

AstroChemical Newsletter #16

February 2017

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

The abundance of C₂H₄ in the circumstellar envelope of IRC+10216

J. P. Fonfria, K. H. Hinkle, J. Cernicharo, M. J. Richter, M. Agundez, L. Wallace

High spectral resolution mid-IR observations of ethylene (C₂H₄) towards the AGB star IRC+10216 were obtained using the Texas Echelon Cross Echelle Spectrograph (TEXES) at the NASA Infrared Telescope Facility (IRTF). Eighty ro-vibrational lines from the 10.5 μ m vibrational mode ν_7 with $J < 30$ were detected in absorption. The observed lines are divided into two groups with rotational temperatures of 105 and 400 K (warm and hot lines). The warm lines peak at ~ -14 km/s with respect to the systemic velocity, suggesting that they are mostly formed outwards from $\sim 20R^*$. The hot lines are centered at -10 km/s indicating that they come from a shell between 10 and $20R^*$. 35% of the observed lines are unblended and can be fitted with a code developed to model the emission of a spherically symmetric circumstellar envelope. The analysis of several scenarios reveal that the C₂H₄ abundance relative to H₂ in the range 5- $20R^*$ is $6.9E-8$ in average and it could be as high as $1.1E-7$. Beyond $20R^*$, it is $8.2E-8$. The total column density is $6.5(3.0)E15$ cm⁻². C₂H₄ is found to be rotationally under local thermodynamical equilibrium (LTE) and vibrationally out of LTE. One of the scenarios that best reproduce the observations suggests that up to 25% of the C₂H₄ molecules at $20R^*$ could condense onto dust grains. This possible depletion would not influence significantly the gas acceleration although it could play a role in the surface chemistry on the dust grains.

Accepted for publication in the Apj

DOI: [10.3847/1538-4357/835/2/196](https://doi.org/10.3847/1538-4357/835/2/196)

Full-text URL: <https://arxiv.org/abs/1612.09307>

Lupus disks with faint CO isotopologues: low gas/dust or large carbon depletion?

A. Miotello, E. F. van Dishoeck, J. P. Williams, M. Ansdell, G. Guidi, M. Hogerheijde, C. F. Manara, M. Tazzari, L. Testi, N. van der Marel, and S. van Terwisga

An era has started in which gas and dust can be observed independently in protoplanetary disks, thanks to the recent surveys with ALMA. The first near-complete high-resolution disk survey in both dust and gas in a single star-forming region has been carried out in Lupus, finding surprisingly low gas/dust ratios. The goal of this work is to fully exploit CO isotopologues observations in Lupus, comparing them with physical-chemical model results, in order to obtain gas masses for a large number of disks. We have employed physical-chemical models to analyze continuum and CO

isotopologues observations of Lupus disks, including isotope-selective processes and freeze-out. Employing also the ALMA ^{13}CO -only detections, disk gas masses have been calculated for a total of 34 sources, expanding the sample of 10 disks studied by Ansdell et al. (2016), where also C^{18}O was detected. We confirm that overall gas-masses are very low, often smaller than 1 M_{J} , if volatile carbon is not depleted. Accordingly, global gas/dust ratios predominantly between 1 and 10. Low CO -based gas masses and gas/dust ratios may indicate rapid loss of gas, or alternatively chemical evolution, e.g. via sequestering of carbon from CO to more complex molecules, or carbon locked up in larger bodies. Current ALMA observations cannot distinguish between these two hypotheses. We have simulated both scenarios, but chemical model results do not allow us to rule out one of the two. Assuming that all Lupus disks have evolved mainly due to viscous processes over the past few Myr, the observed correlation between the current mass accretion rate and dust mass found by Manara et al. (2016) implies a constant gas-to-dust ratio, which is close to 100 based on the observed $M_{\text{disk}}/M_{\text{dot acc}}$ ratio. This in turn points to a scenario in which carbon depletion is responsible for the low CO isotopologue line luminosities.

