AstroChemical Newsletter #27

January 2018

Happy New Year and best wishes for 2018. 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

Detection of HC5N and HC7N Isotopologues in TMC-1 with the Green Bank Telescope

A. M. Burkhardt, E. Herbst, S. V. Kalenskii, M. C. McCarthy, A. J. Remijan, B. A. McGuire

We report the first interstellar detection of DC7N and six 13C-bearing isotopologues of HC7N toward the dark cloud TMC-1 through observations with the Green Bank Telescope, and confirm the recent detection of HC5[15]N. For the average of the 13C isotopomers, DC7N, and HC5[15]N, we derive column densities of 1.9(2)×1e11, 2.5(9)×1e11, and 1.5(4)×1e11 cm−2, respectively. The resulting isotopic ratios are consistent with previous values derived from similar species in the source, and we discuss the implications for the formation chemistry of the observed cyanopolyynes. Within our uncertainties, no significant 13C isotopomer variation is found for HC7N, limiting the significance CN could have in its production. The results further show that, for all observed isotopes, HC5N may be isotopically depleted relative to HC3N and HC7N, suggesting that reactions starting from smaller cyanopolyynes may not be efficient to form HCnN. This leads to the conclusion that the dominant production route may be the reaction between hydrocarbon ions and nitrogen atoms.

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Interstellar dehydrogenated PAH anions: vibrational spectra

Mridusmita Buragohain, Amit Pathak, Peter Sarre and Nand Kishor Gour

Interstellar Polycyclic Aromatic Hydrocarbon (PAH) molecules exist in diverse forms depending on the local physical environment. Formation of ionized PAHs (anions and cations) is favourable in the extreme conditions of the ISM. Besides in their pure form, PAHs are also likely to exist in substituted forms; for example, PAHs with functional groups, dehydrogenated PAHs etc. A dehydrogenated PAH molecule might subsequently form fullerenes in the ISM as a result of ongoing chemical processes. This work presents a Density Functional Theory (DFT) calculation on dehydrogenated PAH anions to explore the infrared emission spectra of these molecules and discuss any possible contribution towards observed IR features in the ISM. The results suggest that dehydrogenated PAH anions might be significantly contributing to the 3.3 μm region. Spectroscopic features unique to dehydrogenated PAH anions are highlighted that may be used for their possible identification in the ISM. A comparison has also been made to see the size effect on spectra of these PAHs.

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Full-text URL: https://arxiv.org/abs/1711.09505

H2 formation on interstellar dust grains: the viewpoints of theory, experiments, models and observations

V. Wakelam, E. Bron, S. Cazaux, F. Dulieu, C. Gry, P. Guillard, E. Habart, L. Hornekær, S. Morisset, G. Nyman, V. Pirronello, S. D. Price, V. Valdivia, G. Vidali, N. Watanabe

Molecular hydrogen is the most abundant molecule in the universe. It is the first one to form and survive photo-dissociation in tenuous environments. Its formation involves catalytic reactions on the surface of interstellar grains. The micro-physics of the formation process has been investigated intensively in the last 20 years, in parallel of new astrophysical observational and modeling progresses. In the perspectives of the probable revolution brought by the future satellite JWST, this article has been written to present what we think we know about the H2 formation in a variety of interstellar environments.

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Carbon chemistry in IRC+10216: infrared detection of diacetylene

J. P. Fonfria, M. Agundez, J. Cernicharo, M. J. Richter, J. H. Lacy

We present the detection of C4H2 for first time in the envelope of the C-rich AGB star IRC+10216 based on high spectral resolution mid-IR observations carried out with the Texas Echelon-cross-Echelle Spectrograph (TEXES) mounted on the Infrared Telescope Facility (IRTF). The obtained spectrum contains 24 narrow absorption features above the detection limit identified as lines of the ro-vibrational C4H2 band nu6+nu8(sigma_u^+). The analysis of these lines through a ro-vibrational

diagram indicates that the column density of C4H2 is 2.4(1.5)1e16 cm^(-2). Diacetylene is distributed in two excitation populations accounting for 20 and 80% of the total column density and with rotational temperatures of 47(7) and 420(120) K, respectively. This two-folded rotational temperature suggests that the absorbing gas is located beyond ~0.4"~20R* from the star with a noticeable cold contribution outwards from ~10"~500R*. This outer shell matches up with the place where cyanoacetylenes and carbon chains are known to form due to the action of the Galactic dissociating radiation field on the neutral gas coming from the inner layers of the envelope.

