Astrochemistry with *AKARI*: the role of ices in the star formation process

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ABSTRACT

In this procedings I will review the role of ices in the context of understanding the physical and chemical charactersitcs of pre-stellar cores as well as young stellar objects. In particular, I will highlight the importance of *AKARI* observations and how it is hoped that a careful interpretation of such observations can help constraining astrochemical modelling.

Keywords: Astrochemistry; ices; young stellar objects; prestellar cores

1. INTRODUCTION

The interstellar medium (ISM) spans a large range of gas and dust components characterized by densities and temperatures ranging from ~ 100 to > 10^6 cm^{-3} and from 10 to > 100 K, respectively. Of these components, of particular interest are the sites where star formation may take place: these are the clouds where most of the material is molecular and where gravitational instabilities may take place, leading eventually to cores so dense that gravitational collapse dominates. Following Olmi et al. (2016), we define a 'clump' as any compact density enhancement with sizes ranging from 0.1 to 1 pc, and densities of the order of 10^4-10^5 cm^{-3}, while cores as substructures, within clumps, of sizes ~ 0.1 pc and densities of > 10^5 cm^{-3}. Cores are where stars will form. Their temperatures are on average ~ 10 K.

During collapse, gas phase atoms and molecules freeze onto the grains, eventually forming layers of ices which are only fully released when the protostar is formed, due to thermal evaporation. Ices are an ideal place for hydrogenated and complex molecules to form. In particular, by comparing gas phase observations of pre-stellar cores with young stellar objects, we know that most of the water and carbon dioxide in star forming regions is formed in the ices via hydrogenation and oxidation of oxygen and carbon monoxide, respectively (see review by Boogert et al. 2015), during the star formation process. The freeze out and surface reaction processes are a direct function of gas density and temperature which spatially as well as temporally vary. Hence the determination of the relative abundance of the gas versus solid form of the most common species is key in the spatial characterization of star forming regions, as well as their evolution.

2. MEASURING THE DEPLETION FACTOR IN STAR FORMING REGIONS

Freeze-out (or depletion) for a particular molecule depends on a complicated chemistry that varies non-linearly with time and physical environment. The strong dependence of freeze outon the age and physical characteristics of a core makes depletion a useful probe of core history. However, depletion is difficult to quantify observationally. It is common to use gas phase emission from molecules such as CO to infer the fraction of the species that is in the ices: his requires a comparison of gas phase molecular line emission with continuum emission from dust and several assumptions need to be made about the gas and dust. This method has been partially successful (e.g., see Caselli et al. 1999; Redman et al. 2002; Duarte-Cabral et al. 2010). Statistical comparisons of maps of CO in molecular clouds can give clues on how depletion depends on the density and age. For example, Christie et al. (2012) performed a statistical comparison of CO depletion in a set of molecular clouds within the Gould Belt and found that in the gas near protostars the levels of depletion are lower than for starless cores with the exception of very dense cores protostellar cores. Although they found a tentative correlation between core mass and core depletion, uncertainties in their temperatures estimation did not allow them to be quantitative in their characterization of the individual CO depletion factors.

In addition to gas-phase studies, one can directly observe molecules in the solid state using, e.g., the absorption of IR emission from background sources (see reviews by van Dishoeck 2004; Öberg et al. 2011). However such studies are much more limited in scope and areas due to the limited availability of near-infrared measurements.

There are several reasons why determining the degree of depletion of even the most abundant species, such as carbon, oxygen and carbon monoxide, is not trivial. First of all, there are many thermal and non thermal mechanisms that can remove molecules from the ices, even while freeze out dominates. Once the protostar is born, thermal evaporation, due to the warm up of the ices by the protostar, and/or ice sputtering, due to non dissociative shocks, are the main removal

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mechanisms (e.g., Viti et al. 2004, 2011). While there are still uncertainties regarding the efficiency of sputtering or the desorption temperatures at which each molecule sublimates, these processes are fast. However non thermal processing of the ices, which is predominant in cold objects, including prestellar cores, is not well characterized yet: we know that species can 'leave' the mantle due to the following mechanisms: (i) chemical desorption, whereby the formation of molecules causes local heating of the surface; (ii) UV photodesorption, whereby either direct UV or UV photons produced as a result of cosmic rays, will impart energy to the grain surface by dissociation of molecules in the mantle; and (iii) cosmic rays that can ionize or excite molecules as they hit the grains. Roberts et al. (2007) theoretically investigated the sensitivity of chemical models to most of these mechanisms and found that cosmic ray desorption, believed to be the most efficient one, is not always the most dominant mechanism and concluded that more studies into the chemical and physical structures of the dust grains and the physical processes which drive desorption are needed in order to quantitatively determine the role of each mechanism at the different evolutionary stages of the star formation process.