Accepted in A&A

DOI: [10.1051/0004-6361/201629556](https://doi.org/10.1051/0004-6361/201629556)

Full-text URL: <https://arxiv.org/abs/1612.01538>

Glycolaldehyde in Perseus young solar analogs

M. De Simone, C. Codella, L. Testi, A. Belloche, A.J. Maury, S. Anderl, Ph. Andre, S. Maret, L. Podio

Aims: In this paper we focus on the occurrence of glycolaldehyde (HCOCH_2OH) in young solar analogs by performing the first homogeneous and unbiased study of this molecule in the Class 0 protostars of the nearby Perseus star forming region. **Methods:** We obtained sub-arcsec angular resolution maps at 1.3mm and 1.4mm of glycolaldehyde emission lines using the IRAM Plateau de Bure (PdB) interferometer in the framework of the CALYPSO IRAM large program. **Results:** Glycolaldehyde has been detected towards 3 Class 0 and 1 Class I protostars out of the 13 continuum sources targeted in Perseus: NGC1333-IRAS2A1, NGC1333-IRAS4A2, NGC1333-IRAS4B1, and SVS13-A. The NGC1333 star forming region looks particularly glycolaldehyde rich, with a rate of occurrence up to 60%. The glycolaldehyde spatial distribution overlaps with the continuum one, tracing the inner 100 au around the protostar. A large number of lines (up to 18), with upper-level energies E_u from 37 K up to 375 K has been detected. We derived column densities $> 10^{15} \text{ cm}^{-2}$ and rotational temperatures T_{rot} between 115 K and 236 K, imaging for the first time hot-corinos around NGC1333-IRAS4B1 and SVS13-A. **Conclusions:** In multiple systems glycolaldehyde emission is detected only in one component. The case of the SVS13-A+B and IRAS4-A1+A2 systems support that the detection of glycolaldehyde (at least in the present Perseus sample) indicates older protostars (i.e. SVS13-A and IRAS4-A2), evolved enough to develop the hot-corino region (i.e. 100 K in the inner 100 au). However, only two systems do not allow us to firmly conclude whether the primary factor leading to the detection of glycolaldehyde emission is the environments hosting the protostars, evolution (e.g. low value of $L_{\text{submm}}/L_{\text{int}}$), or accretion luminosity (high L_{int}).

A&A, in press

DOI: [10.1051/0004-6361/201630049](https://doi.org/10.1051/0004-6361/201630049)

Full-text URL: <http://arxiv.org/abs/1701.00724>

Importance of tunneling in H-abstraction reactions by OH

radicals: The case of CH₄ + OH studied through isotope-substituted analogs

Thanja Lamberts, Gleb Fedoseev, Johannes Kästner, Sergio Ioppolo, Harold Linnartz

We present a combined experimental and theoretical study focussing on the quantum tunneling of atoms in the reaction between CH₄ and OH. The importance of this reaction pathway is derived by investigating isotope substituted analogs. Quantitative reaction rates needed for astrochemical models at low temperature are currently unavailable both in the solid state and in the gas phase. Here, we study tunneling effects upon hydrogen abstraction in CH₄ + OH by focusing on two reactions: CH₄ + OD → CH₃ + HDO and CD₄ + OH → CD₃ + HDO. The experimental study shows that the solid-state reaction rate R(CH₄ + OD) is higher than R(CD₄ + OH) at 15 K. Experimental results are accompanied by calculations of the corresponding unimolecular and bimolecular reaction rate constants using instanton theory taking into account surface effects. From the work presented here, the unimolecular reactions are particularly interesting as these provide insight into reactions following a Langmuir-Hinshelwood process. The resulting ratio of the rate constants shows that the H abstraction (k(CH₄ + OD)) is approximately ten times faster than D-abstraction (k(CD₄ + OH)) at 65 K. We conclude that tunneling is involved at low temperatures in the abstraction reactions studied here. The unimolecular rate constants can be used by the modeling community as a first approach to describe OH-mediated abstraction reactions in the solid phase. For this reason we provide fits of our calculated rate constants that allow the inclusion of these reactions in models in a straightforward fashion.

