Astrochemistry associated with planet formation

Ewine F. van Dishoeck\textsuperscript{1} and Edwin A. Bergin\textsuperscript{2}

\textsuperscript{1}Leiden Observatory, Leiden University, the Netherlands
\textsuperscript{2}Astronomy Department, University of Michigan, USA

1 Introduction

Stars and planets are formed deep inside dense clouds. When these clouds collapse, the surrounding gas and dust become part of the infalling envelopes and rotating disks, thus providing the basic material from which new planetary systems are made. Today we are finding that much of the chemical composition of the planet-building material is likely set in the cold pre- and protostellar stages and preserved en route to planet and comet construction sites. With new observational techniques, astronomers can now zoom into these planet-forming disks and study them on scales comparable with the orbit of Saturn in our own solar system (Andrews 2020).

Astrochemistry, also known as molecular astrophysics, is the study of the formation, destruction and excitation of molecules in astronomical environments. By observing many lines of the same species, molecules are excellent diagnostics of the physical conditions and their high resolution spectral profiles provide unique information on the kinematics in the regions where they reside. More than 200 different molecules have now been detected in interstellar space (McGuire 2018). The main questions in astrochemistry therefore include: how, when and where are these molecules produced? What do they tell us about temperatures, densities, gas masses, ionization rates, radiation fields, and dynamics of the star-forming clouds and planet-forming disks? From these quantities what can be learned about the physics of star and planetary birth? How are they cycled through the various phases of stellar evolution, from birth to death? How far does chemical complexity go? And, most far-reaching, can they form the building blocks for life elsewhere in the Universe? While organics are a central focus of the latter question, water, in the form of ice, stands out as a reservoir of abundant elemental oxygen throughout all phases, hinting that life’s solvent started its journey in space (van Dishoeck et al. 2014).

This brief overview summarizes some of the main results and questions regarding the chemistry along this journey from cloud to disk. References are limited primarily to review papers of the many hundreds of papers in this rapidly growing field; citations to individual papers are mostly to relevant results in the last few years and are highly incomplete. Readers are encouraged to cite original papers.

2 State of the art

Recent overviews of the field of astrochemistry have been given by (Tielens 2013; Yamamoto 2017, and refs cited). Fourteen challenges have been formulated by van Dishoeck (2018).

2.1 How to observe molecules

Molecules can be observed through their electronic, vibrational or rotational transitions at optical/UV, infrared and millimeter wavelengths, respectively. Several of the most powerful new telescopes deployed over the past decades have been particularly well suited to observe interstellar molecules. The bulk of the

\textsuperscript{*}to appear as a book chapter in ExoFrontiers: big questions in exoplanetary science, Ed. N. Madhusudhan (Bristol: IOP Publishing Ltd.), AAS-IOP ebooks, authors’ version
Figure 1: Stages in the formation of a new planetary system from a dark interstellar cloud. Much of the chemistry of planet-forming material is likely set in the cold pre- and protostellar stages. Also, there is strong evidence that the first steps of planetesimal formation take place early, in the embedded protostellar phase of star formation (typically few $\times 10^5$ yr after collapse). Artist impression from Bill Saxton (NRAO/AUI/NSF), annotated by the authors.

molecules are detected through their rotational transitions at millimeter wavelengths, and various single-dish and interferometers at millimeter wavelengths with increasingly sensitive broad-band detectors have become available culminating in the Atacama Large Millimeter/submillimeter Array (ALMA). ALMA has the combined sensitivity and spatial resolution to zoom in on planet-forming disks. Millimeter observations require the molecule to have a permanent dipole moment to be detectable.

Infrared observations are highly complementary. Space missions like the Infrared Space Observatory, Spitzer Space Telescope and the Herschel Space Observatory at mid- and far-infrared wavelengths were particularly well suited to study H$_2$O and molecules like CO$_2$ that are abundant in our Earth’s atmosphere. Moreover, solid state species (silicates, ices), complex molecules (PAHs, fullerenes) and small molecules without a dipole moment like CH$_4$, C$_2$H$_2$ and CO$_2$ can be uniquely observed through their vibrational transitions. Warm H$_2$ can also be detected through mid-infrared lines, but cold H$_2$ in dark clouds is invisible and can only be traced indirectly through other molecules, most notably through far-infrared lines of HD. These space-based data have been complemented by studies of selected molecules using ground-based 8m optical/infrared telescopes equipped with high resolution spectrometers. The James Webb Space Telescope (JWST), to be launched late 2021, will be the next big jump in mid-infrared capabilities.

