AstroChemical Newsletter #21

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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

Chemical segregation in hot cores with disk candidates: An investigation with ALMA

V. Allen, F. F. S. van der Tak, Á. Sánchez-Monge, R. Cesaroni, and M. T. Beltrán

In the study of high-mass star formation, hot cores are empirically defined stages where chemically rich emission is detected toward a massive YSO. It is unknown whether the physical origin of this emission is a disk, inner envelope, or outflow cavity wall and whether the hot core stage is common to all massive stars. We investigate the chemical makeup of several hot molecular cores to determine physical and chemical structure. We use high spectral and spatial resolution submillimeter observations to determine how this stage fits into the formation sequence of a high-mass star. The submillimeter interferometer ALMA (Atacama Large Millimeter Array) was used to observe the G35.20-0.74N and G35.03+0.35 hot cores at 350 GHz in Cycle 0. We analyzed spectra and maps from four continuum peaks (A, B1, B2 and B3) in G35.20-0.74N, separated by 1000-2000 AU, and one continuum peak in G35.03+0.35. We made all possible line identifications across 8 GHz of spectral windows of molecular emission lines down to a 3σ line flux of 0.5 K and determined column densities and temperatures for as many as 35 species assuming local thermodynamic equilibrium (LTE). In comparing the spectra of the four continuum peaks, we find each has a distinct chemical composition expressed in over 400 different transitions. In G35.20, B1 and B2 contain oxygen- and sulfur-bearing organic and inorganic species but few nitrogen-bearing species whereas A and B3 are strong sources of O-, S-, and N-bearing organic and inorganic species (especially those with the CN bond). Column densities of vibrationally excited states are observed to be equal to or greater than the ground state for a number of species. Deuterated methyl cyanide is clearly detected in A and B3 with D/H ratios of 8 and 13%, respectively, but is much weaker at B1 and undetected at B2. No deuterated species are detected in G35.03, but similar molecular abundances to G35.20 were found in other species. We also find co-spatial emission of isocyanic acid (HNCO) and formamide (NH2CHO) in both sources indicating a strong chemical link between the two species. The chemical segregation between N-bearing organic species and others in G35.20 suggests the presence of multiple protostars surrounded by a disk or torus.

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Dehydrogenation effects on the stability of aromatic units in polycyclic aromatic hydrocarbons in the interstellar medium: A computational study at finite temperature

P. Parneix, A. Gambo, C. Falvo, M.A. Bonnin, T. Pino, F. Calvo

Isomerization, ionization and fragmentation of molecular compounds in the interstellar medium can be triggered by stellar radiation and cosmic rays. In the present contribution, we examine the propensity for isomerization and the relative stability of aromatic rings in the pyrene and coronene molecules at various degrees of dehydrogenation by means of molecular modeling. Using the AIREBO reactive force field and advanced Monte Carlo techniques such as the Wang–Landau method based on suitable order parameters, entire free-energy profiles describing the isomerization pathways and equilibrium properties were calculated as a function of temperature or total energy. We generally find that hydrogenation significantly stabilizes the fully polycyclic aromatic hydrocarbon (PAH) structure, even though local dehydrogenation next to an aromatic ring favors ring opening. The formation of pentagonal rings, a typical defect motif in the polycyclic carbon skeleton, is predicted to be actually competitive with the loss of a hydrogen atom. Our investigation emphasizes the likely presence of defects in astrophysical PAHs, whose spectral features remain to be better characterized and understood.

