

AstroChemical Newsletter #35

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Abstracts

Synthetic observations of star formation and the interstellar medium

T. J. Haworth, S. C. O. Glover, C. M. Koepferl, T. G. Bisbas, J. E. Dale

Synthetic observations are playing an increasingly important role across astrophysics, both for interpreting real observations and also for making meaningful predictions from models. In this review, we provide an overview of methods and tools used for generating, manipulating and analysing synthetic observations and their application to problems involving star formation and the interstellar medium. We also discuss some possible directions for future research using synthetic observations.

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Condensed-Phase Photochemistry in the Absence of Radiation Chemistry

Ella Mullikin, Pierce van Mulbregt, Jeniffer Perea, Muhammad Kasule, Jean Huang, Christina Buffo, Jyoti Campbell, Leslie Gates, Helen M. Cumberbatch, Zoe Peeler, Hope Schneider, Julia Lukens, Si Tong Bao, Rhoda Tano-Menka, Subha Baniya, Kendra Cui, Mayla Thompson, Aury Hay, Lily Widdup, Anna Caldwell-Overdier, Justine Huang, Michael C. Boyer, Mahesh Rajappan, Geraldine Echebiri, and Christopher R. Arumainayagam

We report postirradiation photochemistry studies of condensed ammonia using photons of energies below condensed ammonia's ionization threshold of ~ 9 eV. Hydrazine (N_2H_4), diazene (also known as diimide and diimine; N_2H_2), triazane (N_3H_5), and one or more isomers of N_3H_3 are detected as photochemistry products during temperature-programmed desorption. Product yields increase monotonically with (1) photon fluence and (2) film thickness. In the studies reported herein, the energies of photons responsible for product formation are constrained to less than 7.4 eV. Previous post-irradiation photochemistry studies of condensed ammonia employed photons sufficiently energetic to ionize condensed ammonia and initiate radiation chemistry. Such studies typically involve ion–molecule reactions and electron-induced reactions in addition to photochemistry. Although photochemistry is cited as a dominant mechanism for the synthesis of prebiotic molecules in interstellar ices, to the best of our knowledge, ours is one of the first astrochemically relevant studies that has found unambiguous evidence for condensed-phase chemical synthesis induced by photons in the absence of ionization.

Depletion of ^{15}N in the center of L1544: Early transition from atomic to molecular nitrogen?

K. Furuya, Y. Watanabe, T. Sakai, Y. Aikawa, S. Yamamoto

We performed sensitive observations of the $\text{N}^{15}\text{ND}^+(1-0)$ and $\text{N}^{15}\text{NND}^+(1-0)$ lines toward the prestellar core L1544 using the IRAM 30m telescope. The lines are not detected down to 3 sigma levels in 0.2 km/s channels of around 6 mK. The non-detection provides the lower limit of the $^{14}\text{N}/^{15}\text{N}$ ratio for N_2D^+ of $\sim 700\text{-}800$, which is much higher than the elemental abundance ratio in the local ISM of $\sim 200\text{-}300$. The result indicates that N_2 is depleted in ^{15}N in the central part of L1544, because N_2D^+ preferentially traces the cold dense gas, and because it is a daughter molecule of N_2 . In-situ chemistry is unlikely responsible for the ^{15}N depletion in N_2 ; neither low-temperature gas phase chemistry nor isotope selective photodissociation of N_2 explains the ^{15}N depletion; the former prefers transferring ^{15}N to N_2 , while the latter requires the penetration of interstellar FUV photons into the core center. The most likely explanation is that ^{15}N is preferentially partitioned into ices compared to ^{14}N via the combination of isotope selective photodissociation of N_2 and grain surface chemistry in the parent cloud of L1544 or in the outer regions of L1544 which are not fully shielded from the interstellar FUV radiation. The mechanism is the most efficient at the chemical transition from atomic to molecular nitrogen. In other words, our result suggests that the gas in the central part of L1544 already went through the transition from atomic to molecular nitrogen in the earlier evolutionary stage, and that N_2 is currently the primary form of gas-phase nitrogen.

