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Published in:
Laboratory Astrophysics

DOI:
10.1017/S1743921319009153

SESSION 10

Laboratory Astrophysics: from Observations to Interpretation
Proceedings IAU Symposium No. 350, 2019
F. Salama & H. Linnartz, eds.
doi:10.1017/S1743921319009153

Planet forming disks, debris disks and the Solar System

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Abstract. VLT instruments and ALMA with their high spatial resolution have revolutionized in the past five years our view and understanding of how disks turn into planetary systems. This talk will briefly outline our current understanding of the physical processes occurring and chemical composition evolving as these disks turn into debris disks and eventually planetary systems like our own solar system. I will especially focus on the synergy between disk structure/evolution modeling and astrochemical laboratory/theoretical work to highlight the most recent advances, and open questions such as (1) how much of the chemical composition in disks is inherited from molecular clouds, (2) the relevance of snowlines for planet formation, and (3) what is the origin of the gas in debris disks and what can we learn from it. For each of the three, I will outline briefly how the combination of theory/lab astrochemistry, astrophysical models and observations are required to advance our understanding.

Keywords. astrochemistry, planetary systems: protoplanetary disks, comets: general, circumstellar matter

1. Introduction

High spatial resolution and high sensitivity imaging (e.g. ALMA, VLT/SPHERE) of disks around young stars have revolutionized in the past five years our view and understanding of how disks turn into planetary systems. Scattered light and polarized light in near-IR observations show that μm-sized dust remains suspended in the flaring disk surface (e.g. Lagage *et al.* 2006; Avenhaus *et al.* 2018). Thermal emission of mm-sized dust shows that the large grains are settled into a very thin layer in the disk midplane (e.g. Pinte *et al.* 2016). The dust distribution (spatially and in grain sizes) sets the local opacity and hence strongly affects how much radiation enters into the disk (Fig. 1). The $A_{\rm V}$=1 surface (black/white dashed lines) indicate the depth to which optical radiation penetrates the disk.

It is this radiation "leaking" into the disk that is driving the chemistry by setting the gas temperatures, causing photochemistry, photodesorption and processing within ice mantles. In the end, the dust through its opacity determines which molecules/ices reside where and how much ice processing is possible. However, it is the gas pressure that dictates the radial migration, and settling of dust grains (see third moment of the grain size distribution in Fig. 1 for the size sorting) and whether or not dust gets concentrated locally inside pressure maxima (see Birnstiel *et al.* 2016, for a recent review). The resulting spatially dependent gas/dust mass ratio and dust opacities drive changes in the chemical composition. Hence, the interpretation of spatially resolved line and continuum observations often requires a detailed understanding of the intricate ways that gas and dust couple in these planet forming disks. Figure 2 illustrates the various coupling processes that link gas and dust in planet forming disks. One approach to