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Laboratory spectroscopy and astronomical significance of the fully-benzenoid PAH triphenylene and its cation

V. Kofman, P.J. Sarre, R.E. Hibbins, I.L. ten Kate, H. Linnartz

Triphenylene (C18H12) is a highly symmetric polycyclic aromatic hydrocarbon (PAH) molecule with a ‘fully-benzenoid’ electronic structure. This confers a high chemical stability compared with PAHs of similar size. Although numerous infrared and UV-vis experimental spectroscopic and theoretical studies of a wide range PAHs in an astrophysical context have been conducted, triphenylene and its radical cation have received almost no attention. There exists a huge body of spectroscopic evidence for neutral and ionised PAHs in astrophysical sources, obtained principally through detection of infrared emission

features that are characteristic of PAHs as a chemical class. However, it has so far not proved possible to identify spectroscopically a single isolated PAH in space, although PAHs including triphenylene have been detected mass spectrometrically in meteorites. In this work we focus on recording laboratory electronic spectra of neutral and ionised triphenylene between 220 and 780 nm, trapped in H2O ice and solid argon at 12 K. The studies are motivated by the potential for spectroscopic astronomical detection of electronic absorption spectra of PAHs in ice mantles on interstellar grains as discussed by Linnartz (2014), and were performed also in a cold Ar matrix to provide guidance as to whether triphenylene (particularly in its singly positively ionised form) could be a viable candidate for any of the unidentified diffuse interstellar absorption bands. Based on the argon-matrix experimental results, comparison is made with previously unpublished astronomical spectra near 400 nm which contain broad interstellar absorption features consistent with the predictions from the laboratory matrix spectra, thus providing motivation for the recording of gas-phase electronic spectra of the internally cold triphenylene cation.

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Electron-Promoted Desorption from Water Ice Surfaces: Neutral Gas- Phase Products

Ali G. M. Abdulgalil, A. Rosu-Finsen, D. Marchione, J. D. Thrower, M. P. Collings and M. R. S. McCoustra

Electron-promoted desorption (EPD) from compact amorphous solid water (c-ASW) has been studied. Low-energy electron bombardment with 200−300 eV electrons leads to H2O depletion, as monitored by reflection−absorption infrared spectroscopy (RAIRS) of the remaining c-ASW film. Cross- sections for H2O depletion were calculated to be in the range from 1.6 ± 1.0 × 1e−16 to 5.2 ± 3.0 × 1e−16 cm2. However, mass spectrometric measurements identify a major component of the desorbing material as H2, which appears with kinetics similar to those for H2O loss. Molecular H2O is observed as a minor desorption product in the gas phase.

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The chemistry of episodic accretion in embedded objects. 2D radiation thermo-chemical models of the post-burst phase

Ch. Rab, V. Elbakyan, E. Vorobyov, M. Güdel, O. Dionatos, M. Audard, I. Kamp, W.-F. Thi, P. Woitke, A. Postel

Episodic accretion is an important process in the evolution of young stars and their environment. The observed strong luminosity bursts of young stellar objects likely have a long lasting impact on the chemical evolution of the disk and envelope structure. We want to investigate observational signatures of the chemical evolution in the post-burst phase for embedded sources. With such signatures it is possible to identify targets that experienced a recent luminosity burst. We present a new model for episodic accretion chemistry based on the 2D, radiation thermo-chemical disk code ProDiMo. We have extended ProDiMo with a proper treatment for envelope structures. For a representative Class I model, we calculated the chemical abundances in the post-burst phase and produced synthetic observables like intensity maps and radial profiles. During a burst many chemical species, like CO, sublimate from the dust surfaces. As the burst ends they freeze out again (post-burst phase). This freeze-out happens from inside-out due to the radial density gradient in the disk and envelope structure. This inside-out freeze-out produces clear observational signatures in spectral line emission, like rings and distinct features in the slope of radial intensity profiles. We fitted synthetic C18O J=2-1 observations with single and two component fits and find that post-burst images are much better matched by the latter. Comparing the quality of such fits allows identification of post-burst targets in a model-independent way. Our models confirm that it is possible to identify post-burst objects from spatially resolved CO observations. However, to derive proper statistics, like frequencies of bursts, from observations it is important to consider aspects like the inclination and structure of the target and also dust properties as those have a significant impact on the freeze-out timescale.

