The Chemical Picture of Protoplanetary Disk Evolution

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Abstract

Studying chemical evolution of protoplanetary disks has been one of the primary ways to understand planetary formation processes. It has multifaceted effects on the evolution of disks into a planetary systems as it affects processes like pebble accretion and influences disk structure and dynamics by regulating distributions of dust and gas in the disks. All of these processes ultimately have major implications as this chemical make-up will eventually provide the raw materials for all kinds of planets: from rocky worlds to gas giants. This work delves on the both modeling and observational aspects of disk chemistry and how it can help us build theories of planet formation.

Contents

Chapter 1

Introduction

Protoplanetary disks are planet-forming, potentially planet-containing, dust-
and gas-rich disks around young stars. Disk chemistry also provides some
of our best tools to characterize disk structures and dynamics, including the
presence of protoplanets. Developing a predictive theory of planet formation
therefore requires a deep understanding of the chemistry of protoplanetary
disks (Oberg21).

Protoplanetary disks emerge within the context of star formation, when
infalling interstellar cloud material becomes distributed in disk-like structures
to preserve angular momentum (Shun87). It is a gradual process which
involves multiple stages like the interstellar phase, the protostellar phase and
finally the disk phase. The inheritance of chemical compositions across these
phases is of immense importance as it is carried till formation of first planets
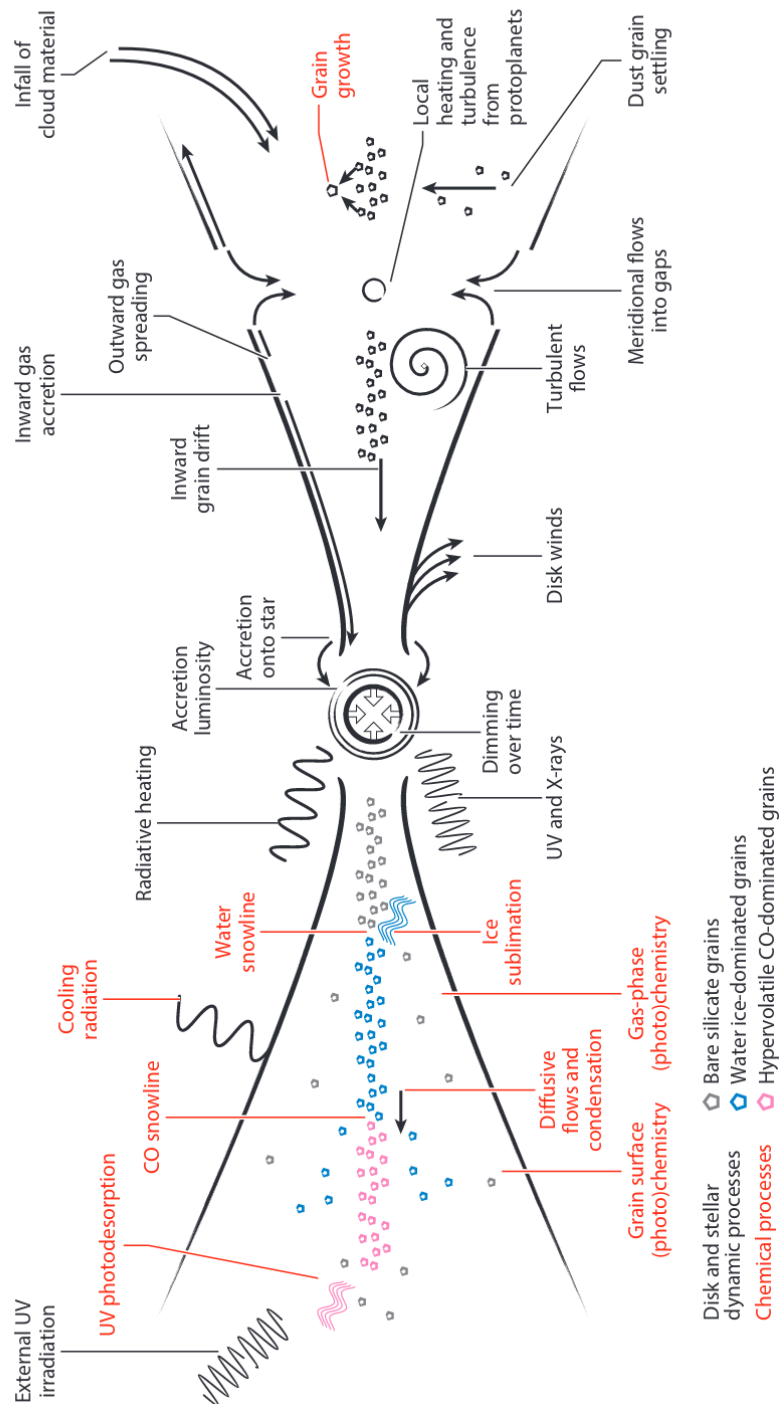as well.