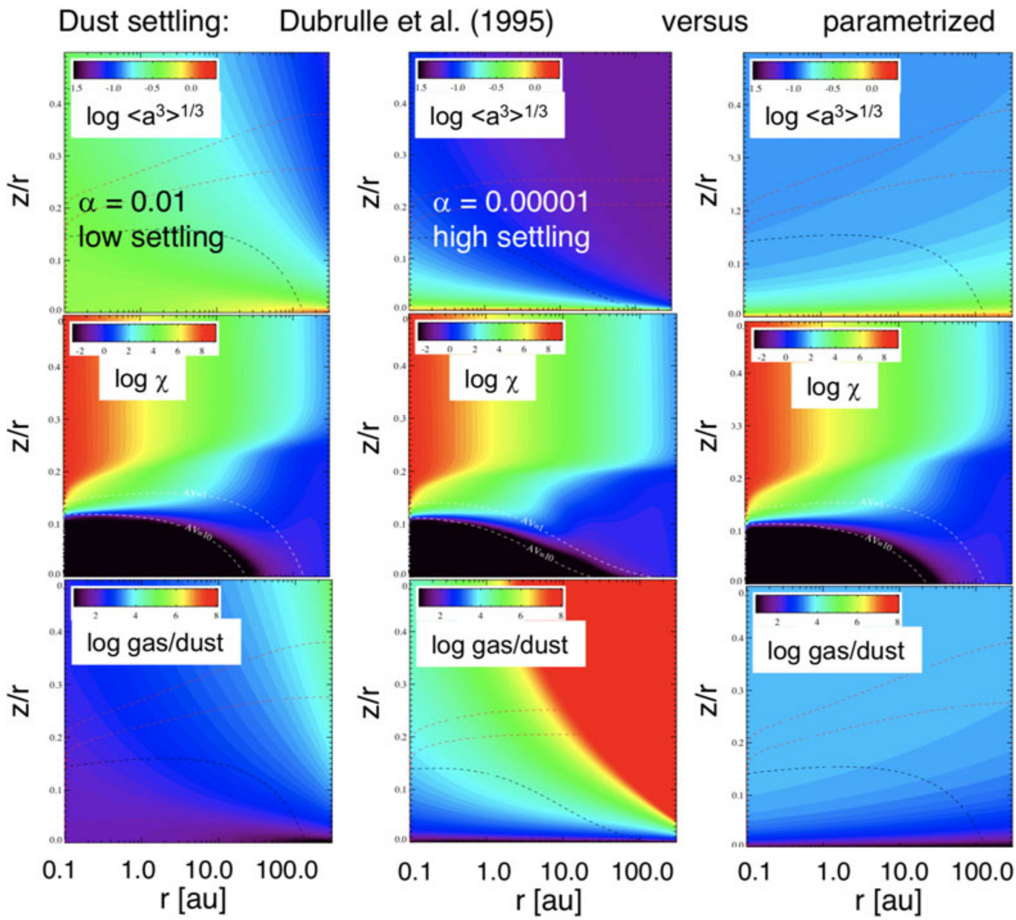

Figure 1. The third moment of the grain size distribution $\langle a^3 \rangle^{1/3}$, the strength of the UV radiation field χ and the dust-to-gas mass ratio in three different ProDiMo (Woitke *et al.* 2009) disk models. Left: dust settling using the Dubrulle *et al.* (1995) prescription with a high turbulence $\alpha{=}10^{-2}$; middle: same with a low turbulence $\alpha{=}10^{-5}$. Right: parametrized settling prescription using a scale height H varying as a function of radius r and grain size a: $H(r,a) \approx H(r)\,(a/1\mu\mathrm{m})^{-1}$. The quantities are extracted from a series of T Tauri disk models from Antonellini *et al.* (2015, 2017).

improve our understanding of those coupling processes is the development of radiation thermo-chemical disk models, i.e. virtual laboratories for planet forming disks.

2. Virtual laboratories for planet forming disks

The need for such virtual laboratories is illustrated by the following example. We learned both from theory and observations that dust grains evolve in the disk over time (see review by Birnstiel *et al.* 2016). Grain growth, destruction, dust settling, and radial transport processes change the local grain size distribution in the disk. Facchini *et al.* (2017) and Greenwood *et al.* (2019) use radiation thermo-chemical disk models to study the impact of this dust evolution on CO sub-mm and mid-IR emission lines in disks. The mid-IR lines of e.g. water, CO_2, HCN, originating from the inner disk ($<$ few au) increase by a factor of a few 100 due to dust evolution within a few Myr (mostly due to an increase in gas-to-dust mass ratio in the surface); yet, CO sub-mm lines originating in the outer disk (beyond 50 au) are hardly affected.