2.2 Astrochemical models

Chemistry in the interstellar medium, where densities are typically $10^3 - 10^6$ cm$^{-3}$, cannot be described by the laws of thermodynamics, except in the densest stellar and planetary atmospheres well shielded from radiation, with densities $> 10^{13}$ cm$^{-3}$. In interstellar space, the chemistry is controlled by two-body reactions and abundances can be obtained through kinetics involving large networks of reactions. These networks contain gas-phase reactions (ion-molecule, neutral-neutral) as well as gas-grain and grain-surface chemistry, with UV photoprocesses playing a role in both gaseous and solid phases. Thanks to many decades of laboratory experiments and quantum chemical calculations by physicists and chemists, deep insight into these processes has been obtained and their reaction rates under different conditions have been quantified.

Compilations of the rate coefficients together with codes that solve the coupled differential equations of these networks include the UMIST 2013 database, the KIDA database, and the UCLCHEM code. Programs tailored to exoplanetary atmospheres include VULCAN and LEVI.

To run an astrochemical model, a prescription of the temperature and density structure of the source,
the incident UV radiation field, the cosmic ray ionization rate, as well as the abundances of the (volatile) elements that are not locked up in refractory solids but that can cycle between the gas and ice phases are needed. Given the uncertainties in each of these parameters as well as in individual rate coefficients, agreement between observations and models at the factor of a few level is generally considered to be good.

3 Important questions + goals: chemistry from clouds to planets

The various stages in the formation of a new planetary system are illustrated in Fig. 1. The first three stages typically take a few million years, with a clear drop in gas and dust content after \( \sim 3 \) Myr. A key recent finding is that planet formation must already start early, in the embedded phase of star formation a few \( \times 10^5 \) yr after cloud collapse, in order to account for the observed mass in exoplanet cores (Tychoniec et al. 2020). This is consistent with the solar system record as Fe-rich meteorites sample the cores of large bodies that formed, in many instances, within the first few 100,000 years (Kruijer et al. 2017). Thus, much of the chemistry of planet-forming material is already set in the cold pre- and protostellar stages. On the other hand, there is clear evidence that molecules and dust were vaporized in the inner young solar nebula and then re-condensed, based on elemental abundance patterns and minerals found in meteorites (Connelly et al. 2012). Key questions therefore include

- What determines the chemical composition of planet-building material: inheritance or full reset? At what disk radius is the cross over (for a given type of star)? Can the composition of the young still-forming protostellar disks be characterized enough to reveal answers to these questions?

- If inherited from the collapsing cloud, to what extent is the gas and ice composition modified en route from cloud to disk (e.g., by accretion shocks), and within the protoplanetary disk midplane?

- Ice rich pebbles drift inwards during the main phase of planetary assembly. What is the fate of pebbles drifting from the outer tens to hundreds of au into the inner disk (\(<10\) au)? How does this impact planet formation and its chemistry?

- How quickly are ices locked up in large planetesimals, and what are the C/O or C/N ratios with radius in the midplane? How are these affected by pebble drift and dust traps? How do the snowlines move with time? How important is vertical mixing?

- Are the majority of the heavy volatile elements in a giant planetary atmosphere accreted as ice or as gas? How are they modified in the atmosphere itself and does a dilute core mix with the envelope? What is the importance of LTE versus kinetic chemistry in the outer layers?

- What can the composition of exo-planetary atmospheres ultimately tell us about their formation location, given the above questions?

- What can we learn about terrestrial planet formation and the delivery of needed volatile elements from astronomical observations?

3.1 Cold dark clouds

Chemistry starts in cold dark clouds prior to star formation with have typical temperatures of 10 K and densities of \( 10^4-10^5 \) cm\(^{-3}\). They exhibit a variety of chemical characteristics, the most important of which are ice formation and heavy deuterium fractionation (Bergin & Tafalla 2007; Caselli & Ceccarelli 2012; Ceccarelli et al. 2014). Most of these chemical signatures are transferred to the protostellar stage where they are observed in the cold outer parts of the collapsing envelope (Fig. 1).

