations each. The CLOUDY program, widely used by the community, has some 5000 citations total. In contrast, the science enabled by CLOUDY has in total well over a million citations. To give credit where credit is due, astronomers should cite as much as possible the essential basic data that went into the analysis, especially since the funding for getting those data is at least loosely correlated with number of citations in many countries.

Public codes and databases. Codes such as CLOUDY, SPEX and CHIANTI illustrate another issue, namely that the cost of writing the initial version is a tiny fraction of the long-term cost for maintenance, improvement, support and training the next generation in the use of such a code (Brickhouse, LAW 2018 workshop). Providing a public code can readily become ones career if the program is widely used and it is tough to get an academic position for what is regarded as just a 'service' to the community. The latter characterization is unfair since the code enables frontline science, including by its

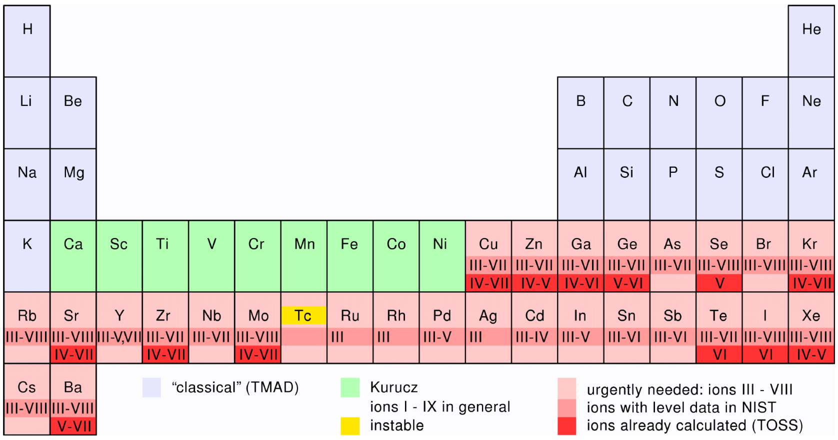

Figure 2. Summary of elements for which accurate oscillator strengths are still lacking. Credit: T. Rauch.

author(s), but the label sticks all too easily and drives such 'service providers' to national centers or institutes, or worse, out of the field so that critical expertise entirely is lost.

Populating the databases with new experiments or calculations requires a critical evaluation of the numbers and their uncertainties: the latest value is not always the best! Also, extrapolations are often needed, for example to lower or higher temperatures. Code comparisons are very time consuming but should be done on a regular basis and can be highly valuable in revealing not only discrepancies but also sensitivities to certain parameters that were not realized before. Integration of databases and codes with astrophysical tools requires teams (and referees!) that understand both aspects.

Organizing the community. To have a voice in policy making and convincing funding agencies to provide more resources where needed, organization of the community is important. This is happening now at various national and international levels. In particular, the IAU has a long-standing tradition in this area, first with the old Commission 14 on 'Atomic and Molecular Data' and after the restructuring in 2012-2015 with Commission B5 on 'Laboratory Astrophysics'. On the molecular side, it has considerable synergy with the former Working Group and now Commission H2 on Astrochemistry.

3. Atomic and nuclear physics

Atomic physics has long been essential in determining and analyzing solar and stellar abundances and opacities, supernova remnants, accretion shocks onto young stars, starburst galaxies and AGN. Extreme wavelength precision of atomic thorium/argon and iodine lines is now also key in providing the reference frame for measuring radial velocities of exoplanets to tens of cm precision.

One recent high energy example is provided by a weak feature around 3.62 keV found in stacked XMM spectra of AGN that was not well fitted with available spectral synthesis packages (Bulbul et al. 2014). This led to speculation: was this a sign of new physics, such as sterile neutrino dark matter? Or could the feature be explained by previously missed dielectronic recombination features, e.g., of Ar XVII? The higher spectral resolution *Hitomi* microcalorimeter spectrum of the Perseus cluster, however, does not show deviations from (updated) spectral packages (Aharonian et al. 2017).

