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Abstracts

Effect of grain size distribution and size-dependent grain heating on molecular abundances in starless and pre-stellar cores

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We present a new gas-grain chemical model to constrain the effect of grain size distribution on molecular abundances in physical conditions corresponding to starless and pre-stellar cores. We simultaneously introduce grain-size dependence for desorption efficiency induced by cosmic rays (CRs) and for grain equilibrium temperatures. The latter were calculated with a radiative transfer code via custom dust models built for the present work. We explicitly tracked of ice abundances on a set of grain populations. We find that the size-dependent CR desorption efficiency affects ice abundances in a highly nontrivial way that depends on the molecule. Species that originate in the gas phase, such as CO, follow a simple pattern in which the ice abundance is highest on the smallest grains and these are the most abundant in the distribution. Some molecules, such as HCN, are instead concentrated on large grains throughout the time evolution; others, such as N2, are initially concentrated on large grains, but at late times on small grains because of grain-size-dependent competition between desorption and hydrogenation. Most of the water ice is on small grains at high medium density (n(H2) higher than 1e6 cm^-3), where the water ice fraction, with respect to the total water ice reservoir, can be as low as ~1e-3 on large (> 0.1 micron) grains. Allowing the grain equilibrium temperature to vary with grain size induces strong variations in relative ice abundances in low-density conditions in which the interstellar radiation field and in particular its ultraviolet component are not attenuated. Our study implies consequences not only for the initial formation of ices preceding the starless core stage, but also for the relative ice abundances on the grain populations going into the protostellar stage. In particular, if the smallest grains can lose their mantles owing to grain-grain collisions as the core is collapsing, the ice composition in the beginning of the protostellar stage could be very different than in the pre-collapse phase because the ice composition depends strongly on the grain size.

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The PDR structure and kinematics around the compact HII regions S235A and S235C with [CII], [13CII], [OI] and HCO+ line profiles

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The aim of the present work is to study structure and gas kinematics in the photodissociation regions (PDRs) around the compact HII regions S235A and S235C. We observe the [CII], [13CII] and [OI] line emission, using SOFIA/upGREAT and complement them by data of HCO+ and CO. We use the [13CII] line to measure the optical depth of the [CII] emission, and find that the [CII] line profiles are influenced by self-absorption, while the [13CII] line remains unaffected by these effects. Hence, for dense PDRs, [13CII] emission is a better tracer of gas kinematics. The optical depth of the [CII] line is up to 10 in S235A. We find an expanding motion of the [CII]-emitting layer of the PDRs into the front molecular layer in both regions. Comparison of the gas and dust columns shows that gas components visible neither in the [CII] nor in low-J CO lines may contribute to the total column across S235A. We test whether the observed properties of the PDRs match the predictions of spherical models of expanding HII region + PDR + molecular cloud. Integrated intensities of the [13CII], [CII] and [OI] lines are well-represented by the model, but the models do not reproduce the double-peaked [CII] line profiles due to an insufficient column density of C+. The model predicts that the [OI] line could be a more reliable tracer of gas kinematics, but the foreground self-absorbing material does not allow using it in the considered regions.

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Prebiotic precursors of the primordial RNA world in space: Detection of NH2OH

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One of the proposed scenarios for the origin of life is the primordial RNA world, which considers that RNA molecules were likely responsible for the storage of genetic information and the catalysis of biochemical reactions in primitive cells, before the advent of proteins and DNA. In the last decade, experiments in the field of prebiotic chemistry have shown that RNA nucleotides can be synthesized from relatively simple molecular precursors, most of which have been found in space. An important exception is hydroxylamine, NH2OH, which, despite several observational attempts, it has not been detected in space yet. Here we present the first detection of NH2OH in the interstellar medium towards the quiescent molecular cloud G+0.693-0.027 located in the Galactic Center. We have targeted the three groups of transitions from the J=2−1, 3−2, and 4−3 rotational lines, detecting 5 transitions that are unblended or only slightly blended. The derived molecular abundance of NH2OH is (2.1±0.9)×1e−10. From the comparison of the derived abundance of NH2OH and chemically related species, with those predicted by chemical models and measured in laboratory experiments, we favor the formation of NH2OH in the interstellar medium via hydrogenation of NO on dust grain surfaces, with possibly a contribution of ice mantle NH3 oxidation processes. Further laboratory studies and quantum chemical calculations are needed to completely rule out the formation of NH2OH in the gas phase.