Accepted for publication in A&A

DOI: [10.1051/0004-6361/201629845](https://doi.org/10.1051/0004-6361/201629845)

Full-text URL: <https://arxiv.org/abs/1612.07027>

13C-substituted C₆₀⁺: Predictions of the rotational spectra

Koichi M.T. Yamada, Stephen C. Ross, Fumiyuki Ito

C₆₀⁺ has recently been identified as the carrier of some of the diffuse interstellar bands (Campbell et al., 2015). Unfortunately, this ion has no dipole moment and therefore no rotational spectrum. We investigate the situation where one of the carbon atoms in this ion is substituted by a ¹³C-atom. This shifts the center of mass away from the center of charge, resulting in a non-zero dipole moment and thus opening the possibility of rotational spectroscopy in the microwave region. That the population of the singly substituted species is comparable to that of the parent isotopologue increases the expected intensity. One complication is that the Jahn-Teller effect may distort the molecule. We use density functional theory to consider this possibility and the rotational properties of the different isomers that would result.

Molecular Astrophysics, Volume 6, March 2017, Pages 9–15

DOI: [10.1016/j.molap.2016.12.001](https://doi.org/10.1016/j.molap.2016.12.001)

Full-text URL: <http://www.sciencedirect.com/science/article/pii/S2405675816300215>

Dissecting the molecular structure of the Orion B cloud: Insight from Principal Component Analysis

Pierre Gratier, Emeric Bron, Maryvonne Gerin, Jérôme Pety, Viviana V. Guzman, Jan Orkisz, Sébastien Bardeau, Javier R. Goicoechea, Franck Le Petit, Harvey Liszt, Karin Öberg, Nicolas Peretto, Evelyne Roueff, Albrecht Sievers and Pascal Tremblin

Context. The combination of wideband receivers and spectrometers currently available in (sub-)millimeter observatories deliver wide-field hyperspectral imaging of the interstellar medium. Tens of spectral lines can be observed over degree wide fields in about fifty hours. This wealth of data calls for restating the physical questions about the interstellar medium in statistical terms. Aims. We aim at gaining information on the physical structure of the interstellar medium from a statistical analysis of many lines from different species over a large field of view, without requiring detailed radiative transfer or astrochemical modeling. Methods. We coupled a nonlinear rescaling of the data with one of the simplest multivariate analysis methods, namely the Principal Component Analysis, to decompose the observed signal into components that we interpret first qualitatively and then quantitatively based on our deep knowledge of the observed region and of the astrochemistry at play. Results. We identify 3 principal components, linear compositions of line brightness temperatures, that are correlated at various levels with the column density, the volume density and the UV radiation field. Conclusions. When sampling a sufficiently diverse mixture of physical parameters, it is possible to decompose the molecular emission in order to gain physical insight on the observed interstellar medium. This opens a new avenue for future studies of the interstellar medium.

Accepted for publication in Astronomy & Astrophysics

Full-text URL: <https://arxiv.org/abs/1701.04205>

Rotational spectroscopy, tentative interstellar detection, and chemical modelling of N-methylformamide

A. Belloche, A. A. Meshcheryakov, R. T. Garrod, V. V. Ilyushin, E. A. Alekseev, R. A. Motiyenko, L. Margulès, H. S. P. Müller, K. M. Menten

N-methylformamide, CH₃NHCHO, may be an important molecule for interstellar pre-biotic chemistry because it contains a peptide bond. The rotational spectrum of the most stable trans conformer of CH₃NHCHO is complicated by strong torsion-rotation interaction due to the low barrier of the methyl torsion. We use two absorption spectrometers in Kharkiv and Lille to measure the rotational spectra over 45--630 GHz. The analysis is carried out using the Rho-axis method and the RAM36 code. We search for N-methylformamide toward the hot molecular core Sgr B2(N2) using a spectral line survey carried out with ALMA. The astronomical results are put into a broader astrochemical context with the help of a gas-grain chemical kinetics model. The laboratory data set for the trans conformer of CH₃NHCHO consists of 9469 line frequencies with $J \leq 62$, including the first assignment of the rotational spectra of the first and second excited torsional states. All these lines are fitted within experimental accuracy. We report the tentative detection of CH₃NHCHO towards Sgr B2(N2). We find CH₃NHCHO to be more than one order of magnitude less abundant than NH₂CHO, a factor of two less abundant than CH₃NCO, but only slightly less abundant than CH₃CONH₂. The chemical models indicate that the efficient formation of HNCO via NH + CO on grains is a necessary step in the achievement of the observed gas-phase abundance of CH₃NCO. Production of CH₃NHCHO may plausibly occur on grains either through the direct addition of functional-group radicals or through the hydrogenation of CH₃NCO. Provided the detection of CH₃NHCHO is confirmed, the only slight underabundance of this molecule compared to its more stable structural isomer acetamide and the sensitivity of the model abundances to the chemical kinetics parameters suggest that the formation of these two molecules is controlled by kinetics rather than thermal equilibrium.

