AstroChemical Newsletter #42

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You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Gas phase reactivity of CH3OH toward OH at interstellar temperatures (11.7 - 177.5 K): experimental and theoretical study

A.J. Ocaña, S. Blázquez, A. Potapov, B. Ballesteros, A. Canosa, M. Antiñolo, L. Vereecken, J. Albaladejo, and E. Jiménez

The reactivity of methanol (CH3OH) toward the hydroxyl (OH) radical was investigated in the temperature range 11.7–177.5 K using the CRESU (French acronym for Reaction Kinetics in a Uniform Supersonic Flow) technique. In the present study, the temperature dependence of the rate coefficient for the OH + CH3OH reaction, k(T), has been revisited and additional experimental and computational data are reported. New kinetic measurements were performed to fill the existing gaps (<22 K, 22–42 K and 88–123 K), reporting k(T o 20 K) for the first time. The lowest temperature ever achieved by a pulsed CRESU has been obtained in this work (11.7 K). k(T) abruptly increases by almost 2 orders of magnitude from 177.5 K to around 100 K. At T o 100 K, this increase is less pronounced, reaching the capture limit at temperatures below 22 K. The pressure dependence of k(T) has been investigated for selected temperatures and gas densities (1.5 x 10^16 to 4.3 x 10^17 cm-3), combining our results with those previously reported. No dependence was observed within the experimental uncertainties below 110 K. The high- and low pressure rate coefficients, kHPL(T) and kLPL(T), were also studied in detail using high-level quantum chemical and theoretical kinetic methodologies, closely reproducing the experimental data between 20 and 400 K. The results suggest that the experimental data are near the high pressure limit at the lowest temperatures, but that the reaction remains a fast and effective source of CH2OH and CH3O at the low pressures and temperatures prevalent in the interstellar medium.

Phys. Chem. Chem. Phys., 21[13], 6942-6957 (2019).
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Full-text URL:
https://pubs.rsc.org/en/content/articlelanding/2019/cp/c9cp00439d#!divAbstract

Ultraviolet Spectroscopy and Photochemistry of SO2/H2O Ices

Robert Hodyss, Paul V. Johnson, Stephen M. Meckler, Edith C. Fayolle

The presence of sulfur dioxide on the trailing hemisphere of Europa’s surface is well-established, and both its presence and its chemistry are influenced by sulfur ion implantation. Particle irradiation is known to be a significant radiolysis source, particularly on the trailing surface, which is subject to particles in Jupiter’s plasma torus. Photochemistry driven by solar ultraviolet (UV) photons is also significant. To date,

most studies have investigated the effects of vacuum UV radiation, while photochemistry at longer wavelengths is less well-studied. This work investigates chemical changes in thin, cryogenic films of SO2/H2O at temperatures and pressures relevant to Europa's surface when subjected to temperature changes and UV radiation at 147, 206, 254, and 284 nm. Spectra were collected in both the mid-infrared range and the UV range, which elucidates electronic transitions that are less diagnostic but perhaps more applicable to reflectance spectra of solar system bodies. These experiments show irreversible red shifting of the B-X absorption peak upon heating likely as a result of crystallization and/or thermal chemical reactions. Further, photons with wavelengths up to 284 nm are shown to induce significant chemistry in SO2/H2O mixtures. This in conjunction with the increased solar flux compared to more energetic wavelengths and the strong C-X and B-X absorption bands in SO2 suggests that far-UV radiation plays a significant role in the sulfur cycle on Europa.