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Full-text URL: http://adsabs.harvard.edu/abs/2017arXiv171110926F

Tunneling Rate Constants for H2CO+H on Amorphous Solid Water Surfaces

Lei Song, Johannes Kästner

Formaldehyde (H2CO) is one of the most abundant molecules observed in the icy mantle covering interstellar grains. Studying its evolution can contribute to our understanding of the formation of complex organic molecules in various interstellar environments. In this work, we investigated the hydrogenation reactions of H2CO yielding CH3O, CH2OH and the hydrogen abstraction resulting in H2 + HCO on an amorphous solid water (ASW) surface using a quantum mechanics/molecular mechanics (QM/MM) model. The binding energies of H2CO on the ASW surface vary broadly from 1000 K to 9370 K. No correlation was found between binding energies and activation energies of hydrogenation reactions. Combining instanton theory with QM/MM modeling, we calculated rate constants for the Langmuir-Hinshelwood and the Eley-Rideal mechanisms for the three product channels of H + H2CO surface reactions down to 59 K. We found that the channel producing CH2OH can be ignored owing to its high activation barrier leading to significantly lower rates than the other two channels. The ASW surface influences the reactivity in favor of formation of CH3O (branching ratio ~80%) and hinders the H2CO dissociation into H2+HCO. In addition, kinetic isotope effects are strong in all reaction channels and vary strongly between the channels. Finally, we provide fits of the rate constants to be used in astrochemical models.

Astrophys. J. 850, 118 (2017)
DOI: 10.3847/1538-4357/aa943e
Full-text URL: http://iopscience.iop.org/article/10.3847/1538-4357/aa943e/meta

Gas-Phase Spectra of MgO Molecules: A Possible Connection from Gas-Phase Molecules to Planet Formation

Katherine A. Kloska and Ryan C. Fortenberry

A more fine-tuned method for probing planet-forming regions, such as protoplanetary discs, could be rovibrational molecular spectroscopy observation of particular premineral molecules instead of more common but ultimately less related volatile organic compounds. Planets are created when grains aggregate, but how molecules form grains is an ongoing topic of discussion in astrophysics and planetary science. Using the spectroscopic data of molecules specifically involved in mineral formation could help to map regions where planet formation is believed to be occurring in order to examine the interplay between gas and dust. Four atoms are frequently associated with planetary formation: Fe, Si, Mg, and O. Magnesium, in particular, has been shown to be in higher relative abundance in planet-hosting stars. Magnesium oxide crystals comprise the mineral periclase making it the chemically simplest magnesium-bearing mineral and a natural choice for analysis. The monomer, dimer, and trimer forms of (MgO)n with n = 1 − 3 are analyzed in this work using high-level quantum chemical computations known to produce accurate results. Strong vibrational transitions at 12.5 μm, 15.0 μm, and 16.5 μm are indicative of magnesium oxide monomer, dimer, and trimer making these wavelengths of particular interest for the observation of protoplanetary discs and even potentially planet-forming regions around stars. If such transitions are observed in emission from the accretion discs or absorptions from stellar spectra, the beginning stages of mineral and, subsequently, rocky body formation could be indicated.

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High-mass Star Formation through Filamentary Collapse and Clump-fed Accretion in G22

J. Yuan, J.-Z. Li, Y. Wu, S. P. Ellingsen, C. Henkel, K. Wang, T. Liu, H. Liu, A. Zavagno, Z. Ren, Y.-F. Huang

How mass is accumulated from cloud-scale down to individual stars is a key open question in understanding high-mass star formation. Here, we present the mass accumulation process in a hub-filament cloud G22 which is composed of four supercritical filaments. Velocity gradients detected along three filaments indicate that they are collapsing with a total mass infall rate of about 440 M⊙ Myr^-1, suggesting the hub mass would be doubled in six free-fall times, adding up to ∼2 Myr. A fraction of the masses in the central clumps C1 and C2 can be accounted for through large-scale filamentary collapse. Ubiquitous blue profiles in HCO+ (3−2) and 13CO (3−2) spectra suggest a clump-scale collapse scenario in the most massive and densest clump C1. The estimated infall velocity and mass infall rate are 0.31 km s^-1 and 7.2×1e-4 M⊙ yr^-1, respectively. In clump C1, a hot molecular core (SMA1) is revealed by the SMA observations and an outflow-driving high-mass protostar is located at the center of SMA1. The mass of the protostar is estimated to be 11−15 M⊙ and it is still growing with an accretion rate of 7×1e-5 M⊙ yr^-1. The coexistent infall in filaments, clump C1, and the central hot core in G22 suggests that pre-assembled mass reservoirs (i.e., high-mass starless cores) may not be required to form high-mass stars. In the course of high-mass star formation, the central protostar, the core, and the clump can simultaneously grow in

mass via core-fed/disk accretion, clump-fed accretion, and filamentary/cloud collapse.

