AstroChemical Newsletter #95

October 2023

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

Linking ice and gas in the Coronet cluster in Corona Australis

G. Perotti, J. K. Jørgensen, W. R. M. Rocha, A. Plunkett, E. Artur de la Villarmois, L. E. Kristensen, M. Sewiło, P. Bjerkeli, H. J. Fraser, S. B. Charnley

During the journey from the cloud to the disc, the chemical composition of the protostellar envelope material can be either preserved or processed to varying degrees depending on the surrounding physical environment. This works aims to constrain the interplay of solid (ice) and gaseous methanol (CH3OH) in the outer regions of protostellar envelopes located in the Coronet cluster in Corona Australis (CrA), and assess the importance of irradiation by the Herbig Ae/Be star R CrA. CH3OH is a prime test-case as it predominantly forms as a consequence of the solid-gas interplay (hydrogenation of condensed CO molecules onto the grain surfaces) and it plays an important role in future complex molecular processing. We present 1.3 mm Submillimeter Array (SMA) and Atacama Pathfinder Experiment (APEX) observations towards the envelopes of four low-mass protostars in the Coronet. Eighteen molecular transitions of seven species are identified. We calculate CH3OH gas-to-ice ratios in this strongly irradiated cluster and compare them with ratios determined towards protostars located in less irradiated regions such as the Serpens SVS 4 cluster in Serpens Main and the Barnard 35A cloud in the λ Orionis region. The CH3OH gas-to-ice ratios in the Coronet vary by one order of magnitude (from 1.2e−4 to 3.e−3) which is similar to less irradiated regions as found in previous studies. We find that the CH3OH gas-to-ice ratios estimated in these three regions are remarkably similar despite the different UV radiation field intensities and formation histories. This result suggests that the overall CH3OH chemistry in the outer regions of low-mass envelopes is relatively independent of variations in the physical conditions and hence that it is set during the prestellar stage.

Accepted for publication in Astronomy & Astrophysics
DOI: 10.1051/0004-6361/202245541
Full-text URL: https://arxiv.org/abs/2308.13598

The unusual 3D distribution of NaCl around the asymptotic giant branch star IK Tau

A. Coenegrachts, T. Danilovich, F. De Ceuster, and L. Decin

Context. Sodium chloride (NaCl) is a diatomic molecule with a large dipole moment, which allows for its detection even at relatively low abundances. It has been detected towards several evolved stars, including the asymptotic giant branch (AGB) star IK Tau, around which it is distributed in several clumps that lie off-centre from the star. Aims. We aim to study the 3D distribution of NaCl around the AGB star IK Tau and determine

the abundance of NaCl relative to H2 for each of the clumps. Methods. First, a new value for the maximum expansion velocity was determined. The observed ALMA channel maps were then de-projected to create a 3D model of the distribution of NaCl. This model was then used as input for the radiative transfer modelling code Magritte. We determined the NaCl abundances of each of the clumps by comparing the observations with the results of the Magritte simulations. Results. We derive an updated value for the maximum expansion velocity of IK Tau: υexp = 28.4 ± 1.7 km s−1. A spiral-like shape can be discerned in our 3D distribution model of NaCl. This spiral lies more or less in the plane of the sky, with the distribution flatter in the line-of-sight direction than in the plane of the sky. We find clump abundances of between 9e-9 and 5e−8 relative to H2; the relative abundance is typically lower for clumps closer to the star. Conclusions. This is the first time de-projection has been used to understand the 3D environment of molecular emission around an AGB star and to calculate the fractional abundance of NaCl in clumps surrounding the star.

Accepted for publication in Astronomy & Astrophysics
DOI: 10.1051/0004-6361/202346116
Full-text URL: https://arxiv.org/abs/2302.06221

The extremely sharp transition between molecular and ionized gas in the Horsehead nebula

C. Hernández-Vera, V. V. Guzmán, J. R. Goicoechea, V. Maillard, J. Pety, F. Le Petit, M. Gerin, E. Bron, E. Roueff, A. Abergel, T. Schirmer, J. Carpenter, P. Gratier, K. Gordon, K. Misselt

(Abridged) Massive stars can determine the evolution of molecular clouds with their strong ultraviolet (UV) radiation fields. Moreover, UV radiation is relevant in setting the thermal gas pressure in star-forming clouds, whose influence can extend from the rims of molecular clouds to entire star-forming galaxies. Probing the fundamental structure of nearby molecular clouds is therefore crucial to understand how massive stars shape their surrounding medium and how fast molecular clouds are destroyed, specifically at their UV-illuminated edges, where models predict an intermediate zone of neutral atomic gas between the molecular cloud and the surrounding ionized gas whose size is directly related to the exposed physical conditions. We present the highest angular resolution (~0.5", corresponding to 207 au) and velocity-resolved images of the molecular gas emission in the Horsehead nebula, using CO J=3-2 and HCO+ J=4-3 observations with ALMA. We find that CO and HCO+ are present at the edge of the cloud, very close to the ionization (H+/H) and dissociation fronts (H/H2), suggesting a very thin layer of neutral atomic gas (<650 au) and a small amount of CO-dark gas (Av=0.006−0.26 mag) for stellar UV illumination conditions typical of molecular clouds in the Milky Way. The new ALMA observations reveal a web of molecular gas filaments with an estimated thermal gas pressure of Pth=(2.3−4.0)×1e6 K cm−3, and the presence of a steep density gradient at the cloud edge that can be well explained by stationary isobaric PDR models with pressures consistent with our estimations. However, in the HII region and PDR interface, we find Pth,PDR>Pth,HII, suggesting the gas is slightly compressed. Therefore, dynamical effects cannot be completely ruled out and even higher angular observations will be needed to unveil their role.

