AstroChemical Newsletter #52

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Abstracts

Detection of vibrational emissions from the helium hydride ion (HeH+) in the planetary nebula NGC 7027

D.A. Neufeld, M. Goto, T. R. Geballe, R. Güsten, K.M. Menten, H. Wiesemeyer

We report the detection of emission in the v=1-0 P(1) (3.51629 micron) and P(2) (3.60776 micron) rovibrational lines of the helium hydride cation (HeH+) from the planetary nebula NGC 7027. These detections were obtained with the iSHELL spectrograph on NASA's Infrared Telescope Facility (IRTF) on Maunakea. They confirm the discovery of HeH+ reported recently by Guesten et al. (2019), who used the GREAT instrument on the SOFIA airborne observatory to observe its pure rotational J=1-0 transition at 149.137 micron. The flux measured for the HeH+ v=1-0 P(1) line is in good agreement with our model for the formation, destruction and excitation of HeH+ in NGC 7027. The measured strength of the J=1-0 pure rotational line, however, exceeds the model prediction significantly, as does that of the v=1-0 P(2) line, by factors of 2.9 and 2.3 respectively. Possible causes of these discrepancies are discussed. Our observations of NGC 7027, covering the 3.26 - 3.93 micron spectral region, have led to the detection of more than sixty spectral lines including nine rovibrational emissions from CH+. The latter are detected for the first time in an astronomical source.

ApJ accepted
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Low-Energy Water−Hydrogen Inelastic Collisions

Astrid Bergeat, Alexandre Faure, Sébastien B. Morales, Audrey Moudens, Christian Naulin

New molecular beam scattering experiments are reported for the water−hydrogen system. Integral cross sections of the first rotational excitations of para- and ortho-H2O by inelastic collisions with normal-H2 were determined by crossing a beam of H2O seeded in He with a beam of H2. H2O and H2 were cooled in the supersonic expansion down to their lowest rotational levels. Crossed-beam scattering experiments were performed at collision energies from 15 cm−1 (below the threshold for the excitation to the lowest excited rotational state of H2O: 18.6 cm−1) up to 105 cm−1 by varying the beam crossing angle. The measured state-to-state cross-sections were compared to the theoretical cross-sections (close-coupling quantum scattering calculations): the good agreement found further validates both the employed potential energy surface describing the H2O−H2 van der Waals interaction and the state-to-state rate coefficients calculated with this potential in the very low temperature range needed for

the modeling of interstellar media.

J. Phys. Chem. A 2020, 124, 2, 259-264
DOI: 10.1021/acs.jpca.9b04753
Full-text URL: https://pubs.acs.org/doi/pdf/10.1021/acs.jpca.9b04753

Dissociative Electron Attachment to MgCN

A. E. Orel and A. Larson

Dissociative electron attachment (DEA) to the molecule MgCN and its isomer MgNC has been proposed as a possible source of CN- in the interstellar media. We have carried out electron scattering calculations using the complex Kohn Variational Method as a function of the internal degrees of freedom of the molecule to obtain the resonance energy surfaces and autoionization widths. We use this data as input to form the Hamiltonian relevant to the nuclear dynamics. The multidimensional time-dependent Schrodinger equation is solved using the MultiConfiguration Time-Dependent Hartree (MCTDH) approach. We compute the DEA cross sections and discuss the implications for CN-formation in circumstellar envelopes.

Eur. Phys. J. D (2020) 74:15
DOI: 10.1140/epjd/e2019-100542-x
Full-text URL: https://link.springer.com/article/10.1140%2Fepjd%2Fe2019-100542-x

Abundant refractory sulfur in protoplanetary disks

M. Kama, O. Shorttle, A.S. Jermyn, C.P. Folsom, K. Furuya, E.A. Bergin, C. Walsh, L. Keller

Sulfur is one of the most abundant elements in the universe, with important roles in astro-, geo-, and biochemistry. Its main reservoirs in planet-forming disks have previously eluded detection: gaseous molecules only account for <1% of total elemental sulfur, with the rest likely in either ices or refractory minerals. We use a new method to measure the refractory component. Mechanisms such as giant planets can filter out dust from gas accreting onto disk-hosting stars. For stars above 1.4 solar masses, this leaves a chemical signature on the stellar photosphere that can be used to determine the fraction of each element that is locked in dust. Here, we present an application of this method to sulfur, zinc, and sodium. We analyze the accretion-contaminated photospheres of a sample of young stars and find (89 ± 8)% of elemental sulfur is in refractory form in their disks. The main carrier is much more refractory than water ice, consistent with sulfide minerals such as FeS.