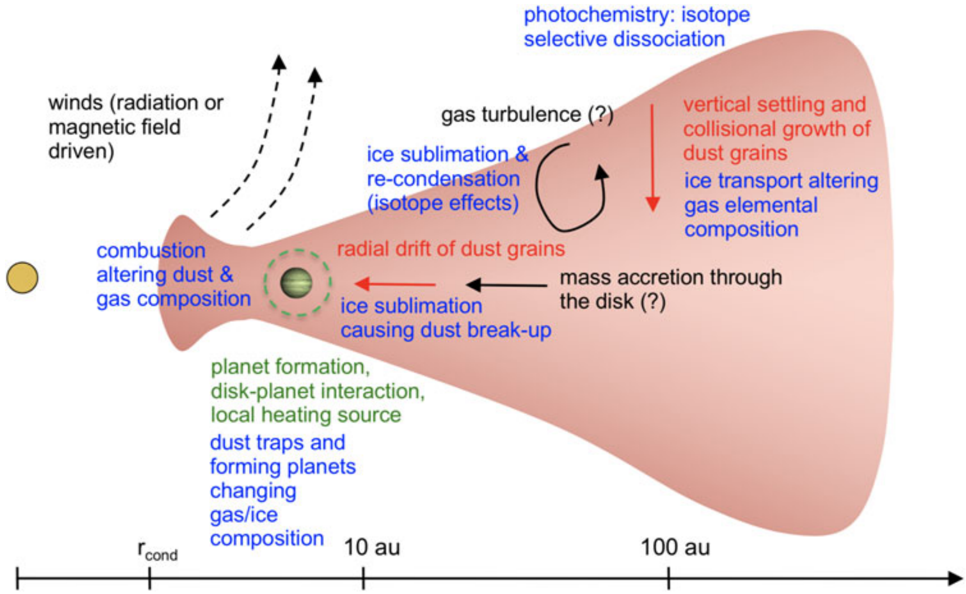

Figure 2. The various coupling processes between gas and dust in planet forming disks displayed in this sketch show that chemistry in an integral part of disk evolution. The color scheme denotes dust (red), gas (black), planets (green) and chemistry (blue).

Thus, a crucial step to infer from observations how planets are forming in disks and how we can link the birth environment to planetary diversity is to link theoretical and laboratory chemistry all the way to astronomical observations. This can be achieved by embedding the chemistry into detailed physical disk structure models that include radiative transfer both for determining the X-ray-to-submm radiation field that permeates the disk and impacts chemical processes as well as for post-processing (ray tracing) to compare directly to observations. Figure 3 illustrates schematically the concept of such virtual laboratories.

3. Synergy of astrochemistry and disk observations

In view of time (space), I present here my personal selection of a few currently debated issues that relate to planet formation and laboratory astrochemistry: (1) How much of the chemical composition in disks is inherited from molecular clouds? (2) Where are the icelines in disks? (3) What is the origin of the gas in debris disks and what does it tell us about planet formation?

3.1. *How much of the chemical composition in disks is inherited from molecular clouds?*

The thermal history of the material forming a disk is very complex. The evolution of young stellar objects proceeds through the collapse of cores to protostars: cloud → pre-stellar core → class 0, I, II and III young stellar object (YSO), where the latter class definitions are based on the slope of the infrared-excess of the YSO (Lada 1987). Class 0 disks are still heavily embedded, while class II disks have barely any remnant cloud material left around them.

Ice mantles start growing in the cloud stage prior to core and disk formation. The ices forming in the molecular cloud phase are likely layered structure with polar water ice underneath a CO rich apolar ice layer (e.g. Bergin *et al.* 2005; Pontoppidan 2006; Öberg *et al.* 2010, polar ices are water rich, non-polar ices are water poor). Grain sizes