Accepted in Astronomy & Astrophysics
DOI: 10.1051/0004-6361/202347206
Full-text URL: https://arxiv.org/abs/2307.09540

Aromatic cycles are widespread in cold clouds

M. Agundez, N. Marcelino, B. Tercero, J. Cernicharo

We report the detection of large hydrocarbon cycles toward several cold dense clouds. We observed four sources (L1495B, Lupus-1A, L483, and L1527) in the Q band (31-50 GHz) using the Yebes 40m radiotelescope. Using the line stack technique, we find statistically significant evidence of benzonitrile (C6H5CN) in L1495B, Lupus-1A, and L483 at levels of 31.8σ, 15.0σ, and 17.2σ, respectively, while there is no hint of C6H5CN in the fourth source, L1527. The column densities derived are in the range (1.7-3.8)×1e11 cm−2, which is somewhat below the value derived toward the cold dense cloud TMC-1. When we simultaneously analyze all the benzonitrile abundances derived toward cold clouds in this study and in the literature, a clear trend emerges in that the higher the abundance of HC7N, the more abundant C6H5CN is. This indicates that aromatic cycles are especially favored in those interstellar clouds where long carbon chains are abundant, which suggests that the chemical processes that are responsible for the formation of linear carbon chains are also behind the synthesis of aromatic rings. We also searched for cycles other than benzonitrile, and found evidence of indene (C9H8), cyclopentadiene (C5H6), and 1-cyano cyclopentadiene (1-C5H5CN) at levels of 9.3σ, 7.5σ, and 8.4σ, respectively, toward L1495B, which shows the strongest signal from C6H5CN. The relative abundances between the various cycles detected in L1495B are consistent -- within a factor of three -- with those previously found in TMC-1. It is therefore likely that not only C6H5CN but also other large aromatic cycles are abundant in clouds rich in carbon chains.

Accepted for publication in A&A Letters.
DOI: 10.1051/0004-6361/202347524
Full-text URL: https://arxiv.org/abs/2308.15951

The abundance and excitation of molecular anions in interstellar clouds

M. Agundez, N. Marcelino, B. Tercero, I. Jimenez-Serra, J. Cernicharo

We report new observations of molecular anions with the Yebes 40m and IRAM 30m telescopes toward the cold dense clouds TMC-1 CP, Lupus-1A, L1527, L483, L1495B, and L1544. We detected for the first time C3N- and C5N- in Lupus-1A and C4H- and C6H- in L483. In addition, we report new lines of C6H- toward the six targeted sources, of C4H- toward TMC-1 CP, Lupus-1A, and L1527, and of C8H- and C3N- in TMC-1 CP. Excitation calculations indicate that the lines of anions accessible to radiotelescopes run from subthermally excited to thermalized as the size of the anion increases, with the degree of departure from thermalization depending on the H2 volume density and the line frequency. We noticed that the collision rate coefficients available for the radical C6H cannot explain various observational facts, which advises for a revisitation of the collision data for this species. The observations presented here, together with observational data from the literature, are used to model the excitation of interstellar anions and to constrain their abundances. In general, the anion-to-neutral ratios derived here agree within 50 % (a factor of two at most) with literature values, when available, except for the C4H-/C4H ratio, which shows higher differences due to a revision of the dipole moment of C4H. From the set of anion-to-neutral abundance ratios derived two conclusions can be drawn. First, the C6H-/C6H ratio shows a tentative trend in which it increases with increasing H2 density, as expected from theoretical grounds. And second, it is incontestable that the higher the molecular size the higher the anion-to-neutral ratio, which supports a formation mechanism based on radiative electron attachment. Nonetheless, calculated rate coefficients for electron attachment to the medium size species C4H and C3N are probably too high and too

low, respectively, by more than one order of magnitude.