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Observations of Cyanopolyynes toward Four High-Mass Star-Forming Regions Containing Hot Cores

Kotomi Taniguchi, Masao Saito, Tomoya Hirota, Hiroyuki Ozeki, Yusuke Miyamoto, Hiroyuki Kaneko, Tetsuhiro Minamidani, Tomomi Shimoikura, Fumitaka Nakamura, Kazuhito Dobashi

We carried out line survey observations at the 26-30 GHz band toward the four high-mass star-forming regions containing hot cores, G10.30-0.15, G12.89+0.49, G16.86-2.16, and G28.28-0.36, with the Robert C. Byrd Green Bank Telescope. We have detected HC5N from all of the sources, and HC7N from the three sources, except for G10.30-0.15. We further conducted observations of HC5N at the 42-46 GHz and 82-103 GHz bands toward the three sources, G12.89+0.49, G16.86-2.16, and G28.28-0.36, with the Nobeyama 45 m radio telescope. The rotational lines of HC5N with the high excitation energies (Eu/k=63-100 K), which are hardly excited in the cold dark clouds, have been detected from the three sources. The rotational temperatures of HC5N are found to be 13-20 K in the three sources. The detection of the lines with

the high excitation energies and the derived rotational temperatures indicate that HC5N exists in the warm gas within 0.07-0.1 pc radii around massive young stellar objects. The column densities of HC5N in the three sources are derived to be (2.0+-2.8) ×10^13 cm^-2 . We compare the ratios between N(HC5N) the column density of HC5N and W(CH3OH) the integrated intensity of the thermal CH3OH emission line among the three high-mass star-forming regions. We found a possibility of the chemical differentiation in the three high-mass star-forming regions; G28.28-0.36 shows the largest N (HC5N)/W (CH3OH) ratio of > 8.0 ×10^14 in units of (K km s^-1)^-1 cm^-2 , while G12.89+0.49 and G16.86-2.16 show the smaller values (~2 ×10^13).

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Kekulene: Structure, stability and nature of H•••H interactions in large PAHs

J. Poater , J. Paauwe, S. Pan, G. Merino, C. Fonseca Guerra, F.M. Bickelhaupt

We have quantum chemically analyzed how the stability of small and larger polycyclic aromatic hydrocarbons (PAHs) is determined by characteristic patterns in their structure using density functional theory at the BLYP/TZ2P level. In particular, we focus on the effect of the nonbonded H•••H interactions that occur in the bay region of kinked (or armchair) PAHs, but not in straight (or zigzag) PAHs. Model systems comprise anthracene, phenanthrene, and kekulene as well as derivatives thereof. Our main goals are: (1) to explore how nonbonded H•••H interactions in armchair configurations of kinked PAHs affect the geometry and stability of PAHs and how their effect changes as the number of such interactions in a PAH increases; (2) to understand the extent of stabilization upon the substitution of a bay Csingle bondH fragment by either C• or N; and (3) to examine the origin of such stabilizing/destabilizing interactions.

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PAH chemistry at eV internal energies. 1. H-shifted isomers

Georges Trinquier, Aude Simon, Mathias Rapacioli, Florent Xavier Gadéa

The PAH family of organic compounds (polycyclic aromatic hydrocarbons), involved in several fields of chemistry, has received particular attention in astrochemistry, where their vibrational spectroscopy, thermodynamics, dynamics, and fragmentation properties are now abundantly documented. This survey aims at drawing trends for low spin-multiplicity surfaces of PAHs bearing internal energies in the range 1–10 eV. It addresses some typical alternatives to the ground-state regular structures of PAHs, making explicit possible intramolecular rearrangements leading to high-lying minima. These isomerisations should be taken into consideration when addressing PAH processing in astrophysical conditions. The first part of this double-entry study focuses on the hydrogen-shifted forms, which bear both a carbene center and a saturated carbon. It rests upon DFT calculations mainly performed on two emblematic PAH representatives, coronene and pyrene, in their neutral and mono- and multi-cationic states. Systematically searched for in neutral species, these H-shifted minima are lying 4–5 eV above the regular all-conjugated forms, and are separated by barriers of about 1 eV. General hydrogen-shifting is found to be easier for cationic species as the relative energies of their H-shifted minima are 1–1.5 eV lower than those for neutral species. As much as possible, classical knowledge and concepts of organic chemistry such as aromaticity and Clar's rules are invoked for result interpretation.

