

AstroChemical Newsletter #85

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Abstracts

Ammonia, carbon dioxide and the non-detection of the 2152 cm⁻¹ CO band

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CO is one of the most abundant ice components on interstellar dust grains. When it is mixed with amorphous solid water (ASW) or located on its surface, an absorption band of CO at 2152 cm⁻¹ is always present in laboratory measurements. This spectral feature is attributed to the interaction of CO with dangling-OH bonds (dOH) in ASW. However, this band is absent in observational spectra of interstellar ices. This raises the question whether CO forms a relatively pure layer on top of ASW or is in close contact with ASW, but not via dangling bonds. We aim to determine whether the incorporation of NH₃ or CO₂ into ASW blocks the dOH and therefore reduces the 2152 cm⁻¹ band. We performed laboratory experiments to simulate the layered structure of the ice mantle, that is, we grew CO ice on top of 1) pure ASW, 2) NH₃:H₂O=10:100 mixed ice, and 3) CO₂:H₂O=20:100 mixed ice. Infrared spectra were measured to quantify the strength of the 2152 cm⁻¹ band. In addition, a second set of experiments were performed to determine how the incorporation of NH₃ into ASW affects the dOH band. We found that annealing the ice reduces the 2152 cm⁻¹ band and that NH₃ blocks the dOH on ASW surface and therefore reduces the 2152 cm⁻¹ band more effectively than CO₂. We suggest that this difference between NH₃ and CO₂ can be ascribed to the polarity of the guest molecule (NH₃ is a polar species, whereas CO₂ is apolar). The polarity implies that the formation of an H-bond between the N atom of ammonia and the dOH is a barrier-less reaction. We also determined the pore surface area of the ice mixtures as a function of the annealing temperature, and found that the nondetection of 2152 cm⁻¹ band does not necessarily exclude the possibility of a porous ice mantle.

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Rotational spectroscopy of mono-deuterated oxirane (c-C₂H₃DO) and its detection towards IRAS 16293–2422 B

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

We prepared a sample of mono-deuterated oxirane and studied its rotational spectrum in the laboratory between 490 and 1060 GHz in order to improve its spectroscopic parameters and consequently the calculated rest frequencies of its rotational transitions. The updated rest frequencies were employed to detect c-C₂H₃DO for the

first time in the interstellar medium in the Atacama Large Millimetre/submillimetre Array Protostellar Interferometric Line Survey (PILS) of the Class 0 protostellar system IRAS 16293–2422. Fits of the detected lines using the rotation diagrams yield a temperature of $T_{\text{rot}} = 103 \pm 19$ K, which in turn agrees well with 125 K derived for the c-C₂H₄O main isotopologue previously. The c-C₂H₃DO to c-C₂H₄O ratio is found to be ~ 0.15 corresponding to a D-to-H ratio of ~ 0.036 per H atom, which is slightly higher than the D-to-H ratio of species such as methanol, formaldehyde, and ketene but lower than those of the larger complex organic species such as ethanol, methyl formate, and glycolaldehyde. This may reflect that oxirane is formed fairly early in the evolution of the prestellar cores. The identification of doubly deuterated oxirane isotopomers in the PILS data may be possibly judged by the amount of mono-deuterated oxirane and the observed trend that multiply deuterated isotopologues have higher deuteration rates than their mono-deuterated variants.

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Near-Threshold and Resonance Effects in Rotationally Inelastic Scattering of D₂O with normal-H₂

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A combined experimental and theoretical study on the rotationally inelastic scattering of heavy water, D₂O, with normal-H₂. Crossed-molecular beam measurements are performed in the collision energy range between 10 and 100 cm⁻¹, corresponding to the near-threshold regime in which scattering resonances are most pronounced. State-to-state excitation cross-sections are obtained by probing three low-lying rotational levels of D₂O using the REMPI technique. These measurements are complemented by quantum close-coupling scattering calculations based on a high-accuracy D₂O–H₂ interaction potential. The agreement between experiment and theory is within the experimental error bars at 95% confidence intervals, leading to a relative difference of less than 7%: the near-threshold rise and the overall shape of the cross-sections, including small undulations due to resonances, are nicely reproduced by the calculations. Isotopic effects (D₂O versus H₂O) are also discussed by comparing the shape and magnitude of the respective cross-sections.

