AstroChemical Newsletter #73

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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

IRMPD spectroscopy of a PAH cation using FELICE: The infrared spectrum and photodissociation of dibenzo[a,l]pyrene

S. D. Wiersma, A. Candian, M. Rapacioli, A. Petrignani

We present the experimental InfraRed Multiple Photon Dissociation (IRMPD) spectrum and fragmentation mass spectrum of the irregular, cationic PAH dibenzo[a,l]pyrene (C24H14+) in the 6–40 μm/250–1650 cm-1 range. The use of the Free-Electron Laser for IntraCavity Experiments (FELICE) enabled us to record its Far-InfraRed (FIR) spectrum for the first time. We aim to understand how irregularity affects the infrared spectrum and fragmentation chemistry of PAHs. Dibenzo[a,l]pyrene is an asymmetric, non-planar molecule, for which all vibrational modes are in principle IR-active. Calculated harmonic Density Function Theory (DFT) and anharmonic Density Functional based Tight Binding Molecular Dynamics (DFTB-MD) spectra show a large wealth of bands, which match the experiment well, but with a few differences. The periphery of the molecule contains several edge geometries, but out of all possible modes in the 11–14 μm out-of-plane C–H bending region, only one band at 13.5 μm is prominent. This fact and the richness of the C–C stretching range make irregular PAHs a possible contributor to D-class interstellar spectra. The fragmentation mass spectra reveal facile 2H-loss and no [2C, 2H]-loss, which is attributed to the sterically hindered, non-planar cove region, which could protect irregular PAHs from radiation damage.

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SOLIS XIII: Nitrogen Fractionation towards the Protocluster OMC-2 FIR4.

L. Evans, F. Fontani, C. Vastel, C. Ceccarelli, P. Caselli, A. Lopez-Sepulcre, R. Neri, F. Alves, L. Chahine, C. Favre, V. Lattanzi

Isotopic fractionation is an important tool to investigate the chemical history of our Solar System. In particular, the isotopic fraction of nitrogen (14N/15N) is lower in comets and other pristine Solar System bodies with respect to the value measured for the protosolar nebula, suggesting a local chemical enrichment of15N during the Solar System formation. Therefore, interferometric studies of nitrogen fractionation in Solar System precursors are imperative for us to obtain clues about our astrochemical origins. In this work, we investigated the variation of the 14N/15N ratio in one of the closest analogues of the environment in which the Solar System was born: the protocluster OMC-2 FIR4. We present the first comparison at high angular resolution between HCN and N2H+ using interferometric data. We analysed observations of the HCN isotopologues H13CN and HC15N in the OMC-2 FIR4 protocluster. Specifically, we observed the transitions H13CN (1−0) and HC15N (1−0) with the NOrthern Extended Millimeter Array (NOEMA) within the context of the IRAM SOLIS (Seeds Of Life In Space) Large Program. We combined our results with analysis of archival data obtained with the Atacama Large Millimeter Array (ALMA) of N2H+ and its15N isotopologues. Our results show a small regional variation in the14N/15N ratio for HCN, from∼250 to 500. The ratios in the central regions of FIR4, where the candidate protostars are located, are largely consistent among them (∼300). They also show little variation from the part of the protocluster known to harbour a high cosmic-ray ionisation rate, to the portion with lower rate. We also found a small variation in the 14N/15N ratio of N2H+ across different regions from ∼200 to ∼400. These results suggest that local changes in the physical parameters occurring on small linear scales probed by our observations in the protocluster do not seem to affect the 14N/15N ratio in either HCN or N2H+ and hence that this is independent of the molecule used. Moreover, the high level of irradiation due to cosmic rays does not affect the N-fractionation either.

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Automated Exploration of Prebiotic Chemical Reaction Space: Progress and Perspectives

Siddhant Sharma, Aayush Arya, Romulo Cruz, Henderson James Cleaves II

Prebiotic chemistry often involves the study of complex systems of chemical reactions that form large networks with a large number of diverse species. Such complex systems may have given rise to emergent phenomena that ultimately led to the origin of life on Earth. The environmental conditions and processes involved in this emergence may not be fully recapitulable, making it difficult for experimentalists to study prebiotic systems in laboratory simulations. Computational chemistry offers efficient ways to study such chemical systems and identify the ones most likely to display complex

properties associated with life. Here, we review tools and techniques for modeling prebiotic chemical reaction networks and outline possible ways to identify self-replicating features that are central to many origin-of-life models.

