AstroChemical Newsletter #93

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Abstracts

Rotational spectroscopy of oxirane-2,2-d2, c-CD2CH2O, and its tentative detection toward IRAS 16293-2422 B

Holger S. P. Müller, Jes K. Jørgensen, Jean-Claude Guillemin, Frank Lewen, Stephan Schlemmer

We prepared a sample of oxirane doubly deuterated at one C atom and studied its rotational spectrum in the laboratory for the first time between 120 GHz and 1094 GHz. Accurate spectroscopic parameters up to eighth order were determined, and the calculated rest frequencies were used to identify c-CD2CH2O tentatively in the interstellar medium in the Atacama Large Millimeter/submillimeter Array Protostellar Interferometric Line Survey (PILS) of the Class 0 protostellar system IRAS 16293−2422. The c-CD2CH2O to c-C2H4O ratio was estimated to be ∼0.054 with Trot = 125 K. This value translates to a D-to-H ratio of ∼0.16 per H atom which is higher by a factor of 4.5 than the ∼0.036 per H atom obtained for c-C2H3DO. Such increase in the degree of deuteration referenced to one H atom in multiply deuterated isotopologs compared to their singly deuterated variants have been observed commonly in recent years.

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Investigation of the rotational spectrum of CD3OD and an astronomical search toward IRAS 16293-2422

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Solar-type prestellar cores and protostars display large amounts of deuterated organic molecules. Recent findings on CHD2OH and CD3OH toward IRAS 16293-2422 suggest that even fully deuterated methanol, CD3OD, may be detectable as well. However, searches for CD3OD are hampered in particular by the lack of intensity information from a spectroscopic model. The objective of the present investigation is to develop a spectroscopic model of CD3OD in low-lying torsional states that is sufficiently accurate to facilitate searches for this isotopolog in space. We carried out a new measurement campaign for CD3OD involving two spectroscopic laboratories that covers the 34 GHz-1.1 THz range. A torsion-rotation Hamiltonian model based on the rho-axis method was employed for our analysis. Our resulting model describes the ground and first excited torsional states of CD3OD well up to quantum numbers J≤51 and Ka≤23. We derived a line list for radio-astronomical observations from this model that is accurate up to at least 1.1 THz and should be sufficient for all types of radio-astronomical searches for this methanol isotopolog. This line list was used to search for CD3OD in data from the Protostellar Interferometric Line Survey of IRAS 16293−2422 obtained with the Atacama Large Millimeter/submillimeter Array. While we found several emission features that can be attributed largely to CD3OD, their number is still not sufficiently high enough to establish a clear detection. Nevertheless, the estimate of 2×1015 cm−2 derived for the CD3OD column density may be viewed as an upper limit that can be compared to column densities of CD3OH, CH3OD, and CH3OH. The comparison indicates that the CD3OD column density toward IRAS 16293-2422 is in line with the enhanced D/H ratios observed for multiply deuterated complex organic molecules.

Astron. Astrophys., in press
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Rotation-tunneling spectrum and astrochemical modeling of dimethylamine, CH3NHCH3, and searches for it in space

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Methylamine has been the only simple alkylamine detected in the interstellar medium for a long time. With the recent secure and tentative detections of vinylamine and ethylamine, respectively, dimethylamine has become a promising target for searches in space. Its rotational spectrum, however, has been known only up to 45 GHz until now. Here we investigate the rotation-tunneling spectrum of dimethylamine in selected regions between 76 and 1091 GHz using three different spectrometers in order to facilitate its detection in space. The quantum number range is extended to J=61 and Ka=21, yielding an extensive set of accurate spectroscopic parameters. To search for dimethylamine, we refer to the spectral line survey ReMoCA carried out with the Atacama Large Millimeter/submillimeter Array toward the high-mass star-forming region Sagittarius B2(N) and a spectral line survey of the molecular cloud G+0.693−0.027 employing the IRAM 30 m and Yebes 40 m radio telescopes. We report nondetections of dimethylamine toward the hot molecular cores Sgr B2(N1S) and Sgr B2(N2b) as well as G+0.693−0.027 which imply that dimethylamine is at least 14, 4.5 and 39 times less abundant than methylamine toward these sources, respectively. The observational results are compared to computational results from a gas-grain astrochemical model. The modeled methylamine to dimethylamine ratios are compatible with the observational lower limits. However, the model produces too much ethylamine compared with methylamine which could mean that the already fairly low levels of dimethylamine in the models may also be too high.