Accepted for publication in A&A. arXiv:2307.04487
DOI: 10.1051/0004-6361/202347077
Full-text URL: https://arxiv.org/abs/2307.04487

ALMA observations of the Extended Green Object G19.01-0.03: II. A massive protostar with typical chemical abundances surrounded by four low-mass prestellar core candidates

G. M. Williams, C. J. Cyganowski, C. L. Brogan, T. R. Hunter, P. Nazari, R. J. Smith

We present a study of the physical and chemical properties of the Extended Green Object (EGO) G19.01-0.03 using sub-arcsecond angular resolution Atacama Large Millimeter/submillimeter Array (ALMA) 1.05mm and Karl G. Jansky Very Large Array (VLA) 1.21cm data. G19.01-0.03 MM1, the millimetre source associated with the central massive young stellar object (MYSO), appeared isolated and potentially chemically young in previous Submillimeter Array observations. In our ~0.4"-resolution ALMA data, MM1 has four low-mass millimetre companions within 0.12pc, all lacking maser or outflow emission, indicating they may be prestellar cores. With a rich ALMA spectrum full of complex organic molecules, MM1 does not appear chemically young, but has molecular abundances typical of high-mass hot cores in the literature. At the 1.05mm continuum peak of MM1, N(CH3OH)=(2.22+/-0.01 x 1e18cm-2 and T_ex = 162.7(+0.3,-0.5)K based on pixel-by-pixel Bayesian analysis of LTE synthetic methanol spectra across MM1. Intriguingly, the peak CH3OH T_ex=165.5+/-0.6K is offset from MM1's millimetre continuum peak by 0.22"~880au, and a region of elevated CH3OH T_ex coincides with free-free VLA 5.01cm continuum, adding to the tentative evidence for a possible unresolved high-mass binary in MM1. In our VLA 1.21cm data, we report the first NH3(3,3) maser detections towards G19.01-0.03, along with candidate 25GHz CH3OH 5(2,3)-5(1,4) maser emission; both are spatially and kinematically coincident with 44GHz Class I CH3OH masers in the MM1 outflow. We also report the ALMA detection of candidate 278.3GHz Class I CH3OH maser emission towards this outflow, strengthening the connection of these three maser types to MYSO outflows.

Accepted for publication in MNRAS
DOI: 10.1093/mnras/stad2677
Full-text URL: https://arxiv.org/abs/2309.01743

Protonated hydrogen cyanide as a tracer of pristine molecular gas

Gong, Y. ; Du, F. J. ; Henkel, C. ; Jacob, A. M. ; Belloche, A. ; Wang, J. Z. ; Menten, K. M. ; Yang, W. ; Quan, D. H. ; Bop, C. T. ; Ortiz-León, G. N. ; Tang, X. D. ; Rugel, M. R. ; Liu, S.

Protonated hydrogen cyanide, HCNH+, plays a fundamental role in astrochemistry because it is an intermediary in gas-phase ion-neutral reactions within cold molecular clouds. However, the impact of the environment on the chemistry of HCNH+ remains poorly understood. With the IRAM-30 m and APEX-12 m observations, we report the first robust distribution of HCNH+ in the Serpens filament and in Serpens South. Our data suggest that HCNH+ is abundant in cold and quiescent regions, but is deficit in active star-forming regions. The observed HCNH+ fractional abundances relative to H2 range from 3.1e−11 in protostellar cores to 5.9×10−10 in prestellar cores, and the HCNH+ abundance generally decreases with increasing H2 column density, which

suggests that HCNH+ coevolves with cloud cores. Our observations and modeling results suggest that the abundance of HCNH+ in cold molecular clouds is strongly dependent on the H2 number density. The decrease in the abundance of HCNH+ is caused by the fact that its main precursors (e.g., HCN and HNC) undergo freeze-out as the number density of H2 increases. However, current chemical models cannot explain other observed trends, such as the fact that the abundance of HCNH+ shows an anti-correlation with that of HCN and HNC, but a positive correlation with that of N2H+ in the southern part of the Serpens South northern clump. This indicates that additional chemical pathways have to be invoked for the formation of HCNH+ via molecules like N2 in regions in which HCN and HNC freeze out. Both the fact that HCNH+ is most abundant in molecular cores prior to gravitational collapse and the fact that low-J HCNH+ transitions have very low H2 critical densities make this molecular ion an excellent probe of pristine molecular gas.

accepted for publication in A&A
DOI: 10.1051/0004-6361/202347409
Full-text URL: https://arxiv.org/abs/2308.15521

