

The dance of elements in space: from clouds to planets, from atoms to life

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Abstract / Resumen / Résumé

This article follows the dance of the atoms created in the interiors of the stars, as they bind together and form molecules of increasing complexity while a star and a planetary system like our Solar System form. From a diffuse cloud and free-floating atoms, this process took about 4.5 billions years to shape the Solar System, and ended up with the most complex molecular structure in the Universe that we know: life.

Este artículo describe el camino recorrido por los átomos creados en el interior de las estrellas, que uniéndose entre sí forman moléculas cada vez más complejas a medida que una estrella como el sol y su sistema planetario se forman. Empezando por una mera nube de gas difuso compuesto por átomos flotantes, han hecho falta 4500 millones de años para construir el Sistema Solar, culminando con la más compleja estructura molecular conocida en el Universo: la vida.

Cet article décrit le chemin suivi par les atomes créés dans l'intérieur des étoiles, et comment ils se réunissent pour former des molécules plus complexes au fur et mesure qu'une étoile comme le soleil et son système planétaire se forment. En commençant par un simple nuage de gaz diffus composé d'atomes flottants, 4.5 milliards d'années ont été requis pour construire le système solaire, aboutissant à la structure moléculaire plus complexe connue dans l'univers: la vie.

Key Words / Palabras clave / Mots-clé

Star formation, molecules, life

Formación estelar, moléculas, vida

Formation stellaire, molécules, vie

The beginning

All started with the Big Bang. After a few minutes, the simplest and lightest atoms were created: hydrogen and

helium with a sparkling of lithium and beryllium. The Universe could have remained as such, a place with no chemistry and no life, were it not that a first star was born. A big star, not one as the many that surround us today, but much bigger than that. She lived little but shone as no other star today, and then exploded ejecting into space the jewels formed in her interior, the first heavy atoms. That was enough. Like an immense domino, this started the birth of other stars that formed other heavy elements, and triggered a whole new generation of stars. While stars burned more and more elements, matter organized itself in galaxies, clusters of galaxies, super-clusters of galaxies: our Universe as we see it today.

The vast majority of the material composing the current Universe is constituted by hydrogen (and some helium) atoms and a few, in number only 1/thousands, heavier atoms: oxygen, carbon, nitrogen, sulfur, silicon, iron... Most of matter in our Galaxy is in stars, but a good fraction, estimated to be around 10-20%, remains in a diffuse, gaseous state, forming atomic or molecular clouds, depending on the state of the H atoms. Some heavy elements, oxygen and carbon, remain prevalently in the gaseous state. Others, like silicon and iron, are mostly condensed into little solid particles, very similar to the sand of our beaches, but thousands of times smaller, namely with sub-micron sizes. Astronomers call them interstellar dust grains. They are only 1/100 in terms of mass with respect to the gas, but they have a huge role for many reasons, some of which will be mentioned in this chapter.

In this ever changing Universe, 4.5 billions years ago, a little star was born, our Sun. Before that, it was a small cloud dispersed in the Milky Way, where atoms floated

free. Until something suddenly happened, maybe the cloud bumped into another cloud or one of the many nearby stars exploded and compressed it. We still don't know for sure what happened, but the small cloud started to collapse. At first, matter slowly accumulated toward the center and then, when the gravitational force was too strong to be resisted, matter started raining on the nascent star, feeding it with new material. Like an ice-skate dancer pirouetting first arms fully extended and then folded, slowly rotating matter falling from a region more than tens of thousands of times the distance Sun-Earth (which is called AU for Astronomical Unit) acquired a huge centrifugal velocity when it approached the nascent Sun. Then, instead of falling directly toward the center, matter formed a disk perpendicular to the rotation axis, from where the vast majority either fell inwards or was expelled outwards in supersonic jets. Some of what remained rotating around the newborn Sun eventually formed the planets. The leftovers became comets and asteroids, some fragments of which reach the Earth and are then called meteorites.

From the moment the cloud started collapsing to the birth of the Earth probably a few tens of million years passed. A ridiculously tiny fraction with respect to the Solar System life, four and half billion years. A tiny fraction of time during which atoms combined together in molecules and complex molecular structures: as tiny as it was, it was of enormous importance because this was the period that paved the road to life.