accepted in A&A

DOI: [10.1051/0004-6361/201629724](https://doi.org/10.1051/0004-6361/201629724)

Full-text URL: <http://xxx.lanl.gov/abs/1701.04640>

Photodissociation and photoionisation of atoms and molecules of astrophysical interest

Alan Heays, A. D. Bosman, E. F. van Dishoeck

A new collection of photodissociation and photoionisation cross sections for 102 atoms and molecules of astrochemical interest has been assembled, along with a brief review of the basic processes involved. These have been used to calculate dissociation and ionisation rates, with uncertainties, in a standard ultraviolet interstellar radiation field (ISRF) and wavelength-dependent radiation fields. The new ISRF rates generally agree within 30% with our previous compilations, with a few notable exceptions. The reduction of rates in shielded regions was calculated as a function of dust, molecular and atomic hydrogen, atomic C, and self-shielding column densities. The relative importance of shielding types depends on the species in question and the dust optical properties. The new data are publicly available from the Leiden photodissociation and ionisation database. Sensitivity of rates to variation of temperature and isotope, and cross section uncertainties, are tested. Tests were conducted with an interstellar-cloud chemical model, and find general agreement (within a factor of two) with the previous iteration of the Leiden database for the ISRF, and order-of-magnitude variations assuming various kinds of stellar radiation. The newly parameterised dust-shielding factors makes a factor-of-two difference to many atomic and molecular abundances relative to parameters currently in the UDfA and KIDA astrochemical reaction databases. The newly-calculated cosmic-ray induced photodissociation and ionisation rates differ from current standard values up to a factor of 5. Under high temperature and cosmic-ray-flux conditions the new rates alter the equilibrium abundances of abundant dark cloud abundances by up to a factor of two. The partial cross sections for H₂O and NH₃ photodissociation forming OH, O, NH₂ and NH are also evaluated and lead to radiation-field-dependent branching ratios.

Accepted in A&A.

Full-text URL: <https://arxiv.org/abs/1701.04459>

Chemical fractionation of deuterium in the protosolar nebula

J. Kalvans, I. Shmeld, J. R. Kalnin, S. Hocuk

Understanding gas-grain chemistry of deuterium in star-forming objects may help to explain their history and present state. We aim to clarify how processes in ices affect the deuterium fractionation. In this regard, we investigate a Solar-mass protostellar envelope using an astrochemical rate-equation model that considers bulk-ice chemistry. The results show a general agreement with the molecular D/H abundance ratios observed in low-mass protostars. The simultaneous processes of ice accumulation and rapid synthesis of HD on grain surfaces in the prestellar core hampers the deuteration of icy species. The observed very high D/H ratios exceeding 10 per cent, i.e., super-deuteration, are reproduced for formaldehyde and dimethyl ether, but not for other species in the protostellar envelope phase. Chemical transformations in bulk ice lower D/H ratios of icy species and do not help explaining the super-deuteration. In the protostellar phase, the D₂O/HDO abundance ratio was calculated to be higher than the HDO/H₂O ratio owing to gas-phase chemistry. Species that undergo evaporation from ices have high molecular D/H ratio and a high gas-phase abundance.