3. THE ROLE OF ICES: TRACERS OF THE CORE EVOLUTION

Given the uncertainties highlighted in the previous section, a comprehensive approach that includes observations and modelling of both the gas phase and the solid phase is needed. Ultimately we can not properly interpret gas phase observations without the knowledge of the time evolution of how the ices form, how they are processed and how they are removed. In the next two subsections I will highlight examples of how useful ices can be in the interpretation of the physical environments of (i) pre-stellar cores as well as (ii) young stellar objects.

3.1. Pre-stellar cores

Pre-stellar cores represent the very early stages of star formation, where the gas accrete towards the centre increasing and decreasing its density and temperature respectively. Submillimeter maps of several gas phase species show a clear chemical inhomogeneity or differentiation across each core (e.g., Ohashi et al. 1999; Williams et al. 1999, see also review by Bergin & Tafalla 2007). One of the most recently studied cores, L1544 in Taurus, is a clear example of a chemical inhomogeneous contracting core. Originally the molecular differentiation in this core was particularly evident when comparing carbon- versus nitrogen-bearing species (e.g., Tafalla et al. 2002; Caselli et al. 2017). However recent studies have shown that this differentiation is not limited to the difference between these two classes of molecules (Spezzano et al. 2016; Jiménez-Serra et al. 2016). Specifically three molecular 'peaks' have been identified: the c-C_3H_2 peak, the methanol peak, and the HNCO peak (see Figure 1 from Spezzano et al. 2017). Each peak 'characterizes' a family of molecules with a different spatial distribution. While attempts at finding chemical links within each family and across families have been made, a thorough comparison with chemical modelling is still missing. In the past it was believed that chemical models were able to accurately predict the composition of pre-stellar cores: after all, these cores are cold and most of the material is frozen on to the grains. However, as explained earlier, we now know that the depletion factor, even for the most abundant species, is not a trivial parameter to determine. Moreover, in recent years observations of complex organic molecules (defined as molecules with at least 6 atoms, and containing carbon atoms) in cold cores (see review by Herbst & van Dishoeck 2009; Caselli & Ceccarelli 2012) have questioned this simple picture: whilst models have tried to solve this puzzle by including non thermal desorption processes, this still does not seem to be enough to maintain the observed abundances in the gas phase. Although alternative hypotheses involving gas-phase reactions have been recently proposed (e.g., Balucani et al. 2015; Rawlings et al. 2013), clearly observations of ices are essential to settle this debate. It is not easy to observe ices in pre-stellar cores. Of partiular importance are the recent observations with *AKARI* (e.g., Noble et al. 2013, 2017) where ices are found to vary across objects, as well as within each core. There is now compelling evidence that the band profile can be used as an evolutionary indicator of both dust and ice mantle properties and that solid species are powerful tracers of 'small-scale' chemical differentiation in pre-stellar cores.

3.2. Young Stellar Objects and Outflows

Once the protostar is born, ices are released back into the gas phase and, as mentioned already, this is mostly due to thermal evaporation and sometimes sputtering if the gas and dust have been shocked. At the very early stages of the YSO, observations of the warm gas can reveal the 'fingerprint' of what was in the ices before the star was born. However, the uncertainties regarding what happens on the grains means that our view of 'history' is riddled with uncertainties. Whilst there is a long history of ices observations before *AKARI*, in particular with the *ISO* and Spitzer satellites (see review by Boogert et al. 2015), it is only with *AKARI* that simultaneous observations of the stretching mode of H_2O, CO_2, and CO can be performed; this together with the possibility of simultaneously being able to observe all objects in the field of view, and its exceptional sensitivity allowed the sampling of different ranges of evolutionary stages (e.g., Aikawa et al. 2012), as well as the possibility to map large fields (Noble et al. 2013). One of the most interesting results from these studies is the correlation between the different ices and the visual extinction, A_V: while both H_2O and CO_2 increase with visual extinction, there is no clear correlation between CO and A_V, possibly a consequence of the fact that CO is only formed in the gas phase and then frozen on to the grains, unlike the other two molecules. Another important conclusion from the *AKARI* observations is related to the relationship among these three species: analysis of their column densities reveal at least a 2-stages CO_2 formation scenario whereby early formation occurs when H_2O forms, while, at a later stage, more CO_2 is formed by energetic routes, when CO has also frozen out.