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Multi-line Herschel/HIFI observations of water reveal infall motions and chemical segregation around high-mass protostars

Floris van der Tak, Russ Shipman, Thierry Jacq, Fabrice Herpin, Jonathan Braine, Friedrich Wyrowski

(Abridged) We use HIFI maps of the 987 GHz H2O 2(02)-1(11) emission to measure the sizes and shapes of 19 high-mass protostellar envelopes. To identify infall, we use HIFI spectra of the optically thin C18O 9-8 and H2O-18 1(11)-0(00) lines. The high-J C18O line traces the warm central material and redshifted H2O-18 1(11)-0(00) absorption indicates material falling onto the warm core. We probe small-scale chemical differentiation by comparing H2O 752 and 987 GHz spectra with those of H2O-18. Our measured radii of the central part of the H2O 2(02)-1(11) emission are 30-40% larger than the predictions from spherical envelope models, and axis ratios are <2, which we consider good agreement. For 11 of the 19 sources, we find a significant redshift of the H2O-18 1(11)-0(00) line relative to C18O 9-8. The inferred infall velocities are 0.6-3.2 km/s, and estimated mass inflow rates range from 7e-5 to 2e-2 M0/yr, with the highest mass inflow rates occurring toward the sources with the highest masses, and possibly the youngest ages. The other sources show either expanding motions or H2O-18 lines in emission. The H2O-18 1(11)-0(00) line profiles are remarkably similar to the "differences" between the H2O 2(02)-1(11) and 2(11)-2(02) profiles, suggesting that the H2O-18 line and the H2O 2(02)-1(11) absorption originate just inside the radius where water evaporates from grains, typically 1000-5000 au from the center. In some sources, the H2O-18 line is detectable in the outflow, where no C18O emission is seen. Together, the H2O-18 absorption and C18O emission profiles show that the water abundance around high-mass protostars has at least three levels: low in the cool outer envelope, high within the 100 K radius, and very high in the outflowing gas. Thus, despite the small regions, the combination of lines presented here reveals systematic inflows and chemical information about the outflows.

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Sulfur chemistry in protoplanetary disks: CS and H2CS

Romane Le Gal, Karin I. Öberg, Ryan Loomis, Jamila Pegues, Jennifer B. Bergner

The nature and abundance of sulfur chemistry in protoplanetary disks (PPDs) may impact the sulfur inventory on young planets and therefore their habitability. PPDs also present an interesting test bed for sulfur chemistry models, since each disk present a diverse set of environments. In this context, we present new sulfur molecule observations in PPDs, and new S-disk chemistry models. With ALMA we observed the CS 5-4 rotational transition toward five PPDs (DM Tau, DO Tau, CI Tau, LkCa 15, MWC 480), and the CS 6-5 transition toward three PPDs (LkCa 15, MWC 480 and V4046 Sgr). Across this sample, CS displays a range of radial distributions, from centrally peaked, to gaps and rings. We also present the first detection in PPDs of 13CS 6-5 (LkCa 15 and MWC 480), C34S 6-5 (LkCa 15), and H2CS 817−716, 919−818 and 918−817 (MWC 480) transitions. Using LTE models to constrain column densities and excitation temperatures, we find that either 13C and 34S are enhanced in CS, or CS is optically thick despite its relatively low brightness temperature. Additional lines and higher spatial resolution observations are needed to distinguish between these scenarios. Assuming CS is optically thin, CS column density model predictions reproduce the observations within a factor of a few for both MWC 480 and LkCa 15. However, the model underpredicts H2CS by 1-2 orders of magnitude. Finally, comparing the H2CS/CS ratio observed toward the MWC 480 disk and toward different ISM sources, we find the closest match with prestellar cores.

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Full-text URL: https://arxiv.org/pdf/1903.11105.pdf

On Simulating the Proton-Irradiation of O2 and H2O Ices Using Astrochemical-type Models, with Implications for Bulk Reactivity