A principal component analysis of the diffuse interstellar bands

Tiffany Ensor, Jan Cami, Neil H. Bhatt, Andrea Soddu

We present a principal component analysis of 23 line of sight parameters (including the strengths of 16 diffuse interstellar bands, DIBs) for a well-chosen sample of single-cloud sightlines representing a broad range of environmental conditions. Our analysis indicates that the majority (~93%) of the variations in the measurements can be captured by only four parameters. The main driver (i.e., the first principal component) is the amount of DIB-producing material in the line of sight, a quantity that is extremely well traced by the equivalent width of the 5797 DIB. The second principal component is the amount of UV radiation, which correlates well with the 5797/5780 DIB strength ratio. The remaining two principal components are more difficult to interpret, but are likely related to the properties of dust in the line of sight (e.g., the gas-to-dust ratio). With our PCA results, the DIBs can then be used to estimate these line of sight parameters.

Accepted for publication in the Astrophysical Journal

Full-text URL: <https://arxiv.org/abs/1701.06180>

Hyperfine interactions and internal rotation in methanol

Boy Lankhaar, Gerrit C. Groenenboom, and Ad van der Avoird

We present a rigorous derivation of the nuclear spin-rotation and spin-torsion coupling terms in the hyperfine Hamiltonian for molecules with internal rotation. Our formulas differ from the expressions derived by Heuvel and Dymanus [J. Mol. Spectrosc. 47, 363 (1973)], which these authors used and which were also applied recently by others to interpret experimental hyperfine spectra of such molecules. In the present work, our theoretical results are applied to methanol. We calculate the nuclear spin-spin magnetic dipole-dipole interactions and the nuclear contribution to the spin-torsion coupling vectors from the nuclear coordinates as functions of the internal rotation angle γ , compute the spin-rotation coupling tensors by ab initio electronic structure methods also as functions of γ , and obtain the missing parameters for the electronic contribution to the spin-torsion coupling from a fit to measured spectra. The resulting hyperfine Hamiltonian is then used to compute hyperfine transition frequencies and intensities for twelve torsion-rotation transitions in methanol. With the use of the ab initio calculated spin-rotation coupling parameters without any modification, and physically reasonable values for the spin-torsion coupling parameters from the fit, we find good agreement with all of the measured spectra.

J. Chem. Phys., 145, 24, 244301, 22 december 2016

DOI: [10.1063/1.4972004](https://doi.org/10.1063/1.4972004)

Full-text URL: <http://aip.scitation.org/doi/abs/10.1063/1.4972004>

Infrared characterisation of acetonitrile and propionitrile aerosols under Titan's atmospheric conditions

C. Ennis, R. Auchetti, M. Ruzi, E. G. Robertson

Pure, crystalline acetonitrile (CH₃CN) and propionitrile (CH₃CH₂CN) particles were formed in a collisional cooling cell allowing for infrared (IR) signatures to be compiled

from 50 to 5000 cm^{-1} . The cell temperature and pressure conditions were controlled to simulate Titan's lower atmosphere (80–130 K and 1–100 mbar), allowing for the comparison of laboratory data to the spectra obtained from the Cassini-Huygens mission. The far-IR features confirmed the morphology of CH_3CN aerosols as the metastable β -phase (monoclinic) ice, however, a specific crystalline phase for $\text{CH}_3\text{CH}_2\text{CN}$ could not be verified. Mie theory and the literature complex refractive indices enabled the experimental spectra to be modelled. The procedure yielded size distributions for CH_3CN (55–140 nm) and $\text{CH}_3\text{CH}_2\text{CN}$ (140–160 nm) particles. Effective kinetic profiles, tracing the evolution of aerosol band intensities, showed that condensation of $\text{CH}_3\text{CH}_2\text{CN}$ proceeded at twice the rate of CH_3CN aerosols. In addition, the rate of $\text{CH}_3\text{CH}_2\text{CN}$ aerosol depletion via lateral diffusion of the particles from the interrogation volume was approximately 50% faster than that of CH_3CN . The far-IR spectra recorded for both nitrile aerosols did not display absorption profiles that could be attributed to the unassigned 220 cm^{-1} feature, which has been observed to fluctuate seasonally in the spectra obtained from Titan's atmosphere.