Infrared observations of ice features toward reddened background stars show that the formation of water ice starts once the cloud extinction \( A_V \) is a few mag (Boogert et al. 2015; Oberg et al. 2011a). The formation of water ice on the surfaces of grains is now well characterized in the laboratory and models, and tested against observations of cold water gas and ice (van Dishoeck et al. 2013, 2014). CH\(_4\), NH\(_3\) and some CO\(_2\) ice are also made in this early phase, with the amount of ice rapidly increasing as the cores become more
centrally concentrated. All of these molecules are made on the grain surfaces, from reactions of atomic O, C and N with atomic hydrogen; they are not accreted from the gas.

At densities around $10^5\text{ cm}^{-3}$, the timescales for freeze-out become shorter than the lifetime of the cloud core, and CO (the dominant form of volatile carbon at these high densities) rapidly depletes from the gas onto the grains. This CO-rich ice can subsequently react with atomic H to form H$_2$CO and CH$_3$OH, a process that has been demonstrated to proceed rapidly at low temperatures in the laboratory. Various other routes can transform CO to CO$_2$ and more complex organic ices, even at very low temperatures.

A clear signature of cold interstellar chemistry are high abundances of deuterated molecules such as DCN, with DCN/HCN ratios at least three orders of magnitude higher than the overall [D]/[H] ratio of $2 \times 10^{-5}$. Even doubly- and triply-deuterated molecules such as D$_2$CO and ND$_3$ have been detected. This huge fractionation has its origin in two factors. First, the zero-point vibrational energy of deuterated molecules is lower than that of their normal counterparts because of their higher reduced mass. This makes their production reactions exothermic. In cold cores, most of the fractionation is initiated by the H$_3^+$ + HD $\leftrightarrow$ H$_2$D$^+$ + H$_2$ reaction which is exothermic by about 230 K. H$_2$D$^+$ then transfers a deuteron to CO or N$_2$ or another species. Since CO is the main destroyer of both H$_3^+$ and H$_2$D$^+$, their abundances are even further enhanced when CO is removed from the gas. Similarly, CH$_2$D$^+$ is enhanced at low temperatures and can enhance deuterium in organic molecules. The second, related effect is that the gaseous atomic D/H ratio is enhanced, which implies that relatively more D than H arrives on the grain to react with CO to make deuterated versions of formaldehyde, methanol and more complex organic molecules, and powering deuteration of water ice.

Key references summarizing this stage are Caselli & Ceccarelli (2012); Boogert et al. (2015).

3.2 Protostellar envelopes and young disks

Once a protostar has formed in the center, its luminosity sets up a temperature gradient in the gas and dust. Temperatures increase from 10 K in the outer envelope to a few hundred K in the innermost region close to the protostar. This can result in numerous chemical changes: radicals become mobile in and on icy surfaces and recombine to form even more complex molecules, whereas increased UV and X-rays from the protostar-disk accretion boundary trigger further chemistry in the ice and gas. When dust temperatures become high enough for ices to sublimate, molecules do so presumably in a sequence according to their binding energies, with volatile species like CO and N$_2$ sublimating first.

Once dust temperatures of $>100$ K are reached, even the strongly-bound water and methanol ice sublime, together with any minor molecules trapped in them, resulting in particularly rich gas-phase millimeter spectra (Fig. 2). This inner 100 K zone is called the ‘hot core’. Here high-temperature gas-phase reactions between sublimated molecules can result in ‘second generation’ complex organic molecules (Balucani et al. 2015).

Much of the extensive chemical complexity seen in hot cores is thought to be largely assembled in ices. A major question is whether this rich chemistry is incorporated in the forming disks (Fig. 1), and if so in what form. Further, the full extent of chemical complexity occurring on grain surfaces is still uncertain. It
is clear that some molecules of ‘pre-biotic’ significance are found in ices, such as simple sugars and peptide bonds (Fig. 2), but these are still small compared with molecules found in biological systems as well as the macromolecular material found in meteorites and comets (§3.5).

The solar system record suggests that there must have been a mixture of material where the chemistry is reset with pre-existing (or less processed) material ‘inherited’ from the interstellar medium (§3.5). In this regard, it is unclear whether the material entering the disk experiences a strong accretion shock, and if so, whether this shock completely resets the chemistry or whether strongly bound ices survive. At face value observations find an interesting transition in the disk seen in hydrocarbon emission and SO, but in general the overall temperature of these systems appears to be rather cool (< 50 K).

Key references for this section include Herbst & van Dishoeck (2009); Ceccarelli et al. (2014); Jørgensen et al. (2020).