From a cloud to a planet, from an atom to a molecule

The formation of the Sun went hand in hand with the increase of the chemical complexity. We know that because we can see and study stars like our Sun that are forming today. We observe them in various stages, like when we are in a forest and see trees of all ages. By observing the young and the old trees, we can reconstruct the likely life of each single tree. The same happens with stars. Actually, when they are young they do not burn hydrogen in their interiors yet, and we call them protostars. By observing protostars in the various stages, we reconstruct what likely was the birth and youth of the Solar System.

We think that the whole process can be represented by five major phases, sketched in Figure 1: 1) Pre-stellar cores, 2) Protostars, 3) Protoplanetary disks, 4) Planetesimal formation, 5) Planet formation.

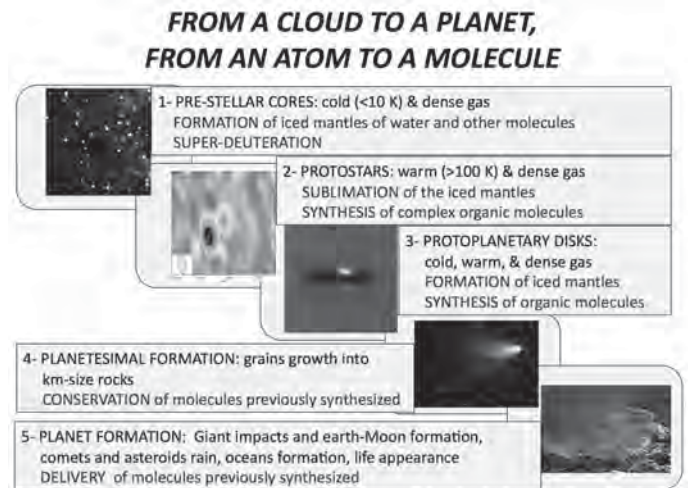


Figure 1: Sketch of the five major phases of the formation of the Solar System.

The following sections will briefly describe what we know about each phase, with emphasis on the dance that occurred between the elements, namely the chemistry.

Phase 1: Pre-stellar cores

Pre-stellar cores are the objects that represent the first step toward the formation of the Solar System. On the sky, they are “boring” black spots like the one shown in Figure 2. When astronomers discovered the first pre-stellar cores, they thought that they were locations of the Galaxy void of matter. Obviously, they were wrong. Indeed, those black spots are the seeds of the Galaxy, where Sun-like stars sprout. And like seeds, they contain in germ how matter will evolve, what it will become: a star like our Sun with few or plenty of planets, or a larger and brighter star that will shine intensely for a short time and will die in gigantic fireworks, or a smaller star that will live longer with less glamour...

In practice, pre-stellar cores are clumps of cold and dense material. Their central temperature is lower than -360°C ($<12\text{ K}$) and their central density is about 1 million

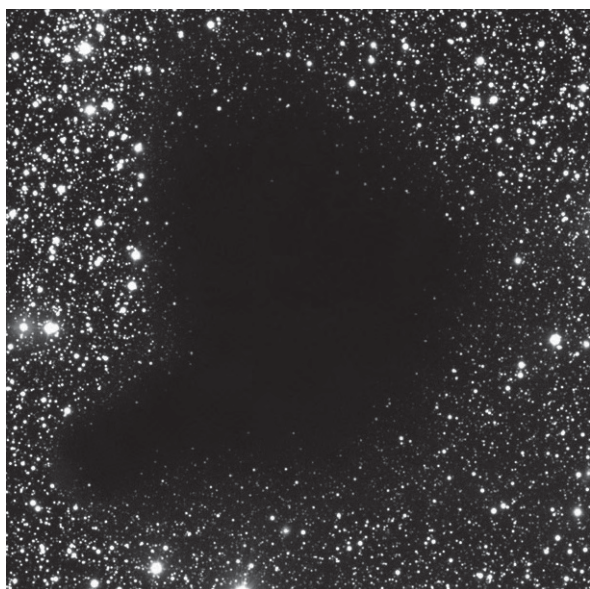


Figure 2: Picture of the pre-stellar core B68. The cold and dense material of the pre-stellar core absorbs the light emitted by the background stars, so that it appears as a black spot in the visible.

particles per cubic centimeter (10^6 pp/cm³), namely more than a thousand times the density of the initial cloud. For terrestrial standards, this is still the void, but when 10^5 - 10^6 pp/cm³ occupy thousands of AUs this makes more than the equivalent of the mass of the Sun, and a huge wall for the light behind to cross.