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A new look at sulphur chemistry in hot cores and corinos

T. H. G. Vidal, V. Wakelam

Sulphur-bearing species are often used to probe the evolution of hot cores since their abundances are particularly sensitive to physical and chemical variations. However, the chemistry of sulphur is not well understood in these regions, notably because observations of several hot cores displayed a large variety of sulphur compositions, and because the reservoir of sulphur in dense clouds, in which hot cores form, is still poorly constrained. In order to help disentangled its complexity, we present a fresh comprehensive review of sulphur chemistry in hot cores along with a study of its sensibility to temperature and pre-collapse chemical composition. In parallel, we analyse the discrepencies that result from the use of two different types of models (static and dynamic) to highlight the sensitivity to the choice of model to be used in astrochemical studies. Our results show that the pre-collapse chemical composition is a critical parameter for sulphur chemistry in hot cores and could explain the different sulphur compositions observed. We also report that differences in abundances for a given species between the static and dynamic models can reach six orders of magnitude in the hot core, which reveals the key role of the choice of model in astrochemical studies.

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Tunneling Reaction Kinetics for the Hydrogen Abstraction Reaction H + H2S -> H2 + HS in the Interstellar Medium

Thanja Lamberts, Johannes Kästner

The hydrogen abstraction reaction between H and H2S, yielding HS and H2 as products, has been studied within the framework of interstellar surface chemistry. High-temperature rate constants up to 2000 K are calculated in the gas phase and are in agreement with previously reported values. Subsequently low-temperature rate constants down to 55 K are presented for the first time that are of interest to astrochemistry, i.e., covering both bimolecular and unimolecular reaction mechanisms. For this, a so-called implicit surface model is used. Strictly speaking, this is a structural gas-phase model in which the restriction of the rotation in the solid state is taken into account. The calculated kinetic isotope effects are explained in terms of difference in activation and delocalization. All rate constants are calculated at the UCCSD(T)-F12/cc-VTZ-F12 level of theory. Finally, we show that the energetics of the reaction is only affected to a small extent by the presence of H2O or H2S molecular clusters that simulate an ice surface, calculated at the MPWB1K/def2-TZVP level of theory.

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Nitrogen oxide in protostellar envelopes and shocks: the ASAI survey

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The high-sensitivity of the IRAM 30-m ASAI unbiased spectral survey in the mm-window allows us to detect NO emission towards both the Class I object SVS13-A and the protostellar outflow shock L1157-B1. We detect the hyperfine components of the 2Pi 1/2 J = 3/2 -> 1/2 (at 151 GHz) and the 2Pi 1/2 J = 5/2 -> 3/2 (250 GHz) spectral pattern. The two objects show different NO profiles: (i) SVS13-A emits through narrow (1.5 km/s) lines at the systemic velocity, while (ii) L1157-B1 shows broad (~5 km/s) blue-shifted emission. For SVS13-A the analysis leads to Tex >= 4 K, N(NO) <= 3 x 1e15 cm-2, and indicates the association of NO with the protostellar envelope. In L1157-B1, NO is tracing the extended outflow cavity: Tex ~= 4-5 K, and N(NO) = 5.5±1.5 x 1e15 cm-2. Using C18O, 13C18O, C17O, and 13C17O ASAI observations we derive an NO fractional abundance less than ~1e-7 for the SVS13-A envelope, in agreement with previous measurements towards extended PDRs and prestellar objects. Conversely, a definite X(NO) enhancement is measured towards L1157-B1, ~ 6e-6, showing that the NO production increases in shocks. The public code UCLCHEM was used to interpret the NO observations, confirming that the abundance observed in SVS13-A can be attained in an envelope with a gas density of 1e5 cm-3 and a kinetic temperature of 40 K. The NO abundance in L1157-B1 is reproduced with pre-shock densities of 1e5 cm-3 subjected to a ~45 km/s shock.

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Efficiency of radial transport of ices in protoplanetary disks probed with infrared observations:

the case of CO2

A. D. Bosman, A.G.G.M. Tielens, E. F. van Dishoeck

The efficiency of radial transport of icy solid material from outer disk to the inner disk is currently unconstrained. Efficient radial transport of icy dust grains could significantly alter the composition of the gas in the inner disk. Our aim is to model the gaseous CO2 abundance in the inner disk and use this to probe the efficiency of icy dust transport in a viscous disk. Features in the simulated CO2 spectra are investigated for their dust flux tracing potential. We have developed a 1D viscous disk model that includes gas and grain motions as well as dust growth, sublimation and freeze-out and a parametrisation of the CO2 chemistry. The thermo-chemical code DALI was used to model the mid-infrared spectrum of CO2, as can be observed with JWST-MIRI. CO2 ice sublimating at the iceline increases the gaseous CO2 abundance to levels equal to the CO2 ice abundance of ∼10^−5, which is three orders of magnitude more than the gaseous CO2 abundances of ∼10^−8 observed by Spitzer. Grain growth and radial drift further increase the gaseous CO2 abundance. A CO2 destruction rate of at least 10^−11 s^−1 is needed to reconcile model prediction with observations. This rate is at least two orders of magnitude higher than the fastest known chemical destruction rate. A range of potential physical mechanisms to explain the low observed CO2 abundances are discussed. Transport processes in disks can have profound effects on the abundances of species in the inner disk. The discrepancy between our model and observations either suggests frequent shocks in the inner 10 AU that destroy CO2, or that the abundant midplane CO2 is hidden from our view by an optically thick column of low abundance CO2 in to the disk surface XDR/PDR. Other molecules, such as CH4 or NH3, can give further handles on the rate of mass transport.

