

AstroChemical Newsletter #105

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Abstracts

The Complex (Organic) Puzzle of the Formation of Hydrogen Cyanide and Isocyanide on Interstellar Ice Analogues

Joan Enrique-Romero, Thanja Lamberts

Aiming to constrain the surface formation of HCN and HNC in the dense interstellar medium on ice-covered dust grains, we investigate the interaction of CN radicals with H₂O and CO ices and their subsequent reactivity with H and H₂. CN radicals can physisorb on both ices. However, on H₂O ice, a hemibond formation is the most common binding mode, while on CO ice, the CN-CO van der Waals complex can form NCCO with a small energy barrier. We show low barrier or barrierless pathways to the formation of HCN and HNC for the reaction H + CN on both ices. Reactivity with H₂ involves activation energy barriers to form HCN, which may be overcome by quantum tunneling, while HNC formation is unlikely. The formation of HCN and HNC competes with the formation of NH₂CHO on H₂O and HCOCN on CO.

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The rapid formation of macromolecules in irradiated ice of protoplanetary disk dust traps

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Organic macromolecular matter is the dominant carrier of volatile elements such as carbon, nitrogen and noble gases in chondrites—the rocky building blocks from which Earth formed. How this macromolecular substance formed in space is unclear. Here we show that its formation could be associated with the presence of dust traps, which are prominent mechanisms for forming planetesimals in planet-forming disks. We demonstrate the existence of heavily irradiated zones in dust traps, where small frozen molecules that coat large quantities of microscopic dust grains could be rapidly converted into macromolecular matter by receiving radiation doses of up to several tens of electronvolts per molecule per year. This allows for the transformation of simple molecules into complex macromolecular matter within several decades. Up to roughly 4% of the total disk ice reservoir can be processed this way and subsequently incorporated into the protoplanetary disk midplane where planetesimals form. This finding shows that planetesimal formation and the production of organic macromolecular matter, which provides the essential elemental building blocks for life, might be linked.

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Cold water emission cannot be used to infer depletion of bulk elemental oxygen [O/H] in disks

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We re-examine the constraints provided by Herschel Space Observatory data regarding cold water emission from protoplanetary disks. Previous disk models that were used to interpret observed water emission concluded that oxygen (O/H) is depleted by at least 2 orders of magnitude if a standard, interstellar gas/dust mass ratio is assumed in the disk. In this work, we use model results from a recent disk parameter survey and show that most of the \textit{Herschel} constraints obtained for cold water (i.e. for transitions with an upper energy level $E_{up} < 200$ K, where the bulk of the disk water lies) can be explained with disk models adopting ISM-like oxygen elemental abundance (i.e. $O/H = 3.2e-4$) and the canonical gas/dust mass ratio of 100. We show that cold water vapor is mainly formed by photodesorption of water ice at the interface between the molecular layer and the midplane, and that its emission is relatively independent of the main disk properties like the disk gas mass and gas/dust mass ratio. We find that the abundance of water vapor in the outer disk is set by photoprocesses and depends on the (constant) vertical column density of water ice needed to attenuate the FUV photon flux, resulting in roughly constant emission for the parameters (gas mass, dust mass, disk radius) varied in our survey. Importantly, water line emission is found to be optically thick and hence sensitive to temperature more than abundance, possibly driving previous inferences of large scale oxygen depletion.

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Binding Energies and Vibrational Spectral Features of Sn Species on Amorphous Water-ice Mantles: A Quantum Mechanical Study