4. MODELLING OF ICES

Astrochemical models simulate the time evolution and space distribution of molecules in star forming regions. Due to the large range of densities and temperatures present in the interstellar medium, significant changes in the energetics and dynamics of the gas can occur, leading to large variations of molecular abundances. Hence, while chemical simulations provide us with predictions of molecular abundances as a function of the physical conditions, their interpretation is not trivial (although it is often trivialised). In particular, while the gas phase chemistry is reasonably well implemented in all astrochemical models, the approach to surface chemistry varies enormously from model to model: among other problems, there is too much uncertainty regarding surface reactions and their rate coefficients and there are no structured ways to explore the solid phase chemical network, beside performing lengthy laboratory experiments. A new approach to astrochemical modelling is clearly needed and it has been explored in Makrymallis & Viti (2014) and in Makrymallis (2015).

4.1. A statistical approach to Astrochemistry

As larger datasets and more complex models are being employed in astrochemistry, the need for novel methodologies will increase. In Makrymallis & Viti (2014) we showed that a Bayesia Metropolis-Hastings (MH) parameter estimation analysis can help to solve a typical ill-posed inverse astrochemical problem (see Figure 1) whereby a large number of different chemical models may all fit the given observations or, viceversa, a small set of very similar models may give very different fits. In (Makrymallis & Viti 2014) we used a a chemical modelling code and solid-phase observations, together with a Bayesian approach based on a Markov chain Monte Carlo (MCMC) method, to infer the values of the physical and chemical parameters that characterize quiescent regions of molecular clouds and we showed that in high-dimensional problems, MCMC algorithms provide a more efficient and complete solution than more classical strategies.

Ultimately, time-dependent chemical codes are great tools to predict and interpret molecular observations, but their potential to explore large physical and chemical parameter spaces is often not exploited either because of the computational complexity or the complexity of the parameter space. This is particularly limiting for the interpretation and modelling of ices due to the complication of the network, the lack of any prior information and the duration of laboratory experiments. On the other hand, sampling techniques can tackle uncertainty about surface reactions and rate coefficients, and assist laboratory astrochemists by guiding experimental techniques probabilistically.

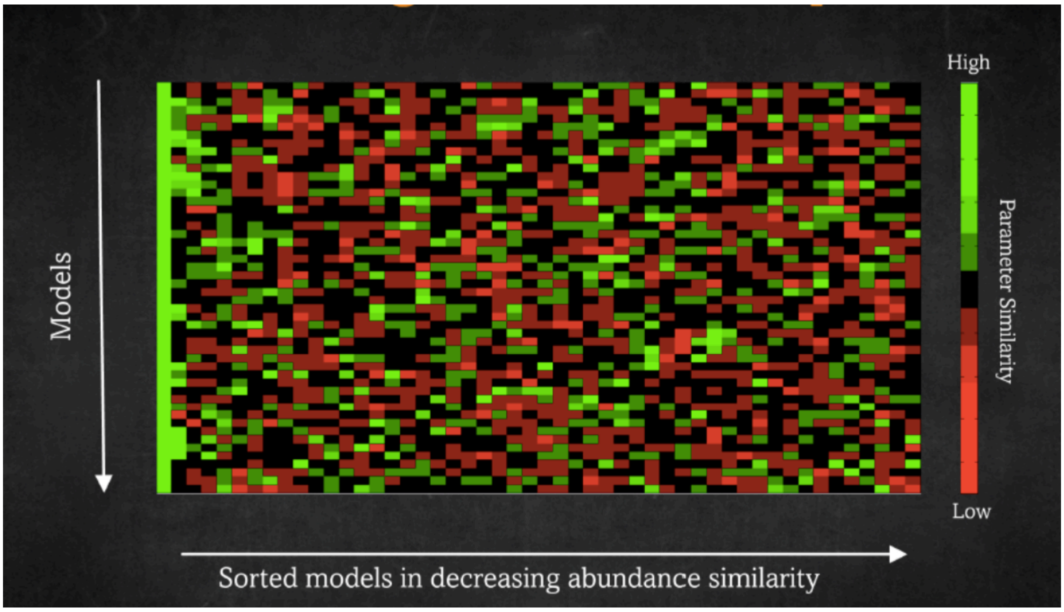

Figure 1. This plot shows the inverse nature of the problems tackled by astrochemical modelling (Makrymallis, private communication)

5. CONCLUSIONS

Molecular data contain information that hold the key to the understanding of the ISM and star forming regions. Synthetic data from chemical codes are a great resource but need to be carefully interpreted, possibly with the use of machine learning and Bayesian techniques. Observational constraints, both gas- and solid-phase, are essential for defining informative priors that can be fed into the models. *AKARI* observations of ices in star forming regions have provided an insight into the chemical diversity and relationship between gas and ices in molecular clouds and Young Stellar Objects.