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ALMA Detection of Interstellar Methoxymethanol (CH3OCH2OH)

Brett A. McGuire, Christopher N. Shingledecker, Eric R. Willis, Andrew M. Burkhardt, Samer El-Abd, Roman A. Motiyenko, Crystal L. Brogan, Todd R. Hunter, Laurent Margulès, Jean-Claude Guillemin, Robin T. Garrod, Eric Herbst, Anthony J. Remijan

We report the detection of interstellar methoxymethanol (CH3OCH2OH) in ALMA Bands 6 and 7 toward the MM1 core in the high-mass star-forming region NGC 6334I at ~0.1" - 1" spatial resolution. A column density of 4(2) x 1e18 cm−2 at Tex = 200 K is derived toward MM1, ~34 times less abundant than methanol (CH3OH), and significantly higher than predicted by astrochemical models. Probable formation and destruction pathways are discussed, primarily through the reaction of the CH3OH photodissociation products, the methoxy (CH3O) and hydroxymethyl (CH2OH) radicals. Finally, we comment on the implications of these mechanisms on gas-phase vs grain-surface routes operative in the region, and the possibility of electron-induced dissociation of CH3OH rather than photodissociation.

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Probing the baryon cycle of galaxies with SPICA mid- and far-infrared observations

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The SPICA mid and far-infrared telescope will address fundamental issues in our understanding of star formation and ISM physics in galaxies. A particular hallmark of SPICA is the outstanding sensitivity enabled by the cold telescope, optimized detectors, and wide instantaneous bandwidth throughout the mid- and far-infrared. The spectroscopic, imaging and polarimetric observations that SPICA will be able to collect will help in clarifying the complex physical mechanisms which underlie the baryon cycle of galaxies. In particular: (i) The access to a large suite of atomic and ionic fine-structure lines for large samples of galaxies will shed light on the origin of the observed spread in star formation rates within and between galaxies. (ii) Observations of HD rotational lines (out to ~10 Mpc) and fine structure lines such as [CII] 158 um (out to ~100 Mpc) will clarify the main reservoirs of interstellar matter in galaxies, including phases where CO does not emit. (iii) Far-infrared spectroscopy of dust and ice features will address uncertainties in the mass and composition of dust in galaxies, and the contributions of supernovae to the interstellar dust budget will be quantified by photometry and monitoring of supernova remnants in nearby galaxies. (iv) Observations of far-infrared cooling lines such as [OI] 63 um from star-forming molecular clouds in our Galaxy will evaluate the importance of shocks to dissipate turbulent energy. The paper concludes with requirements for the telescope and instruments, and recommendations for the observing strategy.

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Accelerated Gillespie Algorithm for Gas-Grain Reaction Network Simulations Using Quasi-Steady-State Assumption

Q. Chang, Y. Lu, D. Quan

Although the Gillespie algorithm is accurate to simulate gas-grain reactions networks, so far its computational cost is so expensive that it cannot be use to simulate chemical reaction networks including molecular hydrogen accretion or the chemical evolution of protoplanatory disks. We present an accelerated Gillespie algorithm that is based on quasi-steady-state assumption with further approximation that the population distribution of transient species depends only on the accretion and desorption processes. The new algorithm is tested against a few reaction networks that are simulated by the regular Gillespie algorithm. We found that the less likely transient species are formed and destroyed on grain surfaces, the more accurate the new method is. We also apply the new method to simulate reaction networks that include molecular hydrogen accretion. The results show that surface chemical reactions involving molecular hydrogen are not important for the production of surface species under standard physical conditions of dense molecular clouds.

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Phosphorus-bearing molecules in the Galactic Center

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Phosphorus (P) is one of the essential elements for life due to its central role in biochemical processes. Recent searches have shown that P-bearing molecules (in particular PN and PO) are present in star-forming regions, although their formation routes remain poorly understood. In this Letter, we report observations of PN and PO towards seven molecular clouds located in the Galactic Center, which are characterized by different types of chemistry. PN is detected in five out of seven sources, whose chemistry is thought to be shock-dominated. The two sources with PN non-detections correspond to clouds exposed to intense UV/X-rays/cosmic-ray radiation. PO is detected only towards the cloud G+0.693−0.03, with a PO/PN abundance ratio of ∼1.5. We conclude that P-bearing molecules likely form in shocked gas as a result of dust grain sputtering, while are destroyed by intense UV/X-ray/cosmic ray radiation.