Figure 1.1: An overview of different physical and chemical processes that go in protoplanetary disks. The processes labelled in black are stellar and/or disk dynamical processes which do not depend on local chemical environment. Processes labelled in red are the chemistry dependent mechanisms.

Chapter 2

Astrochemical Modeling and Observations

Disk chemistry models are used to provide interpretative frameworks for observations, to expand the kinds of species that can be characterized in disks beyond what is directly observable, and to connect different evolutionary phases up until and sometimes including planet formation.

To setup any kind of astrochemical modeling, we need a *physical structure* of the disk; a grid based layout where we will model the spatial points (2-D models which assume a azimuthally symmetric disk and full blown 3-D models both exist) having their own unique physical characteristics (dust/gas densities, dust/gas temperatures) and their own unique chemistry, which is depends on factors like location of that particular point in the grid of the disk and distance from the central star.

2.1   Physical Structure

We start by considering parametric profiles for density distributions. We assume the dust-to-gas mass ratio to be equal to the ISM value of 0.01 and use the single equation to model both the structure of gas and dust. We assume that the disk is static in the vertical direction and is in Keplerian rotation in the azimuthal direction (only needed for the line radiative transfer). The axisymmetric disk density structure we use takes the following parameterized form in cylindrical coordinates (r, z)(refs).

$$\rho(r, z) = \frac{\Sigma}{\sqrt{2\pi}h} \exp\left[\frac{1}{2}\left(\frac{z}{h}\right)^2\right], \qquad (2.1)$$

where

$$\Sigma(r) = \Sigma_c \left(\frac{r}{r_c}\right)^{-\gamma} \exp\left[-\left(\frac{r}{r_c}\right)^{2-\gamma}\right],$$

$$h = h_c \left(\frac{r}{r_c}\right)^{\psi} \tag{2.2}$$

The disk mass (gas or dust) is

$$M_{disk} = \int_{r_{in}}^{r_{out}} \Sigma \, 2\pi r dr,$$

$$= \frac{2}{2-\gamma} \pi r_c^2 \Sigma_c \left[\exp\left(\frac{r_{in}}{r_c}\right)^{2-\gamma} - \left(\frac{r_{out}}{r_c}\right)^{2-\gamma}\right] \tag{2.3}$$

Here, r_{in} and r_{out} are the radii of disk's inner and outer edges respectively (a tapered disk can be assumed by employing an exponential tapering function, but here, we assume a sharp inner edge). r_c is the characteristic radius, or the radius where the we have observationally constrained parameter values. h_c is the scale height at the characteristic radius. γ and ψ are power indices for disk surface density distribution (Σ) and scale height as a function of radius respectively.

2.1.1 Dust species and distribution

We assume two types of dust grains, each with a Mathis–Rumpl–Nordsieck (MRN) size distribution (Mathis et al. 1977). The two dust components are assumed to be spatially coexistent in this fiducial model. The larger population has $r_{min} = 1\,\mu\text{m}$ and $r_{max} = 100\,\mu\text{m}$, with a dust-to-gas mass ratio of 0.01, while the smaller population has $r_{min} = 0.01\,\mu\text{m}$ and $r_{max} = 1\,\mu\text{m}$, with a dust-to-gas mass ratio of 2×10^{-5}. Larger values for r_{max} of the big grains has been used in the literature for fitting the disk spectral energy distribution. However, the chemical processes mainly depends on the total available dust grain surface area, which is more sensitive to the assigned overall mass fractions of the small and big grains than the value of r_{max}. The dust material is assumed to be a 7 : 3 mixture of "smoothed UV astronomical silicate" and graphite. The optical parameters of the dust are taken from the Web site of Bruce T. Draine4 (Draine & Lee 1984; Laor & Draine 1993).