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High-speed molecular cloudlets around the Galactic Center supermassive black hole

J. R. Goicoechea, J. Pety, E. Chapillon, J. Cernicharo, M. Gerin, C. Herrera, M. A. Requena-Torres, M. G. Santa-Maria

We present 1"-resolution ALMA observations of the circumnuclear disk (CND) and the environment around SgrA*. The images unveil the presence of small spatial scale CO ($J=3-2$) molecular "cloudlets" within the central pc of the Milky Way, moving at high speeds, up to 300 km/s along the line-of-sight. The CO-emitting structures show intricate morphologies: extended and filamentary at high negative-velocities ($v_{\text{LSR}} < -150$ km/s), more localized and clumpy at extreme positive-velocities ($v_{\text{LSR}} > +200$ km/s). Based on the pencil-beam CO absorption spectrum toward SgrA* synchrotron emission, we also present evidence for a diffuse gas component producing absorption features at more extreme negative-velocities ($v_{\text{LSR}} < -200$ km/s). The CND shows a clumpy spatial distribution. Its motion requires a bundle of non-uniformly rotating streams of slightly different inclinations. The inferred gas density peaks are lower than the local Roche limit. This supports that CND molecular cores are transient. We apply the two standard orbit models, spirals vs. ellipses, invoked to explain the kinematics of the ionized gas streamers around SgrA*. The location and velocities of the CO cloudlets are inconsistent with the spiral model, and only two of them are consistent with the Keplerian ellipse model. Most cloudlets, however, show similar velocities that are

incompatible with the motions of the ionized streamers or with gas bounded to the central gravity. We speculate that they are leftovers of more massive, tidally disrupted, clouds that fall into the cavity, or that they originate from instabilities in the inner rim of the CND and infall from there. Molecular cloudlets, all together with a mass of several $10 M_{\text{Sun}}$, exist around SgrA*. Most of them must be short-lived: photoevaporated by the intense stellar radiation field, blown away by winds from massive stars, or disrupted by strong gravitational shears.

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High-velocity hot CO emission close to Sgr A*: Herschel/HIFI submillimeter spectral survey toward Sgr A*

Javier R. Goicoechea, M. G. Santa-Maria, D. Teyssier, J. Cernicharo, M. Gerin, J. Pety

The properties of molecular gas, the fuel that forms stars, inside the cavity of the circumnuclear disk (CND) are not well constrained. We present results of a velocity-resolved submillimeter scan (~ 480 to 1250 GHz) and [CII] $158\mu\text{m}$ line observations carried out with Herschel/HIFI toward Sgr A*; these results are complemented by a $\sim 2' \times 2'$ CO ($J=3-2$) map taken with the IRAM 30 m telescope at $\sim 7''$ resolution. We report the presence of high positive-velocity emission (up to about $+300$ km/s) detected in the wings of CO $J=5-4$ to $10-9$ lines. This wing component is also seen in H₂O ($1_{1,0}-1_{0,1}$) a tracer of hot molecular gas; in [CII] $158\mu\text{m}$, an unambiguous tracer of UV radiation; but not in [CI] $492,806$ GHz. This first measurement of the high-velocity CO rotational ladder toward Sgr A* adds more evidence that hot molecular gas exists inside the cavity of the CND, relatively close to the supermassive black hole (< 1 pc). Observed by ALMA, this velocity range appears as a collection of CO ($J=3-2$) cloudlets lying in a very harsh environment that is pervaded by intense UV radiation fields, shocks, and affected by strong gravitational shears. We constrain the physical conditions of the high positive-velocity CO gas component by comparing with non-LTE excitation and radiative transfer models. We infer $T_k \sim 400$ K to 2000 K for $n_H \sim (0.2-1.0) \times 10^5 \text{ cm}^{-3}$. These results point toward the important role of stellar UV radiation, but we show that radiative heating alone cannot explain the excitation of this $\sim 10-60 M_{\text{Sun}}$ component of hot molecular gas inside the central cavity. Instead, strongly irradiated shocks are promising candidates.