The Astrophysical Journal 2019, V885, A114
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Full-text URL: https://arxiv.org/abs/1908.05169

Mass constraints for 15 protoplanetary discs from HD 1-0

M. Kama, L. Trapman, D. Fedele, S. Bruderer, M.R. Hogerheijde, A. Miotello, E.F. van Dishoeck, C. Clarke, E.A. Bergin

Hydrogen deuteride (HD) rotational line emission can provide reliable protoplanetary disk gas mass measurements, but it is difficult to observe and detections have been limited to three T-Tauri disks. No new data have been available since the Herschel Space Observatory mission ended in 2013. We set out to obtain new disk gas mass constraints by analysing upper limits on HD 1-0 emission in Herschel/PACS archival data

from the DIGIT key programme. With a focus on the Herbig Ae/Be disks, whose stars are more luminous than T Tauris, we determine upper limits for HD in data previosly analysed for its line detections. Their significance is studied with a grid of models run with the DALI physical-chemical code, customised to include deuterium chemistry. Nearly all the disks are constrained to Mgas ≤ 0.1 Msun, ruling out global gravitational instability. A strong constraint is obtained for the HD 163296 disk mass, Mgas ≤ 0.067 Msun, implying a gas-to-dust ratio Δg/d ≤ 100. This HD-based mass limit is towards the low end of CO-based mass estimates for the disk, highlighting the large uncertainty in using only CO and suggesting that gas-phase CO depletion in HD 163296 is at most a factor of a few. The Mgas limits for HD 163296 and HD 100546, both bright disks with massive candidate protoplanetary systems, suggest disk-to-planet mass conversion efficiencies of Mp/(Mgas+Mp)~10 to 40% for present-day values. Near-future observations with SOFIA/HIRMES will be able to detect HD in the brightest Herbig Ae/Be disks within 150pc with ~10h integration time.

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Full-text URL: https://arxiv.org/abs/1912.11883

Formation of complex molecules in translucent clouds: Acetaldehyde, vinyl alcohol, ketene, and ethanol via "nonenergetic" processing of C2H2 ice

Ko-Ju Chuang, G. Fedoseev, D. Qasim, S. Ioppolo, C. Jäger, T. Henning, M.E. Palumbo, E.F. van Dishoeck, H. Linnartz

Complex organic molecules (COMs) have been identified toward high- and low-mass protostars as well as molecular clouds, suggesting that these interstellar species originate from the early stage(s) of star formation. The reaction pathways resulting in COMs described by the formula C2HnO are still under debate. In this work, we investigate the laboratory possible solid-state reactions that involve simple hydrocarbons and OH-radicals along with H2O ice under translucent cloud conditions (1<=A_V<=5 and nH~1e3 cm-3). We focus on the interactions of C2H2 with H-atoms and OH-radicals, which are produced along the H2O formation sequence on grain surfaces at 10 K. Ultra-high vacuum (UHV) experiments were performed to study the surface chemistry observed during C2H2 + O2 + H codeposition, where O2 was used for the in-situ generation of OH-radicals. Reflection absorption infrared spectroscopy (RAIRS) was applied to in situ monitor the initial and newly formed species. After that, a temperature-programmed desorption experiment combined with a Quadrupole mass spectrometer (TPD-QMS) was used as a complementary analytical tool. The investigated 10 K surface chemistry of C2H2 with H-atoms and OH-radicals not only results in semi and fully saturated hydrocarbons, such as ethylene (C2H4) and ethane (C2H6), but it also leads to the formation of COMs, such as vinyl alcohol, acetaldehyde, ketene, ethanol, and possibly acetic acid. It is concluded that OH-radical addition reactions to C2H2, acting as a molecular backbone, followed by isomerization (i.e., keto-enol tautomerization) via an intermolecular pathway and successive hydrogenation provides a so far experimentally unreported solid-state route for the formation of these species without the need of energetic input.