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Experimental Determination of the Dissociative Recombination Rate Coefficient for Rotationally Cold CH⁺ and Its Implications for Diffuse Cloud Chemistry

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Observations of CH⁺ are used to trace the physical properties of diffuse clouds, but this requires an accurate understanding of the underlying CH⁺ chemistry. Until this work, the most uncertain reaction in that chemistry was dissociative recombination (DR) of CH⁺. Using an electron-ion merged-beams experiment at the Cryogenic Storage Ring, we have determined the DR rate coefficient of the CH⁺ electronic, vibrational, and rotational ground state applicable for different diffuse cloud conditions.

Our results reduce the previously unrecognized order-of-magnitude uncertainty in the CH⁺ DR rate coefficient to ~20% and are applicable at all temperatures relevant to diffuse clouds, ranging from quiescent gas to gas locally heated by processes such as shocks and turbulence. Based on a simple chemical network, we find that DR can be an important destruction mechanism at temperatures relevant to quiescent gas. As the temperature increases locally, DR can continue to be important up to temperatures of ~600 K, if there is also a corresponding increase in the electron fraction of the gas. Our new CH⁺ DR rate-coefficient data will increase the reliability of future studies of diffuse cloud physical properties via CH⁺ abundance observations.

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Survey of Ices toward Massive Young Stellar Objects: I. OCS, CO, OCN⁻, and CH₃OH

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An important tracer of the origin and evolution of cometary ices is the comparison with ices found in dense clouds and towards Young Stellar Objects (YSOs). We present a survey of ices in the 2-5 micron spectra of 23 massive YSOs, taken with the NASA InfraRed Telescope Facility SpeX spectrometer. The 4.90 micron absorption band of OCS ice is detected in 20 sight-lines, more than five times the previously known detections. The absorption profile shows little variation and is consistent with OCS being embedded in CH₃OH-rich ices, or proton-irradiated H₂S or SO₂-containing ices. The OCS column densities correlate well with those of CH₃OH and OCN⁻, but not with H₂O and apolar CO ice. This association of OCS with CH₃OH and OCN⁻ firmly establishes their formation location deep inside dense clouds or protostellar envelopes. The median composition of this ice phase towards massive YSOs, as a percentage of H₂O, is CO:CH₃OH:OCN⁻:OCS=24:20:1.53:0.15. CS, due to its low abundance, is likely not the main precursor to OCS. Sulfurization of CO is likely needed, although the source of this sulfur is not well constrained. Compared to massive YSOs, low mass YSOs and dense clouds have similar CO and CH₃OH ice abundances, but less OCN⁻ and more apolar CO, while OCS awaits detection. Comets tend to be under-abundant in carbon-bearing species, but this does not appear to be the case for OCS, perhaps signalling OCS production in protoplanetary disks.

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CORINOS I: JWST/MIRI Spectroscopy and Imaging of a Class 0 protostar IRAS 15398-3359

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The origin of complex organic molecules (COMs) in young Class 0 protostars has been one of the major questions in astrochemistry and star formation. While COMs are thought to form on icy dust grains via gas-grain chemistry, observational constraints on their formation pathways have been limited to gas-phase detection. Sensitive mid-infrared spectroscopy with JWST enables unprecedented investigation of COM formation by measuring their ice absorption features. We present an overview of

JWST/MIRI MRS spectroscopy and imaging of a young Class 0 protostar, IRAS 15398-3359, and identify several major solid-state absorption features in the 4.9-28 μm wavelength range. These can be attributed to common ice species, such as H_2O , CH_3OH , NH_3 , and CH_4 , and may have contributions from more complex organic species, such as $\text{C}_2\text{H}_5\text{OH}$ and CH_3CHO . The MRS spectra show many weaker emission lines at 6-8 μm , which are due to warm CO gas and water vapor, possibly from a young embedded disk previously unseen. Finally, we detect emission lines from [Fe II], [Ne II], [S I], and H_2 , tracing a bipolar jet and outflow cavities. MIRI imaging serendipitously covers the south-western (blue-shifted) outflow lobe of IRAS 15398-3359, showing four shell-like structures similar to the outflows traced by molecular emission at sub-mm wavelengths. This overview analysis highlights the vast potential of JWST/MIRI observations and previews scientific discoveries in the coming years.