Christopher N. Shingledecker, Anton Vasyunin, Eric Herbst, Paola Caselli

Many astrochemical models today explicitly consider the species that comprise the bulk of interstellar dust grain ice-mantles separately from those in the top few monolayers. Bombardment of these ices by ionizing radiation - whether in the form of cosmic rays, stellar winds, or radionuclide emission - represents an astrochemically viable means of driving a rich chemistry even in the bulk of the ice-mantle, now supported by a large body of work in laboratory astrophysics. In this study, using an existing rate equation-based astrochemical code modified to include a method of considering radiation chemistry recently developed by us, we attempted to simulate two such studies in which (a) pure O2 ice at 5 K and, (b) pure H2O ice at 16 K and 77 K, were bombarded by keV H+ ions. Our aims are twofold: (1) to test the capability of our newly developed method to replicate the results of ice-irradiation experiments, and (2) to determine in such a well-constrained system how bulk chemistry is best handled using the same gas-grain codes that are used to model the interstellar medium (ISM). We find that our modified astrochemical model is able to reproduce both the abundance of O3 in the 5 K pure O2 ice, as well as both the abundance of H2O2 in the 16 K water ice and the previously noted decrease of hydrogen peroxide at higher temperatures. However, these results require the assumption that radicals and other reactive species produced via radiolysis react quickly and non-diffusively with neighbors in the ice.

ApJ, accepted
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Formation of Acetaldehyde on CO-rich Ices

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The radicals HCO and CH3 on carbon monoxide ice surfaces were simulated using density functional theory. Their binding energy on amorphous CO ice shows broad distributions, with approximative average values of 500 K for HCO and 200 K for CH3. If they are located on the surface close to each other (3 to 4 Ang), molecular dynamics calculations based on density functional theory show that they can form acetaldehyde (CH3CHO) or CH4 + CO in barrier-less reactions, depending on the initial orientation of the molecules with respect to each other. In some orientations, no spontaneous reactions were found, the products remained bound to the surface. Sufficient configurational sampling, inclusion of the vibrational zero point energy, and a thorough benchmark of the applied electronic structure method are important to predict reliable binding energies for such weakly interacting systems. From these results it is clear that complex organic molecules, like acetaldehyde, can be formed by recombination reactions of radicals on CO surfaces.

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On the formation of phosphorous polycyclic aromatics hydrocarbons (PAPHs) in astrophysical environments

Marco Fioroni, Robert E. Savage and Nathan J. DeYonker

The formation of phosphorous-containing polycyclic aromatic hydrocarbons (PAPHs) in astrophysical contexts is proposed and analyzed by means of computational methods [B3LYP-D3BJ/ma-def2-TZVPP, MP2-F12, CCSD-F12b and CCSD(T)-F12b levels of theory]. A ‘‘bottom-up’’ approach based on a radical-neutral reaction scheme between acetylene (C2H2) and the CP radical was used investigating: (a) the synthesis of the first PAPH (C5H5P) ‘‘phosphinine’’; (b) PAPH growth by addition of C2H2 to the C5H4P radical; (c) PAPH synthesis by addition reactions of one CP radical and nC2H2 to a neutral PAH. Results show: (I) the formation of the phosphinine radical has a strong thermodynamic tendency (133.3 kcal mol -1) and kinetic barriers <5.4 kcal mol-1 ; (II) PAPH growth by nC2H2 addition on the radical phosphinine easily and exothermically produces radicals (1a- or 1-phospha-naphtalenes with kinetic barriers <7.1 kcal mol-1 and reaction free energies <102.5 kcal mol-1); (III) the addition of a single CP + nC2H2 to a neutral benzene generates a complex chemistry where the main product is 2-phospha-naphtalene; (IV) because of the CP radical character, its barrierless addition to a PAH produces a resonant stabilized PAPH, becoming excellent candidates for addition reactions with neutral or radical hydrocarbons and PAHs; (V) the same energy trend between all four levels of theory continues a well-calibrated computational protocol to analyze complex organic reactions with astrochemical interest using electronic structure theory.

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Oxygen Atom Reactions with C2H6, C2H4, and C2H2 in Ices

J. Bergner, K. Oberg, M. Rajappan

Oxygen atom addition and insertion reactions may provide a pathway to chemical

complexity in ices that are too cold for radicals to diffuse and react. We have studied the ice-phase reactions of photoproduced oxygen atoms with C2 hydrocarbons under ISM-like conditions. The main products of oxygen atom reactions with ethane are ethanol and acetaldehyde; with ethylene are ethylene oxide and acetaldehyde; and with acetylene is ketene. The derived branching ratio from ethane to ethanol is ~0.74 and from ethylene to ethylene oxide is ~0.47. For all three hydrocarbons, there is evidence of an effectively barrierless reaction with O(1D) to form oxygen-bearing organic products; in the case of ethylene, there may be an additional barriered contribution of the ground-state O(3P) atom. Thus, oxygen atom reactions with saturated and unsaturated hydrocarbons are a promising pathway to chemical complexity even at very low temperatures where the diffusion of radical species is thermally inaccessible.