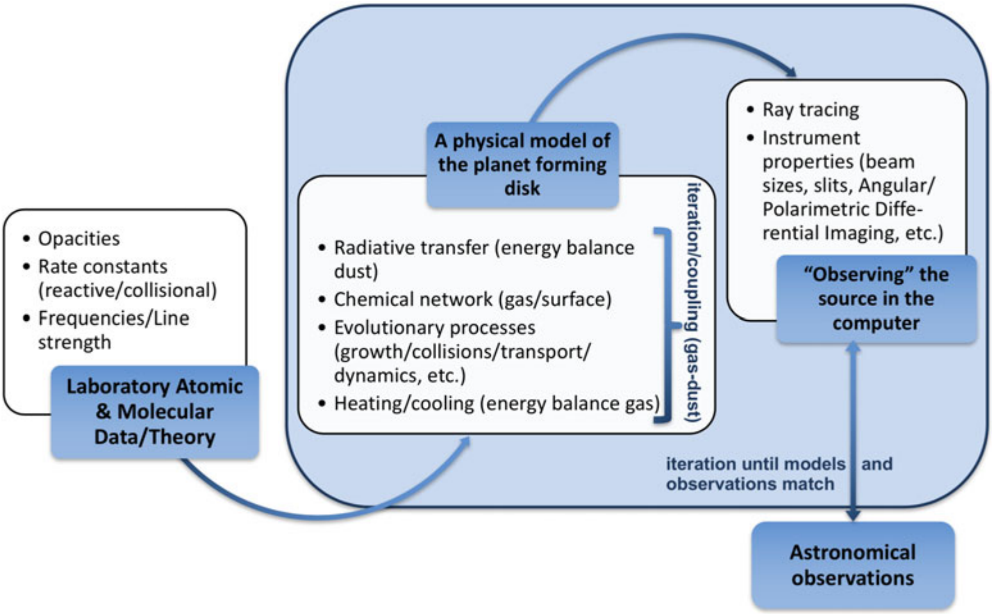

Figure 3. Concept of virtual laboratories for planet forming disks.

can reach at least micrometer sizes in the core phase (e.g. coreshine phenomenon, Pagani *et al.* 2010; Steinacker *et al.* 2015, this process is only sensitive to grain sizes of a few μm). Further processing occurs during the collapse that leads to disk formation (e.g. Chick & Cassen 1997; Visser *et al.* 2009, 2011; Furuya *et al.* 2012; Drozdovskaya *et al.* 2014, 2016, class 0 and I stage). To give an example, methanol ice can be further processed during this phase into more complex organics (Drozdovskaya *et al.* 2016) and the memory of the pre-disk phase is expected to be kept (i.e. ices do not fully sublimate). These chemo-hydrodynamical simulations covered the first 2.5×10^5 yr (mostly class 0 and I stage). However, it remains unclear how much additional processing occurs afterwards in the class II disk stage that can last up to a few Myr; radial and vertical mixing processes as well as photodesorption could play a role. Several works compared comet and class II disk model ice composition (e.g. Chaparro Molano & Kamp 2012; Eistrup *et al.* 2016) neglecting the collapse phase and assuming either atomic (hot start) or molecular cloud (cold start) starting compositions; since the ice composition in the outer disk (beyond 10 au) is neither in thermodynamic equilibrium nor in steady state these initial assumptions play a key role in determining the ice composition at 1 to a few Myr. Deuteration has been explicitly addressed by Mousis *et al.* (2000); Cleeves *et al.* (2014); Furuya & Aikawa (2014); Willacy *et al.* (2015); Taquet *et al.* (2016). Efficient mixing within the disk is required to produce the low D/H observed in comets (Willacy *et al.* 2015). However, Kamp (2019) showed that mixing affects the CH_4/H_2O ratio in disks only beyond 25 au. Such comparisons should be extended to a larger suite of molecules. If comets inherit the composition from the disk, this can help us to constrain the amount of additional chemical processing between the cloud and comet formation phase and possibly also the importance of disk transport processes.

We are only starting to develop a coherent chemical picture all the way from clouds to comets. Many aspects are still discussed and worked at: (1) How much does time variable accretion and episodic outbursts affect the disk composition beyond 10 au? (2) When, where and over which timescale did the comets form? (3) What is the relative contribution of external UV/X-rays, Cosmic Rays (CRs), stellar particles to ionization in disks? How does grain growth/migration affect the chemical composition in disks? What is the relevance of surface processing versus gas phase processes? If ices are indeed layered in small ISM grains, how does this affect the grain growth into the disk phase and how much diffusion occurs inside them?