High-resolution images from *Chandra* combined with data from *NuSTAR* beautifully reveal the production of elements through nuclear fusion in stars and supernovae ejecta,

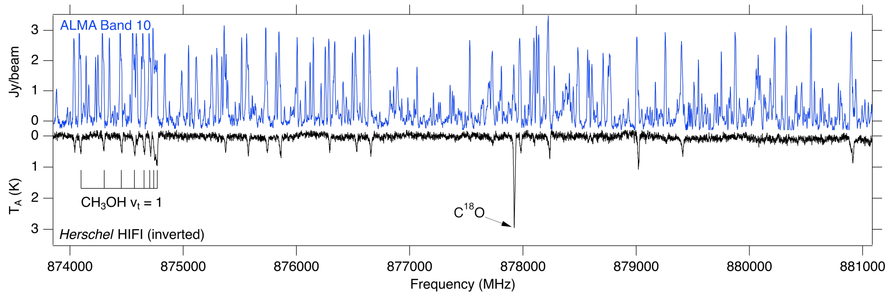

Figure 3. ALMA Band 10 spectrum of the high-mass star-forming region NGC 6334I, compared with the spectrum over the same frequency range obtained with *Herschel*. Note the huge number of lines detected with ALMA due to its much smaller beam. Around 20-70% of ALMA lines are still unidentified, stressing the need for more laboratory spectroscopy. Figure based on McGuire et al. (2018a).

including, for example, ^{44}Ti (Grefenstette et al. 2017). An overview of nuclear astrophysics needs can be found in Wiescher et al. (2012). Particularly exciting are the recent data on neutron star mergers, detected through gravitational waves with optical spectroscopy follow-up, showing that they are indeed a major source of elements heavier than Fe through the rapid $r-$process. More generally, surveys of abundances of heavy elements like Ga and Ge in a wide range of sources (diffuse clouds, white dwarfs, planetary nebulae) can constrain the relative contributions of slow (AGB) vs rapid (supernovae, neutron star mergers) neutron capture processes to current epoch Galactic chemical evolution (e.g., Ritchey et al. 2018). Such studies are only possible, however, with accurate values for the oscillator strengths ($f-$values) of the transitions. Fig. 2 summarizes the data needs for heavy elements.

4. Molecular physics: gas phase

Molecules, both in the gas and in the solid state, are observed throughout the Universe, from the highest redshift galaxies to the comets and planets in our own Solar System. Molecular data are needed to interpret observations of the diffuse interstellar medium, dark clouds, star-forming regions, protoplanetary disks, exoplanetary atmospheres, solar system objects, evolved star envelopes, late type stellar atmospheres, nearby and distant galaxies, and the early Universe. Besides line frequencies, line strengths, and collisional data, molecules have the added complexity of a wide range of chemical reactions that can occur for which rate coefficients are needed over a large range of conditions.

Spectroscopy. High-mass star-forming clouds like Orion-KL and SgrB2(N) are well known as line-rich sources. *Herschel* and ALMA line surveys reveal the rich chemical composition of warm gas, but making a full inventory is hampered by the sometimes large fraction of unidentified lines. For *Herschel*, about 5-12% of the channels are unidentified (Crockett et al. 2014; Neill et al. 2014). This fraction is much higher for ALMA data (Fig. 3). The low-mass source IRAS 16293-2422B has very narrow lines which allows identification of prebiotic molecules toward solar-mass protostars for the first time (Jørgensen et al. 2016, 2018). Interestingly, in the 350 GHz window (ALMA Band 7), the fraction of U-lines is about 20%, but this grows to ∼70% in very deep observations at lower frequencies (230 and 115 GHz, ALMA Band 6 and 3) (Taquet et al. 2018). Most of the lines are likely due to isotopologs and/or vibrationally excited states of known complex organic molecules. For example, the abundant HNCO molecule shows lines of $HN^{13}CO$, $HNC^{18}O$, $HNC^{17}O$, $H^{15}NCO$, DNCO, $DN^{13}CO$, $DNC^{18}O$ and many more combinations, for which laboratory data were still lacking until recently. This, in turn, prevents identification of new species, including amino acids. ALMA spectra of AGB stars also contain a large fraction of U-lines (Cernicharo et al. 2013) that may be due to different types of species (e.g., metal-containing), especially if they are probing the dust formation zone. Databases such as the Cologne Database for Molecular Spectroscopy (Endres et al. 2016) and the JPL molecular database are invaluable resources for identifying lines (see review by Widicus-Weaver 2019).