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Molecular complexity in pre-stellar cores: a 3 mm-band study

of L183 and L1544

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Pre-stellar cores (PSCs) are units of star formation. Besides representing early stages of the dynamical evolution leading to the formation of stars and planets, PSCs also provide a substrate for incipient chemical complexity in the interstellar space. Our aim is to understand the influence of external conditions on the chemical composition of PSCs. For this purpose, we compared molecular column densities in two typical PSCs, L183 and L1544, which are embedded in different environments. Methods. A single-pointing survey of L183 at λ = 3mm was conducted using the IRAM 30-m single-dish antenna. This led to the detection of more than 100 emission lines from 46 molecular species. The molecular column densities and excitation temperatures derived from these lines were compared to the corresponding parameters in L1544. The data for L1544 were obtained from literature or publicly available surveys, and they were analysed using the same procedure as adopted for L183. An astrochemical model, previously developed for the interpretation of organic molecule emissions towards the methanol peak of L1544, was used to interpret the combined data. Our analysis reveals clear chemical differences between the two PSCs. While L1544 is richer in carbon-bearing species, in particular carbon chains, oxygen-containing species are generally more abundant in L183. The results are well-reproduced by our chemical model. The observed chemical differentiation between the two PSCs is caused by the different environmental conditions: the core of L183 is deeply buried in the surrounding cloud, whereas L1544 lies close to the edge of the Taurus Molecular Cloud. The obscuration of L183 from the interstellar radiation field (ISRF) allows the carbon atoms to be locked in carbon monoxide, which ultimately leads to a large abundance of O-bearing species. In contrast, L1544, being more affected by the ISRF, can keep a fraction of carbon in atomic form, which is needed for the production of carbon chains.

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Dissociation dynamics of the diamondoid adamantane upon photoionization by XUV femtosecond pulses

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This work presents a photodissociation study of the diamondoid adamantane using extreme ultraviolet femtosecond pulses. The fragmentation dynamics of the dication is unraveled by the use of advanced ion and electron spectroscopy giving access to the dissociation channels as well as their energetics. To get insight into the fragmentation dynamics, we use a theoretical approach combining potential energy surface determination, statistical fragmentation methods and molecular dynamics simulations. We demonstrate that the dissociation dynamics of adamantane dications takes place in a two-step process: barrierless cage opening followed by Coulomb repulsion-driven fragmentation.

Scientific Reports 10 2884 (2020)
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Full-text URL: https://www.nature.com/articles/s41598-020-59649-1

The effect of CO−H2O collisions in the rotational excitation of cometary CO

Alexandre Faure, François Lique, Jérôme Loreau

We present the first accurate rate coefficients for the rotational excitation of CO by H2O in the kinetic temperature range 5–100 K. The statistical adiabatic channel method (SACM) is combined with a high-level rigid-rotor CO−H2O intermolecular potential energy surface. Transitions among the first 11 rotational levels of CO and the first 8 rotational levels of both para-H2O and ortho-H2O are considered. Our rate coefficients are compared to previous data from the literature and they are also incorporated in a simple non-LTE model of cometary coma including collision-induced transitions, solar radiative pumping and radiative decay. We find that the uncertainties in the collision data have significant influence on the CO population distribution for H2O densities in the range 10^3–10^8 cm−3. We also show that the rotational distribution of H2O plays an important role in CO excitation (owing to correlated energy transfer in both CO and H2O), while the impact of the ortho-to-para ratio of H2O is found to be negligible.

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Constraining the Infalling Envelope Models of Embedded Protostars: BHR 71 and its Hot Corino

Yao-Lun Yang, Neal J. Evans II, Aaron Smith, Jeong-Eun Lee, John J. Tobin, Susan Terebey, Hannah Calcutt, Jes K. Jørgensen, Joel D. Green, and Tyler L. Bourke