Indeed, pre-stellar cores are black spots in the sky because they do not shine –too cold for that– but, instead, their dust intercepts the light from the background stars.

During the pre-stellar core phase, matter slowly accumulates toward the cold and dense center. This causes the first two steps towards the molecular complexity to occur. First, when the atoms and molecules of the gas hit the dust grains, they remain stuck onto them. This is like a storm of little mosquitoes –the atoms and molecules of the gas– hitting an elephant –the dust grain. If the elephant skin is sticky, the mosquitoes remain glued. In the case of the grain, it is so cold that any atom or molecule hitting it remains frozen. The only exceptions are the atoms of hydrogen, which stay stuck on the grains for a short time only. During this short stay, they move on the grain surface, wandering around. Sometimes, an H-atom encounters a frozen atom or molecule and, if it is the right one,

reacts with it forming a new molecule. Two important examples are the reactions with the frozen O-atoms and CO molecules. In the first case, the final product is water, H₂O, a molecule of paramount importance for the terrestrial life (see the article by Podio & Codella, for more details). In the second case, the reactions lead to the formation of two organic molecules: formaldehyde, H₂CO, and methanol, CH₃OH. We will see in the next section, why these two molecules are so important in the way to the molecular complexity. Other important hydrogenated species formed during the pre-stellar core phase are methane, CH₄, and ethene, C₂H₄, which also have an important role in the interstellar organic chemistry.

Another important event occurs during the pre-stellar core phase. The dense and cold conditions cause a very peculiar phenomenon, called “super-deuteration”. Briefly, H-containing molecules become enriched of deuterium¹ atoms, which take the place of the H. In the Universe, there are about 150,000 atoms of H for every one of D. From a chemical point of view, hydrogen and deuterium have exactly the same role, governed by the only electron they have. Therefore, in “normal conditions”, molecules containing one H would have 1/150,000 of them containing one D. But when the gas is very cold, as in the pre-stellar cores, this equilibrium is broken and many more molecules contain deuterium instead. It can go up to 50%, in extreme cases, for example methanol. Mind, this does not mean that new deuterium is created, it just means that D atoms remain more easily attached to molecules than H atoms. Although, as said, this does not have a direct implication on the chemistry, this super-deuteration has a huge diagnostic power, as these “deuterated” molecules bring with them the unambiguous imprint that they were formed in very cold conditions. In other words, molecular deuteration is like the silver halide crystals in photographic films, it fixes images.

In summary, during the pre-stellar core phase, the dust grains become enveloped by mantles of iced molecules, in majority water, for the simple reason that hydrogen and oxygen are the most abundant reactive elements in the Galaxy. Inside the water ice, other hydrogenated species, like

¹ Deuterium is the heavy isotope of hydrogen, namely its nucleus is constituted by one neutron and one proton.

formaldehyde, methanol, methane and ethene, are trapped. These molecules, as water, are highly enriched in deuterium. Everything occurs slowly and smoothly, over a long time, maybe one million years. Indeed, some astronomers call the pre-stellar core phase “the calm before the storm”. As the pre-stellar cores are the seeds of the stars, the hydrogenated species are the seeds of increasingly complex organic molecules.

The process is in route... let's see what happens next.

Phase 2: Protostars

When enough material has been accumulated in the central zone of the pre-stellar core, the gravitational force wins against the pressure and whatever other mechanism may have contrasted it, turbulence, magnetic fields... Nothing can prevent the storm to begin! Matter from the whole core rains freely towards the center, forming first a dense object that will, at the end of the process, become a star. A good fraction of the falling material doesn't reach the center but it is violently expelled toward the interstellar space at supersonic velocities, causing shocks all around and, eventually, even disrupting the molecular cloud where the star formed. Most of the matter, though, joins the central hundred AUs zone, which in the case of the Solar System is called Solar Nebula.

At this stage, the material around the central object, the future star, is called the envelope of the protostar. This envelope, which is what before was called pre-stellar core, contains material more than enough to form one star like the Sun. At the beginning of the process, it is cold and dense. As pre-stellar cores, therefore, protostars are black spots in the photographic plates. The only difference is that, often, they lie in regions where other stars are just born, sometimes bright stars that illuminate the whole region creating among the most beautiful pictures of our Galaxy, as the one shown in Figure 3.

