

# AstroChemical Newsletter #53

April 2020

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

### **Perturbation of the Surface of Amorphous Solid Water by the Adsorption of Polycyclic Aromatic Hydrocarbons**

**E Michoulier, C Toubin, A Simon, J Mascetti, C Aupetit, and JA Noble**

This joint theoretical and experimental study establishes that the adsorption of polycyclic aromatic hydrocarbons (PAHs) onto the amorphous ice surface provokes a broadening and redshift of the “dangling” OH (dOH) ice spectral feature, the redshift increasing with PAH size up to  $\sim 85$   $\text{cm}^{-1}$ . It also reveals that, in certain interaction configurations, adsorption induces substantial reorganization of the hydrogen-bonding network at the ice surface. Comparison with experiments validates the novel theoretical methodology relying on the density functional-based tight binding approach, which offers a compromise between the system size and accuracy, enabling a wide sampling of surface structures. Applied in an astrophysical context, this study suggests that widening of the dOH feature by adsorption of aromatic molecules could explain its absence heretofore in observational ice spectra, offering hope that future missions with higher sensitivity will verify its presence or absence in dense regions.

2020 J Phys Chem C, 124, 2994

DOI: [10.1021/acs.jpcc.9b09499](https://doi.org/10.1021/acs.jpcc.9b09499)

Full-text URL: <https://arxiv.org/abs/2003.02098>

### **An ALMA view of SO and SO<sub>2</sub> around oxygen-rich AGB stars**

**T. Danilovich, A. M. S. Richards, L. Decin, M. Van de Sande, C. A. Gottlieb**

We present and analyse SO and SO<sub>2</sub>, recently observed with high angular resolution and sensitivity in a spectral line survey with ALMA, for two oxygen-rich AGB stars: the low mass-loss rate R Dor and high mass-loss rate IK Tau. We analyse 8 lines of SO detected towards both stars, 78 lines of SO<sub>2</sub> detected towards R Dor and 52 lines of SO<sub>2</sub> detected towards IK Tau. We detect several lines of <sup>34</sup>SO, <sup>33</sup>SO and <sup>34</sup>SO<sub>2</sub> towards both stars, and tentatively S<sup>18</sup>O towards R Dor, and hence derive isotopic ratios for these species. The spatially resolved observations show us that the two sulphur oxides are co-located towards R Dor and trace out the same wind structures in the circumstellar envelope (CSE). Much of the emission is well reproduced with a Gaussian abundance distribution spatially centred on the star. Emission from the higher energy levels of SO and SO<sub>2</sub> towards R Dor provide evidence in support of a rotating inner region of gas identified in earlier work. The new observations allow us to refine the abundance distribution of SO in IK Tau derived from prior observations with single antennas, and confirm the distribution is shell-like with the peak in the fractional abundance not centred on the star. The confirmation of different types of SO abundance distributions will help fine-tune chemical models and allows for an additional

method to discriminate between low and high mass-loss rates for oxygen-rich AGB stars.

Accepted in MNRAS

DOI: [10.1093/mnras/staa693](https://doi.org/10.1093/mnras/staa693)