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Impact of PAH photodissociation on the formation of small hydrocarbons in the Orion Bar and the Horsehead PDRs

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We study whether polycyclic aromatic hydrocarbons (PAHs) can be a weighty source of small hydrocarbons in photo-dissociation regions (PDRs). We modeled the evolution of 20 specific PAH molecules in terms of dehydrogenation and destruction of the carbon skeleton under the physical conditions of two well-studied PDRs, the Orion Bar and the Horsehead nebula which represent prototypical examples of PDRs irradiated by "high" and "low" ultraviolet radiation field. PAHs are described as microcanonical systems. The acetylene molecule is considered as the main carbonaceous fragment of the PAH dissociation as it follows from laboratory experiments and theory. We estimated the rates of acetylene production in gas phase chemical reactions and compared them with the rates of the acetylene production through the PAH dissociation. It is found that the latter rates can be higher than the former rates in the Orion Bar at Av<1 and also at Av>3.5. In the Horsehead nebula, the chemical reactions provide more acetylene than the PAH dissociation. The produced acetylene participate in the reactions of the formation of small hydrocarbons (C2H, C3H, C3H+, C3H2, C4H). Acetylene production via the PAH destruction may increase the abundances of small hydrocarbons produced in gas phase chemical reactions in the Orion Bar only at Av>3.5. In the Horsehead nebula, the contribution of PAHs to the abundances of the small hydrocarbons is negligible. We conclude that the PAHs are not a major source of small hydrocarbons in both PDRs except some locations in the Orion Bar.

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A protostellar system fed by a streamer of 10,500 au length

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Binary formation is an important aspect of star formation. One possible route for close-in binary formation is disk fragmentation. Recent observations show that small-scale asymmetries (<300 au) around young protostars, although not always resolving the circumbinary disk, are linked to disk phenomena. In later stages, resolved circumbinary disk observations (<200 au) show similar asymmetries, suggesting that the asymmetries arise from binary–disk interactions. We observed one of the youngest systems to study the connection between disk and dense core. We find a bright and clear streamer in chemically fresh material (carbon-chain molecular species) that originates from outside the dense core (>10,500 au). This material connects the outer dense core with the region where asymmetries arise near disk scales. This new structure type, ten times larger than those seen near disk scales, suggests a different interpretation of previous observations: large-scale accretion flows funnel material down to disk scales. These results reveal the under-appreciated importance of the local environment on the formation and evolution of disks in early systems and a possible initial condition for the formation of annular features in young disks.

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The surprisingly carbon-rich environment of the S-type star W Aql

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W Aql is an asymptotic giant branch (AGB) star with an atmospheric elemental abundance ratio C/O≈0.98 and reported circumstellar molecular abundances intermediate between those of M-type (C/O<1) and C-type (C/O>1) AGB stars. This intermediate status is considered typical for S-type stars, although our understanding of the chemical content of their circumstellar envelopes (CSEs) is currently rather limited. We performed observations in the frequency range 159-268 GHz with the APEX telescope and make abundance estimates through comparison to available spectra towards some well-studied AGB stars and based on rotational diagram analysis in the case of SiC2. We conclude that W Aql's CSE appears considerably closer to that of a C-type AGB star than to that of an M-type AGB star. In particular, we detect emission from C2H, SiC2, SiN, and HC3N, molecules previously only detected towards the CSEs of C-type stars. This conclusion, based on the chemistry of the gaseous component of the CSE, is further supported by reports in the literature on the presence of atmospheric molecular bands and spectral features of dust species typical for C-type AGB stars. Although our observations mainly trace species in the outer regions of the CSE, our conclusion matches closely that based on recent chemical equilibrium models for the inner wind of S-type stars: the atmospheric and circumstellar chemistry of S-type stars likely resembles that of C-type AGB stars much more closely than that of M-type AGB stars. Further observational investigation of the gaseous circumstellar chemistry of S-type stars is required to characterise its dependence on the atmospheric C/O. Non-equilibrium chemical models of the CSEs of AGB stars need to address the particular class of S-type stars and the chemical variety that is induced by the range in atmospheric C/O.