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Infrared action spectroscopy as tool for probing gas-phase dynamics: protonated dimethyl ether, (CH3)2OH+, formed by the reaction of CH3OH2 + with CH3OH

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Methanol is one of the most abundant interstellar Complex Organic Molecules (iCOMs) and represents a major building block for the synthesis of increasingly complex oxygen-containing molecules. The reaction between protonated methanol and its neutral counterpart, giving protonated dimethyl ether, (CH3)2OH+, along with the ejection of a water molecule, has been proposed as a key reaction in the synthesis of dimethyl ether in space. Here, gas phase vibrational spectra of the (CH3)2OH+ reaction product and the [C2H9O2]+ intermediate complex(es), formed under different pressure and temperature conditions, are presented. The widely tunable free electron laser for infrared experiments, FELIX, was employed to record these vibrational fingerprint spectra using different types of infrared action spectroscopy in the 600-1700 cm−1 frequency range, complemented with measurements using an OPO/OPA system to cover the O−H stretching region 3400 − 3700 cm−1. The formation of protonated dimethyl ether as a product of the reaction is spectroscopically confirmed, providing the first gas-phase vibrational spectrum of this potentially relevant astrochemical ion.

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Early Planet Formation in Embedded Disks (eDisk). III. A First High-resolution View of Submillimeter Continuum and Molecular Line Emission toward the Class 0 Protostar L1527 IRS

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Studying the physical and chemical conditions of young embedded disks is crucial to constrain the initial conditions for planet formation. Here, we present Atacama Large Millimeter/submillimeter Array (ALMA) observations of dust continuum at ~0.06" (8 au) resolution and molecular line emission at ~0.17" (24 au) resolution toward the Class 0 protostar L1527 IRS from the Large Program eDisk (Early Planet Formation in Embedded Disks). The continuum emission is smooth without substructures, but asymmetric along both the major and minor axes of the disk as previously observed. The detected lines of 12CO, 13CO, C18O, H2CO, c-C3H2, SO, SiO, and DCN trace different components of the protostellar system, with a disk wind potentially visible in 12CO. The 13CO brightness temperature and the H2CO line ratio confirm that the disk is too warm for CO freeze out, with the snowline located at ~350 au in the envelope. Both molecules show potential evidence of a temperature increase around the disk-envelope interface. SO seems to originate predominantly in UV-irradiated regions such as the disk surface and the outflow cavity walls rather than at the disk-envelope interface as previously suggested. Finally, the continuum asymmetry along the minor axis is consistent with the inclination derived from the large-scale (100" or 14,000 au) outflow, but opposite to that based on the molecular jet and envelope emission, suggesting a misalignment in the system. Overall, these results highlight the importance of observing multiple molecular species in multiple transitions to characterize the physical and chemical environment of young disks.

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Low NH3/H2O ratio in comet C/2020 F3 (NEOWISE) at 0.7 au from the Sun

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A lower-than-solar elemental nitrogen content has been demonstrated for several comets, including 1P/Halley and 67P/C-G with independent in situ measurements of volatile and refractory budgets. The recently discovered semi-refractory ammonium salts in 67P/C-G are thought to be the missing nitrogen reservoir in comets. The thermal desorption of ammonium salts from cometary dust particles leads to their decomposition into ammonia and a corresponding acid. The NH3/H2O ratio is expected to increase with decreasing heliocentric distance with evidence for this in near-infrared observations. NH3 has been claimed to be more extended than expected for a nuclear source. Here, the aim is to constrain the NH_3/H_2O ratio in comet C/2020 F3 (NEOWISE) during its July 2020 passage. OH emission from comet C/2020 F3 (NEOWISE) was monitored for 2 months with NRT and observed from GBT on 24 July and 11 August 2020. Contemporaneously with the 24 July 2020 OH observations, the NH_3 hyperfine lines were targeted with GBT. The concurrent GBT and NRT observations allowed the OH quenching radius to be determined at (5.96±0.10)×1e4 km on 24 July 2020, which is important for accurately deriving Q(OH). C/2020 F3 (NEOWISE) was a highly active comet with $Q(H_2O) \approx 2e30$ molec/s one day before perihelion. The 3σ upper limit for Q_{NH_3}/Q_{H_2O} is <0.29% at 0.7 au from the Sun. The obtained NH_3/H_2O ratio is a factor of a few lower than measurements for other comets at such heliocentric distances. The abundance of NH_3 may vary strongly with time depending on the amount of water-poor dust in the coma. Lifted dust can be heated, fragmented, and super-heated; whereby, ammonium salts, if present, can rapidly thermally disintegrate and modify the NH_3/H_2O ratio.