2017, Phys. Chem. Chem. Phys.

DOI: [10.1039/C6CP08110J](https://doi.org/10.1039/C6CP08110J)

Full-text URL:

<http://pubs.rsc.org/en/Content/ArticleLanding/2017/CP/C6CP08110J#!divAbstract>

Binding energies: new values and impact on the efficiency of chemical desorption

V. Wakelam, J.-C. Loison, R. Mereau, M. Ruaud

Recent laboratory measurements have confirmed that chemical desorption (desorption of products due to exothermic surface reactions) can be an efficient process. The impact of including this process into gas-grain chemical models entirely depends on the formalism used and the associated parameters. Among these parameters, binding energies are probably the most uncertain ones for the moment. We propose a new model to compute binding energy of species to water ice surfaces. We have also compared the model results using either the new chemical desorption model proposed by Minissale et al. (2016) or the one of Garrod et al. (2007). The new binding energies have a strong impact on the formation of complex organic molecules. In addition, the new chemical desorption model from Minissale produces a much smaller desorption of these species and also of methanol. Combining the two effects, the abundances of CH_3OH and COMs observed in cold cores cannot be reproduced by astrochemical models anymore.

Molecular Astrophysics, Volume 6, March 2017, Pages 22 - 35

DOI: [10.1016/j.molap.2017.01.002](https://doi.org/10.1016/j.molap.2017.01.002)

Full-text URL: <http://lanl.arxiv.org/abs/1701.06492>

Radiative charge transfer in collisions of C with He^+

James F Babb and B M McLaughlin

Radiative charge exchange collisions between a carbon atom $\text{C}(3\text{P})$ and a helium ion $\text{He}^+(2\text{S})$, both in their ground state, are investigated theoretically. Detailed quantum chemistry calculations are carried out to obtain potential energy curves and transition dipole matrix elements for doublet and quartet molecular states of the HeC^+ cation. Radiative charge transfer cross sections and rate coefficients are calculated and are found at thermal and lower energies to be large compared to those for direct charge transfer. The present results might be applicable to modelling the complex interplay of

C II (or C+), C, and CO at the boundaries of interstellar photon dominated regions and in x-ray dominated regions, where the abundance of He+ affects the abundance of CO.

J. Phys. B: At. Mol. Opt. Phys. 50 (2017) 044003

DOI: [10.1088/1361-6455/aa54f4](https://doi.org/10.1088/1361-6455/aa54f4)

Full-text URL: <https://arxiv.org/abs/1610.05989>

The SILCC project --- IV. Impact of dissociating and ionising radiation on the interstellar medium and H α emission as a tracer of the star formation rate

T. Peters, T. Naab, S. Walch, S.C.O. Glover, P. Girichidis, E. Pellegrini, R.S. Klessen, R. Wünsch, A. Gatto, C. Baczynski

We present three-dimensional radiation-hydrodynamical simulations of the impact of stellar winds, photoelectric heating, photodissociating and photoionising radiation, and supernovae on the chemical composition and star formation in a stratified disc model. This is followed with a sink-based model for star clusters with populations of individual massive stars. Stellar winds and ionising radiation regulate the star formation rate at a factor of ~ 10 below the simulation with only supernova feedback due to their immediate impact on the ambient interstellar medium after star formation. Ionising radiation (with winds and supernovae) significantly reduces the ambient densities for most supernova explosions to $\rho < 10^{-25} \text{ g cm}^{-3}$, compared to $10^{-23} \text{ g cm}^{-3}$ for the model with only winds and supernovae. Radiation from massive stars reduces the amount of molecular hydrogen and increases the neutral hydrogen mass and volume filling fraction. Only this model results in a molecular gas depletion time scale of 2 Gyr and shows the best agreement with observations. In the radiative models, the H α emission is dominated by radiative recombination as opposed to collisional excitation (the dominant emission in non-radiative models), which only contributes $\sim 1\text{--}10\%$ to the total H α emission. Individual massive stars ($M \geq 30 M_{\text{sun}}$) with short lifetimes are responsible for significant fluctuations in the H α luminosities. The corresponding inferred star formation rates can underestimate the true instantaneous star formation rate by factors of ~ 10 .