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First Detection of Interstellar S2H

Asunción Fuente, Javier R. Goicoechea, Jérôme Pety, Romane Le Gal, Rafael Martín-Doménech, Pierre Gratier, Viviana Guzmán, Evelyne Roueff, Jean-Christophe Loison, Guillermo M. Muñoz-Caro, Valentine Wakelam, Maryvonne Gerin , Pablo Riviére-Marichalar, and Thomas Vidal

We present the first detection of gas-phase S2H in the Horsehead, a moderately UV-irradiated nebula. This confirms the presence of doubly sulfuretted species in the interstellar medium and opens a new challenge for sulfur chemistry. The observed S2H abundance is ∼5×1e-11, only a factor of 4–6 lower than that of the widespread H2S molecule. H2S and S2H are efficiently formed on the UV-irradiated icy grain mantles. We performed ice irradiation experiments to determine the H2S and S2H photodesorption yields. The obtained values are ∼1.2×1e−3 and <1e−5 molecules per incident photon for H2S and S2H, respectively. Our upper limit to the S2H photodesorption yield suggests that photodesorption is not a competitive mechanism to release the S2H molecules to the gas phase. Other desorption mechanisms such as chemical desorption, cosmic-ray desorption, and grain shattering can increase the gaseous S2H abundance to some extent. Alternatively, S2H can be formed via gas phase reactions involving gaseous H2S and the abundant ions S+ and SH+. The detection of S2H in this nebula therefore could be the result of the coexistence of an active grain-surface chemistry and gaseous photochemistry.

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Influence of galactic arm scale dynamics on the molecular composition of the cold and dense ISM I. Observed abundance gradients in dense clouds

M. Ruaud, V. Wakelam, P. Gratier, I. A. Bonnell

Aims. We study the effect of large scale dynamics on the molecular composition of the dense interstellar medium during the transition between diffuse to dense clouds. Methods. We followed the formation of dense clouds (on sub-parsec scales) through the dynamics of the interstellar medium at galac- tic scales. We used results from smoothed particle hydrodynamics (SPH) simulations from which we extracted physical parameters that are used as inputs for our full gas-grain chemical model. In these simulations, the evolution of the interstellar matter is followed for ~50 Myr. The warm low-density interstellar medium gas flows into spiral arms where orbit crowding produces the shock formation of dense clouds, which are held together temporarily by the external pressure. Results. We show that depending on the physical history of each SPH particle, the molecular composition of the modeled dense clouds presents a high dispersion in the computed abundances even if the local physical properties are similar. We find that carbon chains are the most affected species and show that these differences are directly connected to differences in (1) the electronic fraction, (2) the C/O ratio, and (3) the local physical conditions. We argue that differences in the dynamical evolutio of the gas that formed dense clouds could account

for the molecular diversity observed between and within these clouds. Conclusions. This study shows the importance of past physical conditions in establishing the chemical composition of the dense medium.

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Chemical modelling of glycolaldehyde and ethylene glycol in star-forming regions

A. Coutens, S. Viti, J. M. C. Rawlings, M. T. Beltran, J. Holdship, I. Jiménez-Serra, D. Quénard, and V. M. Rivilla

Glycolaldehyde (HOCH2CHO) and ethylene glycol ((CH2OH)2) are two complex organic molecules detected in the hot cores and hot corinos of several star-forming regions. The ethylene glycol/glycolaldehyde abundance ratio seems to show an increase with the source luminosity. In the literature, several surface-chemistry formation mechanisms have been proposed for these two species. With the UCLCHEM chemical code, we explored the different scenarios and compared the predictions for a range of sources of different luminosities with the observations. None of the scenarios reproduce perfectly the trend. A better agreement is, however, found for a formation through recombination of two HCO radicals followed by successive hydrogenations. The reaction between HCO and CH2OH could also contribute to the formation of glycolaldehyde in addition to the hydrogenation pathway. The predictions are improved when a trend of decreasing H2 density within the core region with T≥100 K as a function of luminosity, is included in the model. Destruction reactions of complex organic molecules in the gas phase would also need to be investigated, since they can affect the abundance ratios once the species have desorbed in the warm inner regions of the star-forming regions.

