From midplane to planets : the chemical fingerprint of a disk

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ENGLISH SUMMARY

Planets and the search for life in space. Humankind has always wondered about its origin. Where do we come from, and are we alone? The latter question concerns life, and how it can erupt. The only life we know of is life here on our own planet, the Earth. The search for life elsewhere in space is thus a search for planets and exoplanets that have environments that are similar to the life-supporting environment we have on the Earth.

The origin of life on our planet may trace as far back in time as the formation of the Earth itself (there is evidence to suggest that there was life of the Earth already 3.6 billion years ago, with the Earth itself being 4.6 billion years old). Life's ingredients originate from the same material that formed the planet, and hence understanding planet formation and which material forms planets is key to understanding, not only the evolution of the Earth, but also of the life on it.

Planet formation. Planets form around stars, which in turn start forming when large regions of space filled with gas and dust collapse due to the pull of gravity from all the material (see "Prestellar Core" in image 5.11, where gravity pulls all the material in the grey cloud inwards, in the directions of the arrows). The formation of planets is an active field of research in astronomy. It attempts to describe, how the process of forming a star from the gas and dust collapsing under gravity can lead to planets forming out of some of this material around the star (illustrated by all six evolution stages in image 5.11). Understanding the size, movements and composition of the resulting planets requires knowledge of both the physical and chemical processes taking place during the formation process.

These processes are studied in several different ways in astronomical research: through theoretically understanding of the processes and predicting what they will lead to, through astronomical observations of space, and through laboratory experiments on the Earth. In the case of planet formation, theoretically understanding of the physical processes taking place has greatly advanced in recent years. Computer simulations have provided predictions about which types of planets form where. Observations of planets, exoplanets and planet-forming regions, in turn, have constrained these predictions. Laboratory experiments have contributed to understanding the molecules that exist in space, how to detect them, and which chemical reactions can happen between them. This all helps to understand the composition of the material that goes into forming planets.

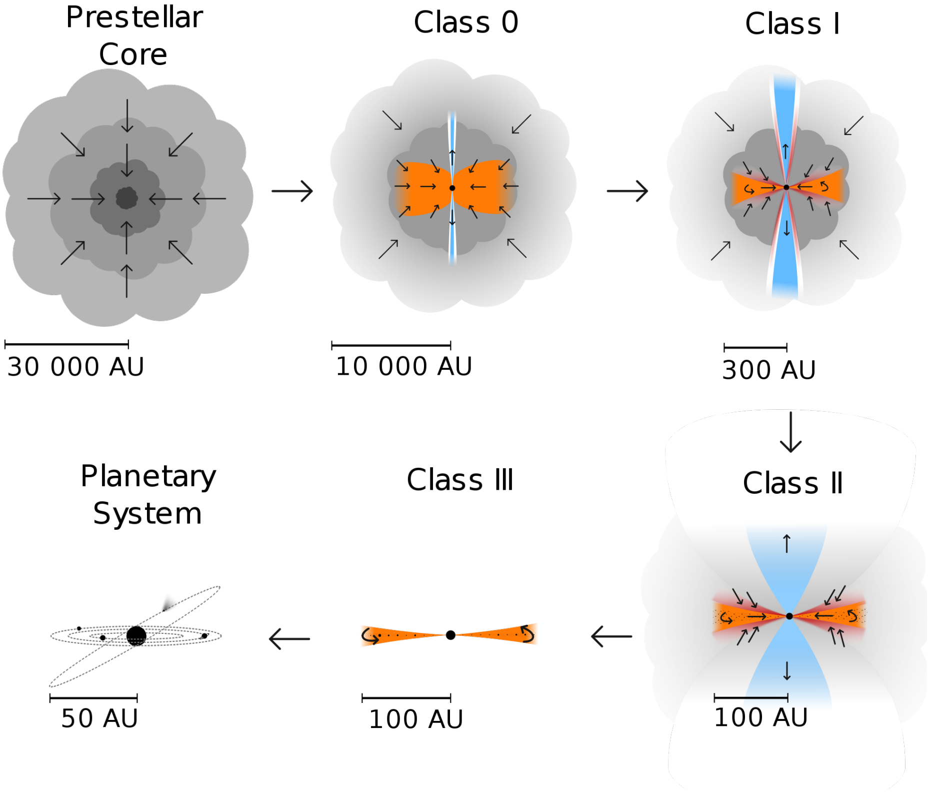

Figure 5.11: Different stages of star and planet formation. The chemical simulations in this thesis focus mostly on classes 2 and 3, but links are made to both the prestellar core, and to the end-product, namely the planetary system. Image credit: "Current view of protostellar evolution" by Dr. Magnus Vilhelm Persson.