A high HDO/H2O ratio in the Class I protostar L1551 IRS5

A. Andreu, A. Coutens, F. Cruz-Sáenz de Miera, N. Houry, J. K. Jørgensen, A. Kóspál, D. Harsono

Water is a very abundant molecule in star-forming regions. Its deuterium fractionation provides an important tool for understanding its formation and evolution during the star and planet formation processes. While the HDO/H2O abundance ratio has been determined toward several young Class 0 protostars and comets, the number of studies toward Class I protostars is limited. Our aim is to study the water deuteration toward the Class I protostellar binary L1551 IRS5 and to investigate the effect of evolutionary stage and environment on variations in the water D/H ratio. Observations were carried out toward L1551 IRS5 using the NOrthern Extended Millimeter Array (NOEMA) interferometer. The HDO (3,1,2–2,2,1) transition at 225.9 GHz and the H182O (3,1,3–2,2,0) transition at 203.4 GHz were covered with a spatial resolution of 0.5″× 0.8″, while the HDO (4,2,2–4,2,3) transition at 143.7 GHz was observed with a resolution of 2.0″ × 2.5". We constrained the water D/H ratio using both local thermodynamic equilibrium (LTE) and non-LTE models. The three transitions are detected. The line profiles display two peaks, one at ∼ 6 km s−1 and one at ∼ 9 km s−1. We derive an HDO/H2O ratio of (2.1 ± 0.8) × 1e−3 for the redshifted component and a lower limit of > 0.3 × 1e−3 for the blueshifted component. This lower limit is due to the blending of the blueshifted H182O component with redshifted CH3OCH3 emission. The HDO/H2O ratio in L1551 IRS5 is similar to the values in Class 0 isolated sources and in the disk of the Class I protostar V883 Ori, while it is significantly higher than in the previously studied clustered Class 0 sources and the comets. This result suggests that the chemistry of protostars that belong to molecular clouds with relatively low source densities, such as L1551, share more similarities with the isolated sources than the protostars of very dense clusters. If the HDO/H2O ratios in Class 0 protostars with few sources around are comparable to those found to date in isolated Class 0 objects, it would mean that there is little water reprocessing from the Class 0 to Class I protostellar stage.

Accepted in A&A
DOI: 10.1051/0004-6361/202347484
Full-text URL: https://arxiv.org/abs/2309.01688

Surface diffusion of carbon atoms as a driver of interstellar organic chemistry

M. Tsuge, G. Molpeceres, Y. Aikawa, N. Watanabe

Many interstellar complex organic molecules (COMs) are believed to be produced on the surfaces of icy grains at low temperatures. Atomic carbon is considered responsible for the skeletal evolution processes, such as C–C bond formation, via insertion or addition reactions. Before reactions, C atoms must diffuse on the surface to encounter reaction partners; therefore, information on their diffusion process is critically important for evaluating the role of C atoms in the formation of COMs. In situ detection of C atoms on ice was achieved by a combination of photostimulated desorption and resonance-enhanced multiphoton ionization methods. We found that C atoms weakly bound to the ice surface diffused above approximately 30 K and produced C2 molecules. The activation energy for C-atom surface diffusion was experimentally determined to be 88 meV (1,020 K), indicating that the diffusive reaction of C atoms is activated at approximately 22 K on interstellar ice. The facile diffusion of C atoms at temperatures above 22 K on interstellar ice opens a previously overlooked chemical regime where the increase in complexity of COMs is driven by C atoms. Carbon addition chemistry can be an alternative source of chemical complexity in translucent clouds and protoplanetary disks with crucial implications in our current understanding on the origin and evolution of organic chemistry in our Universe.

Published in Nature Astronomy
DOI: 10.1038/s41550-023-02071-0
Full-text URL: https://arxiv.org/abs/2308.02181

Deep learning denoising by dimension reduction: Application to the ORION-B line cubes

L. Einig, J. Pety, A. Roueff, P. Vandame, J. Chanussot, M. Gerin, J.H. Orkisz, P. Palud, M.G. Santa-Maria, V. de Souza Magalhaes, I. Bešlić, S. Bardeau, E. Bron, P. Chainais, J.R. Goicoechea, P. Gratier, V.V. Guzman, A. Hughes, J. Kainulainen, D. Languignon, R. Lallement, F. Levrier, D.C. Lis, H.S. Liszt, J. Le Bourlot, F. Le Petit, K. Öberg, N. Peretto, E. Roueff, A. Sievers, P.-A. Thouvenin, P. Tremblin

The availability of large bandwidth receivers for millimeter radio telescopes allows the acquisition of position-position-frequency data cubes over a wide field of view and a broad frequency coverage. These cubes contain much information on the physical, chemical, and kinematical properties of the emitting gas. However, their large size coupled with inhomogenous signal-to-noise ratio (SNR) are major challenges for consistent analysis and interpretation. We search for a denoising method of the low SNR regions of the studied data cubes that would allow to recover the low SNR emission without distorting the signals with high SNR. We perform an in-depth data analysis of the 13CO and C17O (1 − 0) data cubes obtained as part of the ORION-B large program performed at the IRAM 30m telescope. We analyse the statistical properties of the noise and the evolution of the correlation of the signal in a given frequency channel with that of the adjacent channels. This allows us to propose significant improvements of typical autoassociative neural networks, often used to denoise hyperspectral Earth remote sensing data. Applying this method to the 13CO (1 − 0) cube, we compare the denoised data with those derived with the multiple Gaussian fitting algorithm ROHSA, considered as the state of the art procedure for data line cubes. The nature of astronomical spectral data cubes is distinct from that of the hyperspectral data usually studied in the Earth remote sensing literature because the

observed intensities become statistically independent beyond a short channel separation. This lack of redundancy in data has led us to adapt the method, notably by taking into account the sparsity of the signal along the spectral axis. The application of the proposed algorithm leads to an increase of the SNR in voxels with weak signal, while preserving the spectral shape of the data in high SNR voxels. The proposed algorithm that combines a detailed analysis of the noise statistics with an innovative autoencoder architecture is a promising path to denoise radio-astronomy line data cubes. In the future, exploring whether a better use of the spatial correlations of the noise may further improve the denoising performances seems a promising avenue. In addition, dealing with the multiplicative noise associated with the calibration uncertainty at high SNR would also be beneficial for such large data cubes.