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In the denser and colder regions of the interstellar medium (ISM), gas-phase sulfur is depleted by 2 or 3 orders of magnitude with respect to its cosmic abundance. Thus, which species are the main carriers of sulfur is an open question. Recent studies have proposed Sn species as potential sulfur reservoirs. Among the various sulfur allotropes, the most stable one is the S₈ ring, detected in the asteroid Ryugu and Orgueil meteorite. Shorter species, namely S₃ and S₄, have been found in the comet 67P/C-G, but their presence in the ISM remains elusive. In this study, we compute the binding energies (BEs) of Sn ($n = 1-8$) species on an amorphous water-ice surface model and analyze their infrared (IR) and Raman spectral features to provide data for their identification in the ISM. Our computations reveal that these species exhibit lower BEs than previously assumed and that their spectral features experience minimal shifts when adsorbed on water ice, because of the weak and nonspecific Sn-ice interactions. Furthermore, these species display very low IR band intensities and, therefore, very accurate instruments operating in the mid-IR range are required for detecting the presence of these species in dense interstellar environments.

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A framework for incorporating binding energy distribution in gas-ice astrochemical models

K. Furuya

One of the most serious limitations of current astrochemical models with the rate equation (RE) approach is that only a single type of binding site is considered in grain surface chemistry, although laboratory and quantum chemical studies have found that surfaces contain various binding sites with different potential energy depths. When various sites exist, adsorbed species can be trapped in deep potential sites, increasing the resident time on the surface. On the other hand, adsorbed species can be populated in shallow sites, activating thermal hopping and thus two-body reactions even at low temperatures, where the thermal hopping from deeper sites is not activated. Such behavior cannot be described by the conventional RE approach. In this work, I present a framework for incorporating various binding sites (i.e., binding energy distribution) in gas-ice astrochemical models as an extension of the conventional RE approach. I propose a simple method to estimate the probability density function for the occupation of various sites by adsorbed species, assuming a quasi-steady state. By using thermal desorption and hopping rates weighted by the probability density functions, the effect of binding energy distribution is incorporated into the RE approach without increasing the number of ordinary differential equations to be solved. This method is found to be accurate and computationally efficient and enables us to consider binding energy distribution even for a large gas-ice chemical network, which contains hundreds of icy species. The impact of the binding energy distribution on interstellar ice composition is discussed quantitatively for the first time.

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Formation of carbonyl sulfide (OCS) via SH radicals in interstellar CO-rich ice under dense cloud conditions

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Carbonyl sulfide (OCS) is widely observed in the gas phase towards star-forming regions and was the first of the only two sulfur-bearing species detected in interstellar ices so far. However, the chemical network governing its formation is still not fully understood. While the sulfurization of CO and the oxidation of CS are often invoked to form OCS, other mechanisms could have a significant contribution. In particular, the multistep reaction involving CO and SH is a good candidate to forming OCS in dense cloud environments. We aim to constrain the viability of the CO + SH route to forming solid OCS in the interstellar medium, in a similar manner as CO + OH is known to produce CO₂ ice. This is achieved by conducting a systematic laboratory investigation of the targeted reactions on interstellar ice analogues under dense cloud conditions. An ultrahigh vacuum chamber is utilized to simultaneously deposit CO, H₂S, and atomic H at 10 K. SH radicals produced in situ via hydrogen abstraction from H₂S react with CO to form OCS. OCS is efficiently formed through surface reactions involving CO, H₂S, and H atoms. The suggested underlying mechanism behind OCS formation is CO + SH → HSCO followed by HSCO + H → OCS + H₂. The OCS yield reduces slowly, but remains significant with increasing CO:H₂S mixing ratios (CO:H₂S = 1:1, 5:1, 10:1, and 20:1). Our experiments provide unambiguous evidence that OCS can be formed from CO + SH in the presence of H atoms. This route remains efficient for large H₂S dilutions

(5% w.r.t CO), suggesting that it is a viable mechanism in interstellar ices. Given that SH radicals can be created in clouds throughout a wide evolutionary timescale, this mechanism could have a non-negligible contribution to forming interstellar OCS ice.