### 3.3 Planet-forming disks

ALMA has been transformational for studies of planet-forming disks, and will likely remain so for the coming decade(s) (Andrews 2020). ALMA and high contrast infrared imaging of disks are providing striking pictures of the first steps of planet formation: rings, gaps, cavities, asymmetric structures, and / or spiral arms. Although there are many possible interpretations of these structures, they do indicate that growth of dust grains to pebbles and planetesimals is taking place, starting even in the embedded phase.

Disks remain challenging to study both observationally and theoretically, however. Observationally, molecular lines are very weak since disks are small (typically less than 1″ on the sky) and their mass is only 1% of that of the collapsing cloud. Theoretically, they are a challenge since they cover a huge range of densities and temperatures in at least two dimensions, from > 1000 K in the inner disk and upper layers, to 10 K in the outer midplane, and from densities of > 10^{13} cm^{-3} in the inner midplane down to 10^5 cm^{-3} in the upper outer layers. UV radiation fields from the central star impinging on the surface layers can be as high as 10^5 times the interstellar radiation field at 1 au from the star, thereby ionizing atoms and dissociating molecules. Thus, different types of chemistry are important in different parts of the disks (Henning & Semenov 2013; Bergin & Cleeves 2018; Oberg & Bergin 2020) (Fig. 3).

Moreover, gas and dust are largely decoupled (except for the smallest grains): dust grains grow to pebble size (few cm), settle to the midplane and drift in radially (Fig. 3). If they encounter a pressure bump, dust traps can form where particles can grow to even larger, planetesimal sizes. Gas/dust ratios can therefore differ significantly from 100. While ALMA is particularly well suited to study the gas and mm-sized dust in the outer disk (> 10 au for gas, few au for dust), JWST and other mid-infrared facilities probe the important inner 10 au planet-forming zones of disks.

The decreasing temperature in the radial direction sets up a range of snowlines, i.e., radii where molecules...
Figure 4: Left: Midplane C/O ratios in gas and ice as function of disk radius, with major steps occurring at the H₂O, CO₂ and CO snowlines. The ice is oxygen rich, whereas the gas has high C/O but is overall depleted in carbon and oxygen (Oberg et al. 2011b). Right: illustration how abundances in the inner disk can be affected by dust traps locking up volatiles in the outer disk beyond their snowlines, as in this case for the TW Hya disk (Bosman & Banzatti 2019).

freeze-out onto the grains, defined as the half-gas, half-ice point. Because of the vertical temperature gradient, the 2D snow surfaces are actually curved (Fig. 3). Snowlines are thought to play a significant role in planet formation, since ice coating of grains enhances the solid mass, potentially promotes coagulation of grains to larger particles and/or require a higher collision velocity for destruction (Blum 2018; Pinilla & Youdin 2017), effects which are particularly prominent just outside the snowline. Thus it is thought that water ice coated grains grow to larger sizes and provide larger pebbles for planet formation which has implications on growth via pebble accretion (Morbidelli et al. 2015). They also control the bulk elemental composition of the icy planetesimals and gas from which exoplanetary atmospheres are built.

Cold outer disks. Most molecules detected in disks are simple species containing only a few atoms. Only two complex molecules, CH₃CN and CH₃OH, have been detected so far, and only barely. Even the brightest disks do not show rich line forests such as found for hot cores. This lack of gas-phase lines is because the bulk of the disks are cold with molecules frozen out. In fact, the CO snow surface is resolved in highly flared systems - thus the comet-forming zone can essentially be seen by eye in some ALMA images. The most important snowline, that of water, is generally out of reach because it typically occurs at a few au for T Tauri stars, too small for ALMA to pick up. Only systems undergoing luminosity outbursts such as V883 Ori or young disks with enhanced accretion luminosity, for which the water snowlines have moved out to tens of au, offer the opportunity for direct detection and imaging of complex chemistry (Lee et al. 2019).

The overall picture of the outer disk is therefore that much of the volatile oxygen and carbon is locked up in ices in large bodies. Since the dominant H₂O and CO₂ ices have more oxygen than carbon, the ice is oxygen rich, with an overall C/O ratio that is lower than the interstellar or solar abundance (Fig. 4) (Oberg et al. 2011b). In contrast, the gas is carbon rich even though it is overall depleted in carbon and oxygen. Once C/O> 1, the chemistry completely changes and small hydrocarbon molecules become abundant. This can indeed explain the strong observed C₂H and c-C₃H₂ emission in some disks, although models suggest that midplane chemistry tends to evolve toward gaseous C/O significantly less than 1 depending on the level of ionization (Eistrup et al. 2018). JWST will be able to observationally constrain the ice composition in planet-forming zones, but only for a handful of near edge-on disks and then only in the intermediate layers.