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First detection of cyanamide (NH2CN) towards solar-type protostars

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Searches for the prebiotically-relevant cyanamide (NH2CN) towards solar-type protostars have not been reported in the literature. We here present the first detection of this species in the warm gas surrounding two solar-type protostars, using data from the Atacama Large Millimeter/Submillimeter Array Protostellar Interferometric Line Survey (PILS) of IRAS 16293–2422 B and observations from the IRAM Plateau de Bure Interferometer of NGC1333 IRAS2A. We furthermore detect the deuterated and 13C isotopologues of NH2CN towards IRAS 16293–2422 B. This is the first detection of NHDCN in the interstellar medium. Based on a local thermodynamic equilibrium analysis, we find that the deuteration of cyanamide (∼ 1.7%) is similar to that of formamide (NH2CHO), which may suggest that these two molecules share NH2 as a common precursor. The NH2CN/NH2CHO abundance ratio is about 0.2 for IRAS 16293–2422 B and 0.02 for IRAS2A, which is comparable to the range of values found for Sgr B2. We explored the possible formation of NH2CN on grains through the NH2 + CN reaction using the chemical model MAGICKAL. Grain-surface chemistry appears capable of reproducing the gas-phase abundance of NH2CN with the correct choice of physical parameters.

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Announcements

Research Fellow in ALMA Studies of Protoplanetary Disks

The School of Physics and Astronomy at the University of Leeds invites applications for a 2-year fixed-term postdoctoral research fellow in ALMA Studies of Protoplanetary Disks. The post involves working on an STFC-funded project in collaboration with Dr Catherine Walsh in the Astrophysics Group investigating the chemistry of complex organic molecules (COMs) in disks around nearby young stars. You will carry out a research programme to search for emission from COMs in nearby protoplanetary disks using the Atacama Large Millimeter/submillimeter Array (ALMA). You will conduct analyses of the data to derive the distribution and abundance of COMs using molecular line radiative transfer methods. In addition, you will aid interpretation of the data by running astrochemical models to determine the chemical origin of COMs in protoplanetary disks. With a PhD in Astrophysics or a related field (or if you will have submitted your thesis prior to taking up the appointment), you will have experience in the reduction and analysis of observational data at (sub)millimeter or radio wavelengths and a developing track record of peer reviewed publications in international journals. The application deadline is 15th January 2018 and the starting date will be 1st April 2018 or as soon as possible thereafter. For more information and to apply, please follow the link: https://jobs.leeds.ac.uk/Vacancy.aspx?ref=MAPPA1049. For more information on the project, you can also contact Dr Catherine Walsh (c.walsh1@leeds.ac.uk).

Post-doctoral positions at the Virginia Initiative on Cosmic Origins

The University of Virginia invites applications for three or more Postdoctoral Research Associate positions as part of the new interdisciplinary Virginia Initiative on Cosmic Origins (VICO). The incumbents will lead an ambitious, independent research program related to Cosmic Origins science, expected to align with the wide range of research at the University of Virginia, as well as at the National Radio Astronomy Observatory on the grounds of the University. The relevant themes include star formation, planet formation and evolution, planetary science, astrochemistry and astrobiology, from both

theoretical and observational perspectives. See www.cosmicorigins.space for more information. The Postdoctoral Research Associates will participate in departmental activities and promote collaboration both within VICO and with its partner institutes, Chalmers University of Technology, Gothenburg, Sweden and the Center for Astrochemical Studies at the Max Planck Institute for Extraterrestrial Physics (MPE), Garching, Germany. There are three types of research programs: 1) Virginia Cosmic Origins Program; (2) Virginia-Chalmers Cosmic Origins Program; (3) Virginia-MPE Cosmic Origins Program. Applicants should indicate in their cover letter if they have preferences among these research programs. These positions are initially a one-year appointment, with renewal for an additional two one-year increments for the Virginia position contingent upon satisfactory performance and an additional three one-year increments for the Virginia-Chalmers and Virginia-MPE positions contingent upon satisfactory performance and the approval of the Vice President of Research. Applicants are required to have a Ph.D. in astrophysics, astrochemistry, astrobiology or related disciplines by the appointment start date. To apply, please submit a candidate profile on-line through Jobs@UVA(https://jobs.virginia.edu), search on posting number 0622344 . Electronically attach as a single PDF document as "Other 1": cover letter; curriculum vitae; list of publications; summary of previous and current research (limited to 3 pages, including references); research proposal (limited to 3 pages text plus up to 2 pages of references/figures). Applicants should also arrange for 3 letters of recommendation to be submitted to vico-postdoc@virginia.edu A competitive salary and benefits package is offered at University of Virginia. The positions also include travel funds and opportunities for dissemination, networking, and international collaboration. Review of applications will begin on January 15, 2017; however, the position will remain open until filled. Applicants may conduct informational interviews at the AAS Winter Meeting. Questions regarding the position should be directed to: Eric Herbst (eh2ef@virginia.edu), Zhi-Yun Li (zl4h@virginia.edu) or Jonathan Tan (jct6e@virginia.edu). Questions regarding the application process in Jobs@UVA should be directed to: Barbara K. Johnson, 434-924-5070, bk9nx@virginia.edu The University will perform background checks on all new hires prior to making a final offer of employment. The University of Virginia is an equal opportunity and affirmative action employer. Women, minorities, veterans and persons with disabilities are encouraged to apply.