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Desorption Kinetics and Binding Energies of Small Hydrocarbons

Aida Behmard, Edith C. Fayolle, Dawn M. Graninger, Jennifer B. Bergner, Rafael Martín-Doménech, Pavlo Maksyutenko, Mahesh Rajappan, and Karin I. Öberg

Small hydrocarbons are an important organic reservoir in protostellar and protoplanetary environments. Constraints on desorption temperatures and binding energies of such hydrocarbons are needed for accurate predictions of where these molecules exist in the ice versus gas phase during the different stages of star and planet formation. Through a series of temperature programmed desorption experiments, we constrain the binding energies of 2- and 3-carbon hydrocarbons (C2H2—acetylene, C2H4—ethylene, C2H6—ethane, C3H4—propyne, C3H6—propene, and C3H8—propane) to 2200–4200 K in the case of pure amorphous ices, to 2400–4400 K on compact amorphous H2O, and to 2800–4700 K on porous amorphous H2O. The 3-carbon hydrocarbon binding energies are always larger than the 2-carbon hydrocarbon binding energies. Within the 2- and 3-carbon hydrocarbon families, the alkynes (i.e., least-saturated) hydrocarbons exhibit the largest binding energies, while the alkane and alkene binding energies are comparable. Binding energies are ~5%–20% higher on water ice substrates compared to pure ices, which is a small increase compared to what has been measured for other volatile molecules such as CO and N2. Thus in the case of hydrocarbons, H2O has a less pronounced effect on sublimation front locations (i.e., snowlines) in protoplanetary disks.

ApJ, Volume 875, No. 1, 2019, pg. 73-85
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Full-text URL: https://arxiv.org/abs/1903.09720

Dicarbon formation in collisions of two carbon atoms

J. F. Babb, R. T. Smyth, and B. M. Mclaughlin

Radiative association cross sections and rates are computed, using a quantum approach, for the formation of C2 molecules (dicarbon) during the collision of two ground state C(3P) atoms. We find that transitions originating in the C 1 Pi g, d 3 Pi g, and 15 Pi u states are the main contributors to the process. The results are compared and contrasted with previous results obtained from a semi-classical approximation. New ab initio potential curves and transition dipole moment functions have been

obtained for the present work using the multi-reference configuration interaction approach with the Davidson correction (MRCI+Q) and aug-cc-pCV5Z basis sets, substantially increasing the available molecular data on dicarbon. Applications of the current computations to various astrophysical environments and laboratory studies are briefly discussed focusing on these rates.

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ALMA reveals a pseudo-disc in a proto-brown dwarf

Riaz, B.; Machida, M. N.; Stamatellos, D.

We present the observational evidence of a pseudo-disc around the proto-brown dwarf Mayrit 1701117, the driving source of the large-scale HH 1165 jet. Our analysis is based on ALMA 12CO (2-1) line and 1.37 mm continuum observations at an angular resolution of ˜0.4″. The pseudo-disc is a bright feature in the CO position-velocity diagram (PVD), elongated in a direction perpendicular to the jet axis, with a total (gas+dust) mass of ˜0.02 M⊙, size of 165-192 AU, and a velocity spread of ±2 km s-1. The large velocity gradient is a combination of infalling and rotational motions, indicating a contribution from a pseudo-disc and an unresolved inner Keplerian disc. There is weak emission detected in the H2CO (3-2) and N2D+ (3-2) lines. H2CO emission likely probes the inner Keplerian disc where CO is expected to be frozen, while N2D+ possibly originates from an enhanced clump at the outer edge of the pseudo-disc. We have considered various models (core collapse, disc fragmentation, circum-binary disc) that can fit both the observed CO spectrum and the position-velocity offsets. The observed morphology, velocity structure, and the physical dimensions of the pseudo-disc are consistent with the predictions from the core collapse simulations for brown dwarf formation. From the best model fit, we can constrain the age of the proto-brown dwarf system to be ˜30,000-40,000 yr. A comparison of the H2 column density derived from the CO line and 1.37 mm continuum emission indicates that only about 2% of the CO is depleted from the gas phase.