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X-ray photodesorption of complex organic molecules in protoplanetary disks I. Acetonitrile CH_3CN

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Context. X-rays emitted from pre-main-sequence stars at the center of protoplanetary disks can induce nonthermal desorption from interstellar ices populating the cold regions of the disk. This process, known as X-ray photodesorption, needs to be quantified for complex organic molecules (COMs), including acetonitrile CH_3CN, which has been detected in several disks. Aims. The purpose of this work is to experimentally estimate the X-ray photodesorption yields of neutral species from pure CH_3CN ices and from interstellar ice analogs for which CH_3CN is mixed either in a CO-dominated ice or in a H_2O-dominated ice. Methods. The ices, grown in an ultrahigh vacuum chamber, were irradiated at 15 K by soft X-rays from synchrotron light (SOLEIL synchrotron) in the N K edge region (395 - 420 eV) and in the O K edge region (530 - 555 eV). X-ray photodesorption was probed in the gas phase via quadrupole mass spectrometry by monitoring the changes in the mass signals due to the X-ray irradiation of the ices. X-ray photodesorption yields were derived from the mass signals and were extrapolated to higher X-ray energies in order to provide astrophysical yields adapted to astrochemical models. Results. X-ray photodesorption of the intact CH_3CN is detected from pure CH_3CN ices and from mixed $^{13}CO:CH_3CN$ ices, with an experimental yield of about $5e{-4}$ molecules.photon^{-1} at 560 eV. When mixed in H_2O-dominated ices, X-ray photodesorption of the intact CH_3CN at 560 eV is below its detection limit, which is 10^{-4} molecules.photon^{-1}. Yields associated with the desorption of HCN, CH_4 , and CH_3 are also provided. The derived astrophysical yields significantly depend on the local conditions expected in protoplanetary disks, that is, on the ice composition and on the local X-ray irradiation spectrum. They vary from ∼ 1e-4 to ∼ 1e-6 molecules.photon^{-1} for the X-ray photodesorption of intact CH_3CN from CO-dominated ices. Only upper limits varying from ∼ 5e-5 to ∼ 5e-7 molecules.photon^{-1} could be derived for the X-ray photodesorption of intact CH_3CN from H_2O-dominated ices. Conclusions. X-ray photodesorption of intact CH_3CN from interstellar ices might in part explain the abundances of CH_3CN observed in protoplanetary disks. The desorption efficiency is expected to vary with the local physical conditions, hence with the disk region considered.

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Formation of complex organic molecules on interstellar CO ices? Insights from computational chemistry simulations

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Carbon (^3P) atom is a reactive species that, according to laboratory experiments and theoretical calculations, condensates with interstellar ice components. This fact is of uttermost importance for the chemistry in the interstellar medium (ISM) because the condensation reaction is barrierless and the subsequent species formed are still reactive given their open-shell character. Carbon condensation on CO-rich ices forms the C=C=O ($^3\Sigma^-$) species, which can be easily hydrogenated twice to form ketene (H_2CCO). Ketene is very reactive in terrestrial conditions, usually found as an intermediate hard to be isolated in chemical synthesis laboratories. These characteristics suggest that ketene can be a good candidate to form interstellar complex organic molecules (iCOMs) via a two-step process, i.e., its activation followed by a radical-radical coupling. In this work, reactions between ketene and atomic H, and the OH and NH_2 radicals on a CO-rich ice model have been explored by means of quantum chemical calculations complemented by kinetic calculations to evaluate if they are favourable in the ISM. Results indicate that H addition to ketene (helped by tunneling) to form the acetyl radical (CH_3CO) is the most preferred path, as the reactions with OH and NH_2 possess activation energies (≥ 9kJ/mol) hard to surmount in the ISM conditions, unless external processes provide energy to the system. Thus, acetaldehyde (CH_3CHO) and, probably, ethanol (CH_3CH_2OH) formation via further hydrogenations are the possible unique operating synthetic routes. Moreover, from the computed relatively large binding energies of OH and NH_2 on CO ice, slow diffusion is expected, hampering possible radical-radical couplings with CH_3CO. The astrophysical implications of these findings are discussed considering the incoming James Webb Space Telescope observations.