3.2. *Where are the icelines in disks?*

Icelines are defined as the transition between gas phase and solid; for water, this is often referred to as the snowline. These lines are not sharp transitions/jumps because of the freezing of the first layer (e.g. Marseille & Cazaux 2011), photodesorption, and turbulent mixing (e.g. Ciesla & Cuzzi 2006; Furuya & Aikawa 2014; Krijt *et al.* 2016). These lead to an extended region in which icy and bare grains can co-exist in planet forming disks. Cold photodesorbed water vapour has been observed with Herschel/HIFI confirming that photodesorption is active (e.g. Hogerheijde *et al.* 2011; Podio *et al.* 2013). The CO surface iceline has now been directly imaged with ALMA in the disks around TW Hya (inclination of 7^o) and IM Lup (inclination of 48^o) (Schwarz *et al.* 2016; Pinte *et al.* 2018). In the case of the inclined IM Lup disk, the channel maps can be used to infer a CO temperature at each point. After deprojection, the authors find a radial temperature profile for the upper and lower half of the disk, thus bracketing the ice reservoir in the midplane. The optically thin tracer ^{13}CO for the upper half and the ^{12}CO for the lower half show a temperature plateau of 21 K out to $\sim$300 au. This agrees very well with simulation results using the CO adsorption energy measured in the laboratory (Collings *et al.* 2003; Öberg *et al.* 2005). In addition, the channel maps do indicate residual emission in the cold icy regions, thus providing evidence for an incomplete freeze-out. Also here, cold CO gas emission is traced beyond 300 au, indicating photodesorption from ice largely driven by the interstellar UV radiation field. The penetration of stellar, but also interstellar UV radiation, is determined by the distribution of dust grains and their opacity in the disk. Hence, the quantitative interpretation of the CO data requires a good knowledge of the dust properties in these disks, or if we turn it around, the knowledge of the chemical processes governing the gas phase CO allows us to put constraints on the dust, i.e. settling, and grain sizes.

The location of icelines in disks both radially and vertically, evolves in time and they are determined by thermal and non-thermal desorption processes (e.g. photodesorption, cosmic ray induced desorption). Mass accretion heats the disk midplane and thus affects the radius at which water freezes (Lecar *et al.* 2006; Garaud & Lin 2007); this implies that variable accretion will shift the position of icelines in the midplane. Especially in early stages, accretion can happen episodically leading to large bursts in luminosity (FUors, EXors, for a recent review, see Audard *et al.* 2014), which leads to a warm-up of the disk/envelope; Lee *et al.* (2019) have recently detected abundances of complex organic molecules higher than those in quiescent disks around the FUor star V883 Ori; the enhanced COM abundance could be related to the sublimation of ices during outburst. The dust temperatures and thus iceline positions are also strongly affected by the composition of the dust, i.e. the dust opacity (Mulders *et al.* 2015). Min *et al.* (2011) showed that in the presence of accretion, grain composition and the dust equilibrium temperature become an intertwined problem.

More laboratory work is required to understand the processing of ices in the presence of a complex thermal/collisional history (collisional grain growth, radial migration, and vertical settling inside a disk). Recently, laboratory studies by Dupuy *et al.* (2018); Jiménez-Escobar *et al.* (2018) measured yields for X-ray desorption of water ice; these need to be fully implemented now in astrophysical models to study the relevance of this additional desorption process. Also, more recent laboratory works focusing on wavelength dependent photodesorption and desorption from ice mixtures (e.g. Fayolle *et al.* 2013; Paardekooper *et al.* 2016) need to be studied in the icy reservoirs of disks.

For a detailed comparison with observations, we need optical constants of ices (mixed and/or layers ices) across a wide wavelength range (near âĂŞ far-IR; scattered light/thermal emission); first steps in this direction have been set by Rocha *et al.* (2017) who derived these from experiments in which water containing ices have been processed by cosmic ray analogues. The comparison between observations of ice features and thermo-chemical models will again help to decipher the history of ices in disks, but also their role in the formation of COMs. Future missions such as JWST and the proposed SPICA mission will provide access to the near- to far-IR wavelength regime and provide the sensitivity and resolution to study mixed ices.

3.3. *What is the origin of gas in debris disks, what does it tell us about planet formation?*

Debris disks consist of small μm-sized dust grains that originate from recent collisions. Johan Olofsson covered the nature of these objects in his contribution. I am focusing here only on the gas component and the relevant processes.

The gas composition is thought to reflect the composition of the parent bodies (i.e. hydrogen poor). By studying the chemical composition of the gas, we can learn how much carbonaceous material, $CO+CO_2$ and water ice these bodies contain. The gas is thought to be released either through photodesorption or through collisions (see Kral 2016, for a recent review). However, photodissociation timescales are short ($\sim$100 yr) and the molecular content will thus depend on the balance between production and dissociation/ionization. Kral & Latter (2016) show that these debris disks can have a high ionization degree ($\gtrsim$0.1), potentially leading to Magneto Rotational Instabilities (MRI) in the gas.