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PAH chemistry at eV internal energies. 2. Ring alteration and dissociation

Georges Trinquier, Aude Simon, Mathias Rapacioli, Florent Xavier Gadéa

Recognized as important interstellar constituents, polycyclic aromatic hydrocarbons (PAHs) have been intensively studied in astrochemistry and their spectroscopy, thermodynamics, dynamics, and fragmentations are now amply documented. There exists typical alternatives to the ground-state regular planar structures of PAHs, as long as they bear internal energies in the range 1–10 eV. Resulting from intramolecular rearrangements, such high-lying minima on the potential-energy surfaces should be taken into consideration in the studies of PAH processing in astrophysical conditions. Resting upon DFT calculations mainly performed on two emblematic PAH representatives, coronene and pyrene, in their neutral and mono- and multi-cationic states, this second survey addresses the following alternatives: (1) opened forms containing ethynyl or 2-butynyl groups, (2) vinylidene isomers, in which phenanthrene patterns are reorganized into dibenzofulvene ones, (3) “twisted” forms, where external CHdouble bond; length as m-dashCH bonds can be partly twisted, and (4) bicyclobutane forms, in which the latter are integrated in saturated bicyclic forms. A few scenarios for elimination of fragments H, H2, C2H2 and C2H4 are explored. As far as possible, familiar concepts of organic chemistry, such as aromaticity or Clar's rules, are invoked for interpretations.

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Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets

Laboratory spectra of hot molecules: Data needs for hot super-Earth exoplanets

Jonathan Tennyson, Sergei N. Yurchenko

The majority of stars are now thought to support exoplanets. Many of those exoplanets discovered thus far are categorized as rocky objects with an atmosphere. Most of these objects are however hot due to their short orbital period. Models suggest that water is the dominant species in their atmospheres. The hot temperatures are expected to turn these atmospheres into a (high pressure) steam bath containing remains of melted rock. The spectroscopy of these hot rocky objects will be very different from that of cooler objects or hot gas giants. Molecules suggested to be important for the spectroscopy of these objects are reviewed together with the current status of the corresponding spectroscopic data. Perspectives of building a comprehensive database of linelist/cross sections applicable for atmospheric models of rocky super-Earths as part of the ExoMol project are discussed. The quantum-mechanical approaches used in linelist productions and their challenges are summarized.

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Chemical complexity induced by efficient ice evaporation in the Barnard 5 molecular cloud

V. Taquet, E. Wirström, S. B. Charnley, A. Faure, A. López-Sepulcre, C. M. Persson

Cold gas-phase water has recently been detected in a cold dark cloud, Barnard 5 located in the Perseus complex, by targeting methanol peaks as signposts for ice mantle evaporation. Observed morphology and abundances of methanol and water are consistent with a transient non-thermal evaporation process only affecting the outermost ice mantle layers, possibly triggering a more complex chemistry. We present the detection of the Complex Organic Molecules (COMs) acetaldehyde and methyl formate as well as formic acid and ketene, and the tentative detection of di-methyl ether towards the methanol hotspot of Barnard 5 located between two dense cores using the single dish OSO 20m, IRAM 30m, and NRO 45m telescopes. The high energy cis- conformer of formic acid is detected, suggesting that formic acid is mostly formed at the surface of interstellar grains and then evaporated. The detection of multiple transitions for each species allows us to constrain their abundances through LTE and non-LTE methods. All the considered COMs show similar abundances between ∼1 and ∼10 % relative to methanol depending on the assumed excitation temperature. The non-detection of glycolaldehyde, an isomer of methyl formate, with a [glycolaldehyde]/[methyl formate] abundance ratio lower than 6 %, favours gas phase formation pathways triggered by methanol evaporation. According to their excitation temperatures derived in massive hot cores, formic acid, ketene, and acetaldehyde have been designated as "lukewarm" COMs whereas methyl formate and di-methyl ether were defined as "warm" species. Comparison with previous observations of other types of sources confirms that "lukewarm" and "warm" COMs show similar abundances in low-density cold gas whereas the "warm" COMs tend to be more abundant than the "lukewarm" species in warm protostellar cores.