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Isotopic Enrichment Resulting from Differential Condensation of Methane Isotopologues Involving Non-equilibrium Gas–Surface Collisions Modeled with Molecular Dynamics Simulations

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We employ molecular dynamics simulations to understand the energy transfer processes involved during the collisions of CH4 and CD4 with CH4 layered surfaces at 20 K in order to explain our experimental finding of preferential adsorption of CD4 compared to CH4. There is good agreement between our MD simulations and our experimental results. We find that gas–surface collisional energy accommodation is dominated by exchange involving the translational degrees of freedom of the incident molecule and intermolecular vibrations of the interface. This observation allows us to understand that the cause of CD4 preferential sticking arises from its propensity to lose more energy during its first impact with the surface, inducing longer residence times and leading to increased probability of becoming trapped and condensed onto the surface. Systematic trends are seen for sticking probabilities and energy transfer when we explore the behavior of the other H/D-substituted isotopologues of methane. These molecular insights provide context into the adsorption behavior occurring on icy dust grains in our solar system. Because adsorption is often the first step, trapping efficiency differences between isotopologues have notable implications for condensed phase reaction probabilities involving isotopically substituted species and subsequent events leading to increased molecular complexity. Aside from astrophysical significance, our findings have direct implications for novel isotope enrichment mechanisms under non-equilibrium conditions involving the preferential condensation of heavier isotopes and isotopologues during gas–surface collisions under specifically selected substrate, gas mixture, and incident kinematic conditions.

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Polycyclic Aromatic Hydrocarbon Size Tracers

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We examine the dependence of polycyclic aromatic hydrocarbon (PAH) band intensity ratios as a function of the average number of carbon atoms and assess their effectiveness as tracers for PAH size, utilising the data, models, and tools provided by the NASA Ames PAH Infrared Spectroscopic Database. To achieve this, we used spectra from mixtures of PAHs of different ionisation fractions, following a size distribution. Our work, congruent with earlier findings, shows that band ratios that include the 3.3 μm PAH band provide the best PAH size tracers for small-to-intermediate sized PAHs. In addition, we find that band ratios that include the sum of the 15-20 μm PAH features (IΣ15−20) and the 6.2 or 7.7 μm bands also serve as good tracers for PAH size in the case of small-to-intermediate sized PAHs, for objects under a similar PAH size distribution as with the presented models. For different PAH size distributions, the application of a scaling factor to the I6.2/IΣ15−20 ratio can provide estimates for the size of the small-to-intermediate PAH population within sources. Employment of the I6.2/IΣ15−20 and I7.7/IΣ15−20 ratios can be of particular interest for JWST observations limited only to ∼ 5-28 μm MIRI(-MRS) coverage.

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Ryugu's Anhydrous Ingredients and Their Spectral Link to Primitive Dust from the Outer Solar System

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Ryugu is a second-generation C-type asteroid formed by the reassembly of fragments of a previous larger body in the main asteroid belt. While the majority of Ryugu samples returned by Hayabusa2 are composed of a lithology dominated by aqueously altered minerals, clasts of pristine olivine and pyroxene remain in the least-altered lithologies. These clasts are objects of great interest for revealing the composition of the dust from which the original building blocks of Ryugu's parent asteroid formed. Here we show that some grains rich in olivine, pyroxene, and amorphous silicates discovered in one millimeter-sized stone of Ryugu have infrared spectra similar to the D-type asteroid Hektor (a Jupiter Trojan), to comet Hale–Bopp, and to some anhydrous interplanetary dust particles of probable cometary origin. This result indicates that Ryugu's primary parent body incorporated anhydrous ingredients similar to the building blocks of asteroids (and possibly some comets) formed in the outer solar system, and that Ryugu retained valuable information on the formation and evolution of planetesimals at different epochs of our solar system's history.