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Theoretical spectra and energetics for c-C₃H₂, l-C₅H₂, and bipyramidal D_{3h} C₅H₂

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The recent astronomical detection of c-C₃H₂ and l-C₅H₂ has led to increased interest in C₅H₂ isomers and their relative stability. The present work provides the first complete list of anharmonic vibrational spectral data with infrared intensities for three such isomers as well as including the first set of rotational data for the bipyramidal C₅H₂ isomer allowing for these molecules to serve as potential tracers of interstellar carbon. All three isomers have fundamental vibrational frequencies with at least one notably intense fundamental frequency. The l-C₅H₂ isomer has, by far, the highest intensities out of the three isomers at 2076.3 cm^{-1} (738 km mol^{-1}) and 1887.5 cm^{-1} (182 km mol^{-1}). The c-C₃H₂ isomer has one intense peak at 3460.6 cm^{-1} (84 km mol^{-1}), and the bipyramidal C₅H₂ isomer has one intense peak at 489.3 cm^{-1} (78 km mol^{-1}). The relative intensities highlight that while l-C₅H₂ is not the lowest energy isomer, its notable intensities should make it more detectable in the infrared than the lower energy c-C₃H₂ form. The bipyramidal isomer is firmly established here to lie 44.98 kcal mol^{-1} above the cyclic form. The explicitly correlated coupled cluster rovibrational spectral data presented herein should assist with future laboratory studies of these C₅H₂ isomers and aid in detection in astronomical environments especially through the newly operational James Webb Space Telescope.

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Quantum chemical computations of gas-phase glycolaldehyde deuteration and constraints to its formation route

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Despite the detection of numerous interstellar complex organic molecules (iCOMs) for decades, it is still a matter of debate whether they are synthesized in the gas-phase or on the icy surface of interstellar grains. In the past, molecular deuteration has been used to constrain the formation paths of small and abundant hydrogenated interstellar species. More recently, the deuteration degree of formamide, one of the most interesting iCOM, has also been explained in the hypothesis that it is formed by the gas-phase reaction $\text{NH}_2 + \text{HCO}$. In this article, we aim at using molecular deuteration to

constrain the formation of another iCOM, glycolaldehyde, which is an important prebiotic species. More specifically, we have performed dedicated electronic structure and kinetic calculations to establish the glycolaldehyde deuteration degree in relation to that of ethanol, which is its possible parent species according to the suggestion of Skouteris et al. (2018). We found that the abundance ratio of the species containing one D-atom over the all-protium counterpart depends on the produced D isotopomer and varies from 0.9 to 0.5. These theoretical predictions compare extremely well with the monodeuterated isotopomers of glycolaldehyde and that of ethanol measured towards the Solar-like protostar IRAS 16293-2422, supporting the hypothesis that glycolaldehyde could be produced in the gas-phase for this source. In addition, the present work confirms that the deuterium fractionation of iCOMs cannot be simply anticipated based on the deuterium fractionation of the parent species but necessitates a specific study, as already shown for the case of formamide.

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Interpreting molecular hydrogen and atomic oxygen line emission of T Tauri disks with photoevaporative disk-wind models

Ch. Rab, M. Weber, T. Grassi, B. Ercolano, G. Picogna, P. Caselli, W.-F. Thi, I. Kamp, P. Woitke

Winds in protoplanetary disks play an important role in their evolution and dispersal. However, what physical process is driving the winds is still unclear (i.e. magnetically vs thermally driven), and can only be understood by directly confronting theoretical models with observational data. We use hydrodynamic photoevaporative disk-wind models and post-process them with a thermo-chemical model to produce synthetic observables for the o-H₂ at 2.12 micron and [OI] at 0.63 micron spectral lines and directly compare the results to a sample of observations. Our photoevaporative disk-wind model is consistent with the observed signatures of the blueshifted narrow low-velocity component (NLVC), which is usually associated with slow disk winds, for both tracers. Only for one out of seven targets that show blueshifted NLVCs does the photoevaporative model fail to explain the observed line kinematics. Our results also indicate that interpreting spectral line profiles by simple methods, such as the thin-disk approximation, to determine the line emitting region can yield misleading conclusions. The photoevaporative disk-wind models are largely consistent with the studied observational data set, but it is not possible to clearly discriminate between different wind-driving mechanisms. Further improvements to the models, such as consistent modelling of the dynamics and chemistry and detailed modelling of individual targets would be beneficial. Furthermore, a direct comparison of magnetically driven disk-wind models to the observational data set is necessary in order to determine whether or not spatially unresolved observations of multiple wind tracers are sufficient to discriminate between theoretical models.