The collapse of the protostellar envelope results in the growth of the protostar and the development of a protoplanetary disk, playing a critical role during the early stages of star formation. Characterizing the gas infall in the envelope constrains the dynamical models of star formation. We present unambiguous signatures of infall, probed by optically thick molecular lines, toward an isolated embedded protostar, BHR 71 IRS1. The three dimensional radiative transfer calculations indicate that a slowly rotating infalling envelope model following the "inside-out" collapse reproduces the observations of both HCO+ J=4-3 and CS J=7-6 lines, and the low velocity emission of the HCN J=4-3 line. The envelope has a model-derived age of 12000+/-3000 years after the initial collapse. The envelope model underestimates the high velocity emission at the HCN J=4-3 and H13CN J=4-3 lines, where outflows or a Keplerian disk may contribute. The ALMA observations serendipitously discover the emission of complex organic molecules (COMs) concentrated within a radius of 100 au, indicating that BHR 71 IRS1 harbors a hot corino. Eight species of COMs are identified, including CH3OH and CH3OCHO, along with H2CS, SO2 and HCN v2=1. The emission of methyl formate and 13C-methanol shows a clear velocity gradient within a radius of 50 au, hinting at an unresolved Keplerian rotating disk.

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Physical and chemical modeling of a starless core: L1512

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The deuterium fractionation in starless cores gives us a clue to estimate their lifetime scales, thus allowing us to distinguish between different dynamical theories of core formation. Cores also seem to be subject to a differential N2 and CO depletion which was not expected from models. We aim to make a survey of 10 cores to estimate their lifetime scales and depletion profiles in detail. After L183, in Serpens, we present the second cloud of the series, L1512 in Auriga. To constrain the lifetime scale, we perform chemical modeling of the deuteration profiles across L1512 based on dust extinction measurements from near-infrared observations and non-local thermal equilibrium radiative transfer with multiple line observations of N2H+, N2D+, DCO+, C18O, and 13CO, plus H2D+ (1_10-1_11). We find a peak density of 1.1x10^5 cm^{-3} and a central temperature of 7.5+-1 K, which are respectively higher and lower compared with previous dust emission studies. The depletion factors of N2H+ and N2D+ are 27(+17, -13) and 4(+2, -1) in L1512, intermediate between the two other more advanced and denser starless core cases, L183 and L1544. These factors also indicate a similar freeze-out of N2 in L1512, compared to the two others despite a peak density one to two orders of magnitude lower. Retrieving CO and N2 abundance profiles with the chemical model, we find that CO has a depletion factor of ~430-870 and the N2 profile is similar to that of CO unlike towards L183. Therefore, L1512 has probably been living long enough so that N2 chemistry has reached steady state. N2H+ modeling remains compulsory to assess the precise physical conditions in the center of cold starless cores, rather than dust emission. L1512 is presumably older than 1.4 Myr. Therefore, the dominating core formation mechanism should be ambipolar diffusion for this source.

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Questioning the spatial origin of complex organic molecules in young protostars with the CALYPSO survey

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Complex organic molecules (COMs) have been detected in a few Class 0 protostars but their origin is not well understood. Going beyond studies of individual objects, we want to investigate the origin of COMs in young protostars on a statistical basis. We use the CALYPSO survey performed with the IRAM PdBI to search for COMs at high angular resolution in a sample of 26 solar-type protostars, including 22 Class 0 and four Class I objects. Methanol is detected in 12 sources and tentatively in one source, which represents half of the sample. Eight sources (30%) have detections of at least three COMs. We find a strong chemical differentiation in multiple systems with five systems having one component with at least three COMs detected but the other component devoid of COM emission. The internal luminosity is found to be the source parameter impacting the most the COM chemical composition of the sources, while there is no obvious correlation between the detection of COM emission and that of a disk-like structure. A canonical hot-corino origin may explain the COM emission in four sources, an accretion-shock origin in two or possibly three sources, and an outflow origin in three sources. The CALYPSO sources with COM detections can be classified into three groups on the basis of the abundances of oxygen-bearing molecules, cyanides, and CHO-bearing molecules. These chemical groups correlate neither with the COM origin scenarii, nor with the evolutionary status of the sources if we take the ratio of envelope mass to internal luminosity as an evolutionary tracer. We find strong correlations

between molecules that are a priori not related chemically (for instance methanol and methyl cyanide), implying that the existence of a correlation does not imply a chemical link. [abridged]

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Rotational spectroscopy of singly 13C substituted isotopomers of propyne and determination of a semi-empirical equilibrium structure