"Astrochemistry: Past, Present, and Future" - A meeting in celebration of Ewine van Dishoeck - July 10th-13th, 2018, Caltech - Pasadena, CA, USA

Astrochemistry, the study of molecules in astrophysical environments, has become an invaluable part of astrophysical studies ranging from planet forming disks to high-z galaxies. This development was made possible by the arrival of a suite of new telescopes in the past decade — Spitzer, Herschel and ALMA – and was realized by the pioneering work and ongoing leadership by Ewine van Dishoeck. To honor Ewine's outstanding contributions to astrochemistry this 4-day meeting will review the successes in astrochemistry in unveiling star and planet formation, present ongoing astrochemical theoretical and laboratory studies, and observational investigations focused on ALMA, and peer into the future of astrochemistry in the age of JWST. The meeting is organized around five science themes: - The astrochemical water trail - Photon-dominated regions during star and planet formation - Origins of astrochemical complexity - Role of dust and grain growth for planet formation - Chemistry as a tracer of physics in astronomical environments Within each theme, we imagine exploring the past, present, and future questions that characterize(d) it, and discuss how observations, theory, laboratory efforts and new instrumentation contribute(d) to solving these questions. Invited (confirmed) speakers: Ted Bergin, John Black, Paola Caselli, Ilse Cleeves, Neal Evans, Edith Fayolle, Kenji Furuya, Thomas Henning, Eric Herbst, Lars Kristensen, Thanja Lamberts, Harold Linnartz, David Neufeld, Paola Pinilla, Nami Sakai, Leonardo Testi, Xander Tielens, Floris van der Tak & Catherine Walsh For further information and registration - please see the conference website at: http://www.cfa.harvard.edu/events/2018/astrochem18 Please note, there are a limited number of possible attendees due to space restrictions. Registration is therefore on a first come first service basis. In case of questions, please send us an email to: astrochemistry2018@gmail.com Important dates: February 16, 2018 - Abstract submission due for consideration as a contributed talk March 16, 2018 - Conference Registration and Poster Abstract Submission SOC: Karin Oberg, Agata Karska, Jes Jorgensen (co-chairs), Ruud Visser, Nienke van der Marel, Frank Helmich, Michiel Hogerheijde, Maria Drozdovskaya, Geoff Blake LOC: Geoff Blake (chair), Edith Fayolle, Umut Yildiz, Olivia Wilkins, Cam Buzzard, Christine Benoit

Computational Astrochemistry Workshop at ICCSA 2018 (Melbourne, July 2-5, 2018)

This is an invitation to submit a contribution for the Computational Astrochemistry (CompAstro) Workshop of the 18th International Conference on Computational Science and Applications (ICCSA 2018, http://www.iccsa.org/) to be held on July 2 - 5, 2018 in Melbourne (Australia). All accepted papers will be included in the Springer Lecture Notes in Computer Science (LNCS, http://www.springer.com/gp/computer-science/lncs) series and indexed by Scopus, EI Engineering Index, Thomson Reuters Conference Proceedings Citation Index (included in ISI Web of Science), and several other indexing services. The papers will contain linked references, XML versions and citable DOI numbers. Submitted papers will be subject to stringent peer review by at least three experts and carefully evaluated based on originality, significance, technical soundness, and clarity of exposition. The themes of the Workshop include (but are not limited to): - Potential energy surfaces of species relevant in astrochemistry - Thermodynamics of reactions relevant in astrochemistry - Calculation of kinetic parameters associated with reactions relevant in astrochemistry - Modelling dust and icy grain structures and properties - Modelling processes at the grain surfaces Organizers: Marzio Rosi - marzio.rosi@unipg.it (Università degli Studi di Perugia), Dimitrios Skouteris - dimitrios.skouteris@sns.it (Scuola Normale Superiore di Pisa), Albert Rimola - Albert.Rimola@uab.cat (Universitat Autònoma de Barcelona) Program Committee Members: Nadia Balucani, Università degli Studi di Perugia, nadia.balucani@unipg.it; Cecilia Ceccarelli, Université Grenoble Alpes, cecilia.ceccarelli@univ-grenoble-alpes.fr; Piero Ugliengo, Università degli Studi di Torino, piero.ugliengo@unito.it; Daniela Ascenzi, Università degli Studi di Trento, daniela.ascenzi@unitn.it RATIONALE OF THE WORKSHOP: Since their first detection, the presence of relatively complex molecules in the interstellar medium, ISM, has posed the question of how they are formed. The harsh chemical environments of interstellar clouds (namely, very low temperature and very low number density), indeed, challenge the common notions that chemical synthesis requires energy to promote the weakening of the reactant bonds and frequent