Gas studies have been done using ground based spectroscopy (Brandeker et al. 2004), using HST absorption spectroscopy in edge-on debris disks (e.g. Roberge *et al.* 2006), using the Herschel Space Telescope to study the [O I] and [C II] emission lines (e.g. Riviere-Marichalar *et al.* 2012; Roberge *et al.* 2013; Donaldson *et al.* 2013; Cataldi *et al.* 2014; Brandeker *et al.* 2016), and using ALMA to detect CO and [C I] gas emission (e.g. Kóspál *et al.* 2013; Dent *et al.* 2014; Moór *et al.* 2017; Cataldi *et al.* 2018). Recent debris disk models include full non-LTE (e.g. Matrà *et al.* 2015), and viscous spreading of the gas (Kral *et al.* 2019). Cataldi *et al.* (2020) use a consistent modeling approach for CO and its photodissociation products C, C^+, to show that the observations can be inverted to allow timing estimates of the collision event that produced the gas.

These debris disks present a very different astrophysical environment compared to the normal interstellar medium and planet forming disks. The gas is hydrogen poor and highly ionised and the gas emission is likely in non-LTE due to the low densities and strong radiation field of the central star (many debris disks studied in detail with multiple lines are around A-type stars). In such environments, the electrons are likely non-thermal and collision partners other than H, H_2 can become important, such as O, C, or water. Revisiting those collisional rates can help to make the modeling and interpretation of gas observations in debris disks more robust and thus put more stringent constraints on the production mechanism of this gas and the parent body composition.

4. Outlook

Virtual laboratories of astrophysical environments in form of detailed radiation thermo-chemical models provide a key link between laboratory astrochemistry and astronomical

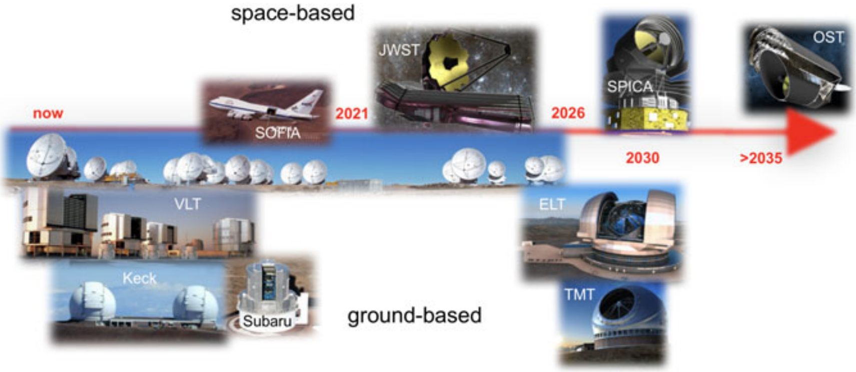

Figure 4. Timeline of existing and upcoming observation facilities that are relevant for astrochemical disk research. The SPace Infrared telescope for Cosmology and Astrophysics (SPICA) is one of the three proposed M5 missions currently under ESA study (joint ESA/JAXA mission); the Origins Space Telescope (OST) has been proposed for the US decadal review. Images show the VLT (Credit: ESO), E-ELT (Credit: ESO/L. Calçada), ALMA (Credit: ALMA (ESO/NAOJ/NRAO)), Subaru (Credit: National Astronomical Observatory of Japan), SOFIA (Credit: DLR), JWST (Credit: NASA/ESA), TMT (Courtesy TMT International Observatory), SPICA (Credit: JAXA/SPICA Team), OST (Credit: NASA/GSFC/Britt Griswold).

observations. They are key elements in the quantitative interpretation of the observations, but can also serve as testbeds to identify the most relevant astrochemical processes that require more in depth studies either from the laboratory or theory side. To maximize the scientific return from existing/future astronomical observatories and missions (Fig. 4), we need all the help we can get from our physical/chemical colleagues.

Ackowledgements

I would like to thank the organizers for their invitation and the Royal Society of Chemistry and the Science and Technology Facility Council for their generosity to support my participation in this meeting. I also thank Wing-Fai Thi for a careful reading of the manuscript.

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