2.2 Chemical Evolution

After setting up the physical structure and performing a Monte-Carlo based dust radiative transfer (Bjorkman), we have the radiation structure of the disk. After establishing the this dust temperature distribution, we evolve the disk chemistry for 1 Myr. Since the heating and cooling processes are coupled with chemistry, the gas temperature is evolved in tandem with chemistry based on the heating and cooling rates. Namely, we solve the following set of ordinary differential equations (ODEs):

$$\frac{d}{dt} X_i = P_i(X;T) - D_i(X;T), \quad i = 1, \ldots, N$$
$$\frac{d}{dt} T = (\Gamma - \Lambda)/C_V,$$

(2.4)

where X_i is is the abundance of species i, P_i and D_i are the production and destruction rates of this species, which are functions of the chemical abundances and temperature (and other physical parameters), and N is the total number of species. $C_V = 3k_B/2$ is the volume-specific heat capacity of an ideal gas, where k_B is the Boltzmann constant. The exact value of C_V is not important because we are only concerned with the equilibrium temperature rather than the rate of temperature change. The heating and cooling rates are contained in Γ and Λ. We do not need a separate set of equations to account for the elemental conservation since elements are automatically conserved within numerical tolerance.

2.2.1 Chemical Network

We use the full KIDA chemical network (Wakelam 2015) for our three-phase chemistry (gas phase, gas-grain surface and grain surface-grain mantle). We consider chemical reactions involving adsorption, thermal desorption, photodesorption, cosmic-ray desorption, H_2 formation, photodissociation of species like H_2O, OH, CO and H_2

2.2.2 Thermochemical modeling

In our thermochemical considerations we have taken following processes into account:

1. Photoelectric heating,

2. Chemical heating and cooling,

3. Heating by formation of H_2,

4. Heating by viscous dissipation,

5. Heating by cosmic ray and X-ray,

6. Energy exchange by gas-dust collision,

7. Heating by photodissociation processes,

8. Heating by ionization of atomic carbon,

9. Cooling by electrons recombine with small dust grains,

10. Cooling by the rotational transitions of H_2, and the rotational and vibrational transitions of CO and H_2O,

11. Heating and cooling by the vibrational transitions of H_2, and cooling by C^+ and O emission,

12. Cooling by Lyα emission, free–bound, and free–free emissions.

2.2.3   Dynamical chemistry

There is a growing list of observations that are difficult to explain with static models, and a frontier in disk chemistry modeling is the comodeling of chemistry and dynamical processes that occur on timescales similar to those of chemical reactions. Simulating the combined effects of all major physical, chemical, and dynamical processes throughout the entire disk is currently too computationally expensive, however, and models therefore need to choose which physical and chemical processes to include and exclude. Several models incorporate aspects of vertical mixing (e.g., Semenov & Wiebe 2011, Furuya & Aikawa 2014), radial gas diffusion (e.g., Aikawa & Herbst 1999, Ilgner et al. 2004, Nomura et al. 2009, Bosman et al. 2018, Price et al. 2020), and dust evolution (e.g., Vasyunin et al. 2011, Akimkin et al. 2013, Krijt et al. 2018, Booth & Ilee 2019, Eistrup & Henning 2022, Van Clepper et al. 2022), but many of them consider a simplified chemistry (i.e., they are not necessarily more complete than static models with larger chemical networks). In addition to local mass transport processes, some models consider how global environmental changes affect the chemistry. The effects of stellar evolution have been explored by solving for chemical abundances while altering the disk environment at specified time steps (Price et al. 2020). The impact of short-lived accretion outbursts from the young star on disk compositions has also been investigated (Cleeves et al. 2017, Rab et al. 2017).

The outbursts generate chemical changes that persist beyond the duration of the event (Molyarova et al. 2018), but the potential for longterm chemical changes or alteration of planetary compositions by such phenomena has yet to be determined.

2.3   Observational techniques

Disk chemistry is observationally characterized through a range of techniques. These observations directly produce molecular line emission fluxes or absorption depths, from which molecular column densities, abundance structures, or higher-level constraints on the disk chemistry and its environment can be retrieved

An observational chemical characterization of protoplanetary disks can be achieved by spectroscopic studies at a wide range of frequencies and energy scales probing electronic, vibrational, and rotational transitions of atoms, molecules, and ions. Each wavelength and technique probes a unique aspect of the disk chemistry, and a comprehensive disk chemical characterization requires observations across the electromagnetic spectrum.