collisions to increase the number of reactive encounters. Since 1% of interstellar clouds is composed by small silicates or vitreous carbonaceous particles, interstellar grains covered by icy mantles are also invoked to play an important role in synthesizing interstellar molecules by acting as interstellar catalysts. One important drawback of astrochemical models, which include several thousands of molecular processes, is due to the uncertainty associated with the parameters which are used to quantitatively account for the importance of every step: many of those processes have never been investigated in laboratory experiments, many others have been investigated but under experimental conditions that do not reproduce the interstellar ones (either regarding the temperature or the pressure). For gas-phase reactions of the first kind, rate coefficients and their temperature dependence are mainly estimated with some chemical intuition or by drawing analogies with similar known processes. Small details in the molecular structure and in the potential energy surfaces, however, can induce a huge change in the chemical behaviour and reasoning by analogy can cause severe mistakes. In the second case, the values obtained as a function of the temperature in a T range that does not encompass those of relevance in ISM are used, but this can also be very risky as a change in the reaction mechanism can alter the temperature dependence in non-Arrhenius reactions. The case of grain-chemistry simulation in laboratory experiments is even more complex, as no experiments are able to reproduce the size of interstellar particles, the exact composition of the grain icy mantle and the flux of particles and/or photons impinging on the grains. A theoretical characterization at the atomic/molecular level can help in extrapolating experimental data at the conditions of ISM or in estimating in a reliable way the kinetic parameters (e.g. cross sections, rate constants, branching ratios) associated with reactions that cannot be investigated in laboratory experiments. These theoretical characterizations, once used to interpret and understand the laboratory data, can assist in the extrapolation to the actual ISM conditions. When laboratory data are not available, instead, they can provide a reliable estimate of the relative parameters. In conclusion, a thorough theoretical characterization can be pivotal to the understanding of chemistry in space either in the presence or absence of experimental data. All these topics are covered by computational astrochemistry, which forms the subject of the present workshop. ICCSA CONFERENCE: The 18th International Conference on Computational Science and Applications (ICCSA 2018) will be held on July 2 - 5, 2018 in Melbourne, Australia in collaboration with the Monash University, Australia. ICCSA 2018 will be the next event in a series of highly successful International Conferences on Computational Science and Its Applications (ICCSA), previously held in Trieste, Italy (2017), Beijing. China (2016), Banff, Canada (2015), Guimaraes, Portugal (2014), Ho Chi Minh City, Vietnam (2013), Salvador de Bahia, Brazil (2012), Santander, Spain (2011), Fukuoka, Japan (2010), Suwon, Korea (2009), Perugia, Italy (2008), Kuala Lumpur, Malaysia (2007), Glasgow, UK (2006), Singapore (2005), Assisi, Italy (2004), Montreal, Canada (2003), and (as ICCS) in Amsterdam, The Netherlands (2002) and San Francisco, USA (2001). The first ICCSA conference was co-organized by C.J.K. Tan (UK) and M. Gavrilova (U of Calgary, Canada) in 2003. Computational Science is a main pillar of most of the present research, industrial and commercial activities and plays a unique role in exploiting Information and Communication Technologies as innovative technologies. The ICCSA Conference offers a real opportunity to discuss new issues, tackle complex problems and find advanced enabling solutions able to shape new trends in Computational Science. This conference is sponsored by: Monash University, Australia; The University of Perugia, Italy; Kyushu Sangyo University, Japan; The University of Basilicata, Italy; University of Minho, Portugal

SOFIA Workshop 2018, 2-4 May 2018, Stuttgart, Germany

This May, Deutsches SOFIA Institut is organising „SOFIA Workshop 2018”. WHEN: 2-4 May 2018 WHERE: Deutsches SOFIA Institut in Stuttgart, Germany WHY: The purpose of the SOFIA Workshop 2018 is to bring together young astronomers, scientists, and experienced SOFIA users mainly from the German community to share information about the current status of the observatory, discuss recent results, and learn to write successful proposals. International participants are also very welcome. The deadline for registration is 28 February 2018. For more information, please, check the website: https://conference.dsi.uni-stuttgart.de/e/sofiaworkshop2018 Main Topics: SOFIA Science Capabilities SOFIA Instruments (GREAT, EXES, FIFI-LS, HAWC+, FORCAST, FPI+) SOFIA Status & Schedule Call for Proposal Cycle 7 Tutorial in proposal writing Tutorial on data reduction SOC: Jochen Eislöffel Alfred Krabbe Jürgen Stutzki Harold Yorke Hans Zinnecker