Life. 2021; 11(11):1140.
DOI: 10.3390/life11111140
Full-text URL: https://www.mdpi.com/2075-1729/11/11/1140/htm

Discovery of two isomers of ethynyl cyclopentadiene in TMC-1: Abundances of CCH and CN derivatives of hydrocarbon cycles

J. Cernicharo, M. Agundez, R. I. Kaiser, C. Cabezas, B. Tercero, N. Marcelino, J. R. Pardo, P. de Vicente

We report the detection of two isomers of ethynyl cyclopentadiene (c-C5H5CCH), namely 1- and 2-ethynyl-1,3-cyclopentadiene, in the direction of TMC-1. We derive column densities of (1.4 +/- 0.2)e12 cm-2, and (2.0 +/- 0.4)e12 cm-2, respectively, for these two cyclopentadiene derivatives, which imply that they are about ten times less abundant than cyclopentadiene. We also report the tentative detection of ethynyl benzene (C6H5CCH), for which we estimate a column density of (2.5 +/-0.4)e12 cm-2. We derived abundances for the corresponding cyano derivatives of cyclopentadiene and benzene and found values significantly lower than previously reported. The rotational temperature of the ethynyl and cyano derivatives of these cycles is about 9 K, that is, very close to the gas kinetic temperature of the cloud. The abundance ratio of the 1- and 2- isomers of ethynyl cyclopentadiene is 1.4 +/-0.5, while for the two isomers of cyano cyclopentadiene it is 2.4 +/- 0.6. The relative abundances of CCH over CN derivatives is 7.7 +/- 2.2 for cyclopentadiene, which probably reflects the abundance ratio of the radicals CCH and CN; this ratio is only 2.1 +/- 0.5 for benzene, which suggests that additional reactions besides cyano radicals with benzene are involved in the formation of benzonitrile. The formation of these cycles is reasonably well accounted for through a chemical scheme based on neutral-neutral reactions. It is predicted that benzene should be as abundant as cyclopentadiene in TMC-1.

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Bottom-up dust nucleation theory in oxygen-rich evolved stars I. Aluminium oxide clusters

David Gobrecht, John M. C. Plane, Stefan T. Bromley, Leen Decin, Sergio Cristallo, Sanjay Sekaran

Aluminum oxide (alumina, Al2O3) is a promising candidate as a primary dust condensate in the atmospheres of oxygen-rich evolved stars. Therefore, alumina seed particles might trigger the onset of stellar dust formation and of stellar mass loss in the wind. However, the formation of alumina dust grains is not well understood. To shed light on the initial steps of cosmic dust formation (i.e. nucleation) in oxygen-rich environments by a quantum-chemical bottom-up approach. Starting with an elemental gas-phase composition, we construct a detailed chemical-kinetic network describing the formation and destruction of aluminium-bearing molecules and dust-forming (Al2O3)n clusters up to the size of dimers (n=2) coagulating to tetramers (n=4). Intermediary species include the prevalent gas-phase molecules AlO and AlOH, and AlxOy clusters with x=1−5, y=1−6. The resulting extensive network is applied to two model stars, representing a semi-regular variable and a Mira-type, and to different circumstellar gas trajectories including a non-pulsating outflow and a pulsating model. The growth of larger-sized (Al2O3)n clusters with n=4−10 is described by the temperature-dependent Gibbs free energies of the most favourable structures (i.e. the global minima clusters) as derived from global optimisation techniques and calculated by density functional theory. We provide energies, bond characteristics, electrostatic properties and vibrational spectra of the clusters as a function of size n and compare these to corundum corresponding to the crystalline bulk limit ($n \rightarrow \infty$). The circumstellar aluminium gas-phase chemistry in oxygen-rich giants is primarily controlled by AlOH and AlO, which are tightly coupled by the reactions AlO+H2, AlO+H2O, and their reverse. Models of ...