Astronomy & Astrophysics, 2023
DOI: 10.1051/0004-6361/202346064
Full-text URL: https://arxiv.org/abs/2307.13009

The Perseus ALMA Chemical Survey (PEACHES). III. Sulfur-bearing species tracing accretion and ejection processes in young protostars

E. Artur de la Villarmois, V. V. Guzman, Y.-L. Yang, Y. Zhang, N. Sakai

(Abridged) Sulfur chemistry is poorly understood in the process of low-mass star and planet formation, where the main carriers of sulfur are still unknown. Despite the fact that simple S-bearing molecules are usually detected toward embedded sources, large surveys of S-bearing molecules with high angular resolution and sensitive observations are currently lacking. The goal of this work is to present an unbiased survey of simple sulfur-bearing species in protostars and provide new statistics. In addition, we investigate the role of S-bearing molecules in accretion processes and the connection between (non-)detection of complex organic molecules (COMs) and S-related species. We present the observations of sulfur-bearing species that are part of the Perseus ALMA Chemical Survey (PEACHES). We analyzed a total of 50 Class 0/I sources with an average angular resolution of about 0.6" (~180 au) in ALMA band 6. We present detection rates for CS, SO, 34SO, and SO2. The SO/34SO ratio is lower than the canonical value of 22 and the lowest values are found for those sources rich in COMs. This ratio, therefore, seems to be a good tracer of the inner high-density envelope. The detection of multiple COMs seems to be related to the presence of collimated outflows and SO2 emission seems to trace the warm gas in those sources where CH3OH is also detected. The SO2 abundances toward the PEACHES sample are, on average, two orders of magnitude lower than values from the Ophiuchus star-forming region and comparable with sources in Taurus, suggesting that the sulfur depletion in the gas-phase could depend on the external UV radiation. Finally, the SO2 emission detected in different evolutionary stages seems to arise from different physical mechanisms: high column density of warm material in Class 0 sources, shocks in Class I/II, and exposure to UV radiation from the protostar in more evolved Class II disks.

Accepted in A&A
DOI: 10.1051/0004-6361/202346728
Full-text URL: https://arxiv.org/abs/2309.05839

HCN emission from translucent gas and UV-illuminated cloud edges revealed by wide-field IRAM 30m maps of the Orion B GMC. Revisiting its role as tracer of the dense gas reservoir

for star formation.

M. G. Santa-Maria, J. R. Goicoechea, J. Pety, M. Gerin, J. H. Orkisz, L. Einig, P. Palud, V. de Souza Magalhaes, I. Bešlić, L. Segal, S. Bardeau, E. Bron, P. Chainais, J. Chanussot, P. Gratier, V. V. Guzmán, A. Hughes, D. Languignon, F. Levrier, D. C. Lis, H.S. Liszt, J. Le Bourlot, F. Le Petit, Y. Oya, K. Öberg, N. Peretto, E. Roueff, A. Roueff, A. Sievers, P.-A. Thouvenin, S. Yamamoto

We present 5 deg2 (~250 pc2) HCN, HNC, HCO+, and CO J=1-0 maps of the Orion B GMC, complemented with existing wide-field [CI] 492 GHz maps, as well as new pointed observations of rotationally excited HCN, HNC, H13CN, and HN13C lines. We detect anomalous HCN J=1-0 hyperfine structure line emission almost everywhere in the cloud. About 70% of the total HCN J=1-0 luminosity arises from gas at A_V < 8 mag. The HCN/CO J=1-0 line intensity ratio shows a bimodal behavior with an inflection point at A_V < 3 mag typical of translucent gas and UV-illuminated cloud edges. We find that most of the HCN J=1-0 emission arises from extended gas with n(H2) < 1e4 cm-3, even lower density gas if the ionization fraction is > 1e-5 and electron excitation dominates. This result explains the low-A_V branch of the HCN/CO J=1-0 intensity ratio distribution. Indeed, the highest HCN/CO ratios (~0.1) at A_V < 3 mag correspond to regions of high [CI] 492 GHz/CO J=1-0 intensity ratios (>1) characteristic of low-density PDRs. Enhanced FUV radiation favors the formation and excitation of HCN on large scales, not only in dense star-forming clumps. The low surface brightness HCN and HCO+ J=1-0 emission scale with I_FIR (a proxy of the stellar FUV radiation field) in a similar way. Together with CO J=1-0, these lines respond to increasing I_FIR up to G0~20. On the other hand, the bright HCN J=1-0 emission from dense gas in star-forming clumps weakly responds to I_FIR once the FUV radiation field becomes too intense (G0>1500). The different power law scalings (produced by different chemistries, densities, and line excitation regimes) in a single but spatially resolved GMC resemble the variety of Kennicutt-Schmidt law indexes found in galaxy averages. As a corollary for extragalactic studies, we conclude that high HCN/CO J=1-0 line intensity ratios do not always imply the presence of dense gas.