Anyway, things are doomed to change quickly, on scales of a few hundred thousand years. This is because the material coming from the external zones of the envelope, namely from thousands of AUs, has to release the gravitational energy that it possesses before stopping and being



Figure 3: Picture of the star forming region Orion, as seen by the European satellite Herschel in the Far Infra-Red (http://www.esa.int/Our_Activities/Space_Science/Embracing_Orion).

part of the central future star. This gravitational energy is converted, in one way or another, into photons that warm up the envelope material. The innermost regions are the hottest, for they are closer to the energy source, while the border of the envelope remains as cold as in a pre-stellar core. Not surprisingly, this has important consequences on the chemical composition of the gas.

First, the warming up of the dust causes the iced mantles to sublime. Indeed, at the densities of the inner zones, a few

10^8 pp/cm³, it is enough that the temperature reaches -272 °C, namely about 100 K, to make the water ice change from ice to gas –remember, the liquid water phase occurs only in a very small interval of pressure and temperature, the one found on the Earth but almost nowhere else in the Universe (see the chapter by Guedel). Therefore, in the inner regions of the protostar envelope, where the temperature is more than 100 K, all the molecules that were formed during the pre-stellar core phase are injected into the gas by the sudden sublimation of the dust grain mantles. How do we know that? Remember what we said about the super-deuteration phenomenon in the pre-stellar phase? This is how we know it, we observe highly deuterated molecules in warm gas, certainly a record of the previous phase.

These zones where the icy mantles sublimate are called “hot corinos” if the future star will be like the Sun, and “hot cores” if it will be much bigger. Let’s focus on the hot corinos, as here we want to reconstruct the youth of the Sun.

Hot corinos have deserved a specific name because they are extremely interesting when it comes to the chemical complexity in space. These objects, indeed, contain a zoo of complex organic molecules, which we also find on Earth: methyl formate (HCOOCH₃: the simplest example of esters, it is used in insecticides, old refrigerators and pharmaceutical products), dimethyl ether (CH₃OCH₃: at present heavily studied because it could be a non-polluting fuel substituting, for example, diesel), formic acid (HCOOH: it owns its name to the fact that it was first discovered in the venom of some ants), acetaldehyde (CH₃HCO: it occurs naturally in coffee, bread, and ripe fruit), just to mention a few examples.

But mind, the abundances of these molecules are very small, never exceeding one over about one million with respect to hydrogen –remember, there is a very little amount of available carbon and oxygen in the Galaxy. In fact, these molecules are called “trace molecules”. Nonetheless, when one considers the total amount of organic molecules in an envelope of about one solar mass, it adds up to the amount of material that makes the Moon!

The obvious questions are: what are the most complex molecules that have been detected so far? Any really biotic or pre-biotic molecule? Any aminoacid?....

Let’s try to give some answers.

The longest molecule so far discovered is the cyanodecapentayne, HC₁₁N, a chain of eleven carbons with one atom of nitrogen and another of hydrogen at the two extremities. It belongs to the family of the cyanopolynes, a family of molecules very difficult to reproduce in terrestrial laboratories because they are very unstable, but easily formed in interstellar clouds! These molecules may have had a role in the synthesis of some biotic molecules, for example pyrimidines (key components of nucleic acids), in the very young Earth.

Among the complex organic molecules with a prebiotic value discovered so far are glycolaldehyde (HOCH₂CHO: the simplest sugar), amino acetonitrile (NH₂CH₂CN: it can be hydrolyzed into the simplest amino acid, glycine), urea ((NH₂)₂CO: discovered more than two centuries ago in human urines). We should mention also the case of a smaller molecule, formamide (NH₂HCO), which may have had a primordial role in synthesizing both metabolic and genetic molecules, according to some experts. This molecule is found in (relatively!) large quantities, namely up to about the mass of the Moon, in the envelopes of solar type protostars. Of course, whether it really had a role in the appearance of life on Earth is a whole different story.

The point we want to make here is that complex chemical reactions occur in hot corinos that lead to the synthesis of complex organic molecules. We do not know yet exactly how this happens, what are the exact pathways that lead to these molecules. We have theories, which we try to verify on Earth with laboratory experiments and complex computations involving quantum chemistry. But we haven’t a complete and solid theory yet. What we know is that, very likely, the answer to the question what are the most complex molecules synthesized in the interstellar medium will come once we have fully understood how these molecules are formed rather than observing them... because we will always be limited by the telescopes used to detect these molecules, while a good theory can predict also what we cannot detect for years to come: the Higgs boson teaches!