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Cracking the Puzzle of CO2 Formation on Interstellar Ices. Quantum Chemical and Kinetic Study of the CO + OH --> CO2 + H Reaction

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Context. CO2 is one of the dominant components of the interstellar ice. Recent observations show CO2 exists more abundantly in polar (H2O-dominated) ice than in apolar (H2O-poor) ice. CO2 ice formation is primarily attributed to the reaction between CO and OH, which has a barrier. Aims. We investigate the title reaction in H2O ice and CO ice to quantify the efficiency of the reaction in polar ice and apolar ice. Methods. Highly accurate quantum chemical calculations were employed to analyze the stationary points of the potential energy surfaces of the title reaction in the gas phase on a H2O and CO clusters. Microcanonical transition state theory was used as a diagnostic tool for the efficiency of the reaction under ISM conditions. We simulate the kinetics of ice chemistry, considering different scenarios involving non-thermal processes and energy dissipation. Results. The CO + OH reaction proceeds through the remarkably stable intermediate HOCO radical. On the H2O cluster, the formation of this intermediate is efficient, but the subsequent reaction leading to CO2 formation is not. Conversely, HOCO formation on the CO cluster is inefficient without external energy input. Thus, CO2 ice cannot be formed by the title reaction alone either on H2O cluster or CO cluster. Conclusions. In the polar ice, CO2 ice formation is possible via CO + OH --> HOCO, followed by HOCO + H −−> CO2 + H2, as demonstrated by abundant experimental literature. In apolar ice, CO2 formation is less efficient because HOCO formation requires external energy. Our finding is consistent with the JWST observations. Further experimental work is encouraged using low-temperature OH radicals.

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Collision-induced excitation of ammonia in warm interstellar and circumstellar environments

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Abstract Ammonia (NH3) is the first polyatomic molecule detected in the interstellar medium. Both its spectroscopic and collisional properties have been extensively studied earlier, and NH3 was often used in laboratory astrophysics studies to compare high-level scattering calculations with state-of-the-art experiments. Nevertheless, some of its important collisional properties remain unresolved. In this paper we report state-to-state and thermally averaged collisional data for the rotational excitation of NH3 by H2 calculated with the close-coupling quantum theory. Both nuclear spin symmetries (ortho/para) of the colliders are studied. Similar research has been carried out previously, providing rate coefficients up to temperature of 200 K for rotational states with internal energy up to ~420 cm−1. Here we have computed cross sections for collision energies up to 4700 cm−1 and rate coefficients up to 500 K. Most of the rotation-inversion levels of ammonia have been considered below the first vibrational excitation threshold, leading to a total of 33 ortho- and 62 para-NH3 states. We have compared our results with the most accurate data for He and H atoms available in the literature. The propensity rules have also been analysed in the case of high rotational levels of NH3. The rate coefficients obtained by averaging over the thermal H2 relative populations exhibit significantly larger magnitudes than the state-to-state collisional data in the case of NH3 transitions with large internal energy difference, when the rotational energy transfer between the colliders is strong.

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Photodissociation and photoionization of molecules of astronomical interest. Updates to the Leiden photodissociation & photoionization cross section database

H. R. Hrodmarsson & E. F. van Dishoeck

Context. Vacuum-ultraviolet (VUV) photons are important drivers of chemical processes in space. Thus, it is important to accurately characterize and constrain photorates in different radiation fields, via the photodissociation and photoionization cross sections of individual atoms and molecules. These have been available in the Leiden VUV photodissocation and photoionization cross section database. Aims. Experimental and theoretical advances in the past decade or so have allowed multiple new cross sections to be obtained, particularly photoionization cross sections of radicals. The database is hereby updated by including these more recent cross sections and is also expanded with several astronomically relevant species. Methods. The cross sections have been used to calculate photodissociation and photoionization rates in several different radiation fields as well as from cosmic-ray-induced VUV fluxes. The reduction of rates in shielded regions was calculated as a function of dust, molecular and atomic hydrogen, atomic carbon, and self-shielding column densities. The relative importance of these shielding types is molecule and atom dependent, as well as the assumed dust absorbance. All the data are publicly available from the Leiden VUV cross section database. Results. The Leiden VUV cross section database has been updated with 14 new astrophysically relevant molecular species and 16 updates to previous entries. The database update is accompanied by a brief review of the basic physical processes, particularly photoionization processes which have not been reviewed in the context of previous database updates.