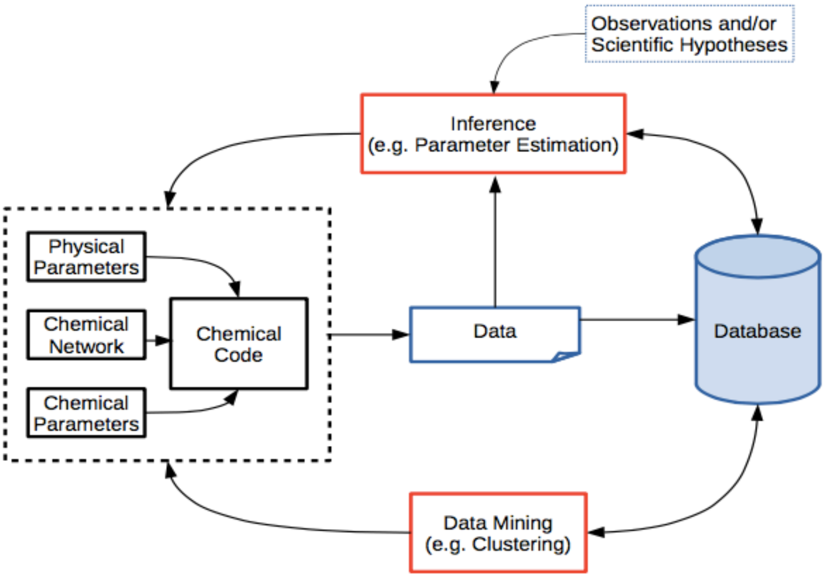

Figure 2. Process diagram of the new approach to astrochemical modelling (from Makrymallis 2015, PhD Thesis)

REFERENCES

Aikawa, Y., Kamuro, D., Sakon, I., et al. 2012, A&A, 538, A57
Balucani, N., Ceccarelli, C., & Taquet, V. 2015, MNRAS, 449, L16
Bergin, E. A., & Tafalla, M. 2007, ARA&A, 45, 339
Boogert, A. C. A., Gerakines, P. A., & Whittet, D. C. B. 2015, ARA&A, 53, 541
Caselli, P., Walmsley, C. M., Tafalla, M., Dore, L., & Myers, P. C. 1999, ApJL, 523, L165
Caselli, P., Bizzocchi, L., Keto, E., et al. 2017, A&A, 603, L1
Caselli, P., & Ceccarelli, C. 2012, A&A Rv, 20, 56
Duarte-Cabral, A., Fuller, G. A., Peretto, N., et al. 2010, A&A, 519, A27
Jiménez-Serra, I., Vasyunin, A. I., Caselli, P., et al. 2016, ApJL, 830, L6
Herbst, E., & van Dishoeck, E. F. 2009, ARA&A, 47, 427
Makrymallis, A., & Viti, S. 2014, ApJ, 794, 45
Makrymallis, A., 2015, PhD Thesis, UCL
Noble, J. A., Fraser, H. J., Aikawa, Y., Pontoppidan, K. M., & Sakon, I. 2013, ApJ, 775, 85
Noble, J. A., Fraser, H. J., Pontoppidan, K. M., & Craigon, A. M. 2017, MNRAS, 467, 4753
Öberg, K. I., Boogert, A. C. A., Pontoppidan, K. M., et al. 2011, ApJ, 740, 109
Ohashi, N., Lee, S. W., Wilner, D. J., & Hayashi, M. 1999, ApJL, 518, L41
Olmi, L., Cunningham, M., Elia, D., & Jones, P. 2016, A&A, 594, A58
Rawlings, J. M. C., Williams, D. A., Viti, S., & Cecchi-Pestellini, C. 2013, MNRAS, 436, L59
Roberts, J. F., Rawlings, J. M. C., Viti, S., & Williams, D. A. 2007, MNRAS, 382, 733
Redman, M. P., Rawlings, J. M. C., Nutter, D. J., Ward-Thompson, D., & Williams, D. A. 2002, MNRAS, 337, L17
Spezzano, S., Bizzocchi, L., Caselli, P., Harju, J., & Brünken, S. 2016, A&A, 592, L11
Spezzano, S., Caselli, P., Bizzocchi, L., Giuliano, B. M., & Lattanzi, V. 2017, A&A, 606, A82
Tafalla, M., Myers, P. C., Caselli, P., Walmsley, C. M., & Comito, C. 2002, ApJ, 569, 815
van Dishoeck, E. F. 2004, ARA&A, 42, 119
Viti, S., Collings, M. P., Dever, J. W., McCoustra, M. R. S., & Williams, D. A. 2004, MNRAS, 354, 1141
Viti, S., Jimenez-Serra, I., Yates, J. A., et al. 2011, ApJL, 740, L3
Williams, J. P., Myers, P. C., Wilner, D. J., & Di Francesco, J. 1999, ApJL, 513, L61