Collisional rate coefficients. Considerable progress continues to be made in this area through quantum chemical calculations, thanks also to coordinated efforts maintaining a close link with observers. State-to-state collisional rate coefficients with H_2 for pure rotational transitions have been computed in the last decade for H_2O, H_2CO, HCN, HNC, CN, CS, SO, SO_2, CH, CH_2, HF, HCl, OH^+, NH_2D, HC_3N, CH_3CN, and CH_3OH, among others. For ions and molecules with large dipole moments such as HF, CH^+ and ArH^+, collisions with electrons are also important. Driven by infrared spectra from *ISO* and *Spitzer*, and with *JWST* on the horizon, there is now also attention to the calculation of rate coefficients for vibration-rotation transitions. For example, new data have been provided for CO with H_2 and H (Song et al. 2015). All of these data are very time consuming to compute, sometimes taking nearly a decade per species (e.g., H_2O). The data can be accessed through the BASECOL database (Dubernet et al. 2013) and the LAMDA database (Schöier et al. 2005; van der Tak et al. 2007).

Chemical reactions. Rate coefficients for gas-phase chemical reactions are derived from experiments and from theory. The main databases are UMIST (McElroy et al. 2013) and KIDA (Wakelam et al. 2015), which continue to be updated with new results from the chemical physics literature. An interesting example is the associative detachment reaction, $H^- + H \rightarrow H_2 + e$, which controls the amount of H_2 in the early Universe and thus its cooling. This reaction was studied in the 1970s but never again until this decade (e.g., Kreckel et al. 2010); the new values significantly reduce the uncertainty in the masses of the first stars found in hydrodynamical simulations.

Photodissociation. UV radiation is one of the main destruction routes of molecules. Heays et al. (2017) have provided an update of the wavelength dependent photodissociation and photoionization cross sections for many astrophysically important molecules and atoms. Rates are provided both for the interstellar radiation field, for cool stars and the Sun, as well as for the cosmic ray induced field (important inside dark cores and disks). The photodissociation of CO and N_2 and their isotopologs continues to be studied experimentally, leading to refinements in self- and mutual shielding factors (Visser et al. 2009; Heays et al. 2014). Taking the wavelength dependence into account is particularly important for the chemistry in protoplanetary disks around different types of stars.

Other types of data. One example are Landé factors, needed to measure magnetic fields in interstellar clouds through Zeeman splitting of molecules. In star-forming regions, methanol is particularly abundant and has strong lines, both thermally excited and as masers. Calculation of the CH_3OH Landé factors by Lankhaar et al. (2018) allowed the magnetic field in the Cep A cloud to be measured at 7.7 ± 1.0 mG. Other examples can be found in § 7.

5. Molecular physics: PAHs, fullerenes

Strong and broad emission features at mid-infrared wavelengths have been seen since the 1970s throughout the ISM and are most plausibly ascribed to a collection of Polycyclic Aromatic Hydrocarbons (PAHs) of 50–100 carbon atoms each (see review by Tielens 2008). Since these features can even be detected out to high redshift and are excited

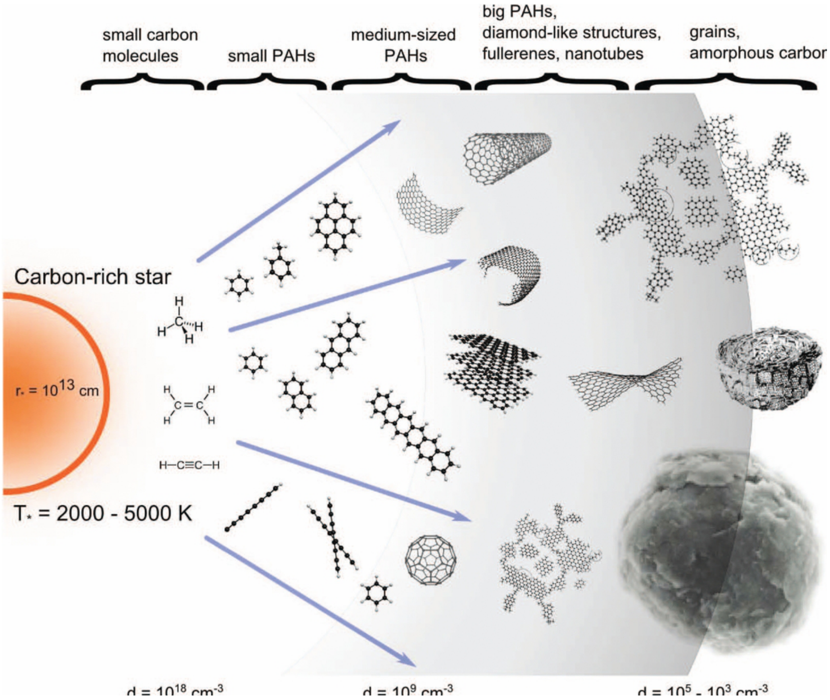

Figure 4. Illustration of growth of carbonaceous molecules and solids in the envelopes of evolved stars. Figure from Contreras & Salama (2013) with permission.