Phase 3: Protoplanetary disks

Matter continues to rain on the future star, to be expelled with violence, to plan into the disk rotating around the future star. As time passes the envelope becomes thinner and thinner, until only the disk and the newborn star remain (see Figure 4). Matter continues to be transferred from the disk to the star and to swell it, but at a rate hundred times smaller than during the protostellar phase. It will take some ten millions years to finish the process.

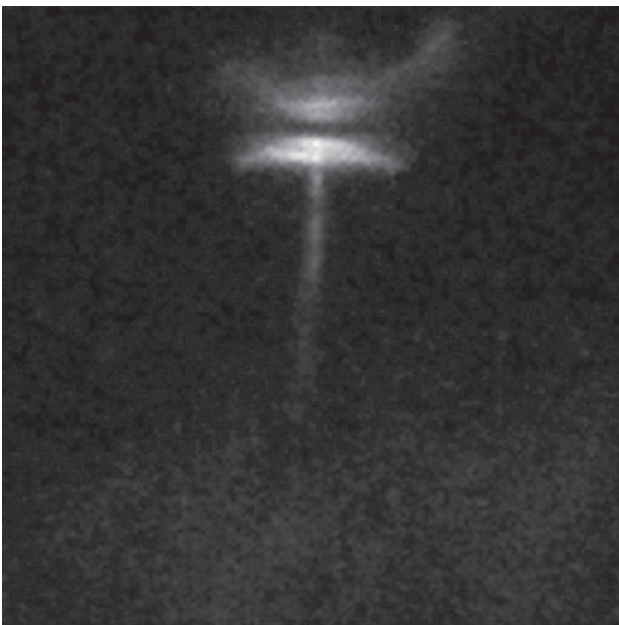


Figure 4: Picture of the protoplanetary disk HH30. The disk is only indirectly observable as the black band in between the two nebulosities, which are due to the light emitted by the star, obscured by the disk itself, and scattered by the disk dust.

The two lines perpendicular to the disk show a jet of material expelled at supersonic velocities.

The star at this stage is “big” enough to burn some fuel at its interior, not yet hydrogen but only deuterium, the heavier form of hydrogen. Yet, this is what makes it finally shine in the sky. Its light is irregular, it goes up and down as on a roller coaster, and all sorts of violent processes occur close to the star surface. For example, a large fraction, up to 10%, of photons are emitted in the X-rays, namely more than ten thousand times the Sun today! These moody stars are often called “T Tauri stars” in honor of the first member of this class of objects discovered more than 150 years ago by an asteroid hunter.

The disks also have a specific name, they are called “protoplanetary” because we believe that planets are formed there. In other words, protoplanetary disks are the nurseries of planets. Needless to say, what happens to the chemical composition of matter during this phase is of paramount importance. But we do not know much, as observations of these objects have been extremely difficult in the past. We can, however, partially complement what we know for sure with what we have learned from the pre-stellar and protostellar phases, for reasons that will become apparent in the next few lines.

We know that, at the beginning, the disk is composed of the same material that made up the protostar envelope, and, more specifically, the hot corino: H_2 gas with a sprinkle of other molecules, and dust, about one hundred times less in mass than the gas. The temperature and density gradients across the disk plane and surface are extreme. The density increases going inward and from the surface to the plane of the disk. In the “planet forming” zone, the density reaches 10^{10} - 10^{12} pp/cm³, whereas on the disk surface and far from the star the gas is rarefied, with densities smaller than 10^2 pp/cm³. The situation is not very different in temperature. At the surface of the disk, which is exposed to the immediate irradiation (from X-rays to optical) from the star, the temperature can reach 1000 K. No molecule survives to the UV photons in those regions. On the disk plane close to the star, in planet forming regions, the matter is still warm, a few hundred K, and the conditions are similar to those in hot corinos, also from a chemical point of view. On the contrary, far away from the star and the disk surface matter is very cold, like in pre-stellar cores, both in terms of temperature and chemistry.