Astronomy & Astrophysics, 2023
DOI: 10.1051/0004-6361/202346598
Full-text URL: https://arxiv.org/abs/2309.03186

Neural network-based emulation of interstellar medium models

P. Palud, L. Einig, F. Le Petit, E. Bron, P. Chainais, J. Chanussot, J. Pety, P.-A. Thouvenin, D. Languignon, I. Bešlíc, M.G. Santa-Maria, J.H. Orkisz, L.E. Ségal, A. Zakardjian, S. Bardeau, M. Gerin, J.R. Goicoechea, P. Gratier, Viviana V. Guzman, A. Hughes, F. Levrier, H.S. Liszt, J. Le Bourlot, A. Roueff, and A. Sievers

The interpretation of observations of atomic and molecular tracers in the galactic and extragalactic interstellar medium (ISM) requires comparisons with state-of-the-art astrophysical models to infer some physical conditions. Usually, ISM models are too time-consuming for such inference procedures, as they call for numerous model evaluations. As a result, they are often replaced by an interpolation of a grid of precomputed models. We propose a new general method to derive faster, lighter, and more accurate approximations of the model from a grid of precomputed models for use in inference procedures. These emulators are defined with artificial neural networks (ANNs) with adapted architectures and are fitted using regression strategies instead of interpolation methods. The specificities inherent in ISM models need to be addressed to

design and train adequate ANNs. Indeed, such models often predict numerous observables (e.g., line intensities) from just a few input physical parameters and can yield outliers due to numerical instabilities or physical bistabilities and multistabilities. We propose applying five strategies to address these characteristics: 1) an outlier removal procedure; 2) a clustering method that yields homogeneous subsets of lines that are simpler to predict with different ANNs; 3) a dimension reduction technique that enables us to adequately size the network architecture; 4) the physical inputs are augmented with a polynomial transform to ease the learning of nonlinearities; and 5) a dense architecture to ease the learning of simpler relations between line intensities and physical parameters. Results. We compare the proposed ANNs with four standard classes of interpolation methods, nearest-neighbor, linear, spline, and radial basis function (RBF), to emulate a representative ISM numerical model known as the Meudon PDR code. Combinations of the proposed strategies produce networks that outperform all interpolation methods in terms of accuracy by a factor of 2 in terms of the average error (reaching 4.5% on the Meudon PDR code) and a factor of 3 for the worst-case errors (33%). These networks are also 1 000 times faster than accurate interpolation methods and require ten to forty times less memory. This work will enable efficient inferences on wide-field multiline observations of the ISM.

Astronomy & Astrophysics, 2023
DOI: 10.1051/0004-6361/202347074
Full-text URL: https://arxiv.org/abs/2309.01724

Carbonates and ices in the z = 0.89 galaxy-absorber towards PKS 1830-211 and within star-forming regions of the Milky Way

Bowey, J. E.

A pair of 6.0 and 6.9 μm absorption features are frequently observed in Milky Way (MW) molecular-clouds and YSOs; they also occur in the z = 0.886 rest-frame of a molecule-rich spiral galaxy obscuring blazar PKS 1830-211. I calibrate χ2-fitting methods, which match observations with two or three laboratory spectra. The 6.0-μm component is dominated by H2O ice, as expected. Included MW sources were selected using opacity criteria which limit the range of explored H2O-ice column densities to 1.6 - 2.4 × 1e18 molecules cm-2, while the H2O-ice density in the galaxy absorber is (2.7 ± 0.5) × 1e18 molecules cm-2. CH3OH ice and / or small (< 0.1-μm-sized) Ca- and Mg-bearing carbonates contribute at 6.9 μm. The 41 per cent CH3OH:H2O molecular ratio in the PKS 1830-211 absorber is significantly higher than in the molecular cloud towards Taurus-Elias 16 (<7.5 per cent) and similar to the highest value in MW YSOs (35 per cent in AFGL 989). Fitted carbonate (-CO3):H2O ratios in the galaxy absorber of 0.091 per cent are low in comparison to most of the ratios detected in the MW sample (0.2 per cent-0.4 per cent; ~0 per cent in AFGL 989). Inorganic carbonates could explain the increased oxygen depletion at the diffuse-medium-to-molecular-cloud transition, which Jones and Ysard associated with unobserved organic carbonates or materials with a C:O ratio of 1:3.