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Electron-induced Chemistry: Preliminary Comparative Studies of Hydrogen Production from Water, Methanol and Diethyl Ether

Demian Marchione and Martin R. S. McCoustra

Binary, layered ices comprising of benzene (C6H6) on water (H2O), on methanol (CH3OH) and on diethyl ether (CH3CH2OCH2CH3) have been irradiated with 250 eV electrons. Molecular hydrogen (H2) production is observed by quadrupole mass spectrometry to be competitive with (in the case of H2O), and dominate over (in the case of the organic substrates), C6H6 desorption. While very preliminary, these results suggest that chemical change (in the form of dehydrogenation) induced by interaction of organic-rich icy solids with ionising particle radiation may significantly contribute to hydrogen recycling in cold dense environments.

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First detection of THz water maser in NGC7538-IRS1 with SOFIA and new 22 GHz e-MERLIN maps

F. Herpin (LAB-France), A. Baudry (LAB), A.M.S. Richards (Univ. of,Manchester), M.D. Gray (Univ. of Manchester), N. Schneider (University of Cologne), K.M. Menten (MPIfR-Bonn), F. Wyrowski (MPIfR-Bonn), S. Bontemps (LAB), R. Simon (University of Cologne), and H. Wiesemeyer (MPIfR-Bonn)

The formation of massive stars is still not well understood. Accumulating a large amount of mass infalling within a single entity in spite of radiation pressure is possible if, among several other conditions, enough thermal energy is released. Despite numerous water line observations, with the Herschel Space Observatory, in most of the sources observations were not able to trace the emission from the hot core around the newly forming protostellar object. We want to probe the physical conditions and water abundance in the inner layers of the host protostellar object NGC7538-IRS1 using a highly excited H2O line. Water maser models predict that several THz water masers should be detectable in these objects. We present SOFIA observations of the o-H2O 8(2,7)-7(3,4) line at 1296.41106 GHz and a 6(1,6)-5(2,3) 22 GHz e-MERLIN map of the region (first-ever 22 GHz images made after the e-MERLIN upgrade). In order to be able to constrain the nature of the emission - thermal or maser - we use near-simultaneous observations of the 22 GHz water maser performed with the Effelsberg radiotelescope and e-MERLIN. A thermal water model using the RATRAN radiative transfer code is presented based on HIFI pointed observations. Molecular water abundances are derived for the hot core. The H2O 8(2,7)- 7(3,4) line is detected toward NGC7538-IRS1 with one feature at the source velocity (-57.7 km/s) and another one at -48.4 km/s. We propose that the emission at the source velocity is consistent with thermal excitation and is excited in the innermost part of the IRS1a massive protostellar object's closest circumstellar environment. The other emission is very likely the first detection of a water THz maser line, pumped by shocks due to IRS1b outflow, in a star-forming region. Assuming thermal excitation of the THz line, the water abundance in NGC7538-IRS1's hot core is estimated to be 5.2x10^{-5} with respect to H2.

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SH stretching vibration of propanethiol ice—a signature for its identification in the interstellar icy mantles

S. Pavithraa, D. Sahu, G. Seth, J.-I. Lo, B.N. Raja Sekhar, B.-M. Cheng, A. Das, N.J. Mason, B. Sivaraman

Among the most commonly existing thiol molecules, methanethiol and ethanethiol were discovered in the interstellar medium and identification of the next larger thiol molecule, propanethiol, is long awaited. By simulating icy astrochemical conditions and probing propanethiol ices under infrared spectroscopy we propose the use of SH stretching vibrations observed in the propanethiol molecular ice as a probe towards its identification in the interstellar medium. Though there are conformational changes within the ice (as observed in both VUV and IR spectra), the SH stretching vibration of propanethiol is observed to be unique among the set of thiol molecules, methanethiol and ethanethiol, which enables the detection of propanethiol ice in interstellar dust mantles using the James Webb Space Telescope.