Holger S. P. Müller, Sven Thorwirth, Frank Lewen

Submillimeter spectra of three isotopomers of propyne containing one 13C atom were recorded in natural isotopic composition in the region of 426 GHz to 785 GHz. Additional measurements were carried out near 110 GHz. Combining these with earlier data resulted in greatly improved spectroscopic parameters which permit reliable extrapolations up to about 1.5 THz. Coupled cluster quantum-chemical calculations were carried out in order to assess the differences between equilibrium and ground state rotational parameters of these and many other isotopic species to evaluate semi-empirical equilibrium structural parameters. In addition, we estimated the main spectroscopic parameters of the isotopomers of propyne with two 13C atoms, which have not yet been studied in the laboratory, but which may be detectable in astronomical sources with a large amount of 13C compared to the dominant 12C.

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The influence of molecular vicinity (expressed in terms of dielectric constant) on the infrared spectra of embedded species in ices and solid matrices

Sergio Pilling, Víctor Bonfim

In this theoretical work we evaluate how the chemical environment influences some features presented in the infrared spectrum, such as band intensities and band location of embedded species in icy matrices. The calculations were performed employing the Polarized Continuum Model (PCM) approach with the second-order Møller–Plesset perturbation theory (MP2) level using the Gaussian 09 package. Here, we simulate the effects of molecular vicinity around embedded species in terms of the effects of the dielectric constant (ε) of the icy and solid samples. Gas phase calculation was also performed for comparison purpose. The investigated embedded single molecules were CO, CO2, CH4, NH3, SO2, HCOOH, CH3OH and also H2O. The results suggest that for most vibrational modes, the strengths of IR bands show an increase with ε, which implies they also decrease with respect to porosity. The frequency shifts showed opposite behavior in relation to the band strengths, with few exceptions. A correlation between calculated band intensities with the band strengths A (taken from literature) was determined and described by a linear function I ~ 6 × 1e18 A [km mol−1], with A in unity of cm per molecule. Since astrophysical ice mantles over cold dust grains can vastly vary in composition in space (having different dielectric constants) they are a challenge to be well characterized. Therefore, this work can help the astrochemistry community to better understand astrophysical ices and its observations in the infrared.

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https://pubs.rsc.org/en/content/articlelanding/2020/RA/C9RA10136E#!divAbstract

No nitrogen fractionation on 600 au scale in the Sun progenitor analogue OMC-2 FIR4

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We show the first interferometric maps of the 14N/15N ratio obtained with the Atacama Large Millimeter Array (ALMA) towards the Solar-like forming protocluster OMC-2 FIR4. We observed N2H+, 15NNH+, N15NH+ (1-0), and N2D+ (2-1), from which we derive the isotopic ratios 14N/15N and D/H. The target is one of the closest analogues of the environment in which our Sun may have formed. The ALMA images, having synthesised beam corresponding to ~600 au, show that the emission of the less abundant isotopologues is distributed in several cores of ~10" (i.e. ~0.02~pc or 4000 au) embedded in a more extended N2H+ emission. Overall, our results indicate that: (1) 14N/15N does not change across the region at core scales, and (2) 14N/15N does not depend on temperature variations. Our findings also suggest that the 14N/15N variations found in pristine Solar System objects are likely not inherited from the protocluster stage, and hence their reason has to be found elsewhere.

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Seeds of Life in Space (SOLIS).VII. Discovery of a cold dense methanol blob toward the L1521F VeLLO system

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The SOLIS (Seeds Of Life In Space) IRAM/NOEMA Large Program aims at studying a set of crucial complex organic molecules in a sample of sources, with well-known physical structure, covering the various phases of Solar-type star formation. One representative object of the transition from the prestellar core to the protostar phases has been observed toward the Very Low Luminosity Object (VeLLO) called L1521F. This type of source is important to study to make the link between prestellar cores and Class 0 sources and also to constrain the chemical evolution during the process of star formation. Two frequency windows (81.6-82.6 GHz and 96.65-97.65 GHz) were used to observe the emission from several complex organics toward the L1521F VeLLO. These set-ups cover transitions of ketene (H2CCO), propyne (CH3CCH), formamide (NH2CHO), methoxy (CH3O), methanol (CH3OH), dimethyl ether (CH3OCH3) and methyl formate (HCOOCH3). Only 2 transitions of methanol (A+, E2) have been detected in the narrow window centered at 96.7 GHz (with an upper limit on E1) in a very compact emission blob (~7" corresponding to ~1000 au) toward the North-East of the L1521F protostar. The CS 2-1 transition is also detected within the WideX bandwidth. Consistently, with what has been found in prestellar cores, the methanol