by UV radiation, they can be widely used as diagnostics, for example to measure star-formation rates in obscured regions. More subtle variations in band shapes and relative strengths are seen in local sources, such as PDRs versus disks or evolved stars (Peeters et al. 2002, 2017). To unlock the potential of PAHs as diagnostics, a large range of data is needed, from spectra of individual PAHs (Boersma et al. 2014; Mackie et al. 2015) to their ionization and electron recombination/attachment rates (e.g., Le Page et al. 2001) and dehydrogenation rates (e.g., Bouwman et al. 2019).

Individual PAHs have not yet been identified through infrared spectroscopy: only their ionization stage (positively or negatively charged vs. neutral) and their global size and molecular structure have been characterized. Small PAHs with a side group and dipole moment also have strong radio spectra, however. The recent GBT detection of one of the smallest PAHs, C_6H_5CN (benzonitrile), at centimeter wavelengths in a cold dark cloud, TMC-1, therefore caused considerable excitement (McGuire et al. 2018). This detection opens the door for searches for other PAHs and also raises interesting questions on its formation, which is most likely bottom-up starting from C_2H_2, rather than top down. In addition to experiments, quantum chemical studies can be useful to identify reaction paths and stable structures starting from C_2H_2 (e.g. Peverati et al. 2016).

A subset of infrared bands between 5 and 22 μm can be uniquely assigned to fullerenes, C_{60} and C_{70} (Cami et al. 2010). Initially identified in a young planetary nebula, they are now seen in a wide variety of sources. Interstellar C_{60}^+, originally proposed by Foing & Ehrenfreund (1994), is now firmly detected at optical wavelenths (Cordiner et al. 2019). In fact, there is now good observational evidence for the transformation of PAHs to fullerenes under the influence of UV radiation, a process that is also understood theoretically (Berné & Tielens 2012) and simulated experimentally (Zhen et al. 2014).

6. Condensed matter physics: solids, ices

Carbonaceous grains. When PAHs, fullerenes and other carbon-containing species grow to large enough sizes (few hundred atoms), they start to behave like solids rather than individual molecules (Contreras & Salama 2013, Fig. 4). The structure of interstellar carbonaceous material is amorphous but the details and composition are under discussion, such as the fraction of aromatic vs. aliphatic bonds: does the material resemble coal or hydrogenated amorphous carbon? A related question is how and where they are formed. It has been known for some time that the destruction rates of interstellar grains are larger than their production rates in envelopes of evolved stars. Thus, some (re-)formation of grains must also take place in the low density cold ISM. Laboratory experiments are now starting to provide some proof that this indeed can happen (Fulvio et al. 2017).

Silicate grains. The same issue also holds for the formation of silicate grains. SiO polymerization has been shown to take place without barriers in experiments using the He-droplet technique to confine SiO molecules. This then provides a route for producing silicate grains in the cold ISM by accretion onto a kernel (Krasnokutski et al. 2014).

Most interstellar silicate grains are amorphous but a distinct set of peaks have been observed in protoplanetary disks and evolved stars, that can be ascribed to crystalline silicates such as forsterite (Mg_2SiO_4). Much laboratory work has been carried out to make these identifications (see review by Henning 2010) and more work is needed since some of the longer wavelength features are highly sensitive to precise composition and/or temperature (Sturm et al. 2010).

Ices: freeze out and sublimation. At low dust temperatures of $\sim$10 K, the probability for atoms and molecules to freeze out on dust grains is unity on every collision, thus forming an icy layer on top of the silicate or carbonaceous core. Once on the grain, new molecules can form, ranging from simple species like H_2O to complex organic molecules (see below). When the grain heats up, these molecules will sublimate back into the gas in a sequence according to their binding energies. Thus, laboratory determinations of binding energies of ices, either as pure or mixed ices, are essential for understanding of observations of star- and planet-forming regions (Collings et al. 2004).