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Complex organic molecules in strongly UV-irradiated gas

S. Cuadrado, J. R. Goicoechea, J. Cernicharo, A. Fuente, J. Pety, and B. Tercero

We investigate the presence of COMs in strongly UV-irradiated interstellar molecular gas. We have carried out a complete millimetre line survey using the IRAM-30m telescope towards the edge of Orion Bar photodissociation region (PDR), close to the H2 dissociation front, a position irradiated by a very intense FUV radiation field. These observations have been complemented with 8.5 arcsec resolution maps of the H2CO 5(1,5)-4(1,4) and C18O 3-2 emission at 0.9 mm. Despite being a harsh environment, we detect more than 250 lines from COMs and related precursors: H2CO, CH3OH, HCO, H2CCO, CH3CHO, H2CS, HCOOH, CH3CN, CH2NH, HNCO, H2-13CO, and HC3N (in decreasing order of abundance). For each species, the large number of detected lines allowed us to accurately constrain their rotational temperatures (Trot) and column densities (N). Owing to subthermal excitation and intricate spectroscopy of some COMs (symmetric- and asymmetric-top molecules such as CH3CN and H2CO, respectively), a correct determination of N and Trot requires building rotational population diagrams of their rotational ladders separately. We also provide accurate upper limit abundances for chemically related molecules that might have been expected, but are not conclusively detected at the edge of the PDR (HDCO, CH3O, CH3NC, CH3CCH, CH3OCH3, HCOOCH3, CH3CH2OH, CH3CH2CN, and CH2CHCN). A non-LTE LVG excitation analysis for molecules with known collisional rate coefficients, suggests that some COMs arise from different PDR layers but we cannot resolve them spatially. In particular, H2CO and CH3CN survive in the extended gas directly exposed to the strong far-UV flux (Tk = 150-250 K and Td > 60 K), whereas CH3OH only arises from denser and cooler gas clumps in the more shielded PDR interior (Tk = 40-50 K). We find a HCO/H2CO/CH3OH=1/5/3 abundance ratio. These ratios are different from those inferred in hot cores and shocks.

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The L1157-B1 astrochemical laboratory: testing the origin of DCN

G. Busquet, F. Fontani, S. Viti, C. Codella, B. Lefloch, M. Benedettini, C. Ceccarelli

L1157-B1 is the brightest shocked region of the large-scale molecular outflow, considered the prototype of chemically rich outflows, being the ideal laboratory to study how shocks affect the molecular gas. Several deuterated molecules have been previously detected with the IRAM 30m, most of them formed on grain mantles and then released into the gas phase due to the shock. We aim to observationally investigate the role of the different chemical processes at work that lead to formation of the DCN and test the predictions of the chemical models for its formation. We performed high-angular-resolution observations with NOEMA of the DCN(2-1) and H13CN(2-1) lines to compute the deuterated fraction, Dfrac(HCN).We detected emission of DCN(2-1) and H13CN(2-1) arising from L1157-B1 shock. Dfrac(HCN) is ~4x10−3 and given the uncertainties, we did not find significant variations across the bow-shock. Contrary to HDCO, whose emission delineates the region of impact between the jet and the ambient material, DCN is more widespread and not limited to the impact region. This is consistent with the idea that gas-phase chemistry is playing a major role in the deuteration of HCN in the head of the bow-shock, where HDCO is undetected as it is a product of grain-surface chemistry. The spectra of DCN and H13CN match the spectral signature of the outflow cavity walls, suggesting that their emission results from shocked gas. The analysis of the time-dependent gas-grain chemical model UCL-CHEM coupled with a C-type shock model shows that the observed Dfrac(HCN) is reached during the post-shock phase, matching the dynamical timescale of the shock. Our results indicate that the presence of DCN in L1157-B1 is a combination of gas-phase chemistry that produces the widespread DCN emission, dominating in the head of the bow-shock, and sputtering from grain mantles toward the jet impact region.