emission appears ~1000 au away from the dust peak. The location of the methanol blob coincides with one of the filaments previously reported in the literature. The excitation temperature of the gas inferred from methanol is (10±2) K, while the H2 gas density (estimated from the detected CS 2-1 emission and previous CS 5-4 ALMA observations) is a factor >25 higher than the density in the surrounding environment (n(H2) ≥10^7 cm−3). From its compactness, low excitation temperature and high gas density, we suggest that the methanol emission detected with NOEMA is i) either a cold and dense shock-induced blob, recently formed (≤ few hundred years) by infalling gas or ii) a cold and dense fragment that may have just been formed as a result of the intense gas dynamics found within the L1521F VeLLO system.

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Photolysis-induced scrambling of PAHs as a mechanism for deuterium storage

S.D. Wiersma, A. Candian, J.M. Bakker, G. Berden, J. Oomens, W-J. Buma, A. Petrignani

Aim. We investigate the role of PAHs as a sink for deuterium in the interstellar medium and study UV photolysis as a potential process in the variations of the deuterium fractionation in the ISM. Methods. The UV photo-induced fragmentation of various isotopologues of D-enriched, protonated anthracene and phenanthrene ions was recorded in a FTICR mass spectrometer. IRMPD spectroscopy using FELIX provided the IR spectra that were compared to DFT vibrational spectra; reaction barriers and rates were also calculated and related to the product abundances. Results. The mass spectra for both UV and IRMPD photolysis show the loss of H from [D-C14H10]+, whereas [H-C14D10]+ shows a strong preference for D loss. Calculations reveal facile 1,2-H and -D shift reactions, with barriers lower than the energy supplied by the photo-excitation process. Together with confirmation of the ground-state structures via the IR spectra, we determined that the photolytic processes in the 2 PAHs are largely governed by scrambling where the H and the D atoms relocate between different peripheral C atoms. The ~0.1 eV difference in zero-point energy between C-H and C-D bonds ultimately leads to faster H scrambling than D scrambling, and increased H atom loss compared to D. Conclusion. Scrambling is common in PAH cations under UV radiation. Upon photoexcitation of deuterium-enriched PAHs, the scrambling results in a higher probability for the aliphatic D atom to migrate to an aromatic site, protecting it from elimination. This could lead to increased deuteration as a PAH moves towards more exposed interstellar environments. Also, large, compact PAHs with an aliphatic C-HD group on solo sites might be responsible for the majority of aliphatic C-D stretching bands seen in astronomical spectra.

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Announcements

EAS 2020 SS11 - The molecular journey from stars to disks

The Special Session “The molecular journey: from stars to disk (and exoplanets)” will take place on June 29, 2020 at the EAS2020 in Leiden. AIM & SCOPE. In this special

session we will focus on the study of molecules and their isotopologues and what they can teach us about the journey of molecules in our Galaxy. The scope is to bring the community together to showcase molecular insights in the evolution of matter from old stars to the ISM and into newly formed planets, to highlight recent advances in molecular astrophysics, to design strategies to best exploit the new astronomical facilities, and to provide fertile ground for future, interdisciplinary collaborations. INVITED SPEAKERS Leen Decin (KULeuven, Belgium) Paola Caselli (MPIE, Germany) Catherine Walsh (University of Leeds, UK) More information and registration through the EAS 2020 website: https://eas.unige.ch//EAS_meeting/session.jsp?id=SS11 Deadline for abstract submissions (talk and poster): March 2 2020. Limited financial support may be available for early career researchers (PhD students and postdocs). For information and/or question: a.candian@uva.nl On behalf of the SOC Alessandra Candian (UvA) Annemieke Petrignani (UvA) Marie Van de Sande (KULeuven) Serena Viti (UCL/ U Leiden) Tom Millar (QUB) Francesco Fontani (INAF)