2.3.1   X-ray, UV and Optical regimes

Starting at the high-energy end of the spectrum, X-ray and UV transitions are used to probe the elemental abundances of gas and dust that are being accreted onto the stellar surface, providing access to the composition of inner disk refractories (e.g., Drake et al. 2005, Ardila et al. 2013, Kama et al. 2016, Günther et al. 2018). UV observations of fluorescent H2 and CO transitions are also used to probe hot gas in the innermost disk region, including its C/O/H ratio (France et al. 2012, Arulanantham et al. 2021). Optical spectroscopy can be used to constrain the elemental composition of the innermost disk regions (e.g., Facchini et al. 2016) and to characterize the compositions and dynamics of disk winds from the upper layers of the inner disk regions (Pascucci et al. 2022 and references therein).

2.3.2   NIR-MIR regimes

The near- to mid-infrared (NIR–MIR) regime enables observations of rovibrational and highly excited rotational lines of simple molecules in the upper layers of the inner few astronomical units of disks, where temperatures and densities are high enough to collisionally excite these transitions (Pontoppidan et al. 2014 and references therein). From space, the *Spitzer* mission

was instrumental in surveying numerous disks in MIR emission lines (e.g., Carr & Najita 2008, Salyk et al. 2011b), but at fairly low spectral resolution ($\lambda/\Delta\lambda < 700$). Observations at these wavelengths are set to be transformed by the *James Webb Space Telescope* (JWST).

2.3.3 FIR regime

In the far infrared (FIR), most spectroscopic surveys have been performed with the *Herschel* mission because of the prohibitive atmospheric transmission at these wavelengths. But since the it being defunct, there is a need for a new FIR mission which can probe molecules like HD which is crucial chemical tracer of H_2, so that we can estimate the gas content in the disk.

2.3.4 Sub-millimeter and Millimeter regime

These enable the spectroscopic characterization of cold gas, which includes most of the disk gas reservoir. Many small and abundant molecules present rotational transitions at these wavelengths, with typical upper energy levels of 5–500 K. Depending on line and dust optical depths, these observations can probe all the way to the disk midplane, but more often access the outer disk upper layers. In 2011–2014, (sub)millimeter observations of disks were transformed by the arrival of the Atacama Large Millimeter and Submillimeter Array (ALMA), whose collecting area and long baselines enable the detection of rarer molecules and the study of disk chemistry at higher spatial resolution down to scales of 10 AU (Öberg et al. 2015b, Huang et al. 2018a). So far, disk chemistry has not been accessible at longer wavelengths, but in the future a more sensitive radio array may provide access to NH_3 and large organic molecules in the disk midplane.

Chapter 3

Work done

After running a model with a fiducial set of parameters, we found that in the disk upper layer heating is dominated by photoelectric effect, followed by H2 formation heating in the photodissociation layer, and viscous heating in the deep region. Cooling is dominated by O i and C ii lines in the upper layer, and by accommodation on the dust grains in the lower dense layers. Overall the distribution of the dominant heating and cooling mechanisms is similar to what is shown in Woitke et al. (2009).
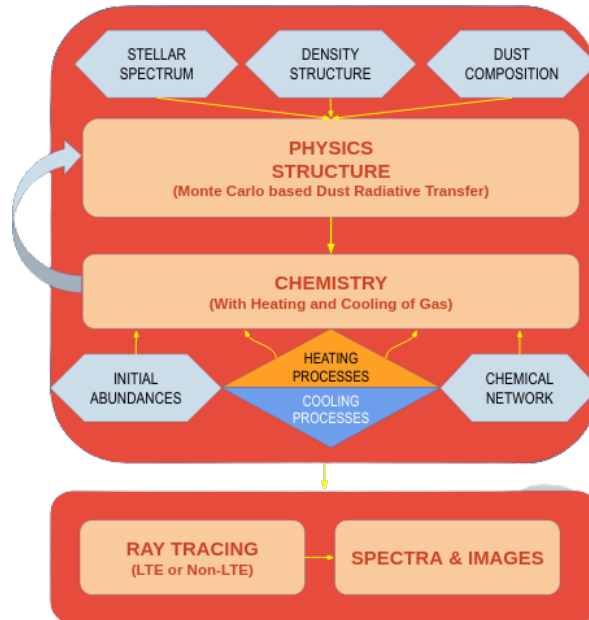