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Discovery of interstellar 3-cyano propargyl radical, CH2CCCN

C. Cabezas, M. Agundez, N. Marcelino, B. Tercero, J.. R. Pardo, P. de Vicente, J. Cernicharo

We report the first detection in interstellar space of the 3-cyano propargyl radical (CH2C3N). This species was observed in the cold dark cloud TMC-1 using the Yebes 40m telescope. A total of seven rotational transitions for both ortho- and para-CH2C3N species were observed in the 31.0-50.4 GHz range. We derive a total column density of (1.6 +/- 0.4)e11 cm-2 and an ortho/para ratio of 2.4 +/- 1.2, which implies an abundance ratio CH2C3N/CH3C3N around 0.1, in sharp contrast with the smaller analogues, in which case CH2CN/CH3CN = 3. This indicates that the chemistry of the cyanides CH2C3N and CH3C3N behaves differently to that of the smaller analogues CH2CN and CH3CN. According to our chemical model calculations, the radical CH2C3N is mostly formed through the neutral-neutral reactions C + CH2CHCN, C2 + CH3CN, and CN + CH2CCH together with the dissociative recombination of the CH3C3NH+ ion with electrons. The neutral-neutral reaction N + C4H3 could also lead to CH2C3N, although its role is highly uncertain. The identified radical CH2C3N could play a role in the synthesis of large organic N-bearing molecules, such as benzonitrile (c-C6H5CN) or nitrogen heterocycles.

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ALMA chemical survey of disk-outflow sources in Taurus (ALMA-DOT) VI: Accretion shocks in the disk of DG Tau and HL Tau

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Planet-forming disks are not isolated systems. Their interaction with the surrounding medium affects their mass budget and chemical content. In the context of the ALMA-DOT program, we obtained high-resolution maps of assorted lines from six disks that are still partly embedded in their natal envelope. In this work, we examine the SO and SO2 emission that is detected from four sources: DG Tau, HL Tau, IRAS 04302+2247, and T Tau. The comparison with CO, HCO+, and CS maps reveals that the SO and SO2 emission originates at the intersection between extended streamers and the planet-forming disk. Two targets, DG Tau and HL Tau, offers clear cases of inflowing material inducing an accretion shock on the disk material. The measured rotational temperatures and radial velocities are consistent with this view. In contrast to younger Class 0 sources, these shocks are confined to the specific disk region impacted by the streamer. In HL Tau, the known accreting streamer induces a shock in the disk outskirt, and the released SO and SO2 molecules spiral toward the star in a few hundreds years. These results suggest that shocks induced by late accreting material may be common in the disks of young star-forming regions with possible consequences on the chemical composition and mass content of the disk. They also highlight the importance of SO and SO2 line observations to probe accretion shocks from a larger sample.

Astronomy and Astrophysics, in press
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Anomalous HCN emission from warm giant molecular clouds

Goicoechea, J. R. , Lique, F. , Santa-Maria, M. G.

HCN is considered a good tracer of the dense molecular gas that serves as fuel for star formation. However, recent large-scale surveys of giant molecular clouds (GMCs) have detected extended HCN line emission. Such observations often resolve the HCN J=1-0 hyperfine structure (HFS). A precise determination of the physical conditions of the gas requires treating the HFS line overlap effects. Here, we study the HCN HFS excitation and line emission using nonlocal radiative transfer models that include line overlaps and new HFS-resolved collisional rate coefficients for inelastic collisions of HCN with both para-H2 and ortho-H2 (computed via the scaled-IOS approximation up to Tk=500 K). In addition, we account for the role of electron collisions in the HFS level excitation. We find that line overlap and opacity effects frequently produce anomalous HCN J=1-0 HFS line intensity ratios (inconsistent with the common assumption of the same Tex for all HFS lines) as well as anomalous HFS line width ratios. Line overlap and electron collisions also enhance the excitation of the higher J rotational lines. Electron excitation becomes important for molecular gas with H2 densities below a few 1e5 cm-3 and electron abundances above ~1e-5. In particular, electron excitation can produce low-surface-brightness HCN emission from very extended but low-density gas in GMCs. The existence of such a widespread HCN emission component may affect the interpretation of the extragalactic relationship HCN luminosity versus star-formation rate. Alternatively, extended HCN emission may arise from dense star-forming cores and become resonantly scattered by large envelopes of lower density gas. There are two scenarios - namely, electron-assisted (weakly) collisionally excited versus scattering - that lead to different HCN J=1-0 HFS intensity ratios, which can be tested on the basis of observations.