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Merged H/H2 and C+/C/CO transitions in the Orion Bar

Maria S. Kirsanova, Dmitri S. Wiebe

High-resolution ALMA images towards the Orion Bar show no discernible offset between the peak of H2 emission in the photodissociation region (PDR) and the 13CO(3-2) and HCO+(4-3) emission in the molecular region. This implies that positions of H2 and CO dissociation fronts are indistinguishable in the limit of ALMA resolution. We use the chemo-dynamical model MARION to show that the ALMA view of the Orion Bar, namely, no appreciable offset between the 13CO(3-2) and HCO+(4-3) peaks, merged H2 and CO dissociation fronts, and high intensity of HCO+(4-3) emission, can only be explained by the ongoing propagation of the dissociation fronts through the molecular cloud, coupled to the dust motion driven by the stellar radiation pressure, and are not reproduced in the model where the dissociation fronts are assumed to be stationary. Modelling line intensities, we demonstrate that after the fronts have merged, the angular separation of the 13CO(3-2) and HCO+(4-3) peaks is indeed unresolvable with the ALMA observations. Our model predictions are consistent with the results of the ALMA observations about the relation of the bright HCO+(4-3) emission to the

compressed gas at the border of the PDR in the sense that the theoretical HCO+(4-3) peak does correspond to the gas density enhancement, which naturally appears in the dynamical simulation, and is located near the H2 dissociation front at the illuminated side of the CO dissociation front.

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Full-text URL: https://arxiv.org/abs/1904.04423

Direct estimation of the electron density in the Orion Bar PDR from mm-wave carbon recombination lines

S. Cuadrado, P. Salas, J. R. Goicoechea, J. Cernicharo, A. G. G. M. Tielens, A. Baez-Rubio

A significant fraction of the molecular gas in star-forming regions is irradiated by stellar UV photons. In these environments, the electron density (n_e) plays a critical role in the gas dynamics, chemistry, and collisional excitation of certain molecules. We determine n_e in the prototypical strongly-irradiated photodissociation region (PDR), the Orion Bar, from the detection of new millimeter wave carbon recombination lines (mmCRLs) and existing far-IR [13CII] hyperfine line observations. We detect twelve mmCRLs (including alpha, beta, and gamma transitions) observed with the IRAM 30m telescope, at ~25" angular resolution, toward the H/H2 dissociation front (DF) of the Bar. We also present a mmCRL emission cut across the PDR. These lines trace the C+/C/CO gas transition layer. As the much lower frequency carbon radio recombination lines, mmCRLs arise from neutral PDR gas and not from ionized gas in the adjacent HII region. This is readily seen from their narrow line profiles (dv=2.6+/-0.4 km/s) and line peak LSR velocities (v_LSR=+10.7+/-0.2 km/s). Optically-thin [13CII] hyperfine lines and molecular lines - emitted close to the DF by trace species such as reactive ions CO+ and HOC+ - show the same line profiles. We use non-LTE excitation models of [13CII] and mmCRLs and derive n_e = 60-100 cm^-3 and T_e = 500-600 K toward the DF. The inferred electron densities are high, up to an order of magnitude higher than previously thought. They provide a lower limit to the gas thermal pressure at the PDR edge without using molecular tracers. We obtain P_th > (2-4)x10^8 cm^-3 K assuming that the electron abundance is equal or lower than the gas-phase elemental abundance of carbon. Such elevated thermal pressures leave little room for magnetic pressure support and agree with a scenario in which the PDR photoevaporates.