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Deuterium fractionation of the starless core L 1498

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Molecular deuteration is commonly seen in starless cores and is expected to occur on a timescale comparable to that of the core contraction. Thus, the deuteration serves as a chemical clock, allowing us to investigate dynamical theories of core formation. We aim to provide a 3D cloud description for the starless core L 1498 located in the nearby low-mass star-forming region Taurus and explore its possible core formation mechanism. We carried out nonlocal thermal equilibrium radiative transfer with multi-transition observations of the high-density tracer N₂H⁺ to derive the density and temperature profiles of the L 1498 core. By combining these observations with the spectral observations of the deuterated species, ortho-H₂D⁺, N₂D⁺, and DCO⁺, we derived the abundance profiles for the observed species and performed chemical modeling of the deuteration profiles across L 1498 to constrain the contraction timescale. We present the first ortho-H₂D⁺ (110-111) detection toward L 1498. We find a peak molecular hydrogen density of 1.6e5 cm⁻³, a temperature of 7.5K, and a N₂H⁺ deuteration of 0.27(-0.15+0.12) in the center. We derived a lower limit of the core age for L 1498 of 0.16Ma, which is compatible with the typical free-fall time, indicating that L 1498 likely formed rapidly.

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The role of point defect reconstructions and Polycyclic Aromatic Hydrocarbons (PAHs) in silicate dust preservation

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Forsterite is a primary constituent of interstellar dust and planetary systems. It is believed to originate from the outflows of oxygen-rich stars and undergo further processing within the interstellar medium (ISM) through the action of cosmic rays and shocks. Under these harsh conditions, point defects may form, such as MgO Schottky vacancies. These vacancies can then undergo atom reconstruction as part of a chemical process to maintain the system's crystalline structure. Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitously observed interstellar molecules and are thought to form through gas phase reactions akin to sooting flames. However, their role and impact on dust stability remain unknown. In this study, we employ an atomistic Artificial Intelligence (AI)-based method, surrogate machine learning trained directly by density functional theory (DFT). Specifically, we utilize Global Optimization with First-principle Energy Expressions (GOFEE) to predict possible reconstructions of MgO vacancies on a crystalline forsterite (010) surface as an important component of interstellar dust and planetary systems. We identify nine possible reconstructions involving the formation of unbound Si and O atoms. We investigate their energy stability and find that the reconstruction of Si-O atoms stabilizes the vacancy by about 0.54 eV. Additionally, if

PAHs bind with the unbound O and Si atoms of the vacancy, the vacancy is stabilized by approximately 1.76 eV. We demonstrate that PAHs, along with the reconstruction of unbound atoms on the dust surface, affect the stability of the dust, which might open up avenues for diverse chemistry.

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JOYS+: link between ice and gas of complex organic molecules. Comparing JWST and ALMA data of two low-mass protostars

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A rich inventory of complex organic molecules (COMs) has been observed in high abundances in the gas phase toward Class 0 protostars. These molecules are suggested to form in ices and sublime in the warm inner envelope close to the protostar. However, only the most abundant COM, methanol (CH₃OH), has been firmly detected in ices before the era of James Webb Space Telescope (JWST). Now it is possible to detect the interstellar ices of other COMs and constrain their ice column densities quantitatively. We aim to determine the column densities of several oxygen-bearing COMs (O-COMs) in both gas and ice for two low-mass protostellar sources, NGC 1333 IRAS 2A and B1-c, as case studies in our JWST Observations of Young protoStars (JOYS+) program. By comparing the column density ratios w.r.t. CH₃OH between both phases measured in the same sources, we can probe into the evolution of COMs from ice to gas in the early stages of star formation. We are able to fit the fingerprints range of COM ices between 6.8 and 8.8 μ m in the JWST/MIRI-MRS spectra of B1-c using similar components as recently used for IRAS 2A. We claim detection of CH₄, OCN-, HCOO-, HCOOH, CH₃CHO, C₂H₅OH, CH₃OCH₃, CH₃OCHO, and CH₃COCH₃ in B1-c, and upper limits are estimated for SO₂, CH₃COOH, and CH₃CN. The comparison of O-COM ratios w.r.t CH₃OH between ice and gas shows two different cases. 1) the column density ratios of CH₃OCHO and CH₃OCH₃ match well between the two phases, which may be attributed to a direct inheritance from ice to gas or strong chemical links with CH₃OH. 2) the ice ratios of CH₃CHO and C₂H₅OH w.r.t. CH₃OH are higher than the gas ratios by 1-2 orders of magnitudes. This difference can be explained by the gas-phase reprocessing following sublimation, or different spatial distributions of COMs in the envelope.