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High-resolution SOFIA/EXES Spectroscopy of Water Absorption Lines in the Massive Young Binary W3 IRS 5

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We present in this paper mid-infrared (5-8 μm) spectroscopy toward the massive young binary W3 IRS 5, using the EXES spectrometer in high-resolution mode (R∼50,000) from the NASA Stratospheric Observatory for Infrared Astronomy (SOFIA). Many (∼180) ν2=1--0 and (∼90) ν2=2-1 absorption rovibrational transitions are identified. Two hot components over 500 K and one warm component of 190 K are identified through Gaussian fittings and rotation diagram analysis. Each component is linked to a CO component identified in the IRTF/iSHELL observations (R=88,100) through their kinematic and temperature characteristics. Revealed by the large scatter in the rotation diagram, opacity effects are important, and we adopt two curve-of-growth analyses, resulting in column densities of ∼1e19 cm−2. In one analysis, the model assumes a foreground slab. The other assumes a circumstellar disk with an outward-decreasing temperature in the vertical direction. The disk model is favored because fewer geometry constraints are needed, although this model faces challenges as the internal heating source is unknown. We discuss the chemical abundances along the line of sight based on the CO-to-H2O connection. In the hot gas, all oxygen not locked in CO resides in water. In the cold gas, we observe a substantial shortfall of oxygen and suggest that the potential carrier could be organics in solid ice.

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Evidence for Ubiquitous Carbon Grain Destruction in Hot Protostellar Envelopes

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Earth is deficient in carbon and nitrogen by up to ~4 orders of magnitude compared with the Sun. Destruction of (carbon- and nitrogen-rich) refractory organics in the high-temperature planet-forming regions could explain this deficiency. Assuming a refractory cometary composition for these grains, their destruction enhances nitrogen-containing, oxygen-poor molecules in the hot gas (>300 K) after the initial formation and sublimation of these molecules from oxygen-rich ices in the warm gas (~150 K). Using observations of 37 high-mass protostars with the Atacama Large Millimeter/submillimeter Array, we find that oxygen-containing molecules (CH3OH and HNCO) systematically show no enhancement in their hot component. In contrast, nitrogen-containing, oxygen- poor molecules (CH3CN and C2H3CN) systematically show an enhancement of a factor ~5 in their hot component, pointing to additional production of these molecules in the hot gas. Assuming only thermal excitation conditions, we interpret these results as a signature of destruction of refractory organics, consistent with the cometary composition. This destruction implies a higher C/O and N/O in the hot gas than the warm gas, while the exact values of these ratios depend on the fraction of grains that are effectively destroyed. This fraction can be found by future chemical models that constrain C/O and N/O from the abundances of minor carbon, nitrogen, and oxygen carriers presented here.

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Formation of H2 on polycyclic aromatic hydrocarbons under conditions of the ISM: an ab initio molecular dynamics study

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Understanding how the H2 molecule is formed under the chemical conditions of the interstellar media (ISM) is critical to the whole chemistry of it. Formation of H2 in the ISM requires a third body acting as a reservoir of energy. Polycyclic aromatic hydrocarbons (PAH's) are excellent candidates to play that role. In this work we simulated the collisions of hydrogen atoms with coronene to form H2 via the Eley-Rideal mechanism. To do so, we used Born-Oppenheimer (ab initio) Molecular Dynamics simulations. Our results show that that adsorption of H atoms and subsequent release of H2 readily happen on coronene for H atoms with kinetic energy as large as 1 eV. Special attention is paid to dissipation and partition of the energy released in the reactions. The capacity of coronene to dissipate collision and reaction energies depends varies with the reaction site. Inner sites dissipate energy easier and faster than edge sites, thus evidencing an interplay between the potential energy surface around the reaction center and its ability to cool the projectile. As for the the recombination of H atoms and the subsequent formation of H2, it is observed that ∼15% of the energy is dissipated by the coronene molecule as vibrational energy and the remaining energy is carried by H2. The H2 molecules desorb from coronene with an excited vibrational state (υ≥3), a large amount of translational kinetic energy (≥ 0.4 eV) and with a small activation of the rotational degree of freedom.