MNRAS 466, 3293-3308, 2017

DOI: [10.1093/mnras/stw3216](https://doi.org/10.1093/mnras/stw3216)

Full-text URL: <https://doi.org/10.1093/mnras/stw3216>

THE PAH EMISSION CHARACTERISTICS OF THE REFLECTION NEBULA NGC 2023

Els Peeters, Charles W. Bauschlicher, Jr., Louis J. Allamandola, Alexander G.G.M. Tielens, Alessandra Ricca, Mark G. Wolfire

We present 5-20 micron spectral maps of the reflection nebula NGC2023 obtained with the Infrared Spectrograph SL and SH modes on board the Spitzer Space Telescope which reveal emission from polycyclic aromatic hydrocarbons (PAHs), C₆₀, and H₂ superposed on a dust continuum. We show that several PAH emission bands correlate with each other and exhibit distinct spatial distributions revealing a spatial sequence with distance from the illuminating star. We explore the distinct morphology of the 6.2, 7.7 and 8.6 micron PAH bands and find that at least two spatially distinct components contribute to the 7--9 micron PAH emission in NGC2023. We report that the PAH features behave independently of the underlying plateaus. We present spectra of compact oval PAHs ranging in size from C₆₆ to C₂₁₀, determined computationally using density functional theory, and investigate trends in the band positions and relative

intensities as a function of PAH size, charge and geometry. Based on the NASA Ames PAH database, we discuss the 7--9 micron components in terms of band assignments and relative intensities. We assign the plateau emission to very small grains with possible contributions from PAH clusters and identify components in the 7--9 micron emission that likely originates in these structures. Based on the assignments and the observed spatial sequence, we discuss the photochemical evolution of the interstellar PAH family as they are more and more exposed to the radiation field of the central star in the evaporative flows associated with the PDRs in NGC2023.

42 pages, 25 figures, 2 animations, accepted for ApJ

Full-text URL: <http://adsabs.harvard.edu/abs/2017arXiv170106585P>

Announcements

Workshop: Current and future perspectives of chemical modelling in astrophysics

We are pleased to announce the Workshop on "Current and Future Perspectives of Chemical Modelling in Astrophysics" to be held in Hamburg, Germany July 17-19, 2017. In the ALMA era it is fundamental to include chemistry and the related microphysics in computational studies aimed at understanding and probing the physical conditions of the different astrophysical environments. This requires to build accurate, well optimised, state-of-the-art models to be included in hydrodynamical simulations. It is then important to provide a platform connecting the different experts to stimulate an exchange of ideas, and to work towards a coherent understanding of chemical modelling in astrophysics. This workshop aims at experts on the calculations and measurements of rates for chemical processes relevant in astrophysics, both in the gas phase as well as on dust, and astrophysicists who develop tools and/or employ chemistry and microphysics in hydrodynamical simulations of the interstellar medium. The workshop will cover the following topics: - Computational Astrochemistry: Numerical Codes and Databases - Chemistry/Microphysics in Hydrodynamical Simulations - Modelling Observations - Gas/Dust phase processes: theory and experiments Conference poster: www.hs.uni-hamburg.de/astromodel2017/flyer.pdf More information and registration <http://www.hs.uni-hamburg.de/astromodel2017> Important dates: May 1st, 2017: End of abstract submission End of May, 2017: Announcement of the selected talks and posters June 11th, 2017: End of registration Invited Speakers: Stephanie Cazaux, Cecilia Ceccarelli, Paul Clark, Dieter Gerlich, Troels Haugboelle, Guillermo Munoz-Caro, David Neufeld, Dmitry Semenov, Alexander Tielens, Valentine Wakelam, Laurent Wiesenfeld, Simon Portegies Zwart Scientific Organizing Committee: Robi Banerjee, Stefano Bovino, Paola Caselli, Daniele Galli, Tommaso Grassi Bastian Kortgen, Daniel Seifried, Dominik Schleicher, Wing-Fai Thi Local Organizing Committee: Robi Banerjee, Stefano Bovino, Bastian Körtgen We are looking forward to meet you in Hamburg.