Physical and chemical effects during planet formation. The understanding of the physics of planet formation has come far. Alongside that, observations of planet-forming regions, especially with the Atacama Large Millimeter/submillimeter Array-observatory (ALMA) in Chile, have provided a wealth of information on the structure and molecular composition of such regions. ALMA consists of 66 of radio antennas situated at 5000 meters altitude in the driest desert on the Earth. In this environment, ALMA is the best observatory in the world for observing electromagnetic radiation at wavelenghts around 1 millimeter. This makes ALMA optimal for many observations, including observing regions of star and planet formation, and also for detecting signatures of specific molecules in these regions. Amongst other, several so-called icelines have been detected using ALMA. An iceline is the radius in a planet-forming region inside of which it is close enough to the star to be warm enough for a molecule (e.g. carbon monoxide) to be in the gas-phase, but outside of which it is so cold that the molecule exists as ice on the surfaces of dust grains. However, the theoretical understanding of the chemical processes taking place during planet formation, especially in the planet-forming regions before planets start forming, are less well-understood. Chemical reactions between molecules are likely to happen, both in the gas, and when the molecules are in the ice-phase on the surfaces of small grains of dust.

This thesis attempts to understand how chemical reactions in the material that forms planets changes this material over time. How the amounts of different common molecules change over time, and how much material, in particular how much carbon and oxygen, is in the gas and ice-phases, respectively, when planets start forming. Since planet formation models thus far have considered only unchanging chemical compositions of this material, or somewhat simplified chemistry, the goal of this thesis is to explore the trends in which chemical changes occur in planet-forming material before planets start forming. The results could potentially be useful, both for research in planet formation, but also for understanding the presence of certain molecules in the atmospheres of planets and exoplanets, and on comets. These molecules all tell stories about formation and evolution of these planets and comets, and the results here could be used to connect the planets and comets that are observed today to where and how they were formed.

Chapter 2 makes use of a computer code (the BADASS code) that can simulate chemical reactions in space. The code is given information about the physical environment found in planet-forming regions, such as temperature, density, and the level of ionisation (the amount of new ions created from neutral atoms or molecules reacting with energetic cosmic ray particles per second). The code is set to either only simulate chemical reactions in the gas-phase, or to also account for reactions taking place between molecules in the ice-phase on the surfaces of grains of dust. The code simulates an astronomical timescale of 1 million years. The timescale from the beginning of star formation and until the star and surrounding planets are all formed is estimated to be around 10 million years. The question is: will chemical reactions change the composition of the material over time?

It is found there are no significant chemical changes seen to the material only, when the ionisation level is low, and the simulations start off with neutral molecules. Significant changes are seen for all other setups of the simulation,

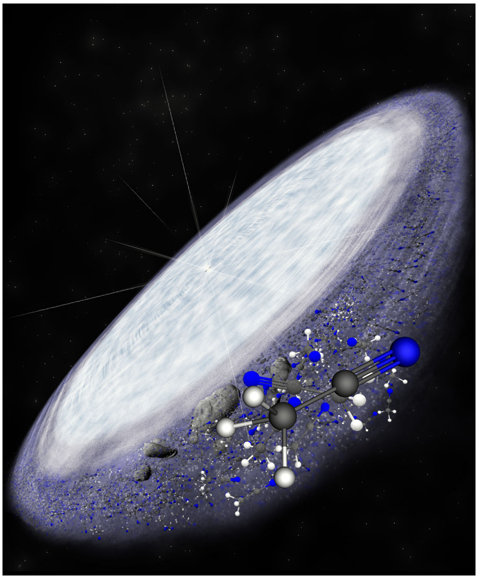

Figure 5.12: A star forming in the middle of a disk of molecules and dust grains (the latter may may appear as rocks). The molecules can react with each other, both in the gas-phase, and when frozen out as ices on the surfaces of the dust grains. Image credit: B. Saxton (NRAO/AUI/NSF).

and both chemical reactions on the surfaces of the dust grains, and the level of ionisation show important effects.