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The formation of peptide-like molecules on interstellar dust grains

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Molecules with an amide functional group resemble peptide bonds, the molecular bridges that connect amino acids, and may thus be relevant in processes that lead to the formation of life. In this study, the solid state formation of some of the smallest amides is investigated in the laboratory. To this end, CH₄:HNCO ice mixtures at 20 K are irradiated with far-UV photons, where the radiation is used as a tool to produce the radicals required for the formation of the amides. Products are identified and

investigated with infrared spectroscopy and temperature programmed desorption mass spectrometry. The laboratory data show that NH_2CHO , CH_3NCO , $\text{NH}_2\text{C}(\text{O})\text{NH}_2$, $\text{CH}_3\text{C}(\text{O})\text{NH}_2$ and CH_3NH_2 can simultaneously be formed. The NH_2CO radical is found to be key in the formation of larger amides. In parallel, ALMA observations towards the low-mass protostar IRAS 16293-2422B are analysed in search of CH_3NHCHO (N-methylformamide) and $\text{CH}_3\text{C}(\text{O})\text{NH}_2$ (acetamide). $\text{CH}_3\text{C}(\text{O})\text{NH}_2$ is tentatively detected towards IRAS 16293-2422B at an abundance comparable with those found towards high-mass sources. The combined laboratory and observational data indicates that NH_2CHO and $\text{CH}_3\text{C}(\text{O})\text{NH}_2$ are chemically linked and form in the ice mantles of interstellar dust grains. A solid-state reaction network for the formation of these amides is proposed.

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The ALMA-PILS survey: Stringent limits on small amines and nitrogen-oxides towards IRAS 16293-2422B

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Hydroxylamine (NH_2OH) and methylamine (CH_3NH_2) have both been suggested as precursors to the formation of amino acids and are therefore of interest to prebiotic chemistry. Their presence in interstellar space and formation mechanisms, however, are not well established. We aim to detect both amines and their potential precursor molecules NO , N_2O and CH_2NH towards the low-mass protostellar binary IRAS 16293--2422, in order to investigate their presence and constrain their interstellar formation mechanisms around a young Sun-like protostar. ALMA observations from the unbiased, high angular resolution and sensitivity Protostellar Interferometric Line Survey (PILS) are used. Spectral transitions of the molecules under investigation are searched for with the CASSIS line analysis software. CH_2NH and N_2O are detected for the first time towards a low-mass source, the latter molecule through confirmation with the single-dish TIMASSS survey. NO is also detected. CH_3NH_2 and NH_2OH are not detected and stringent upper limit column densities are determined. The non-detection of CH_3NH_2 and NH_2OH limits the importance of formation routes to amino acids involving these species. The detection of CH_2NH makes amino acid formation routes starting from this molecule plausible. The low abundances of CH_2NH and CH_3NH_2 compared to Sgr B2 indicate that different physical conditions influence their formation in low- and high-mass sources.

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First Results of an ALMA Band 10 Spectral Line Survey of NGC 6334I: Detections of Glycolaldehyde ($\text{HC}(\text{O})\text{CH}_2\text{OH}$) and a New Compact Bipolar Outflow in HDO and CS

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We present the first results of a pilot program to conduct an ALMA Band 10 spectral

line survey of the high-mass star-forming region NGC 6334I. The observations were taken in exceptional weather conditions (0.19 mm precipitable water) with typical system temperatures $T_{\text{sys}} < 950$ K at ~ 890 GHz. A bright, bipolar north-south outflow is seen in HDO and CS emission, driven by the embedded massive protostar MM1B. This has allowed, for the first time, a direct comparison of the thermal water in this outflow to the location of water maser emission from prior 22 GHz VLA observations. The maser locations are shown to correspond to the sites along the outflow cavity walls where high velocity gas impacts the surrounding material. We also compare our new observations to prior Herschel HIFI spectral line survey data of this field, detecting an order of magnitude more spectral lines (695 vs 65) in the ALMA data. We focus on the strong detections of the complex organic molecule glycolaldehyde (HC(O)CH₂OH) in the ALMA data that is not detected in the heavily beam-diluted HIFI spectra. Finally, we stress the need for dedicated THz laboratory spectroscopy to support and exploit future high-frequency molecular line observations with ALMA.