Full-text URL: <https://arxiv.org/abs/2003.04334>

## **PORTAL: Three-dimensional polarized (sub)millimeter line radiative transfer**

**Boy Lankhaar, Wouter Vlemmings**

**Context.** Magnetic fields are important to the dynamics of many astrophysical processes and can typically be studied through polarization observations. Polarimetric interferometry capabilities of modern (sub)millimeter telescope facilities have made it possible to obtain detailed velocity resolved maps of molecular line polarization. To properly analyze these for the information they carry regarding the magnetic field, the development of adaptive three-dimensional polarized line radiative transfer models is necessary. **Aims.** We aim to develop an easy-to-use program to simulate the polarization maps of molecular and atomic (sub)millimeter lines in magnetized astrophysical regions, such as protostellar disks, circumstellar envelopes, or molecular clouds. **Methods.** By considering the local anisotropy of the radiation field as the only alignment mechanism, we can model the alignment of molecular or atomic species inside a regular line radiative transfer simulation by only making use of the converged output of this simulation. Calculations of the aligned molecular or atomic states can subsequently be used to ray trace the polarized maps of the three-dimensional simulation. **Results.** We present a three-dimensional radiative transfer code, POLarized Radiative Transfer Adapted to Lines (PORTAL), that can simulate the emergence of polarization in line emission through a magnetic field of arbitrary morphology. Our model can be used in stand-alone mode, assuming LTE excitation, but it is best used when processing the output of regular three-dimensional (nonpolarized) line radiative transfer modeling codes. We present the spectral polarization map of test cases of a collapsing sphere and protoplanetary disk for multiple three-dimensional magnetic field morphologies.

Accepted in A&A

DOI: [10.1051/0004-6361/202037509](https://doi.org/10.1051/0004-6361/202037509)

Full-text URL: <https://arxiv.org/abs/2003.04331>

## **Do defects in PAHs promote catalytic activity in space? Stone-Wales pyrene as a test case**

**D. Campisi and A. Candian**

Using density functional theory (DFT), we studied the formation of Stone–Wales defects in pyrene, as a prototype PAH molecule. In addition, we studied the reactivity of the defective and pristine pyrenes toward hydrogenation, a process that can occur in some regions of the interstellar medium. We found that the formation of the defect requires overcoming energies of the order of 8.4 eV, but the defective structure is stable due to the high reverse reaction barrier (approx. 6 eV). We also found that the presence of the defect decreases the sticking barrier for the first hydrogenation and promotes more stable singly and doubly hydrogenated intermediates with respect to that of the pristine pyrene. Finally, our results show that both Stone–Wales pyrene and pristine pyrenes can lead to the formation of H<sub>2</sub> through an extraction mechanism involving H atoms attached on distal carbon atoms with energy barriers below 2 eV.

## Exploring molecular complexity with ALMA (EMoCA): Complex isocyanides in Sgr B2(N)

**E. R. Willis, R. T. Garrod, A. Belloche, H. S. P. Müller, C. J. Barger, M. Bonfand, K. M. Menten**

We used the EMOCA survey data to search for isocyanides in Sgr B2(N2) and their corresponding cyanide analogs. We then used the coupled three-phase chemical kinetics code MAGICKAL to simulate their chemistry. Several new species, and over 100 new reactions have been added to the network. In addition, a new single-stage simultaneous collapse/warm-up model has been implemented, thus eliminating the need for the previous two-stage models. A variable, visual extinction-dependent  $\zeta$  was also incorporated into the model and tested. We report the tentative detection of CH<sub>3</sub>NC and HCCNC in Sgr B2(N2), which represents the first detection of both species in a hot core of Sgr B2. Our updated chemical models can reproduce most observed NC:CN ratios reasonably well depending on the physical parameters chosen. The model that performs best has an extinction-dependent cosmic-ray ionization rate that varies from  $\sim 2 \times 10^{-15} \text{ s}^{-1}$  at the edge of the cloud to  $\sim 1 \times 10^{-16} \text{ s}^{-1}$  in the center. Models with higher extinction-dependent  $\zeta$  than this model generally do not agree as well, nor do models with a constant  $\zeta$  greater than the canonical value of  $1.3 \times 10^{-17} \text{ s}^{-1}$  throughout the source. Radiative transfer models are run using results of the best-fit chemical model. Column densities produced by the radiative transfer models are significantly lower than those determined observationally. Inaccuracy in the observationally determined density and temperature profiles is a possible explanation. Excitation temperatures are well reproduced for the true "hot core" molecules, but are more variable for other molecules such as HC<sub>3</sub>N, for which fewer lines exist in ALMA Band 3.