The radius at which the dust icy mantles sublimate, namely around 100 K, has a profound importance in the evolution of the disk and it is called, not surprisingly, the “snow line”. Inward the snow line an active organic chemistry takes place, whereas outward, especially beyond the radius where also CO remain frozen onto the grain surfaces, the chemistry is dominated by the hydrogenation of the molecules trapped in the grain mantles, and the phenomenon of the super-deuteration occurs again.

Both zones are important, because both leave an imprint in the nascent planetary system. On the one hand, the warm

zone will leave organic molecules ready to be used in the next step of the evolution. On the other hand, molecules will have the imprint of the enhanced molecular deuteration, a heritage difficult to hide.

Phase 4: Planetesimal formation

As we just saw, at the beginning, protoplanetary disks contain one hundred times more gas than dust. Yet, after a few million years, the situation is inverted: there is almost no gas left in the disk, only dust. Such disks are called “debris disks”, and a beautiful example is shown in Figure 5. Also the Solar System possesses some dust in the ecliptic plane, even though this is likely due to the continuum replenishment from fragments of comets of the Kuiper belt, beyond Neptune. By the way, this dust is responsible for the faint glow called “zodiacal light”, visible in the dark nights with no Moon and no pollution...



Figure 5: Picture of the debris disk Fomalhaut, as observed by the European satellite Herschel in the Far Infra-Red.

How did the situation change so drastically? What happened to the gaseous disk?

Two major processes take place in this fourth phase. First, the gas is either trapped in giant gaseous planets, like Jupiter and Saturn in the Solar System, or it is dispersed by

the pressure of the photons emitted by the newborn star. Second, the initially sub-micron dust grains coagulate into larger solid particles called “planetesimals”.

We will focus here on this second process, which has an enormous importance in the formation of the Earth and the rocky planets of our Solar System, as well as in the chemical composition of the matter making them.

As said in the previous section, in a protoplanetary disk equatorial plane, the density is very high, 10^{10} - 10^{12} pp/cm³, so that encounters between dust grains are more frequent than before. Both terrestrial laboratory experiments and computer simulations have shown that, when the sub-micron grains meet with moderate velocities, they stick together because of the van der Waals force, namely because of the electrostatic attraction between the two grains, the same that makes the sand grains stick on our skin in the beach. The sub-micron grains stick together form larger grains, which continue to glue to other grains and to grow in sizes. The process goes on until what were sub-micron grains become rocks of about 1 meter. Then the van der Waals force is not anymore enough to stick together meter-size rocks (this is known in the specialized literature as “the meter-size barrier”) and, in principle, the growth should stop. But it does not, as demonstrated by the existence of the rocky planet! Therefore, in a way or another, the planetesimals continue to swell up to the kilometer sizes. When the planetesimal reaches this limit, the gravitational force takes over and finishes the job to grow up to what is called “planet embryos”, namely bodies of a few thousand kilometers in diameter, a bit less than the size of Mars.

What happens to the chemical composition of matter during this period? The most important phenomenon is the “conservation” of what has been produced during the earlier phases. The grains that gently stick together to form planetesimals are coated by icy mantles that contain the organic molecules previously synthesized. Some of those mantles will be lost in space, but some will be trapped in the interiors of the planetesimals, which act, therefore, as strong boxes. It is very difficult to say how much it is conserved and how much it is lost. More laboratory experiments and numerical computations will be necessary to answer this question.

However, we have a hint of an answer from the observations of the chemical composition of the matter in the rocky leftovers of the process in the Solar System: comets, asteroids and meteorites (see the article by Beck and Bonal). Remember the phenomenon of the super-deuteration? The molecular deuteration is our “Ariadne’s thread”, the link between the first and the last phases of the Solar System formation. This link tells us that something has been inherited from the very first phases, as water is highly deuterated in comets (article by Codella and Podio), and water and organics –even amino acids!– in pristine meteorites have ten times more D atoms than the D/H elemental ratio, as shown in Figure 6.