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H₂ chemistry in interstellar ices: The case of CO ice hydrogenation in UV irradiated CO:H₂ ice mixtures

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Context. In dense clouds, hydrogenation reactions on icy dust grains are key in the formation of molecules, like formaldehyde, methanol and complex organic molecules (COMs). These species form through the sequential hydrogenation of CO ice. Although molecular hydrogen (H₂) abundances can be four orders of magnitude higher than those of free H-atoms in dense clouds, H₂ surface chemistry has been largely ignored; several laboratory studies show that H₂ does not actively participate in “non-energetic” ice chemistry because of the high activation energies required. **Aims.** For the example of CO ice hydrogenation, we experimentally investigated the potential role of H₂ molecules on the surface chemistry when “energetic” processing (i.e., UV photolysis) is involved. We test whether additional hydrogenation pathways become available upon UV irradiation of a CO:H₂ ice mixture and whether this reaction mechanism also applies to other chemical systems. **Methods.** Ultra-high vacuum (UHV) experiments were performed at 8–20 K. A pre-deposited solid mixture of CO:H₂ was irradiated with UV-photons. Reflection absorption infrared spectroscopy (RAIRS) was used as an in situ diagnostic tool. Single reaction steps and possible isotopic effects were studied by comparing results from CO:H₂ and CO:D₂ ice mixtures. **Results.** After UV-irradiation of a CO:H₂ ice mixture, two photon-induced products, HCO and H₂CO, are unambiguously detected. The proposed reaction mechanism involves electronically excited CO in the following reaction steps: $\text{CO} + h\nu \rightarrow \text{CO}^*$, $\text{CO}^* + \text{H}_2 \rightarrow \text{HCO} + \text{H}$ where newly formed H-atoms are then available for further hydrogenation reactions. The HCO formation yields have a strong temperature dependence for the investigated regime, which is most likely linked to the H₂ sticking coefficient. Moreover, the derived formation cross section reflects a cumulative reaction rate that mainly determined by both the H-atom diffusion rate and initial concentration of H₂ at 8-20 K and that is largely determined by the H₂ sticking coefficient. Finally, the astronomical relevance of this photo-induced reaction channel is discussed.

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Formation and Destruction of SiS in Space

A. Zanchet, O. Roncero, M. Agúndez, J. Cernicharo

The presence of SiS in space seems to be restricted to a few selected types of astronomical environments. It is long known to be present in circumstellar envelopes around evolved stars and it has also been detected in a handful of star-forming regions with evidence of outflows, like Sgr B2, Orion KL, and more recently, L1157-B1. The kinetics of reactions involving SiS is very poorly known and here we revisit the chemistry of SiS in space by studying some potentially important reactions of the formation and destruction of this molecule. We calculated ab initio potential energy surfaces of the SiOS system and computed rate coefficients in the temperature range of 50-2500 K for the reaction of the destruction of SiS in collisions with atomic O, and of its formation, through the reaction between Si and SO. We find that both of the reactions are rapid, with rate coefficients of a few times $1e-10 \text{ cm}^3 \text{ s}^{-1}$, almost independent of temperature. In the reaction between Si and SO, SiO production is 5-7 times more efficient than SiS formation. The reaction of SiS with O atoms can play an important role in destroying SiS in envelopes around evolved stars. We built a simple chemical model of a postshock gas to study the chemistry of SiS in protostellar outflows and we found that SiS forms with a lower abundance and later than SiO, that SiS is efficiently destroyed through reaction with O, and that the main SiS-forming reactions are $\text{Si} + \text{SO}$ and $\text{Si} + \text{SO}_2$.

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Infrared Spectrum of Protonated Corannulene $\text{H}^+\text{C}_{20}\text{H}_{10}$ in Solid para-Hydrogen and its Potential Contribution to Interstellar Unidentified Infrared Bands

Pavithraa Sundararajan, Masashi Tsuge, Masaaki Baba, and Yuan-Pern Lee

Polycyclic aromatic hydrocarbons (PAH) and their derivatives, including protonated and cationic species, are suspected to be carriers of the unidentified infrared (UIR) emission bands observed from the galactic and extragalactic sources. We extended our investigations of infrared (IR) spectra of protonated planar PAH to a nonplanar PAH, corannulene ($\text{C}_{20}\text{H}_{10}$), which is regarded as a fragment of a fullerene, C_{60} . The protonated corannulene $\text{H}^+\text{C}_{20}\text{H}_{10}$ was produced on bombarding a mixture of corannulene and para-hydrogen ($p\text{-H}_2$) with electrons during deposition at 3.2 K. During maintenance of the electron-bombarded matrix in darkness the intensities of IR lines of protonated corannulene decreased because of neutralization by electrons that was slowly released from the trapped sites. The observed lines were classified into two groups according to their responses to secondary irradiation at 365 nm. Eighteen lines in one group are assigned to the lowest-energy species among five possible isomers, hub- $\text{H}^+\text{C}_{20}\text{H}_{10}$, and seventeen in another group to rim- $\text{H}^+\text{C}_{20}\text{H}_{10}$, the species of second lowest energy. Spectral assignments were derived based on a comparison of the observed spectra with those predicted with the B3PW91/6-311++G(2d,2p) method. The observed IR spectrum of hub- $\text{H}^+\text{C}_{20}\text{H}_{10}$ resembles several bands of the Class-A UIR bands.