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Detection of the elusive carbonic acid (HOCOOH) in space

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After a quarter century since the detection of the last interstellar carboxylic acid, acetic acid (CH3COOH), we report the discovery of a new one, the cis-trans form of carbonic acid (HOCOOH), toward the Galactic Center molecular cloud G+0.693-0.027. HOCOOH stands as the first interstellar molecule containing three oxygen atoms and also the third carboxylic acid detected so far in the interstellar medium. Albeit the limited available laboratory measurements (up to 65 GHz), we have also identified several pairs of unblended lines directly in the astronomical data (between 75-120 GHz), which allowed us to slightly improve the set of spectroscopic constants previously obtained in the laboratory. We derive a column density for cis-trans HOCOOH of N = (6.4 ± 0.4) × 1e12 cm-2, which yields an abundance with respect to molecular hydrogen of 4.7e-11. Meanwhile, the extremely low dipole moment (about fifteen times lower) of the lower-energy conformer, cis-cis HOCOOH, precludes its detection. We obtain an upper limit to its abundance with respect to H_2 of ≤ 1.2e-9, which suggests that cis-cis HOCOOH might be fairly abundant in interstellar space (abundance of the same order as that of trans-formic acid, t-HCOOH) , although it is nearly undetectable by radio astronomical observations. We derive a cis-cis/cis-trans ratio ≤ 25, consistent with the smaller energy difference between both conformers compared with the relative stability of trans- and cis-formic acid (c-HCOOH). We also compare the abundance of formic acid (HCOOH) and acetic acid (CH_3COOH) in different astronomical environments (including star forming regions, asteroids and comets), further suggesting a relationship between the chemical content found in the interstellar medium and the chemical composition of the minor bodies of the Solar System, which could be inherited during the star formation process.

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First glycine isomer detected in the interstellar medium: glycolamide (NH2C(O)CH2OH)

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We report the first detection in the interstellar medium of a C2H5O2N isomer: syn-glycolamide (NH2C(O)CH2OH). The exquisite sensitivity at sub-mK levels of an ultra-deep spectral survey carried out with the Yebes 40m and IRAM 30m telescopes towards the G+0.693-0.027 molecular cloud have allowed us to unambiguously identify multiple transitions of this species. We derived a column density of (7.4 +- 0.7)1e12 cm-2, which implies a molecular abundance with respect to H2 of 5.5e−11. The other C2H5O2N isomers, including the higher-energy anti conformer of glycolamide, and two conformers of glycine, were not detected. The upper limit derived for the abundance of glycine indicates that this amino acid is surely less abundant than its isomer glycolamide in the ISM. The abundances of the C2H5O2N isomers cannot be explained in terms of thermodynamic equilibrium, and thus chemical kinetics need to be invoked. While the low abundance of glycine might not be surprising, based on the relative low abundances of acids in the ISM compared to other compounds (e.g. alcohols, aldehydes or amines), several chemical pathways can favour the formation of its isomer glycolamide. It can be formed through radical-radical reactions on the surface of dust grains. The abundances of these radicals can be significantly boosted in an environment affected by a strong ultraviolet field induced by cosmic rays, such as that expected in G+0.693-0.027. Therefore, as shown by several recent molecular detections towards this molecular cloud, it stands out as the best target to discover new species with carbon, oxygen and nitrogen with increasing chemical complexity.

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Detection of monothioformic acid towards the solar-type protostar IRAS 16293–2422

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In the interstellar medium (ISM), the complex organic molecules that contain the thiol group (–SH) play an important role in the polymerization of amino acids. We look for SH-bearing molecules in the chemically rich solar-type protostar IRAS 16293–2422. After extensive spectral analysis using the local thermodynamic equilibrium (LTE) model, we have detected the rotational emission lines of trans-isomer monothioformic acid (t-HC(O)SH) towards the IRAS 16293 B using the Atacama Large Millimeter/Submillimeter Array (ALMA). We did not observe any evidence of cis-isomer monothioformic acid (c-HC(O)SH) towards the IRAS 16293 B. The column density of t-HC(O)SH towards the IRAS 16293 B was (1.02±0.6)×10^15 cm^{−2} with an excitation temperature of 125±15 K. The fractional abundance of t-HC(O)SH with respect to H2 towards the IRAS 16293 B is 8.50×10^−11. The column density ratio of t-HC(O)SH/CH3SH towards the IRAS 16293 B is 0.185. We compare our estimated abundance of t-HC(O)SH towards the IRAS 16293 B with the abundance of t-HC(O)SH towards the galactic center quiescent cloud G+0.693–0.027 and hot molecular core G31.41+0.31. After the comparison, we found that the abundance of t-HC(O)SH towards the IRAS 16293 B is several times of magnitude lower than G+0.693–0.027 and G31.41+0.31. We also discussed the possible formation mechanism of t-HC(O)SH in the ISM.