Warm inner disk. The warm gas in the upper layers of the inner disk (<10 au) emits strongly at mid-infrared wavelengths. Indeed, a dense forest of lines due to simple molecules has been detected by Spitzer and ground-based infrared telescopes, providing a glimpse of the chemistry in that region (Pontoppidan et al. 2014). Here the high temperatures can completely ‘reset’ the chemistry. Key abundant molecules without a dipole moment such as CO₂ and C₂H₂ are observed, together with H₂O, OH and HCN, allowing tests of major C, O and N reservoirs and high temperature chemistry. The degree to which these data can probe the disk midplane chemistry and ice sublimation, relevant for planet formation models, is still unclear however, since they can only be observed if effective vertical mixing takes place. On the other hand, the recent observational evidence for meridional flows suggests that giant planets accrete a significant fraction
of their gas from the upper disk layers (Teague et al. 2019). JWST will be poised to provide much deeper searches for CH$_4$, NH$_3$ and minor species, and detect isotopologues to constrain line optical depth, and follow the inner disk chemistry (at least in the surface layers) from the youngest embedded disks to the debris disk stage, and across the stellar type range.

Key references for this stage include Henning & Semenov (2013); Pontoppidan et al. (2014); Andrews (2020); Oberg & Bergin (2020).

3.4 Disk evolution and planetesimal formation

Disk structure and chemistry is not static but evolving, due to grain growth and inward drift of dust particles (Fig. 3) (Pinilla & Youdin 2017). At the same time, mass and angular momentum transport in disks, both inward and outward, are still poorly understood. How does this affect the chemistry? Recent ALMA data indicate either surprisingly low gas/dust ratios or a large fraction (up to a factor of 100) of volatile carbon, carried by CO, missing from the gas phase. The latter case, that CO is missing from layers with temperatures >20 K (the CO sublimation temperature), has support in terms of consistency with accretion rates, the mass needed to make planetary systems, and, in a handful of instances, detections of HD to constrain the gas mass (Bergin & Williams 2018). Thus, at face value, it appears that planet formation removes volatiles from the gas.

The first clue actually came from Herschel-HIFI observations which revealed surprisingly weak gaseous H$_2$O lines in disks. Since cold H$_2$O vapor in the outer disks results from UV photodesorption of water ice coating small grains in intermediate layers, the observed weak emission indicates that this water ice is spatially confined to only a part of the disk: radially, vertically or both. The most plausible interpretation is that most of the water is locked up in large icy bodies (at least pebble size) in the midplane (Du et al. 2017). A second clue comes from models of dust coagulation and growth which suggest that water and CO on the surface can be caught up in the grain evolution and locked within icy pebbles and planetesimals (Krijt et al. 2020). In the case of CO it may be combined with an active disk chemistry transforming CO into CH$_3$OH, CO$_2$ or hydrocarbons.

Do these heavy elements return to the gas when the pebbles drift inward and cross the snowlines (Fig. 3)? If so, one would expect inner disk abundances inside the water snowline to be similar to, or even higher than, the stellar abundances. This is not always the case: there is significant evidence that dust traps located beyond the major snowlines in the outer disk can lock up large fractions of carbon and oxygen preventing these pebbles to drift inward and resulting in inner disks that are depleted in these elements (Fig. 4, right) (Kama et al. 2015; McClure et al. 2020).

So how do we then determine the disk chemical composition just prior to planet formation? Much of the chemistry of planet formation is unfortunately hidden from our view, including the bulk C- and O-containing species. One option is to observe warmer, younger disks where less of the material is frozen out and fewer planetesimals have formed, such as the outbursting case described above. Observational studies show that only the youngest, deeply embedded sources have high enough temperatures to reveal the full chemical richness (§3.2) (van’t Hoff et al. 2020). The forming disks around Class 0 sources, like those for IRAS16293-2422 (Fig. 2), may therefore well provide the most detailed information of chemistry on solar-system scales, even if the material has not yet settled into a Keplerian structure. That chemistry, in turn, may have been set already to a large degree in the dense cold core just prior to and during collapse, arguing for an ‘inheritance’ rather than a ‘reset’ scenario, at least in the outer disk.