Figure 3.1: Flowchart depicting the working of the model
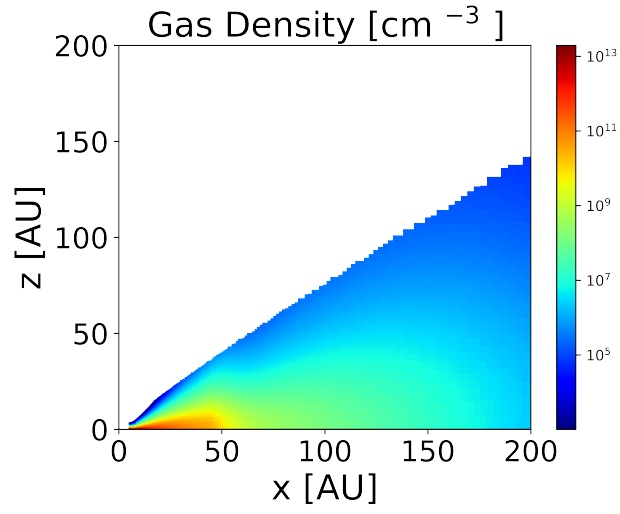
3.1 Results

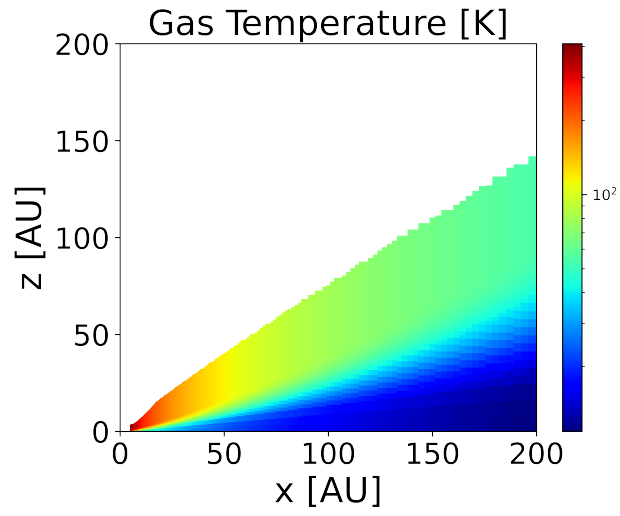Figure 3.2: Parametric gas number density structure
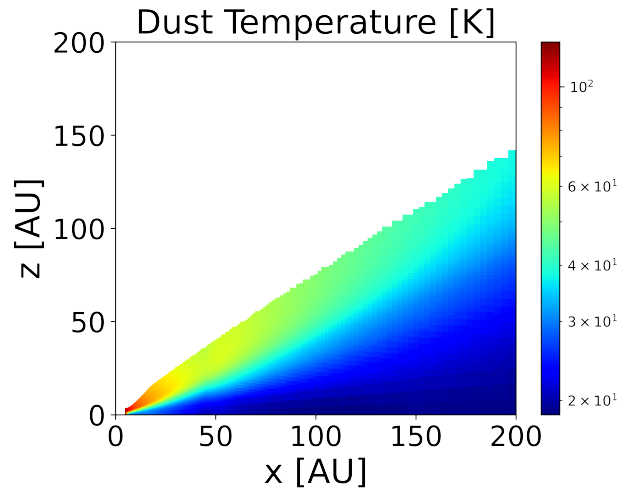

Figure 3.3: Parametric gas temperature structure

Figure 3.4: Dust temperature structure after dust radiative transfer
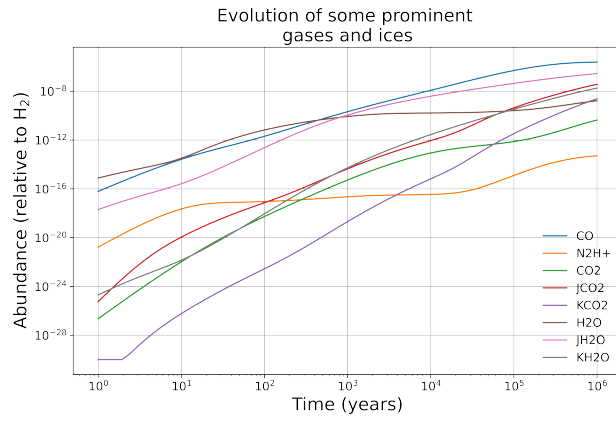

Figure 3.5: Time evolution of some prominent chemical species

Chapter 4

Linking Chemistry to Planetary Formation

To start with, snowline locations may affect the architectures of planetary systems. Snowlines of different volatiles are predicted to affect the grain coagulation rate, resulting in higher (or lower) rates of planet formation in the vicinity of snowline locations. In the Solar System, the presence of Jupiter at 5 au has long been associated with gas giant formation just outside the water snowline in the Solar Nebula (e.g., Stevenson & Lunine 1988). There is also evidence for a pileup of gas giant exoplanets around 2 au (Fernandes et al. 2019), which may coincide with the location of the water snowline during the relevant disk evolutionary stage. Better exoplanet statistics, as well as observations of snowline locations in samples of disks, are needed to establish such links between planet formation and snowline locations with confidence.