2023 MNRAS, Volume 524, Issue 2, pp.2446-2459 September 2023
DOI: 10.1093/mnras/stad1928
Full-text URL: https://arxiv.org/abs/2307.09586

Combined model for 15N, 13C, and spin-state chemistry in molecular clouds

O. Sipilä, L. Colzi, E. Roueff, P. Caselli, F. Fontani, E. Wirström

We present a new gas-grain chemical model for the combined isotopic fractionation of carbon and nitrogen in molecular clouds. To this end, we have developed gas-phase and grain-surface chemical networks where the isotope chemistry of carbon and nitrogen is coupled with a time-dependent description of spin-state chemistry, which is important for nitrogen chemistry at low temperatures. We updated the rate coefficients of some isotopic exchange reactions considered previously in the literature, and here we present a set of new exchange reactions involving molecules substituted in 13C and 15N simultaneously. We applied the model to a series of zero-dimensional simulations representing a set of physical conditions across a prototypical prestellar core, exploring the deviations of the isotopic abundance ratios in the various molecules from the elemental isotopic ratios as a function of physical conditions and time. We find that the 12C/13C ratio can deviate from the elemental ratio to a high factor depending on the molecule, and that there are highly time-dependent variations in the ratios. The HCN/H13CN ratio, for example, can obtain values of less than ten depending on the simulation time. The 14N/15N ratios tend to remain close to the assumed elemental ratio within approximately ten percent, with no clearly discernible trends for the various species as a function of the physical conditions. Abundance ratios between 13C-containing molecules and 13C+15N-containing molecules however show somewhat increased levels of fractionation as a result of the newly included exchange reactions, though they still remain within a few tens of percent of the elemental 14N/15N ratio. Our results imply the existence of gradients in isotopic abundance ratios across prestellar cores, suggesting that detailed simulations are required to interpret observations of isotopically substituted molecules correctly, especially given that the various isotopic forms of a given molecule do not necessarily trace the same gas layers.

Accepted to A&A
DOI: 10.1051/0004-6361/202347106
Full-text URL: https://arxiv.org/abs/2309.02066

Deep search for glycine conformers in Barnard 5

Tadeus Carl, E S Wirström, P Bergman, S B Charnley, Y-L Chuang, Y-J Kuan

One of the most fundamental hypotheses in astrochemistry and astrobiology states that crucial biotic molecules like glycine (NH2CH2COOH) found in meteorites and comets are inherited from early phases of star-formation. Most observational searches for glycine in the interstellar medium have focused on warm, high-mass molecular cloud sources. However, recent studies suggest that it might be appropriate to shift the observational focus to cold, low-mass sources. We aim to detect glycine towards the so-called methanol hotspot in the Barnard (B)5 dark cloud. The hotspot is a cold source (Tgas ≈ 7.5 K) with yet high abundances of complex organic molecules (COMs) and water in the gas phase. We carried out deep, pointed observations with the Onsala 20m telescope, targeting several transitions of glycine conformers I and II (Gly-I and Gly-II) in the frequency range 70.2 - 77.9 GHz. No glycine is detected at the targeted position, but we use a line-stacking procedure to derive sensitive upper limit abundances w.r.t. H2 for Gly-I and Gly-II, i.e. < (2-5) x 1e-10 and < (0.7-3) x 1e-11, respectively. The obtained Gly-II upper limits are the most stringent for a cold source, while the Gly-I upper limits are mostly on the same order than previously measured limits. The measured abundances w.r.t. H2 of other COMs at the B5 methanol hotspot range from 2e-10 (acetaldehyde) to 2e-8 (methanol). Hence, based on a total glycine upper limit of (2-5) x 1e-10, we cannot rule out that glycine is present but undetected.

MNRAS, Volume 524, Issue 4, October 2023, Pages 5993–6003
DOI: 10.1093/mnras/stad2017
Full-text URL: https://arxiv.org/abs/2306.17713

Predicting Observable Infrared Signatures of Nanosilicates in the Diffuse Interstellar Medium

Sascha T. Zeegers, Joan Mariñoso Guiu, Francisca Kemper, Jonathan P. Marshall, Stefan T. Bromley

The destruction time scale of dust in the diffuse interstellar medium is estimated to be an order of magnitude shorter than its residence time. Nevertheless, dust is observed in the interstellar medium, leading to the conclusion that reformation and grain growth must take place. Direct observations of nanometre-sized silicate grains, the main constituent of interstellar dust, would provide a smoking gun for the occurrence of grain condensation in the diffuse interstellar medium. Here we employ quantum chemical calculations to obtain the mid-infrared (IR) optical properties of a library of Mg-end member silicate nanoparticles with olivine (Mg2SiO4) and pyroxene (MgSiO3) stoichiometries. We use this library as an input for a foreground-screen model to predict the spectral appearance of the absorption profile due to mixtures of bulk and nanoparticle silicates towards bright background sources. The mid-IR spectrum observed towards an O8V star or a carbon-rich Wolf–Rayet star starts to change when ~3% of the silicate mass is in the form of nanosilicates. We predict that a 3–10% nanosilicate fraction can be detected with the James Webb Space Telescope (JWST) using the mid-IR instrument (MIRI). With our upcoming JWST observations using MIRI, we will be able to detect or place limits on the nanosilicate content in the diffuse interstellar medium, and thus potentially directly confirm interstellar dust formation.