Accepted in Astronomy & Astrophysics

DOI: [10.1051/0004-6361/201936489](https://doi.org/10.1051/0004-6361/201936489)

Full-text URL: <https://arxiv.org/abs/2003.07423>

## The infrared view of dust and molecules around V4334 Sgr (Sakurai's object): a 20-yr retrospective

**A. Evans, R. D. Gehrz, C. E. Woodward, D. P. K. Banerjee, T. R. Geballe, G. C. Clayton, P. J. Sarre, S. Starrfield, K. Hinkle, R. R. Joyce, Foteini Lykou, L. A. Helton, S. P. S. Eyres, H. Worters, E. J. Montiel, T. Liimets, A. Zijlstra, M. Richter J. Krautter**

We present an analysis of the evolution of circumstellar dust and molecules in the environment of the very late thermal pulse object V4334 Sgr (Sakurai's object) over a 20-yr period, drawing on ground-, airborne-, and space-based infrared photometry and spectroscopy. The dust emission, which started in 1997, resembles a blackbody that cooled from  $\sim 1200 \text{ K}$  in 1998 August to  $\sim 180 \text{ K}$  in 2016 July. The dust mass, assuming amorphous carbon, was  $\sim 5 \times 10^{-10} \text{ M}_{\text{sun}}$  in 1998 August, and we estimate that the total dust mass was  $\sim 2 \times 10^{-5} \text{ M}_{\text{sun}}$  by  $\sim 2016$ . The appearance of a near-infrared excess in 2008 suggests that a new episode of (or renewed) mass-loss began then. We infer lower limits on the bolometric luminosity of the embedded star from that of the dust shell, which rose to  $\sim 16\,000 \text{ L}_{\text{sun}}$  before declining to  $\sim 3000 \text{ L}_{\text{sun}}$ . There is evidence for weak 6-7 micron absorption, which we attribute to hydrogenated amorphous

carbon formed in material ejected by Sakurai's object during a mass ejection phase that preceded the 1997 event. We detect small hydrocarbon and other molecules in the spectra, and trace the column densities in hydrogen cyanide (HCN) and acetylene (C<sub>2</sub>H<sub>2</sub>). We use the former to determine the <sup>12</sup>C/<sup>13</sup>C ratio to be 6.4±0.7, 14 times smaller than the Solar system value.

Monthly Notices of the RAS, vol. 493, pp 2020, 1277-1291 (2020)

DOI: [10.1093/mnras/staa343](https://doi.org/10.1093/mnras/staa343)

Full-text URL: <https://arxiv.org/abs/2002.00907>

## An imaging line survey of OMC-1 to OMC-3

**N. Brinkmann, F. Wyrowski, J. Kauffmann, D. Colombo, K. M. Menten, X. D. Tang, R. Güsten**

**Aims:** Our aim is to identify the dominant molecular cooling lines and characteristic emission features in the 1.3 mm window of distinct regions in the northern part of the Orion A molecular cloud. By defining and analysing template regions, we also intend to help with the interpretation of observations from more distant sources which cannot be easily spatially resolved. **Methods:** We analyse an imaging line survey covering the area of OMC-1 to OMC-3 from 200.2 to 281.8 GHz obtained with the PI230 receiver at the APEX telescope. Masks are used to define regions with distinct properties (e.g. column density or temperature ranges) from which we obtain averaged spectra. Lines of 29 molecular species (55 isotopologues) are fitted for each region to obtain the respective total intensity. **Results:** We find that strong sources like Orion KL have a clear impact on the emission on larger scales. Although not spatially extended, their line emission contributes substantially to spectra averaged over large regions. Conversely, the emission signatures of dense, cold regions like OMC-2 and OMC-3 (e.g. enhanced N<sub>2</sub>H<sup>+</sup> emission and low HCN/HNC ratio) seem to be difficult to pick up on larger scales, where they are eclipsed by signatures of stronger sources. In all regions, HCO<sup>+</sup> appears to contribute between 3% and 6% to the total intensity, the most stable value for all bright species. N<sub>2</sub>H<sup>+</sup> shows the strongest correlation with column density, but not with typical high-density tracers like HCN, HCO<sup>+</sup>, H<sub>2</sub>CO, or HNC. Common line ratios associated with UV illumination, CN/HNC and CN/HCO<sup>+</sup>, show ambiguous results on larger scales, suggesting that the identification of UV illuminated material may be more challenging. The HCN/HNC ratio may be related to temperature over varying scales.