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A cold accretion flow onto one component of a multiple protostellar system

Nadia M. Murillo, Ewine F. van Dishoeck, Alvaro Hacar, Daniel Harsono, Jes K. Jørgensen

Context: Gas accretion flows transport material from the cloud core onto the protostar. In multiple protostellar systems, it is not clear if the delivery mechanism is preferential or evenly distributed among the components. Aims: Gas accretion flows within IRAS16293 is explored out to 6000 AU. Methods: ALMA Band 3 observations of low-J transitions of HNC, cyanopolyynes (HC3N, HC5N), and N2H+ are used to probe the cloud core structure at ~100 AU resolution. Additional Band 3 archival data provide low-J HCN and SiO lines. These data are compared with the corresponding higher-J lines from the PILS Band 7 data for excitation analysis. The HNC/HCN ratio is used as a temperature tracer. Results: The low-J transitions of HC3N, HC5N, HNC and N2H+ trace extended and elongated structures from 6000 AU down to ~100 AU, without accompanying dust continuum emission. Two structures are identified: one traces a flow that is likely accreting toward the most luminous component of the system IRAS16293 A. Temperatures inferred from the HCN/HNC ratio suggest that the gas in this flow is cold, between 10 and 30 K. The other structure is part of an UV-irradiated cavity wall entrained by one of the outflows. The two outflows driven by IRAS16293 A present different molecular gas distributions. Conclusions: Accretion of cold gas is seen from 6000 AU scales onto IRAS16293 A, but not onto source B, indicates that cloud core material accretion is competitive due to feedback onto a dominant component in an embedded multiple protostellar system. The preferential delivery of material could explain the higher luminosity and multiplicity of source A compared to source B. The results of this work demonstrate that several different molecular species, and multiple transitions of each species, are needed to confirm and characterize accretion flows in protostellar cloud cores.

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C18O emission as an effective measure of gas masses of protoplanetary disks

M. Ruaud, U. Gorti, D. Hollenbach

Many astrochemical models of observed CO isotopologue line emission, earlier considered a good proxy measure of H2 and hence disk gas mass, favor large deviations in the carbon and oxygen gas phase abundances and argue that severe gas phase CO depletion makes it a poor mass tracer. Here, we show that C18O line emission is an effective measure of the gas mass, and despite its complex chemistry, a possibly better tracer than HD. Our models are able to reproduce C18O emission from recent ALMA surveys and the TW Hya disk to within a factor of ~2-3 using carbon and oxygen abundances characteristic of the interstellar medium (C/H=1.4e-4; O/H=3.2e-4) without having to invoke unusual chemical processing. Our gas and dust disk structure calculations considering hydrostatic pressure equilibrium and our treatment of the CO conversion on grains are primarily responsible for the very different conclusions on disk masses and CO depletion. As did previous studies, we find that a gas phase C/O of ~1-2 can explain observed hydrocarbon emission from the TW Hya disk; but significantly, we find that CO isotopologue emission is only marginally affected by the C/O ratio. We therefore conclude that C18O emission provides estimates of disk masses that are uncertain only to within a factor of a few, and describe a simplified modeling procedure to obtain gas disk masses from C18O emission lines.