Post-doctoral position in observational IR astronomy

Applications are invited for a post-doctoral position in observational infrared astronomy in the Department of Physics and Astronomy at The University of Western Ontario. The successful candidate will pursue projects with Prof. Els Peeters. These projects will be related to studies of Polycyclic Aromatic Hydrocarbons (PAHs) and dust in various environments, with an emphasis on (galactic and extragalactic) star-forming regions and photodissociation regions (PDRs), and will utilize Spitzer, SOFIA, ground-based and future JWST observations. The successful applicant will be expected to participate in the preparation for the upcoming JWST mission and in the analysis of JWST Early Release

Science data. Candidates must have a PhD in astrophysics or related fields. Preference will be given to candidates with a strong background in IR astronomy and astronomical data reduction. Prior research experience with PAHs and dust is desirable but not required. The appointment is for 2 years with an additional year dependent upon performance and continued funding. The start date is flexible but is expected to be summer 2017. Applicants should send (preferably electronically) a cover letter, CV, a statement of research interests, and arrange for three letters of recommendation to be sent directly to Dr. Peeters by March 1, 2017. The University of Western Ontario is committed to employment equity.

Post-doctoral position in Interstellar Optical Spectroscopy

Prof. Jan Cami invites applications for a post-doctoral research position in interstellar optical spectroscopy in the Department of Physics and Astronomy and the Centre for Planetary Science and Exploration (CPSX) at the University of Western Ontario. The successful applicant will work on the Diffuse Interstellar Band (DIB) problem and lead much of the data analysis efforts to exploit the EDIBLES (ESO DIB Large Exploration Survey) data set, an unprecedented collection of high signal-to-noise and high spectral resolution observations obtained with VLT/UVES. He or she will also have the possibility to participate in other research programs as well as carrying out independent research. Candidates must have a PhD in astrophysics or related fields, and preferably a background in astronomical spectroscopy and/or data analysis. Expertise in studies of the interstellar medium or in data analysis using advanced statistical methods and/or machine learning techniques would be advantageous. The initial appointment is for 1 year with the expectation of one or two additional years dependent upon performance and continued funding. The start date is flexible, but preferably not later than the summer of 2017. Support for research and observing travel as well as publications will be provided. Applicants should send a cover letter, CV with bibliography, a brief statement of research interests, and arrange for three letters of recommendation to be sent directly to Prof. Cami. The position will remain open until filled. For full consideration, complete applications should be received by March 1, 2017. The University of Western Ontario is committed to employment equity. Prof. Jan Cami Department of Physics and Astronomy, PAB 203 The University of Western Ontario 1151 Richmond St London, ON N6A 3K7 Canada e-mail : jcami@uwo.ca

James Webb Space telescope “Early Release Science” programs

The James Webb Space telescope (NASA/ESA/CSA) will be launched in 2018. During the first months of operations, 500 hours of director's time will be allocated to 10 to 15 “Early Release Science” programs. The goals of these programs will be 1) to provide first-look public data to a wide community as soon as possible after launch, 2) to test the instruments and observing modes, 3) to help prepare the community for the open time proposals. A proposal to obtain ERS observations of dense photodissociation regions is in preparation, coordinated by an international “tiger” team of 15 scientists and with the support from members of the guaranteed time. Since the goals of the ERS proposals are community oriented, it is important that the final proposals can be representative of the needs of this community, and therefore the tiger team would like to involve its members in the definition of this proposal. The science goals have been divided in 5 topics, namely : - Dust, amorphous carbon and aliphatics - PAHs, fullerenes - Physics of H₂ (formation & excitation) - Molecular and atomic astrophysics of PDRs - Propyls and photoevaporation The tiger team is planning to organise several telecons in order to obtain inputs and guidance from the community, for the finalization of these science goals, requirements for target selection and observing modes. Scientists with interests in the above topics and who would like to participate (or keep informed) are

welcome to register through the webpage dedicated to this project : <http://jwst-ism.org>