Surprisingly, some molecules produced on grain surfaces are observed in the gas at temperatures well below that for thermal sublimation (e.g., Bacmann et al. 2012). How to get molecules off the grains at low temperatures intact is a major puzzle which is being addressed by experiments and theory. One option is photodesorption by UV radiation although this process often also dissociates the molecule (except for CO and N_2) resulting in desorbing fragments (see review by Öberg 2016). Other options are chemical desorption, in which part of the energy liberated by formation of the chemical bond is used to desorb the molecule (Minissale et al. 2016), or impulsive spot heating by cosmic rays (Ivlev et al. 2015).

Ices: formation of complex organic molecules. Many complex molecules can be produced by reactions occuring on and in ices. Ultra-high vacuum solid-state laboratory experiments have demonstrated that complex molecules like methanol and ethylene glycol can indeed be formed at temperatures as low as 10 K without any energy input, as long as some H atoms are available (e.g., Chuang et al. 2016). Starting from CO, the sequence may even go as far as tri-carbon molecules like glycerol and real 'sugars' (Fedoseev et al. 2017) (Fig. 5). UV irradiation of ices breaks bonds and produces radicals which become mobile upon heating, leading to further molecular complexity (e.g., Öberg 2016). High energy particle irradiation produces many of the same species, with the difference that the strong CO and N_2 bonds can also be broken for energies >11 eV.

The translation of these experiments into numbers that can be used in astrochemical

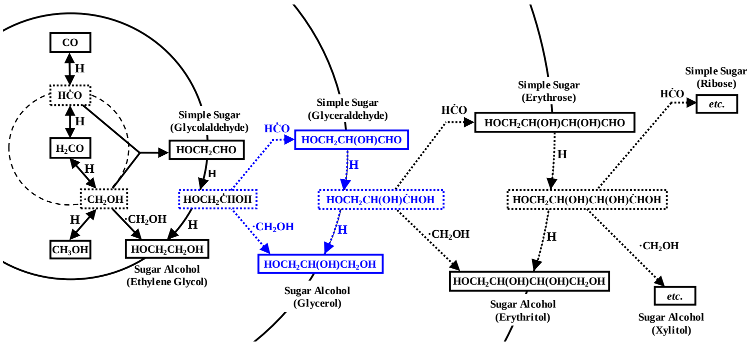

Figure 5. Reaction scheme leading to complex sugars in ices at low temperatures (10-15 K), without the need for UV radiation or cosmic rays. Figure from Fedoseev et al. (2017).

gas-grain models (e.g., Garrod et al. 2008), such as binding energies and diffusion and reaction barriers, is far from simple, however. Diffusion of at least one of the two reactants is particularly important to make the reaction go, unless the two reactants happen to be next to each other. If not, a prescription to hop from site to site is needed, in which the crucial parameter is the barrier $E_{\rm hop}$. Usually $E_{\rm hop} = c^{\rm st} \times E_{\rm bind}$ is assumed with c^{st} varying between 0.3 and 0.7, depending on species and surface site. The importance of tunneling at low temperatures is still debated. A detailed overview of these issues is presented in Cuppen et al. (2017) and highlights the fact that some fundamental chemical physics questions regarding surface chemistry are still poorly understood.

7. Planetary sciences: from dust to exoplanets

From dust to pebbles and planetesimals. Laboratory experiments using drop towers and other set-ups have characterized and quantified the collisional growth of dust grains from sub-μm size to pebbles and beyond over the past 25 years (Blum 2018). Small silicate particles of various sizes are made to collide with each other, with the outcome monitored as a function of collision speed. Besides sticking, bouncing and fragmentation, other processes such as erosion or mass transfer occur. When these lab results are put into coagulation simulations, it is found that μm-sized dust grains can indeed grow to mm- to cm-sized aggregates before they encounter the bouncing barrier. The effects of ice-covered grains are still being debated and more experiments are needed, ideally carried out in zero gravity. To grow beyond pebble size, other processes such as gravitational collapse of dust "pebbles" by the streaming instability is often invoked.