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Mechanism of Prebiotic Uracil Synthesis from Urea and HC₃O⁺ in Space

Joong Chul Choe

The potential energy surface for the formation of protonated uracil (UH⁺) from urea and HC3O⁺ was explored by performing quantum chemical complete basis set-QB3 calculations. A barrierless pathway was found for the formation of UH⁺, which was estimated to occur in the interstellar medium (ISM) much faster than the timescale of chemical revolution of typical dense interstellar clouds. Investigation of further reactions of UH⁺ formed through the obtained pathway led to the conclusion that uracil could be produced on icy grain surfaces but not in the gas phase of the ISM.

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Ion irradiation triggers the formation of the precursors of complex organics in space. The case of formaldehyde and acetaldehyde

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Context. Cosmic rays and solar energetic particles induce changes in the composition of compounds frozen onto dust grains in the interstellar medium (ISM), in comets, and on the surfaces of atmosphere-less small bodies in the outer Solar System. This induces the destruction of pristine compounds and triggers the formation of various species, including the precursors of complex organics. **Aims.** We investigate the role of energetic ions in the formation of formaldehyde (H₂CO) and acetaldehyde (CH₃CHO), which are observed in the ISM and in comets, and which are thought to be the precursors of more complex compounds such as hexamethylenetetramine (HMT), which is found in carbonaceous chondrites and in laboratory samples produced after the irradiation and warm-up of astrophysical ices. **Methods.** We performed ion irradiation of water, methanol, and ammonia mixtures at 14-18 K. We bombarded frozen films with 40-200 keV H⁺ that simulate solar energetic particles and low-energy cosmic rays. Samples were analysed by infrared transmission spectroscopy. **Results.** Among other molecules, we observe the formation of H₂CO and CH₃CHO, and we find that their abundance depends on the dose and on the stoichiometry of the mixtures. We find that the H₂CO abundance reaches the highest value after a dose of 10 eV/16u and then it decreases as the dose increases. **Conclusions.** The data suggest that surfaces exposed to high doses are depleted in H₂CO. This explains why the amount of HMT in organic residues and that formed after irradiation of ices depends on the dose deposited in the ice. Because the H₂CO abundance decreases at doses higher than 10 eV/16u, a lower quantity of H₂CO is available to form HMT during the subsequent warm-up. The H₂CO abundances caused by ion bombardment are insufficient to explain the ISM abundances, but ion bombardment can account for the abundance of CH₃CHO towards the ISM and comets.

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PDFchem: A new fast method to determine ISM properties and infer environmental parameters using probability distributions

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Determining the atomic and molecular content of the interstellar medium (ISM) as a function of environmental parameters is of fundamental importance to understand the star-formation process across the epochs. Although there exist various three-dimensional hydro-chemical codes modelling the ISM at different scales and redshifts, they are computationally expensive and inefficient for studies over a large parameter space. Building on our earlier approach, we present PDFchem, a novel algorithm that models the cold ISM at moderate and large scales using functions connecting the quantities of the local ($A_{v,eff}$) and the observed ($A_{v,obs}$) visual extinctions, and the local number density, n_H , with probability density functions (PDF) of $A_{v,obs}$ on cloud scales typically tens-to-hundreds of pc as an input. For any given $A_{v,obs}$ -PDF, sampled with thousands of clouds, the algorithm instantly computes the average abundances of the most important species (HI, H₂, CII, CI, CO, OH, OH⁺, H₂O⁺, CH, HCO⁺) and performs radiative transfer calculations to estimate the average emission of the most commonly observed lines ([CII] 158 μ m, both [CI] fine-structure lines and the first five rotational transitions of ¹²CO). We examine two $A_{v,obs}$ -PDFs corresponding to a non star-forming and a star-forming ISM region, under a variety of environmental parameters combinations. These cover FUV intensities in the range of $x/x_0=0.1--1e3$, cosmic-ray ionization rates in the range of $\zeta_{cr}=1e-17--1e-13$ s⁻¹ and metallicities in the range of $Z=0.1--2 Z_{sun}$. PDFchem is fast, easy to use, reproduces the PDR quantities of the time-consuming hydrodynamical models and can be used directly with observed data to understand the evolution of the cold ISM chemistry.

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