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Transport of CO in Protoplanetary Disks: Consequences of Pebble Formation, Settling, and Radial Drift

S. Krijt, K. R. Schwarz, E. A. Bergin, F. J. Ciesla

Current models of (exo)planet formation often rely on a large influx of so-called 'pebbles' from the outer disk into the planet formation region. In this paper, we investigate how the formation of pebbles in the cold outer regions of protoplanetary disks and their subsequent migration to the inner disk can alter the gas-phase CO distribution both interior and exterior to the midplane CO snowline. By simulating the resulting CO abundances in the midplane as well as the warm surface layer, we identify observable signatures of large-scale pebble formation and migration that can be used as 'smoking guns' for these important processes. Specifically, we find that after 1 Myr, the formation and settling of icy pebbles results in the removal of up to 80% of the CO vapor in the warm ($T > 22$ K) disk layers outside the CO snowline, while the radial migration of pebbles results in the generation of a plume of CO vapor interior the snowline, increasing the CO abundance by a factor ~ 2 -6 depending on the strength of the turbulence and the sizes of the individual pebbles. The absence of this plume of CO vapor in young nearby disks could indicate efficient conversion of CO into a more refractory species, or a reduction in the radial mass flux of pebbles by, for example, disk inhomogeneities or early planetesimal formation.

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Announcements

PhD Position in Astrochemistry, Star and Planet Formation

A full-time, 4-year PhD position in astrochemistry, star and planet formation is open at the Center for Space and Habitability (CSH), Universität Bern. Brutto salary of 47 000 – 50 000CHF per year (as set by the SNSF). A full package of social benefits is included. Starting date: between November 1st, 2018 and April 30th, 2019. Under the guidance of Dr. Maria Drozdovskaya, a PhD research project is available, which aims to understand the chemical processes that link the different stages of star and planet formation, and that determine the composition of forming cometary and planetary embryos. The insights gained during this project will enhance our understanding of the early history of our Solar System. The work is funded by a Swiss National Science Foundation (SNSF) Ambizione grant (PI: Drozdovskaya) entitled "The Planetary Cookbook: Chemical Composition of Volatiles and Refractories from Star-Forming Regions to Comets and Planetesimals". Primary features of the project include theoretical physicochemical modelling work; possibility of working with observational data from, e.g., ALMA, JWST; active participation in the scientific life of the CSH; exposure to the largest group of planetary scientists in the world via associate membership in the NCCR PlanetS; sufficient funds for participation in national and international conferences, and collaborator visits. Must-haves of candidates are a Master-level degree (or analog) in quantitative science or engineering (e.g., astronomy, physics, chemistry, mathematics, computer science or a related field) by the starting date; and competence in spoken and written English. Nice-to-haves of candidates are programming experience, and exposure to at least basic astronomy. However,

applications from students in other fields of quantitative science or engineering that are interested in learning astronomy are very welcomed. Work-life balance is important; and the Canton of Bern offers 5 weeks of vacation per year (excluding national and cantonal holidays). The CSH is dedicated to equal opportunities, geographical and gender balance, and inclusivity. Applicants should send all application materials in one PDF file to maria.drozdovskaya@csh.unibe.ch by the deadline of November 1st, 2018. Note that applications are considered on a rolling basis, implying that the position may be filled earlier or that late applications may also receive partial consideration. A complete application consists of: cover letter (max. 1 page); curriculum vitae (CV); personal statement detailing, but not limited to: past research experience and the skills obtained, reasons for pursuing a 4-year PhD in general and this research project in specific, aspirations for the future (max. 2 pages); a full list and transcripts (grades) of all university-level courses (Bachelor- and Master-level) and a translated version, if not in English, German, French, Russian or Dutch (notarized translation is not needed); up-to-date contact information of two references that may be contacted for a reference letter.