Key references for this section include Pinilla & Youdin (2017); Du et al. (2017); Bergin & Williams (2018); Krijt et al. (2020).

3.5 Clues from our solar system: comets and meteorites

The solar system record shows evidence of both a full reset of the chemistry as well as inheritance from the interstellar medium. The pattern of elemental abundances in the Earth’s lithosphere and in meteorites suggests that this material formed within a hot (>1500 K) atomic gas in which all original interstellar material was vaporized, followed by a sequence of mineral condensation as the gas cooled (McDonough & Sun 1995). This cannot be the case for all solar system materials, however, as the deuterium enrichment
in Earth’s water, and indeed all solar system water, implies a cold (<30 K) source and cometary abundances appear to follow that of the interstellar medium (Altwegg et al. 2019).

Comets and other icy bodies in our own solar system provide the best clues to the chemistry in the cold part of the natal solar nebula disk and the level of change since their formation 4.5 billion years ago. Comparisons between cometary and interstellar abundances, including those from the Rosetta mission to comet 67P/C-G, have shown some tantalizing similarities (Mumma & Charnley 2011, Drozdovskaya et al. 2019). The organic complexity in comets goes further than has been detected so far in young disks, with even 4- or 5-carbon organic molecules, alkanes, aromatics and even the simplest amino acid, glycine, detected (Altwegg et al. 2019). More bright comets like Hale-Bopp that can be probed with ALMA and modern infrared instruments will provide further insight into their origin, including through determining their D/H ratio in water.

Primitive carbonaceous meteorites also have a rich organic composition, but much of that inventory is either macromolecular or altered via aqueous reactions in liquid water (Alexander et al. 2007). Thus, in terms of the origins of biology and the importance of molecules produced via cold chemistry in the interstellar medium, a key question is the amount of material that was supplied to the Earth that originated in the asteroid belt or beyond. The fate of this material on the Earth itself is, of course, a central issue (see §3.6).

Key references for this section include McDonough & Sun (1995); Altwegg et al. (2019); Alexander et al. (2007).

3.6 Exoplanets and their atmospheres

Detection of young exoplanets with molecules. One new frontier is the use of ALMA to infer the presence of hidden planets, first using dust emission (Andrews 2020) followed by constraints from CO emission showing deep gas cavities and gaps (van der Marel et al. 2016). Even more recently, the presence of hidden planets based on kinematical information has been gleaned from ALMA CO emission maps (Teague et al. 2018, Pinte et al. 2018, and other work by their teams). Fig. 5 provides an example of the overall emission (dust and CO) along with the exquisite measured velocity field. This topic is very much in its infancy but has promise to potentially isolate the locations of hidden planets, set unique constraints on the H$_2$ gas pressure, and reveal the presence of ordered gas motions.

A central aspect of this work is the close collaboration with dynamical theorists. Indeed, the wealth of dust substructures in disks points to a larger number of giant exoplanets than found by direct imaging at 10–100 au distance, suggesting a so-far unseen population of sub-Jupiter mass planets that needs independent confirmation (Zhang et al. 2018, Lodato et al. 2019). The kinematical work is pure molecular astrophysics, but has interesting astrochemical links. Different molecular tracers probe different layers and one might use this information to study the overall physics and chemistry of material directly related to forming planets.

Exoplanet atmospheres. The chemical composition and origin of exoplanet atmospheres, from Super-Earths to mini-Neptunes and Jovian planets, is clearly a new frontier for Astrochemistry (Madhusudhan 2019) and discussed in other chapters in this book. One of the ultimate goals is to link the planetary atmosphere composition with its formation history in the natal protoplanetary disk. On the one hand, the changing C/O ratio with disk radius could provide such a probe of the formation location (Fig. 4). However, the route from disk gas+dust to a mature planet is long and involves many steps, each of them with significant uncertainties (e.g., Mordasini et al. 2016, Cridland et al. 2019). For example, are the heavy elements (i.e., other than H and He) in a giant planet atmosphere accreted mostly from the gas or delivered by icy pebbles? How does the migration history affect the outcome? How about dust traps? It is also clear that individual molecule abundances will be fully reset in giant planet atmospheres, preserving only the overall C/O, C/N, O/H etc. abundance ratios. And even those could be affected if part of the atmosphere material is cycled to the planetary core.