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Linking ice and gas in the Serpens low-mass star-forming region

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The interaction between dust, ice, and gas during the formation of stars produces complex organic molecules. While observations indicate that several species are formed on ice-covered dust grains and are released into the gas phase, the exact chemical interplay between solid and gas phases and their relative importance remain unclear. Our goal is to study the interplay in regions of low-mass star formation through ice- and gas-mapping and by directly measuring gas-to-ice ratios. This provides constraints on the routes that lead to the chemical complexity that is observed in both phases. We present observations of gas-phase methanol (CH3OH) and carbon monoxide at 1.3 mm towards ten low-mass young protostars in the Serpens SVS4 cluster from the SubMillimeter Array and the Atacama Pathfinder EXperiment telescope. We used archival data from the Very Large Telescope to derive abundances of ice H2O, CO, and CH3OH towards the same region. Finally, we constructed gas-ice maps of SVS4 and directly measured CO and CH3OH gas-to-ice ratios. The CH3OH gas-to-ice ratio agrees with values that were previously reported for embedded Class 0/I low-mass protostars. The CO gas-maps trace an extended gaseous component that is not sensitive to the

effect of freeze-out. We find that there is no straightforward correlation between CO and CH3OH gas with their ice counterparts in the cluster. This is likely related to the complex morphology of SVS4: the Class 0 protostar SMM4 and its envelope lie in the vicinity, and the outflow associated with SMM4 intersects the cluster. This study serves as a pathfinder for future observations with ALMA and the James Webb Space Telescope that will provide high-sensitivity gas-ice maps of molecules more complex than methanol. Such comparative maps will be essential to constrain the chemical routes that regulate the chemical complexity in star-forming regions.

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Physicochemical models: source-tailored or generic?

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Physicochemical models can be powerful tools to trace the chemical evolution of a protostellar system and allow to constrain its physical conditions at formation. The aim of this work is to assess whether source-tailored modelling is needed to explain the observed molecular abundances around young, low-mass protostars or if, and to what extent, generic models can improve our understanding of the chemistry in the earliest stages of star formation. The physical conditions and the abundances of simple, most abundant molecules based on three models are compared. After establishing the discrepancies between the calculated chemical output, the calculations are redone with the same chemical model for all three sets of physical input parameters. With the differences arising from the chemical models eliminated, the output is compared based on the influence of the physical model. Results suggest that the impact of the chemical model is small compared to the influence of the physical conditions, with considered timescales having the most drastic effect. Source-tailored models may be simpler by design; however, likely do not sufficiently constrain the physical and chemical parameters within the global picture of star-forming regions. Generic models with more comprehensive physics may not provide the optimal match to observations of a particular protostellar system, but allow a source to be studied in perspective of other star-forming regions.

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Measuring elemental abundance ratios in protoplanetary disks at millimeter wavelengths

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Over million years of evolution, gas dust and ice in protoplanetary disks can be chemically reprocessed. There is evidence that the gas-phase carbon and oxygen abundances are subsolar in disks belonging to nearby star forming regions. These findings have a major impact on the composition of the primary atmosphere of giant planets (but it may also be valid for super-Earths and sub-Neptunes) as they accrete their gaseous envelopes from the surrounding material in the disk. In this study, we performed a thermochemical modeling analysis with the aim of testing how reliable and robust are the estimates of elemental abundance ratios based on (sub)millimeter observations of molecular lines. We created a grid of disk models for the following

different elemental abundance ratios: C/O, N/O, and S/O, and we computed the line flux of a set of carbon-nitrogen and sulphur-bearing species, namely CN, HCN, NO, C2H, c-C3H2, H2CO, HC3N, CH3CN, CS, SO, H2S, and H2CS, which have been detected with present (sub)millimeter facilities such as ALMA and NOEMA. We find that the line fluxes, once normalized to the flux of the 13CO J = 2-1 line, are sensitive to the elemental abundance ratios. On the other hand, the stellar and disk physical parameters have only a minor effect on the line flux ratios. Our results demonstrate that a simultaneous analysis of multiple molecular transitions is a valid approach to constrain the elemental abundance ratio in protoplanetary disks.