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PO and PN in the Envelope of VY Canis Majoris: Elucidating the Chemistry and Origin of Phosphorus

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The J = 5.5 \rightarrow 4.5 and J = 5 \rightarrow 4 transitions of PO and PN, respectively, have been imaged in the envelope of hypergiant star VY Canis Majoris (VY CMa) using the Atacama

Large Millimeter/submillimeter Array with angular resolutions of 0.2" and 1.5" and data from the Submillimeter Telescope of the Arizona Radio Observatory. These maps are the first high-fidelity images of PO and PN in a circumstellar envelope. Both molecules are primarily present in a spherical, star-centered region with a radius $\sim 60 R^*$ (0.5"), indicating formation by LTE chemistry and then condensation into grains. PN, however, shows additional, fan-shaped emission 2" southwest of the star, coincident with dust features resolved by Hubble Space Telescope (HST), as well as four newly identified distinct structures 1"-2" toward the north, east, and west (Cloudlets I-IV), not visible in HST images. The "SW Fan" and the cloudlets are also prominent in the $J = 5.5 \rightarrow 4.5$ transition of NS. The correlation of PN with NS, SiO, and dust knots in the SW Fan suggests a formation in shocked gas enhanced with nitrogen. Excess nitrogen is predicted to favor PN synthesis over PO. Abundances for PN and PO in the spherical source are $f \sim 4.4 \times 10^{-8}$ and 1.4×10^{-7} , respectively, relative to H₂. Given a cosmic abundance of phosphorus, an unusually high fraction ($\sim 35\%$) is contained in PO and PN. Alternatively, the stellar winds may be enriched in P (and N) by dredge-up from the interior of VY CMa.

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Detection of antifreeze molecule ethylene glycol in the hot molecular core G358.93-0.03 MM1

Arijit Manna, Sabyasachi Pal, Serena Viti

The identification of complex pre-biotic molecules using millimetre and submillimetre telescopes allows us to understand how the basic building blocks of life are formed in the universe. In the interstellar medium, ethylene glycol ((CH₂OH)₂) is the simplest sugar alcohol molecule, and it is the reduced alcohol of the simplest sugar-like molecule, glycolaldehyde (CH₂OHCHO). We present the detection of the rotational emission lines of aGg' conformer of ethylene glycol ((CH₂OH)₂) towards the hot molecular core G358.93-0.03 MM1 using the Atacama Large Millimeter/Submillimeter Array. The estimated column density of aGg'-(CH₂OH)₂ towards the G358.93-0.03 MM1 is $(4.5 \pm 0.1) \times 10^{16} \text{ cm}^{-2}$ with an excitation temperature of $155 \pm 35 \text{ K}$. The abundance of aGg'-(CH₂OH)₂ with respect to H₂ is $(1.4 \pm 0.5) \times 10^{-8}$. Similarly, the abundances of aGg'-(CH₂OH)₂ with respect to CH₂OHCHO and CH₃OH are 3.1 ± 0.5 and $(6.1 \pm 0.3) \times 10^{-3}$. We compare the estimated abundance of aGg'-(CH₂OH)₂ with the existing three-phase warm-up chemical model abundance of (CH₂OH)₂, and we notice the observed abundance and modelled abundance are nearly similar. We discuss the possible formation pathways of aGg'-(CH₂OH)₂ towards the hot molecular cores, and we find that aGg'-(CH₂OH)₂ is probably created via the recombination of two CH₂OH radicals on the grain surface of G358.93-0.03 MM1.

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