Rocky exoplanets, lessons from Earth. The atmospheres of rocky terrestrial planets may have an even more complicated history. Well outside the water snowline, the planets are built up largely from planetesimals that are roughly half rock and half ice. When these planets move inward, water becomes liquid, resulting in ocean planets or water worlds. Inside the snowline, the planets are usually thought to be very dry. Computing the atmospheric composition of terrestrial exoplanets is significantly more complex than that of giant exoplanets (Kaltenegger 2017). In this light, a central conundrum lies in the Earth’s carbon content which is orders of magnitude below the carbon content seen in cometary material and the Sun.
Figure 5: High spatial resolution ALMA image of the 1.3 mm dust emission from the HD 163296 disk ($d=101$ pc) showing several dust rings (left) and $^{12}$CO $J=2–1$ emission (middle) published by Isella et al. (2018). The right-hand panel is the H$_2$ gas velocity field in $^{12}$CO 2–1 taken from Teague et al. (2019). The rough (inclination not removed) locations and masses of planets estimated to be present are shown at the bottom of the middle panel as yellow circles. The circles on the left side of the figure (white/black) represent the angular resolution of the data.

Overall, this hints at loss of the main carriers of carbon (and also nitrogen) in Earth’s planetary building blocks in the inner few au of the presolar nebula, and in disks more generally. It also requires consideration of many additional processes that are operative during each stage of the formative process of terrestrial worlds (e.g. Bergin et al. 2015; Gail & Triloff 2017), followed by billions of years of evolution on a living active planet (Foley 2019).

A secondary atmosphere can however be formed through impacts of (icy) planetesimals in the late formation stages, including by comets such as 67P/C-G which can deliver water and organics to the young planet. Given the architecture of the solar system it is not clear if significant mass from comet-forming zones can be brought to Earth (van Dishoeck et al. 2014). However, the giant planets could have migrated and noble gas analyses of 67P are consistent with some cometary supply to the young Earth including most of the organic material, even if not the water (Marty et al. 2017). The survival of these organics depends on planetesimal size and impact speed, and whether the volatile material can perhaps be shielded by a protective layer on the parent body. If they do, there would indeed be a direct link between interstellar molecules and the building blocks for life on new planets.

Key references for this section include Disk Dynamics Collaboration et al. (2020); Mordasini et al. (2016); Madhusudhan (2019); Bergin et al. (2015).

4 Opportunities

There are several frontiers in front of us. On short timescales ALMA remains a pioneering instrument and JWST is on the horizon. The combination of these two observatories will be quite powerful as we describe below.

- ALMA will be able to survey hundreds of young disks in the embedded phase for their chemical composition and thus search for similarities and differences in the chemistry prior to planet formation across stellar mass and age range. ALMA will also reveal whether substructures in young disks are common or not, which could point to locations where planets are typically formed.

- ALMA has inferred the presence of volatile depletion in disk systems beyond the CO snowline, and in a few instances interior to the CO snowline. JWST will be able to probe the inner disk composition (within a few AU, including O and C budgets) in the upper disk atmosphere as well as that of ices in the intermediate layer for a few near edge-on disks. Will ALMA and JWST tell the same story?
• In a handful of systems the stellar abundances, and that of accreted/ejected material, provide a crucial link to explore the composition of gas in the inner disk that reaches the star. Linking these studies to ALMA/JWST analyses may provide unique information on the composition of hidden material.

• Models of grain growth to pebble size and their radial drift are becoming increasingly sophisticated and are being coupled with chemistry. Since pebble accretion is believed to be a primary mode of planetary growth, these models (combined with observations) are a needed step.

• ALMA has just begun to explore the kinematical landscape of planet formation. A clear question is whether any planets inferred to be present by molecular kinematics, or emission structures, are confirmed by ground-based or space-based direct detection. Within this landscape the link between chemistry and 3D kinematics presents an inviting field to explore the composition of gas that is being supplied from the surface to the planet-forming zone.

• High spectral resolution infrared spectrometers on future extremely large telescopes, such as ELT/METIS, will be able to spatially resolve the chemistry and kinematics of warm gas down to a few au and also image, in tandem with ALMA, gas and dust in circumplanetary disks. VLTI/Gravity(+) provides new opportunities to obtain spatially resolved spectra of young exoplanets and their disks on even smaller scales.

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