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Confirming interstellar C60+ using the Hubble Space Telescope

Cordiner, M. A., Linnartz, H., Cox, N. L. J., Cami, J., Najarro, F., Proffitt, C. R., Lallement, R., Ehrenfreund, P., Foing, B. H., Gull, T. R., Sarre, P. J., Charnley, S. B.

Recent advances in laboratory spectroscopy lead to the claim of ionized Buckminsterfullerene (C60+) as the carrier of two diffuse interstellar bands (DIBs) in the near-infrared. However, irrefutable identification of interstellar C60+ requires a match between the wavelengths and the expected strengths of all absorption features detectable in the laboratory and in space. Here we present Hubble Space Telescope (HST) spectra of the region covering the C60+ 9348, 9365, 9428 and 9577 Å

absorption bands toward seven heavily-reddened stars. We focus in particular on searching for the weaker laboratory C60+ bands, the very presence of which has been a matter for recent debate. Using the novel STIS-scanning technique to obtain ultra-high signal-to-noise spectra without contamination from telluric absorption that afflicted previous ground-based observations, we obtained reliable detections of the (weak) 9365, 9428 Å and (strong) 9577 Å C60+ bands. The band wavelengths and strength ratios are sufficiently similar to those determined in the latest laboratory experiments that we consider this the first robust identification of the 9428 Å band, and a conclusive confirmation of interstellar C60+.

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Full-text URL: https://arxiv.org/abs/1904.08821

First astrophysical detection of the helium hydride ion (HeH+)

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During the dawn of chemistry when the temperature of the young Universe had fallen below ~4000 K, the ions of the light elements produced in Big Bang nucleosynthesis recombined in reverse order of their ionization potential. With its higher ionization potentials, He++ (54.5 eV) and He+ (24.6 eV) combined first with free electrons to form the first neutral atom, prior to the recombination of hydrogen (13.6 eV). At that time, in this metal-free and low-density environment, neutral helium atoms formed the Universe's first molecular bond in the helium hydride ion HeH+, by radiative association with protons (He + H+ → HeH+ + hν). As recombination progressed, the destruction of HeH+ (HeH+ + H → He + H+2) created a first path to the formation of molecular hydrogen, marking the beginning of the Molecular Age. Despite its unquestioned importance for the evolution of the early Universe, the HeH+ molecule has so far escaped unequivocal detection in interstellar space. In the laboratory, the ion was discovered as long ago as 1925, but only in the late seventies was the possibility that HeH+ might exist in local astrophysical plasmas discussed. In particular, the conditions in planetary nebulae were shown to be suitable for the production of potentially detectable HeH+ column densities: the hard radiation field from the central hot white dwarf creates overlapping Strömgren spheres, where HeH+ is predicted to form, primarily by radiative association of He+ and H. With the GREAT spectrometer onboard SOFIA, the HeH+ rotational ground-state transition at λ149.1 µm is now accessible. We report here its detection towards the planetary nebula NGC7027.

2019 Nature 568, 357 - 359
DOI: 10.1038/s41586-019-1090-x
Full-text URL: https://arxiv.org/abs/1904.09581

Chemical significance of different temperature regimes for cosmic-ray-induced heating of whole interstellar grains

J. Kalvāns, J. R. Kalnin

Cosmic-ray-induced whole-grain heating induces evaporation and other processes that affect the chemistry of interstellar clouds. With recent data on grain heating frequencies as an input for a modified rate-equation astrochemical model, this study examines which whole-grain heating temperature regime is the most efficient at altering the chemical composition of gas and ices. Such a question arises because low-temperature heating, albeit less effective at inducing evaporation of adsorbed species,

happens much more often than high-temperature grain heating. The model considers a delayed gravitational collapse of a Bonnor-Ebert sphere, followed by a quiescent cloud core stage. It was found that the whole-grain heating regimes can be divided into three classes, depending on their induced physico-chemical effects. Heating to low-temperature thresholds of 27 and 30 K induce desorption of the most volatile of species - N2 and O2 ices, and adsorbed atoms. The medium-temperature thresholds 40, 50, and 60 K allow effective evaporation of CO and CH4, delaying their accumulation in ices. We find that the 40 K threshold is the most effective cosmic-ray-induced whole-grain heating regime because its induced evaporation of CO promotes major abundance changes also for other compounds. An important role in grain cooling may be played by molecular nitrogen as the most volatile of the abundant species in the icy mantles. Whole-grain heating determines the sequence of accretion for different molecules on to grain surface, which plays a key role in the synthesis of complex organic molecules.