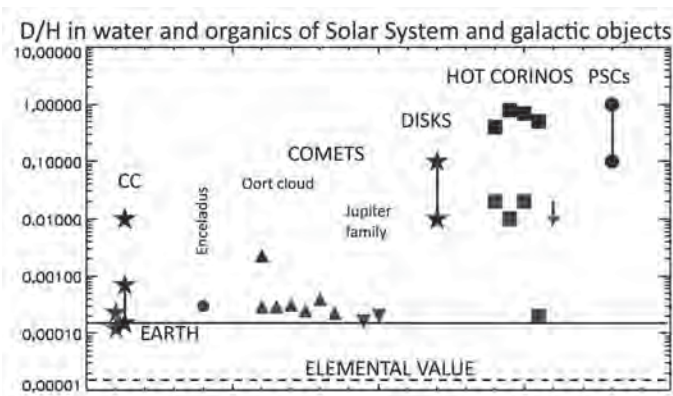


Figure 6: Molecular deuteration in different objects of the Solar System and in forming stars that will eventually become like it. The elemental value shows the ratio of D-containing over H-containing molecules when the “super-deuteration” process is not at work.

Phase 5: Planet formation

We arrive to the last stop of our voyage, the formation of planets. Under the gravitational force the giant gaseous planets form: Jupiter, Saturn and Neptune, in the Solar System. The theories differ in some important details, on when exactly they formed and whether this was triggered by instabilities in the protoplanetary disk, the Solar Nebula. These instabilities, which may have been caused by the viscosity of the material spiraling inward and outward the central star, probably confined large quantities of matter in small zones, and there the gravitational force would have made the gas collapse towards the center, similarly to what happened to the Sun during the protostellar phase.

The formation of the rocky planets followed a slightly different path. After planetesimals reached the thousand kilometer sizes, in the Solar System the period of the “giant impacts” started, when some embryos of planets collided destroying some and swelling others. This was probably the case of the proto-Earth and the protoplanet Theia. They smashed against each other about 4.4-4.5 billions years ago. Theia was completely vaporized in the impact, while a large fraction of the proto-Earth melted creating an ocean of magma. In the gigantic splash, a fraction of the Theia and Earth molten material was ejected in space where, almost instantaneously, condensed and formed the Moon. Numerical simulations predict that it took only five hours to create our beloved satellite, so important for the terrestrial life appearance.

What happened to the molecules synthesized during the very early phases of the Solar System formation? The story becomes more and more confused now, because we do not have other systems so well studied as the Solar System and we have to answer that question based primarily on that. First, we suspect that comets and asteroids rained on Earth at a much higher rate than today. We have evidence of this also in some exo-planetary systems, so this is probably a common phenomenon. Remember that these comets and asteroids are made of the planetesimals described in the previous section. Therefore, they have trapped in their rocks the iced molecules synthesized during the pre-stellar core, protostar and protoplanetary disk phases. When they impact the Earth some of these molecules may reach the surface, while some remain trapped in the rocks of the meteorites.

In any case, the story continues with the Earth that cools down after the gigantic impact with Theia. Very likely, the early Earth had a structure similar to the present one, “core, mantle, crust”, even though the mantle temperature was larger by about 200 °C and it was more heterogeneous, and the oceanic crust was likely five times thicker than today. Most relevant for the context of this article, when the Earth temperature decreased to 1200 °C, the silicates in the atmosphere condensed and fell onto the solid surface. The gases emitted by the volcanoes and brought by the raining comets and asteroids –water, carbon dioxide (CO₂), methane (CH₄) and ammonia (NH₃)– filled the atmosphere. Note that all those molecules are also the components of

the dust mantles formed during the first phases of the Solar System formation.

As the Earth continued to cool down, the water vapor of the atmosphere condensed into the oceans and caused the dissolution of carbon dioxide, which built up carbonate sediments. Then, about 2 billion years ago, a new drastic change occurred: the Great Oxygenation Event, the sudden increase of molecular oxygen (O₂) caused by the appearance of life. What exactly happened is matter of intense study and debate, and discussing it is beyond the scope of this article and certainly the expertise of its author.

What matters here is that the atoms created by the stars and the molecules synthesized during the very first moments of the Solar System life, found a way to combine into complex molecular structures, able to metabolize energy and reproduce themselves, what Dawin called the “first replicator”. At the end, it was just “chemistry at work”, the same chemistry that produces formic acid and formamide in interstellar space, and amino acids in meteorites. The basic ingredients for life are present in the whole Galaxy and probably in the Universe, in the regions where stars form. As the Nobel Prize De Duve stated, *the building blocks of life form naturally in our Galaxy and, most likely, also elsewhere in the cosmos. The chemical seeds of life are universal.*

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For an update list of the molecules discovered in the interstellar space look at http://www.astrochymist.org/astrochymist_ism.html or <http://www.astro.uni-koeln.de/cdms/molecules>