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Chemical survey of Class I protostars with the IRAM-30m

S. Mercimek, C. Codella, L. Podio, E. Bianchi, L. Chahine, M. Bouvier, A. Lopez-Sepulcre, R. Neri, C. Ceccarelli

Class I protostars are a bridge between Class 0 protostars, and Class II protoplanetary disks. Recent studies show gaps and rings in the dust distribution of disks younger than 1 Myr, suggesting that planet formation may start already at the Class I stage. To understand what chemistry planets will inherit, it is crucial to characterize the chemistry of Class I sources and to investigate how chemical complexity evolves from Class 0 protostars to protoplanetary disks. The goal is twofold: to obtain a census of the molecular complexity in a sample of four Class I protostars, and to compare it with the chemical compositions of earlier and later phases of the Sun-like star formation process. We performed IRAM-30m observations towards Class I objects (L1489-IRS, B5-IRS1, L1455-IRS1, and L1551-IRS5). The column densities of the detected species are derived assuming LTE or LVG. We detected 27 species: C-chains, N-bearing, S-bearing, Si-bearing species, deuterated molecules, and iCOMs. Different spectral profiles are observed: narrow lines towards all the sources, broader lines towards L1551-IRS5, and line wings due to outflows. Narrow c-C3H2 emission originates from the envelope. The iCOMs in L1551-IRS5 reveal the occurrence of hot corino chemistry, with CH3OH and CH3CN lines originating from a compact and warm region. Finally, OCS and H2S seem to probe the circumbinary disks in the L1455-IRS1 and L1551-IRS5 binary systems. The deuteration in terms of elemental D/H in the molecular envelopes and hot corino are derived. In addition, B5 IRS1, L1455-IRS1 and L1551-IRS5 show a low excitation methanol line, suggesting an origin from an extended structure, plausibly UV illuminated. The abundance ratios of iCOMs with respect CH3OH measured towards the L1551-IRS5 hot corino and the deuteration in our sample are comparable to that estimated at earlier stages, as well as to that found in comets. These findings support the inheritance scenario from prestellar cores to the Class I phase when planets start forming.

43 Pages, accepted by A&A
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The impact of stellar companion UV photons on the chemistry of the circumstellar environments of AGB stars

M. Van de Sande & T. J. Millar

Spherical asymmetries are prevalent within the outflows of AGB stars. Since binary interaction with a stellar or planetary companion is thought to be the underlying mechanism behind large-scale structures, we included the effects of UV radiation originating from a stellar companion in our chemical kinetics model. The one-dimensional model provides a first approximation of its effects on the chemistry throughout the outflow. The presence of a close-by stellar companion can strongly influence the chemistry within the entire outflow. Its impact depends on the intensity of the radiation (set by the stellar radius and blackbody temperature) and on the extinction the UV radiation experiences (set by the outflow density, density structure, and assumed radius of dust formation). Parent species can be photodissociated by the companion, initiating a rich photon-driven chemistry in the inner parts of the outflow. The outcome depends on the balance between two-body reactions and photoreactions. If two-body reactions dominate, chemical complexity within the outflow increases. This can make the abundance profiles of daughters appear like those of parents, with a larger inner abundance and a gaussian decline. If photoreactions dominate, the outflow can appear molecule-poor. We model three stellar companions. The impact of a red dwarf companion is limited. Solar-like companions show the largest effect, followed by a white dwarf. A stellar companion can also lead to the formation of unexpected species. The outflow's molecular content, especially combined with abundance profiles, can indicate a stellar companion's presence. Our results pave the way for further outflow-specific (three-dimensional) model development.

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High-level ab initio quartic force fields and spectroscopic characterization of C2N-

C. M. R. Rocha and H. Linnartz

While it is now well established that large carbon chain species and radiative electron attachment (REA) are key ingredients triggering interstellar anion chemistry, the role played by smaller molecular anions, for which REA appears to be an unlikely formation pathway, is as yet elusive. Advancing this research undoubtedly requires the knowledge of their astronomical abundances which, for the case of C2N−, is largely hindered by a lack of accurate spectroscopic signatures. In this work, we provide such data for both ground ℓ-CCN−(3Σ−) and low-lying c-CNC−(1A1) isomers by means of state-of-the-art rovibrational quantum chemical techniques. Their quartic force fields are herein calibrated using a high-level composite energy scheme that accounts for extrapolations to both one-particle and (approximate) N-particle basis set limits, in addition to relativistic effects, with the final forms being subsequently subject to nuclear motion calculations. Besides standard spectroscopic attributes, the full set of computed properties includes fine and hyperfine interaction constants and can be readily introduced as guesses in conventional experimental data reduction analyses through effective Hamiltonians. On the basis of benchmark calculations, the target accuracies are determined to be better than 0.1% of experiment for rotational constants and 0.3% for vibrational fundamentals. Apart from laboratory investigations, the results here presented are expected to also prompt future astronomical surveys on C2N−. Using the theoretically-predicted spectroscopic constants, the rotational spectra of both ℓ-CCN−(3Σ−) and c-CNC−(1A1) are also derived and their likely detectability in the interstellar medium is further explored in connection with working frequency ranges of powerful astronomical facilities.