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Announcements

COST Action CA22133 : The birth of solar systems

A COST Action is an interdisciplinary research network that enables re- searchers to interact and investigate a specific topic, in our case, planet formation (https: //www.cost.eu/cost-actions/what-are-cost-actions/). The mission of this Action is to “Build an interdisciplinary network, with expertise in experimental studies, observations, and models, to advance our understanding of planet formation, by determining the computational and data needs of the community, and how to best exploit current and future observations.” COST Actions provide funding over four years to fund meetings, training schools, attendance at conferences (to report research results under the remit of the Action), short-term scientific missions (to visit international collaborators or build new collaborations) and dissemination (e.g., publications) and public engagement material (https://www.cost.eu/what-do-we-fund/).

We aim to recruit researchers (both theorists and observers) working in the areas of protoplanetary disks, planet formation, habitability, and exoplanets (including studies of exoplanet host stars), as well as researchers working in laboratory experiments related to planet formation and habitability. COST Actions are fully open for anyone to join: the only requirement is that you are affiliated with a legal entity such as a university or scientific organisation. If you are based in a COST member state (https://www.cost.eu/about/members/), it is possible to apply for membership of the management committee to represent your country. We especially encourage applications from young researchers and innovators (< 40 years old) to join the management committee. Please contact your Country National Coordinator (CNC) who can guide through the nomination process: https://www.cost.eu/about/who-is-who/national-coordinators/

Applications to join the Action working groups (listed below) are also now open to all:

- WG1: Planet formation: laboratory perspectives
- WG2: Advancing planet formation models
- WG3: Planet formation theory confronts observations
- WG4: Emerging habitable environments
- WG5: Dissemination, public engagement, and outreach
- WG6: Training the next generation of researchers
- WG7: Towards the first database on planet-forming discs

We encourage everyone to join at least two working groups to have good linkage and coverage between and across the groups. You can apply at the COST Action webpage below: look for the “How can I participate?” information on the right-hand side. If you do not already have an eCOST profile you will need to first register.

For more information, please visit the Action page (link below), or you can contact me for any further information (address below). Download/Website: https://www.cost.eu/actions/CA22133/ Contact: c.walsh1@leeds.ac.uk

Tenure Track Assistant Professor in Astronomy and Astrophysics at the University of Groningen

The Kapteyn Astronomical Institute of the University of Groningen invites applications for an Assistant Professor who will strategically strengthen our research in the field of exoplanets. The ideal candidate has a strong background in Planetary Atmosphere Sciences. As an Assistant Professor, you will develop your own research line/group, supervise PhD students, acquire external funding, teach courses, and contribute to the organization of the faculty.

The mission of the Kapteyn Astronomical Institute is to perform front-line research in astronomy, astrophysics and related fields, aided by the proximity of NWO institutes ASTRON and SRON and the NOVA labs, and to provide an excellent educational environment for both graduate and undergraduate studies. The University of Groningen is currently in or near the top 100 on several influential international ranking lists.

We encourage you to apply if you have a PhD degree in Astronomy or closely aligned field and at least two years of postdoctoral experience, a relevant international network, excellent research qualities, and a good track record in teaching (appropriate for your career stage), organizational competences and cross-cultural sensitivity.

We offer a full-time position as Assistant Professor in our faculty's tenure track system Career Paths in Science with a salary, depending on qualifications and work experience, from 3.974€ up to a maximum of 6.181€ gross per month (according to the CAO Dutch Universities). The position includes a pension scheme, paid maternity and parental leave, and the possibility to work part-time (0,9 fte or 0,8 fte).

A complete application consists of a single pdf file including a cover letter in which you describe your motivation and qualifications for the position, a CV, including a list of your publications and a list with names of at least three references, a list of five self-selected key papers, a statement of your teaching goals and experience, and a description of your scientific interest and plans. Please also arrange for three letters of reference to be sent directly to VacancyKapteynNW2@astro.rug.nl. The deadline for applications for this position is 11:59 pm CEST on September 15, 2023.

More details concerning the description of the position, working conditions, pre-requisites and how to apply can be found at https://www.rug.nl/about-ug/work-with-us/job-opportunities/?details=00347-02S000AACP