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Full-text URL: https://arxiv.org/abs/1904.11368

The Case of H2C3O Isomers, Revisited: Solving the Mystery of the Missing Propadienone

Christopher N. Shingledecker, Sonia Álvarez-Barcia, Viktoria H. Korn, Johannes Kästner

To date, two isomers of H2C3O have been detected, namely, propynal (HCCCHO) and cylclopropenone (c-H2C3O). A third, propadienone (CH2CCO), has thus far eluded observers despite the fact that it is the lowest in energy of the three. This previously noted result is in contradiction of the minimum energy principle, which posits that the abundances of isomers in interstellar environments can be predicted based on their relative stabilities - and suggests, rather, the importance of kinetic over thermodynamic effects in explaining the role of such species. Here, we report results of \textit{ab initio} quantum chemical calculations of the reaction between H and (a) HC3O, (b) H2C3O (both propynal and propadienone), and (c) CH2CHCO. We have found that, among all possible reactions between atomic hydrogen and either propadienone or propynal, only the destruction of propadienone is barrierless and exothermic. That this destruction pathway is indeed behind the non-detection of CH2CCO is further suggested by our finding that the product of this process, the radical CH2CHCO, can subsequently react barrierlessly with H to form propenal (CH2CHCHO) which has, in fact, been detected in regions where the other two H2C3O isomers are observed. Thus, these results not only shed light on a previously unresolved astrochemical mystery, but also further highlight the importance of kinetics in understanding the abundances of interstellar molecules.

ApJ, accepted
Full-text URL: https://arxiv.org/abs/1904.11396

Announcements

PhD positions in astrochemistry at University of Le Havre Normandie

Two PhD positions in the field of astrochemistry and molecular astrophysics are available at University of Le Havre Normandie (France) under the supervision of

François Lique.
The first PhD project will be devoted to the study of the collisional excitation of reactive hydrides in the framework of the COLLEXISM project. COLLEXSIM is an ERC consolidator Grant project set to develop a new theoretical approach to study the collisional energy transfer in reactive systems of astrophysical interest. In this project, we plan to set up a new methodology based on quantum approach that allows obtaining accurate collisional rate coefficients, essential for accurately determining the molecular abundance in the interstellar medium. We will carry out the determination of interaction potentials using quantum chemistry ab initio methods while the treatment of the dynamics of the nuclei will primarily be done using quantum time-independent reactive and non-reactive approaches. The new collisional data will then be used in radiative transfer models and the predictions will be finally compared to observations in order to derive the abundances of reactive radicals with unprecedented accuracy.
The second PhD project will be devoted to the study of the spectroscopy and collisional energy transfer in water containing aggregates. Water is the dominant species in the coma of comets and is ubiquitous in the interstellar medium. It is then crucial to study the interaction of water with interstellar and cometary molecules. We plan to spectroscopically characterize the X-H2O (X=CO, HF, CN) van der Waals complexes and to study the collisional energy transfer in these complexes. As for the first project, we will carry out the determination of interaction potentials using quantum chemistry ab initio methods. The dynamics will be studied using both quantum and statistical approaches.
The two projects will be performed in close collaborations with Alexandre Faure and Pierre Hily Blant from the observatory of Grenoble (France).
The successful candidates will have a strong background in fundamental physics or astrophysics. He/She must have a good knowledge of atomic and molecular physics and a good knowledge of programming tools.
Starting September 2019 for a period of 3 years.
Salary: 1400 euros / month - health insurance included
Inquiries and applications, including a CV should be addressed to François Lique

3-years postdoc position in the field of astrochemistry and molecular astrophysics