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Full-text URL: https://pubs.rsc.org/en/content/articlelanding/2021/cp/d1cp03505c

[CII] 158μm emission from Orion A. II. Photodissociation region physics

C. H. M. Pabst, J. R. Goicoechea, A. Hacar, D. Teyssier, O. Berné, M. G. Wolfire, R. D. Higgins, E. T. Chambers, S. Kabanovic, R. Güsten, J. Stutzki, C. Kramer, A. G. G. M. Tielens

The [CII] 158μm fine-structure line is the dominant cooling line of moderate-density photodissociation regions (PDRs) illuminated by moderately bright far-ultraviolet (FUV) radiation fields. We aim to understand the origin of [CII] emission and its relation to other tracers of gas and dust in PDRs. One focus is a study of the heating efficiency of interstellar gas as traced by the [CII] line to test models of the photoelectric heating of neutral gas by polycyclic aromatic hydrocarbon (PAH) molecules and very small grains. We make use of a one-square-degree map of velocity-resolved [CII] line emission toward the Orion Nebula complex, and split this out into the individual spatial components, the expanding Veil Shell, the surface of OMC4, and the PDRs associated with the compact HII region of M43 and the reflection nebula NGC 1977. We employed Herschel far-infrared photometric images to determine dust properties. Moreover, we compared with Spitzer mid-infrared photometry to trace hot dust and large molecules, and velocity-resolved IRAM 30m CO(2-1) observations of the molecular gas. The [CII] intensity is tightly correlated with PAH emission in the IRAC 8μm band and far-infrared emission from warm dust. The correlation between [CII] and CO(2-1) is very different in the four subregions and is very sensitive to the detailed geometry. Constant-density PDR models are able to reproduce the observed [CII], CO(2-1), and integrated far-infrared (FIR) intensities. We observe strong variations in the photoelectric heating efficiency in the Veil Shell behind the Orion Bar and these variations are seemingly not related to the spectral properties of the PAHs. The [CII] emission from the Orion Nebula complex stems mainly from moderately illuminated PDR surfaces. Future observations with the James Webb Space Telescope can shine light on the PAH properties that may be linked to these variations.

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Full-text URL: https://arxiv.org/abs/2111.12363

Announcements

Postdoc in Univ. Tokyo

One postdoctoral position is available in the group of Yuri Aikawa at Department of Astronomy, University of Tokyo in Japan. The group focuses on physical and chemical processes in the star/planet formation. A successful candidate is expected to carry out numerical simulations of physical and chemical processes in interstellar clouds, star-forming cores, and protoplanetary disks in collaboration with the grant group described in the attached file. The candidates must have fundamental knowledge on star/planet formation and/or astrochemistry. The candidates with research experience in chemical reaction network models, Monte-Carlo simulations of grain-surface reactions, radiation hydrodynamics, radiation transfer calculations for synthetic observations are particularly welcome. The candidate should have finished his/her doctoral thesis before taking up the position. Japanese language skill is not required. The position is initially for one year with the annual extension depending on performance, up until March 31, 2025. The position is open from January 2022, but the exact starting date is flexible.
Details about the position, required documents, and contact information can be found in the following page. The application deadline is Dec 31, 2021.
https://www.next-astrochem.com/news/%5Brecruitment%5D-postdoctoral-position-at-u.-tokyo-%5Bdeadline%3A-dec.-

31%2C-2021%5D

Postdoc at Saitama Univ.