Analyzing samples from space. Extraterrestrial samples provide a wealth of information on the formation processes in the early Solar System, including time scales for specific rock formation events, the size distribution of particles, and the level of compositional mixing on small and large scales. Studies can range from in-situ analyses, such as done for comet 67P/C-G with the *Rosetta* mission, to detailed characterization of interplanetary dust particles collected with airplanes and meteorites that have fallen on Earth. Sample return missions that bring back rocks on Earth, ranging from the Lunar Missions to the *Stardust* mission to comet Wild-2 and culminating now with the *Hayubusa2* and *Osiris-Rex* missions to asteroids, provide unique in-depth insight. This is because these samples can be analyzed with increasingly sophisticated experiments that can image and study the composition of the material on nanometer scales: big machines such as NanoSIMS

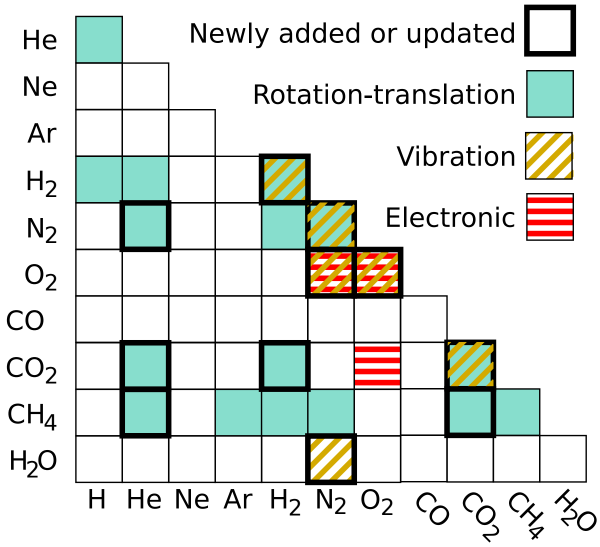

Figure 6. Overview of systems for which collisional induced absorption data are available from calculations. Figure adapted from Karman et al. (2019).

cannot be flown in space. This of course also requires laboratories that are committed to the long-duration (>50 yr!) curation of the extraterrestrial samples.

(Exo)planetary atmosphere studies. Studies of the atmospheres of our Solar System planets and their moons (e.g., Titan) have long recognized the importance of various molecular processes such as high-temperature (photo-)chemistry and pressure broadening in modeling the data collected by various missions. These needs are now (re-)emphasized for exoplanetary atmosphere studies, which cover an even wider range of physical conditions than found in our own Solar System (Moses 2014; Fortney et al. 2019). This includes (i) High-resolution molecular line lists; (ii) Pressure broadening; (iii) Collision-induced absorption, dimers; (iv) Haze and condensate formation and associated opacities; (v) Chemical reaction rates; and (vi) Photodissociation cross sections at high temperatures.

To illustrate a few examples, consider the line lists. The ExoMol program uses computational chemistry (quantum calculation of potential surfaces with associated energy levels and transition probabilities) to provide high accuracy line lists for an increasing list of molecules (Tennyson et al. 2016). Each molecule has billions of lines and may take a few years work of an experienced researcher to compute. The larger the molecule, the more time-consuming the calculations become. Alternative, faster but less accurate methods are now being developed (Sousa-Silva, priv. comm.). The HITRAN database collecting experimental data remains invaluable as well (Gordon et al. 2017).

Collision-induced absorption is a process that contributes significantly to the total absorption of radiation in dense planetary atmospheres. Fig. 6 provides an overview of systems for which such data are now available Karman et al. (2019). It also shows that data for a large number of important species are still missing.

The formation of clouds and hazes significantly affects the detection of molecular bands in exoplanet and brown dwarf atmosphere spectra, making them look 'flat' or 'grey' (e.g., Kreidberg et al. 2014). Exactly how these particles form and under which conditions is still poorly understood, and their opacities are largely unknown (Marley & Robinson 2015). This will be a major challenge for future laboratory experiments.

8. Outlook

The Universe continues to provide a unique laboratory in which to study basic physical and chemical processes, raising fundamental questions and new insight into these fields, off the well-beaten track. Conversely, the deluge of data from new observational facilities across a wide range of wavelengths continues to require accurate atomic, molecular, particle and solid-state data under a huge range of physical conditions. Continued interdisciplinary collaborations between these fields are important to reap the full scientific benefit from these billion $, Euro or Yen facilities. A comparatively small investment can go a long way, but prioritization of data requirements are needed. Also, astronomers have to come to terms with the fact that a significant fraction funding for such experiments have to be provided by astronomy rather than physics or chemistry. Joint approaches to funding agencies may be needed.

In the next 25+ years, with JWST and XRISM being launched in 2021–2022, Ariel in 2028 and Extremely Large Telescopes becoming operational in the mid-2020s, there is a growing data need. The IAU, and in particular Commission B5 on Laboratory Astrophysics and Commission H2 on Astrochemistry †, can play a role in bringing astronomers, chemists and physicists together to make all these experiments and calculations happen!

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