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First Detection of HC5(15N) in the Interstellar Medium

Kotomi Taniguchi and Masao Saito

We report the first detection of HC5(15N) with the J=9−8 rotational line from the cyanopolyyne peak in Taurus Molecular Cloud-1 (TMC-1 CP) using the 45-m radio telescope of the Nobeyama Radio Observatory. The column density of HC5(15N) is derived to be (1.9 +- 0.5)*10(11) cm−2 (1 sigma). We apply the double isotope method to derive the 14N/15N ratios of HC5N and HC3N in TMC-1 CP. The 14N/15N ratios are calculated to be 344 +- 53 and 257 +- 54 for HC5N and HC3N, respectively. The 14N/15N ratio of HC5N is lower than the elemental ratio in the local interstellar medium (~440) and slightly higher than that of HC3N in TMC-1 CP. Since HC3N is formed via the neutral-neutral reaction between C2H2 and CN, the slightly higher 14N/15N ratio of HC5N may support our previous suggestions that the main formation mechanism of HC5N is the ion-molecule reactions between hydrocarbon ions (C5Hn+) and nitrogen atoms.

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Announcements

PhD scholarship in astrochemistry in Ventspils International Radio Astronomy Center (Latvia)

Ventspils International Radio astronomy Center of Ventspils University College (http://venta.lv/en/) announces competition for a four year 1420 €/month PhD scholarship award in astrochemistry. The research will include (theoretical) astrochemistry with VIRAC's leading researcher Dr. phys. Juris Kalvans as thesis supervisor in VUC. The applicant has to demonstrate a high scientific potential as outlined in the Announcement (see the link below). Documents shall be submitted at Ventspils University College, Inzenieru 101, Ventspils, LV-3601, Latvia before July 30, 2017. Scanned copies may also be e-mailed to venta[at]venta.lv. The results will be announced before August 15. The successful applicant has to be employed by VUC for three years after the completion of the thesis. For details, please see the full text of the Announcement: http://venta.lv/en/2017/06/20/ventspils-university-college-announces-an-international-competition-for-doctoral-scholarship/. It has also been posted in the EAS jobs page (http://eas.unige.ch/jobs.jsp). The Regulations of the Competition can be found at http://venta.lv/wp-content/uploads/Doct_regulations_2_0_parveidots1.pdf.

postdoc positions are available to work at the Institute of Physics, Rennes, France,

Up to two postdoc positions are available to work at the Institute of Physics, Rennes, France, on the ERC Advanced Grant Project CRESUCHIRP Applications are invited for postdoctoral research associate positions at the Institute of Physics Rennes (IPR) to conduct experimental research in fundamental chemical physics and reaction kinetics, with particular application to molecular astrophysics and astrochemistry. The project, supported by the European Research Council (ERC Advanced Grant to Ian Sims, Acronym CRESUCHIRP), aims to develop a combination of a chirped-pulse (sub)mm-wave rotational spectrometer with uniform supersonic flows generated by expansion of gases through Laval nozzles and apply it to problems at the frontiers of reaction kinetics. The CRESU (Reaction Kinetics in Uniform Supersonic Flow) technique, combined with laser photochemical methods, has been applied with great success to perform research in gas-phase chemical kinetics at low temperatures, of particular interest for astrochemistry and cold planetary atmospheres. Recently, we have been involved in a collaboration with Arthur Suits (U. Missouri) and Bob Field (MIT) to develop a new combination of the revolutionary chirped pulse broadband rotational spectroscopy technique invented by Brooks Pate and co-workers with a novel pulsed CRESU, which we have called Chirped Pulse in Uniform Flow (CPUF). We propose to exploit the exceptional quality of the Rennes CRESU flows to build an improved CPUF instrument, and use it for the quantitative determination of product branching ratios in elementary chemical reactions over a wide temperature range (data which are sorely lacking as input to models of gas-phase chemical environments), as well as the detection of reactive intermediates and the testing of modern reaction kinetics theory. The successful candidate(s) will work closely with Ian Sims and the CRESUCHIRP team at the IPR (including Abdessamad Benidar, Ludovic Biennier, Robert Georges and Sébastien Le Picard) as well as a team of internationally renowned external experts. The project is fully funded by the ERC as well as the Brittany Region and Rennes Metropole, and benefits from new, dedicated laboratory and office space. The positions are available immediately (initially for 12 months, renewable for two further periods of 12 months by mutual agreement) and a competitive salary will be offered. Candidates should possess a PhD in experimental physics or physical chemistry, and experience in the use of microwave spectroscopy, pulsed lasers, vacuum and gas handling techniques and computer interfacing and programming are highly desirable. Experience in supervision of research (e.g. undergraduate projects) would also be advantageous. Knowledge of the French language, while advantageous, is not essential, and language lessons can be arranged if desired. Inquires and applications, including a detailed CV citing grades, a letter of intent, and the names and contact details of three potential referees, should be addressed to Prof. Ian Sims (ian.sims@univ-rennes1.fr). Review of candidatures will begin immediately, and the call will remain open until suitable candidates have been appointed. Keywords: Chirped Pulse Fourier Transform Microwave Spectroscopy (CPFTMW), CRESU, Chirped Pulse in Uniform supersonic Flow (CPUF), Low Temperature Reaction Kinetics, Product Branching Ratios, Elementary Reactions, Molecular Astrophysics, Experimental Astrochemistry, Chemical Physics, Gas-Phase Physical Chemistry For further details on the host research group and the project, please see https://perso.univ-rennes1.fr/ian.sims/ PhD positions are also available starting in October 2017, please see the website for details and pass the information on to any suitable candidates.