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The family of amide molecules toward NGC 6334I

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Amide molecules produced in space could play a key role in the formation of biomolecules on a young planetary object. However, the formation and chemical network of amide molecules in space is not well understood. In this work, ALMA observations are used to study a number of amide(-like) molecules toward the high-mass star-forming region NGC 6334I. The first detections of cyanamide (NH2CN), acetamide (CH3C(O)NH2) and N-methylformamide (CH3NHCHO) are presented for this source. These are combined with analyses of isocyanic acid (HNCO) and formamide (NH2CHO) and a tentative detection of urea (carbamide; NH2C(O)NH2). Abundance correlations show that most amides are likely formed in related reactions occurring in ices on interstellar dust grains in NGC 6334I. However, in an expanded sample of sources, large abundance variations are seen for NH2CN that seem to depend on the source type, which suggests that the physical conditions within the source heavily influence the production of this species. The rich amide inventory of NGC 6334I strengthens the case that interstellar molecules can contribute to the emergence of biomolecules on planets.

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Temperature structures of embedded disks: young disks in Taurus are warm

Merel L.R. van 't Hoff, Daniel Harsono, John J. Tobin, Arthur D. Bosman, Ewine F. van Dishoeck, Jes K. J{\o}rgensen, Anna Miotello, Nadia M. Murillo, Catherine Walsh

The chemical composition of gas and ice in disks around young stars set the bulk composition of planets. In contrast to protoplanetary disks (Class II), young disks that are still embedded in their natal envelope (Class 0 and I) are predicted to be too warm for CO to freeze out, as has been confirmed observationally for L1527 IRS. To establish whether young disks are generally warmer than their more evolved counterparts, we observed five young (Class 0/I and Class I) disks in Taurus with the Atacama Large Millimeter/submillimeter Array (ALMA), targeting C17O 2-1, H2CO 3(1,2)-2(1,1), HDO 3(1,2)-2(2,1) and CH3OH 5K-4K transitions at 0.48" x 0.31" resolution. The different freeze-out temperatures of these species allow us to derive a global temperature structure. C17O and H2CO are detected in all disks, with no signs of CO freeze-out in

the inner ~100 au, and a CO abundance close to ~1e-4. H2CO emission originates in the surface layers of the two edge-on disks, as witnessed by the especially beautiful V-shaped emission pattern in IRAS 04302+2247. HDO and CH3OH are not detected, with column density upper limits more than 100 times lower than for hot cores. Young disks are thus found to be warmer than more evolved protoplanetary disks around solar analogues, with no CO freeze-out (or only in the outermost part of > ~100 au disks) or CO processing. However, they are not as warm as hot cores or disks around outbursting sources, and therefore do not have a large gas-phase reservoir of complex molecules.

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Carbon-grain sublimation: a new top-down component of protostellar chemistry

Merel L.R. van 't Hoff, Edwin A. Bergin, Jes K. Jörgensen, & Geoffrey A. Blake

Earth's carbon deficit has been an outstanding problem in our understanding of the formation of our Solar System. A possible solution would be the sublimation of carbon grains at the so-called soot line (~300 K) early in the planet-formation process. Here, we argue that the most likely signatures of this process are an excess of hydrocarbons and nitriles inside the soot line, and a higher excitation temperature for these molecules compared to oxygen-bearing complex organics that desorb around the water snowline (~100 K). Such characteristics have been reported in the literature, for example, in Orion KL, although not uniformly, potentially due to differences in observational settings and analysis methods of different studies or related to the episodic nature of protostellar accretion. If this process is active, this would mean that there is a heretofore unknown component to the carbon chemistry during the protostellar phase that is acting from the top down - starting from the destruction of larger species - instead of from the bottom up from atoms. In the presence of such a top-down component, the origin of organic molecules needs to be re-explored.

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