A 3-years postdoc position in the field of astrochemistry and molecular astrophysics is available at University of Le Havre Normandie (France) under the supervision of François Lique.
The research project will be devoted to the study of the collisional excitation of reactive hydrides in the framework of the COLLEXISM project. In particular, the research work of the selected postdoc will focus on the calculation of new potential energy surfaces (PES) to study the collisional energy transfer in OH+/H2O+/H3O+ - H/H2 systems. Highly correlated quantum chemistry methods will be used to generate global PESs and these PESs will then be used in quantum scattering calculations. COLLEXSIM is an ERC consolidator Grant project set to develop new theoretical approach to study the collisional energy transfer in reactive systems of astrophysical interest. In this project, we plan to set up a new methodology based on quantum approach that allows obtaining accurate collisional rate coefficients, essential for accurately determining the molecular abundance in the interstellar medium. We will carry out the determination of interaction potentials using quantum chemistry ab initio methods while the treatment of the dynamics of the nuclei will primarily be done using quantum time-independent reactive and non-reactive approaches. The new collisional data will then be used in radiative transfer models and the predictions will be finally compared to observations in order to derive the abundances of reactive radicals with unprecedented accuracy.
The research project will be performed in close collaborations with Alexandre Faure and

Pierre Hily Blant from the observatory of Grenoble (France).
Candidates should have a strong background in quantum chemistry.
Starting September 2019 for a period of 3 years.
Salary: 2500 euros / month - health insurance included
Inquiries and applications, including a CV, statement of research interests, and the names and addresses of two references should be addressed to François Lique
francois.lique@univ-lehavre.fr

17 PhD fellowships in Astrochemistry

We are pleased to announce the opening of 17 Early Stage Researchers (ESRs) positions to carry out PhD thesis in astrochemistry within the Astro-Chemical Origins (ACO) project. ACO is a European Training Network (ETN) funded by European Commission under the Horizon 2020 Marie Sklodowska-Curie Action.
The scientific goal of ACO is to unveil the early history of the Solar System, using the chemical composition of today forming Solar-like planetary systems and comparing it with that of the Solar System primitive bodies. To achieve this goal, ACO is constituted by a multidisciplinary network of twenty-one academic and non-academic partners in four different countries and covering the following major different areas: millimeter wavelengths instrumentation, astronomical observations and modeling, star formation, theoretical and experimental chemistry, and advanced data modeling analysis tools.
The project ACO will recruit 17 ESRs in thirteen institutes of the four countries (France, Italy, United Kingdom and Spain) that form the network.
All the information is reported in the ACO web site: https://aco-itn.oapd.inaf.it/job-opportunities
The list of the 17 offered position can be found at: https://aco-itn.oapd.inaf.it/job-opportunities/aco-esr-positions
Successful applicants will be offered a 36-month employee contract at one of the thirteen beneficiaries, and receive a salary for ESRs set out by the Marie Skłodowska-Curie Actions (MSCA) regulations. The salary includes a living allowance, a mobility allowance and, if appropriate, a family allowance.
In order to apply, please send a mail to the email address aco-esrN@univ-grenoble-alpes.fr, where N is the number of the ESR (see https://aco-itn.oapd.inaf.it/job-opportunities/aco-esr-positions), within the 2nd June 2019.
In the mail, please include a letter of interest, a CV in pdf format and at least one recommendation letter.
European and non-European students are invited to apply to any of the seventeen fellowships. To be eligible, the candidate needs to:
- be in the first four years of her/his research career, since, e.g., completion of master degree, and not have been awarded a doctoral degree;
- must not have resided or carried out their main activity (work, studies, etc...) in the country of the institution that recruits the student for more than 12 months in the 3 years immediately before the recruitment date;
- be willing to spend at least 6 months in another institute/country of the network during the PhD thesis period.

John H. Black Symposium, 24-28 June, 2019

The registration deadline for “Astrochemistry: From nanometers to megaparsecs - A symposium in honour of John H. Black” is coming up: 17 May 2019.
For more information please visit the website:
http://www.chalmers.se/en/conference/JHBlacksymp2019/