Faraday Discussions, 2023, 245, 609 - 619
DOI: 10.1039/d3fd00055a
Full-text URL: https://pubs.rsc.org/en/content/articlelanding/2023/fd/d3fd00055a

CoCCoA: Complex Chemistry in hot Cores with ALMA. Selected oxygen-bearing species

Y. Chen, M. L. van Gelder, P. Nazari, C. L. Brogan, E. F. van Dishoeck, H. Linnartz, J. K. Jørgensen, T. R. Hunter, O. H. Wilkins, G. A. Blake, P. Caselli, K.-J. Chuang, C. Codella, I. Cooke, M. N. Drozdovskaya, R. T. Garrod, S. Ioppolo, M. Jin, B. M. Kulterer, N. F. W. Ligterink, A. Lipnicky, R. Loomis, M. G. Rachid, S. Spezzano, and B. A. McGuire

Complex organic molecules (COMs) have been observed to be abundant in the gas phase toward protostars. Deep line surveys have been carried out only for a limited number of well-known high-mass star forming regions using the Atacama Large Millimeter/submillimeter Array (ALMA), which has unprecedented resolution and sensitivity. Statistical studies on oxygen-bearing COMs (O-COMs) in high-mass protostars using ALMA are still lacking. With the recent CoCCoA survey, we are able to determine the column density ratios of six O-COMs with respect to methanol (CH3OH) in a sample of 14 high-mass protostellar sources to investigate their origin through ice and/or gas-phase chemistry. The selected species are: acetaldehyde (CH3CHO), ethanol (C2H5OH), dimethyl ether (DME, CH3OCH3), methyl formate (MF, CH3OCHO), glycolaldehyde (GA, CH2OHCHO), and ethylene glycol (EG, (CH2OH)2). DME and MF have the highest and most constant ratios within one order of magnitude, while the other four species have lower ratios and exhibit larger scatter by 1-2 orders of magnitude. We compare the O-COM ratios of high-mass CoCCoA sources with those of

5 low-mass protostars available from the literature, along with the results from experiments and simulations. We find that the O-COM ratios with respect to methanol are on the same level in both the high- and low-mass samples, which suggests that these species are mainly formed in similar environments during star formation, probably in ice mantles on dust grains during early pre-stellar stages. Current simulations and experiments can reproduce most observational trends with a few exceptions, and hypotheses exist to explain the differences between observations and simulations/experiments, such as the involvement of gas-phase chemistry and different emitting areas of molecules.

Accepted in A&A
DOI: 10.1051/0004-6361/202346491
Full-text URL: https://arxiv.org/abs/2308.02688

Revised gas-phase formation network of methyl cyanide: the origin of methyl cyanide and methanol abundance correlation in hot corinos

Lisa Giani, Cecilia Ceccarelli, Luca Mancini, Eleonora Bianchi, Fernando Pirani, Marzio Rosi, Nadia Balucani

Methyl cyanide (CH3CN) is one of the most abundant and widely spread interstellar complex organic molecules (iCOMs). Several studies found that, in hot corinos, methyl cyanide and methanol abundances are correlated suggesting a chemical link, often interpreted as a synthesis of them on the interstellar grain surfaces. In this article, we present a revised network of the reactions forming methyl cyanide in the gas-phase. We carried out an exhaustive review of the gas-phase CH3CN formation routes, propose two new reactions and performed new quantum mechanics computations of several reactions. We found that 13 of the 15 reactions reported in the databases KIDA and UDfA have incorrect products and/or rate constants. The new corrected reaction network contains 10 reactions leading to methyl cyanide. We tested the relative importance of those reactions in forming CH3CN using our astrochemical model. We confirm that the radiative association of CH3+ and HCN, forming CH3CNH+, followed by the electron recombination of CH3CNH+, is the most important CH3CN formation route in both cold and warm environments, notwithstanding that we significantly corrected the rate constants and products of both reactions. The two newly proposed reactions play an important role in warm environments. Finally, we found a very good agreement between the CH3CN predicted abundances with those measured in cold (~10 K) and warm (~90 K) objects. Unexpectedly, we also found a chemical link between methanol and methyl cyanide via the CH3+ ion, which can explain the observed correlation between the CH3OH and CH3CN abundances measured in hot corinos.

Accepted in MNRAS
DOI: 10.1093/mnras/stad2892
Full-text URL: https://arxiv.org/abs/2309.12745