4.1 Chemical Inheritance

Protostars form through the collapse of cloud cores. In our understanding of the chemistry of planet formation, this stage plays a key role because, first, it is during the warm-up of infalling cloud material towards the central protostar that much of the icy molecular cloud chemistry described in the previous section is revealed. Second, warm-up of interstellar grains in the protostellar envelope activates new chemical pathways that changes the compositions of the future solid building blocks of planetesimals and planets. Third, the protostellar disk that forms at this stage is the precursor to the planet-forming disks treated in the next section, and the balance between preservation or inheritance and reset at this stage provides the initial chemical conditions for planet formation. In this section we review the protostellar

organic chemistry, and the chemistry or protostellar disks, after a brief review of the chemical structures of low-mass protostars (analogs to the protosun) and their surrounding environment.

4.2   Composition of Planetary Atmospheres

Most research linking disk and planet composition has focused on the formation of giant planets and the elemental composition of their atmospheres, but in the near future the study of Earth analog atmospheres will become feasible. The atmospheres and hydrospheres of rocky planets are shaped by a range of processes, including outgassing of magma, the length of a magma ocean phase, plate tectonics (e.g., Lichtenberg et al. 2022 and references therein), and impacts of meteorites and comets. The last two connect the disk molecular inventories with rocky planet compositions; therefore, comprehensive data sets on the distribution of key organics in asteroid and cometforming disk environments are needed to predict the prebiotic chemistry on young rocky planets.

4.3   Isotopic Ratios

Finally, isotopic ratios in gas and solids provide a tool to map the origins of cometary and planetary volatiles. So far, these ratios have been applied almost exclusively to the Solar System to constrain the origin of water on Earth and other planets, as well as in comets and asteroids (for reviews, see Ceccarelli et al. 2014, Altwegg et al. 2019). The first isotopic ratio in an exoplanet atmosphere was recently reported, potentially unlocking isotopic ratios as a complementary tool to elementary ratios when extracting a planet's formation history (Y. Zhang et al. 2021). The deployment of this method, however, requires a detailed understanding of the isotopic composition and fractionation chemistry of disks, which is currently incomplete. Additional observations, modeling, and experiments are needed to establish a comprehensive interpretative framework for planetary volatile isotopic compositions.

Chapter 5

Conclusions

We have modeled the formation of warm water vapor in protoplanetary disks with a comprehensive model. The radiative transfer of UV continuum and Lyα photons and the associated heating of dust grains are calculated with a Monte Carlo method. The density structure is described in a parameterized manner, and the gas temperature structure is solved based on the balance between heating and cooling mechanisms. The chemical evolution is followed for 1 Myr.

The final step is how to connect chemical compositions of gas and pebbles in disks with the compositions of young planets. This requires a better understanding of disk midplane compositions (see above), but also on how volatiles can be added to planets post-formation. The latter is especially important to predict the water and organic content of temperate, Earth-like planets. It is currently not clear under which conditions Earth-like planets can sample volatiles formed or preserved in outer disk regions, beyond the water snowline. More in-depth cometary studies are key to assess their formation zones, as well as their relationship to terrestrial volatiles. A frontier in the connection between astrochemistry and planet composition regards the carbon content of inner disks; in the ISM, 50% of carbon resides in refractories, which appears preserved in comets, but seems to have been lost in the inner solar system. Depending on the nature of the refractory carbon removal mechanism, terrestrial planets may be generally carbon-poor, and depend on impacts both for water and organic delivery.

Finally, we note that Astrochemistry is an inherently interdisciplinary field. Its past and future successes depend on a combination of astronomical observations, chemical physics laboratory experiments, quantum calculations, molecular dynamics theory, and astrochemical models. We are entering an exciting era where astrochemistry is connecting with planetary and exoplanetary science to explore the formation of planets and the evolution of

their hydrospheres and atmospheres. While the chemistry of planet formation sets the initial conditions of planets, the atmospheric chemistry and geochemistry determines how these initial conditions develop, and how often we may expect the complex chemistry we believe preceded life here on Earth.

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