Chapter 3 is an expansion of the simulation setup in Chapter 2. A longer astronomical timescale is assumed (7 millions years), and the physical conditions, such as the temperature, are assumed to evolve (it gets colder) during the 7 million years, whereas in Chapter 2 they were kept static. Taking a changing physical environment into account does complicate the calculations, but this is a more realistic scenario, as not just the chemistry, but also the physical environment in the planet-forming region changes over time.

It is found that chemical evolution changes the chemical composition of the planet-forming material continuously up until at least 7 million year. The evolving physical conditions do not cause much different effects from the static conditions from Chapter 2, except that when the temperature decreases with time, then more molecules will become ices on dust grain. Only close to the star, where it is warm enough, will most molecules be in the gas-phase. It also turns out that the chemical composition of the material by 7 million years of evolution has evolved towards a steady state in which the composition is independent of what chemical composition (purely atoms or purely stable molecules) the simulation starts out with. This steady state chemical composition, in turn, is found to be very different than the typical compositions assumed in traditional planet formation models with a more simple treatment of chemistry.

The idea for **Chapter 4** is triggered by the detection of large amounts of molecular O_2 ice in comets 1P and 67P in the Solar System, and the fact that the simulations in Chapter 2 (for certain model setups) shows that O_2 ice is produced in similar amounts as those detected in the comets. In this chapter it is investigated how and under which conditions O_2 ice can be produced on the surfaces of dust grains in the region where comets formed at the time, when our Solar System was still under construction. Several chemical parameters for how reactions between ice molecules take place were explored, and O_3 ice is included into the chemical code, which is not included in Chapter 2.

The results show that after including O_3 ice into the code, O_3 ice, and not O_2 ice is produced in large amounts, which does not match with the detected amounts of those molecules in the two comets. It turns out that the results from the code only agree with the comet detections for a very specific simulation setup, and it is therefore more likely that the O_2 ice was already there in the comet-forming region around the Sun, before chemical reactions took place there, instead of being produced by these reactions. However, chemical reactions on the surfaces of dust grains are less well-understood than reactions in the gas-phase, and the chemical interactions between O_2 ice, O_3 ice and some other chemically related atoms and molecules may need to be understood better before ruling out that that the O_2 ice could have been produced via chemical reaction on the surfaces of the grains, leading to the detected amounts in the comets.

Chapter 5 continues in the cometary track. Chapter 3 provides simulated amounts of many different icy molecules both as a function of astronomical evolution time, and as a function of distance (radius) from the star. The idea is to statistically match these relative amounts of each icy molecule to the amounts of each molecule detected in different comets. Such data on the amounts of each molecule in different comets are available in the scientific literature. A χ^2-method is used for this statistical comparison. The goal is to check if this investigation, using the molecular amounts of several different icy molecules, both detected and simulated, would will result in pointing out where in the planet -and comet-forming region around the Sun the comets were most likely to have formed.

Using a set of 15 different comets with detected amounts of various icy molecules, this statistical analysis points to 14 of the comets to likely have formed in the vicinity of the iceline of carbon monoxide (CO), although probably at different times during the evolution of the Solar System. This method showcases a possible new way of categorising comets: instead of categorising them directly based on the amounts of each molecule that are detected in them, this new method takes into account the chemical changes that can happen to the material during the evolution of the Solar System, and the new method shows that 14 out of 15 comets may have formed around the same iceline, although at different times.

Main conclusions drawn from this thesis:

- Chemical evolution in planet -and comet-forming regions can change the chemical composition of its material significantly over time. Ionisation of this material, as well as chemical reactions between molecules in the ice-phase, are both important factors contributing to the chemical evoution. The evolution may influence the chemical compositions of the planet, exoplanets and comets, that form. Models that simulate planet formation and composition would therefore benefit from incorporating better treatments of chemical reactions in planet-forming material.

- The amount of O_2 ice detected in comets 1P and 67P remains best explained by the O_2 ice having formed before the chemical simulations were run. That is to say, the O_2 ice was most likely already present, before the Solar System started forming.
- Chemical evolution models can be used to speak about the formation histories of, not only planet, but also comets. With a statistical comparison between detected molecules in comets in the Solar System, and simulated amounts of molecules in a comet-forming region, almost all the investigated comets show likely formation around the CO iceline.
- Chemical reactions between icy molecules on the surfaces of dust grains play an important role in changing the chemical composition of material in regions of planet formation. However, these reactions are less well-understood than reactions in the gas-phase. Future laboratory experiments on the Earth will help to better understand these reactions, and this improved understanding will be valuable in codes simulating chemical evolution in space.