Research Fellow in Astrochemistry

vacancy: https://jobs.leeds.ac.uk/Vacancy.aspx?ref=MAPCH1067 Are you an ambitious researcher looking for your next challenge? Do you have an established background in experimental chemical kinetics, reaction dynamics, photochemistry or astrochemistry? Do you want to further your career in one of the UK's leading research intensive universities? We are looking for an exceptional researcher to work on our project 'Astrochemistry of old stars: direct probing of unique chemical laboratories (AEROSOL)', with Professors Dwayne Heardand John Plane. This interdisciplinary project on the stellar winds around evolved stars is funded by the ERC Consolidator Grant AEROSOL(Principal Investigator: Professor Leen Decin, University of Leuven). The aim of the project is to boost our understanding of the physics and chemistry characterizing the stellar winds around evolved stars. The project builds upon novel observations, detailed theoretical wind models, and targeted laboratory experiments. Our experimental research concerns the determination of rate coefficients and product distributions of elementary gas-phase reactions involving key reactive species (OH, C2H, HCHO, etc.) in stellar winds for which data are currently lacking. Specifically, several advanced laser-spectroscopic and chemiluminescence techniques will be employed to follow photolytically-generated reactive species in real time in a state-of-the-art low-temperature Laval-nozzle apparatus, and also other apparatus, with the aim to obtain the rates of gas-phase reactions at temperatures below 200K. You will perform research on the AEROSOL project, working in collaboration with a team of astrophysicists, chemists and computational mathematicians in both Leeds and Leuven. You will also have opportunities for training in science and people management, science communication, and grant application writing, with the aim to develop a personal independent career track. You will have a PhD in Astrochemistry, Astrophysics, Physical Chemistry or a closely aligned discipline, together with experience in laboratory studies of chemical kinetics, reaction dynamics or photochemistry. You'll also have excellent communication skills and the ability to work under pressure and meet deadlines. There is also a potential opportunity for you to be employed and funded by Leuven University, Belgium, for a subsequent one year period following the two year appointment at Leeds. Both Universities have modern and fully equipped research laboratories, and both groups enjoy and encourage further close collaboration with researchers in departments employing high-level quantum chemical calculations on species related to this project. To explore the post further or for any queries you may have, please contact: Professor Dwayne Heard, Professor of Atmospheric Chemistry Tel: +44 (0)113 343 6471, email: D.E.Heard@leeds.ac.uk Professor John Plane, Professor of Atmospheric Chemistry Tel: +44 (0)113 343 8044, email: J.M.C.Plane@leeds.ac.uk