Accepted by A&A

DOI: [10.1051/0004-6361/201936885](https://doi.org/10.1051/0004-6361/201936885)

Full-text URL: <https://arxiv.org/abs/2003.06842>

## Adsorption of H<sub>2</sub> on Amorphous Solid Water Studied with Molecular Dynamics Simulations

**G. Molpeceres, J. Kästner**

We investigated the behavior of H<sub>2</sub>, main constituent of the gas phase in dense clouds, after collision with amorphous solid water (ASW) surfaces, one of the most abundant chemical species of interstellar ices. We developed a general framework to study the adsorption dynamics of light species on interstellar ices. We provide binding energies and their distribution, sticking probabilities for incident energies between 1 meV and 60 meV, and thermal sticking coefficients between 10 and 300 K for surface temperatures from 10 to 110 K. We found that the sticking probability depends strongly on the adsorbate kinetic energy and the surface temperature, but hardly on the angle of

incidence. We observed finite sticking probabilities above the thermal desorption temperature. Adsorption and thermal desorption should be considered as separate events with separate time scales. Laboratory results for these species have shown a gap in the trends attributed to the differently employed experimental techniques. Our results complement observations and extend them, increasing the range of gas temperatures under consideration. We plan to employ our method to study a variety of adsorbates, including radical and charged species.

Accepted in PCCP

DOI: [10.1039/D0CP00250J](https://doi.org/10.1039/D0CP00250J)

Full-text URL: <https://arxiv.org/abs/2003.08873>

## A new proxy to estimate the cosmic-ray ionisation rate in dense cores

**S. Bovino, S. Ferrada-Chamorro, A. Lupi, D. R. G. Schleicher, P. Caselli**

Cosmic rays are a global source of ionisation, and the ionisation fraction represents a fundamental parameter in the interstellar medium. Ions couple to magnetic fields, affect the chemistry, and the dynamics of star-forming regions as well as planetary atmospheres. However, the cosmic-ray ionisation rate represents one of the bottlenecks for astrochemical models, and its determination is one of the most puzzling problems in astrophysics. While for diffuse clouds reasonable values have been provided from H3<sup>+</sup> observations, for dense clouds, due to the lack of rotational transitions, this is not possible, and estimates are strongly biased by the employed model. We present here an analytical expression, obtained from first principles, to estimate the cosmic-ray ionisation rate from observational quantities. The theoretical predictions are validated with high-resolution three-dimensional numerical simulations and applied to the well known core L1544; we obtained an estimate of  $\zeta \sim 2 - 3 \times 10^{-17} \text{ s}^{-1}$ . Our results and the analytical formulae provided represent the first model-independent, robust tool to probe the cosmic-ray ionisation rate in the densest part of star-forming regions (on spatial scales of  $R \leq 0.05 \text{ pc}$ ). An error analysis is presented to give statistical relevance to our study.

MNRAS Letters Accepted

DOI: [10.1093/mnras/sla048](https://doi.org/10.1093/mnras/sla048)

Full-text URL: <https://arxiv.org/pdf/2003.05416.pdf>

## Announcements

### **PhD opportunity, School of Chemistry, University of Leeds**

The kinetics of astrochemical and planetary reactions studied at very low temperatures. We advertise a PhD opportunity (funded by STFC) in Astrochemistry in the School of Chemistry at the University of Leeds.

Neutral – neutral reactions are important in low temperature environments such as the interstellar medium (ISM), dense molecular clouds of star forming regions and planetary atmospheres. However, the chemical databases used to model such environments contain a relatively small number of this class of reaction and the low-temperature chemistry is poorly understood. We have recently shown [1-4] that despite the presence of an energy barrier, the reaction between the OH radical and ketones, alcohols and ethers can proceed to products rapidly at very low temperatures, which we interpret via a mechanism involving the formation of a weak hydrogen bonded association adduct, and quantum mechanical tunnelling. We propose that this

behaviour may be widespread under the low temperature conditions found in space. The successful candidate will measure rate constants and product branching ratios at very low temperatures using laser flash-photolysis combined with a variety of laser-based spectroscopic detection methods. They will use a pulsed Laval nozzle apparatus to study the kinetics of reactions between ~40 and 150 K representative of the atmospheres of other planets and moons, for example Titan, as well as in star-forming regions, stellar outflows and the interstellar medium. Large molecular clouds of acetone, methanol and ethanol have been observed in space, and the large rate constants can be rationalised by the formation of a hydrogen-bonded complex, which can either be stabilised or undergo quantum mechanical tunnelling through the activation barrier to form products.

The successful candidate will interpret the laboratory measurements using theoretical methods, making use of ab initio potential energy surfaces and master equation calculations (using the MESMER program, developed in Leeds) to calculate rate constants as a function of temperature and pressure. These experiments use laser flash-photolysis combined with laser-induced fluorescence (LIF) spectroscopy, and will be extended to study further reactions of OH, CH<sub>2</sub>, C<sub>2</sub>H, NH<sub>2</sub> and other radicals, and will monitor both reactants and products, using LIF.

The PhD will provide a broad spectrum of training in the use of high power lasers, vacuum systems, optics, computer controlled data acquisition systems and numerical calculations. The successful candidate will work in a well equipped laboratory and be part of the active, thriving and well-funded Atmospheric and Planetary Chemistry group within the School of Chemistry. You will be supported to attend both national and international conferences, and will receive a wide range of training, for example in communication skills and other technical aspects.

For further information please contact Professor Dwayne Heard:

D.E.Heard@leeds.ac.uk

#### References

- [1] R. J. Shannon, M. A. Blitz, A. Goddard & D. E. Heard, *Nature Chemistry*, 5, 745-749, 2013
- [2] R. J. Shannon, S. Taylor, A. Goddard, M. A. Blitz & D. E. Heard, *Phys. Chem. Chem. Phys.*, 2010, 12, 13511-13514
- [3] R.J. Shannon, R. L. Caravan, M.A. Blitz & D.E. Heard, *Phys. Chem. Chem. Phys.*, 16, 3466, 2014
- [4] R.L. Caravan, R. J. Shannon, T. Lewis, M. A. Blitz & D. E. Heard, *J. Phys. Chem.*, DOI: 10.1021/jp505790m, 2014.

## **Chemical Processes in Solar-Type Star Forming Regions**

jointly organized by the Department of Chemistry of the University of Torino and INAF Astrophysical Observatory of Arcetri in the context of the EU H2020 ITN project AstroChemical Origins (ACO).

The meeting will consist of invited reviews, invited and contributed talks, and posters. Support for PhD and young students is also planned.

Conference site: Department of Chemistry, University of Torino, Italy

Conference dates: 13th - 17th September 2021

Registration deadline: 20th May 2021

Abstract submission deadline: 1st May 2021

The announcement of the conference is available on the web at:

<https://sites.google.com/inaf.it/aco-conference/>

Rationale:

How the chemical complexity evolves during the process leading to the formation of a Sun and its planetary system? Is the chemical richness of a Solar-like planetary system, at least partially, inherited from the earliest stages or is there a complete chemical

reset? A powerful way to answering these questions is by comparing the chemical content in young protostars and primitive bodies of the Solar System, using astrochemistry as a tool. Yet, to do so, we need to fully understand the processes that govern the chemical evolution of a molecular cloud into a young planetary system. The goal of the conference is to gather together the actors of this intrinsically interdisciplinary endeavor: astronomers, chemists and modelers. The recent huge progresses in the three areas make the time ripe for these communities to join and ride this scientific wave.

We invite all of you to join the Conference.

The Scientific Organizing Committee

P. Ugliengo, C. Codella, A. Barucci, C. Ceccarelli, L. Piccirillo, A. Rimola, C. Vastel, S. Viti, S. Yamamoto