One postdoctoral position is available in the group of Toshiyuki Takayanagi at Department of Chemistry, Saitama University in Japan. The group focuses on physical/chemical processes in the star/planet formation. A successful candidate is expected to carry out numerical calculations of potential energy surfaces and reaction dynamics of both gas-phase and grain-surface reactions relevant to astrochemistry in collaboration with the grant group. The candidates must have fundamental knowledge on quantum chemistry and interests in astrochemistry. The candidates with research experience in potential energy surface development are particularly welcome. The candidate should have finished his/her doctoral thesis before taking up the position. Japanese language skill is not required. The position is initially for one year with the annual extension depending on performance, up until March 31, 2025. The position is open from January 2022, but the exact starting date is flexible.
Details about the position, required documents, and contact information can be found in the following page. The application deadline is Dec 31, 2021.
https://www.next-astrochem.com/news/%5Brecruitment%5D-postdoctoral-position-at-saitama-u.-%5Bdeadline%3A-dec.-31%2C-2021%5D

PhD and PDRA opportunities in Astrochemistry and Exoplanets at the University of Leeds

The School of Physics and Astronomy and the School of Chemistry at the University of Leeds have several positions at both PhD and PDRA level currently accepting applications from candidates interested in working in the areas of astrochemistry, planet formation, or exoplanet atmospheres. Please follow the links below for further information on each project, including application deadlines and how to apply. If you have any questions, please contact the lead project supervisor. Note that there are funding restrictions for PhD applicants at UK institutions. Please contact the lead supervisor to enquire on the funding status of each project in advance of applying.

PhD in Astrochemical Modelling of Planet-forming Regions
https://phd.leeds.ac.uk/project/1097-chemistry-in-planet-forming-regions-revealed-by-alma
Dr Catherine Walsh, School of Physics and Astronomy (c.walsh1@leeds.ac.uk)
The researcher will develop new models of protoplanetary disk chemistry that include the effects of dust evolution and sub-structure, radial transport, and mixing, motivated by current theories on the origin of dust sub-structure in disks. The researcher will use these models to simulate observations to directly compare with the results from ALMA (the Atacama Large Millimeter/submillimeter Array), and will produce suites of diagnostics that will be used to motivate future ALMA proposals. The researcher will have a first class or upper second class degree in physics, astrophysics, or astronomy.

PhD in Laboratory Astrochemistry for Chemical Kinetics at Very Low Temperatures
Prof Dwayne Heard, School of Chemistry (d.e.heard@leeds.ac.uk)
The researcher will use a pulsed Laval nozzle apparatus coupled with laser-based spectroscopic methods to measure kinetic parameters at temperatures as low as 25 K for gas-phase reactions of astrochemical interest. The work is motivated by the lack of knowledge of the formation and destruction mechanisms of complex organic molecules observed by modern telescopes such as ALMA. The laboratory work will be accompanied by rate theory calculations and the new kinetic parameters will be used as input into astrochemical models. The researcher will have a first class or upper second class degree in chemistry, physics, or a related discipline.

Research Fellow (3 years, fixed term) in the Climates of Exoplanets
https://jobs.leeds.ac.uk/Vacancy.aspx?ref=EPSPA1046
Dr Catherine Walsh, School of Physics and Astronomy (c.walsh1@leeds.ac.uk)
The fellow will work on a UKRI-funded project to investigate the role of impacts from volatile-rich small bodies on the chemistry and climate of terrestrial exoplanets. The fellow will simulate the structure and composition of the atmospheres of rocky planets and will produce simulated observations to make predictions with future facilities. The fellow will have a PhD (or will have submitted the thesis prior to taking up the appointment) in astronomy, astrophysics, or atmospheric science, and will have experience in the simulation of planetary atmospheres.

Research Fellow (3 years, fixed term) in Computational Astrochemistry
https://jobs.leeds.ac.uk/Vacancy.aspx?ref=EPSPA1045
Dr Catherine Walsh, School of Physics and Astronomy (c.walsh1@leeds.ac.uk)
The fellow will work on a UKRI-funded project to investigate the role of stellar radiation on the chemistry of ices in the planet- and comet-building regions around young stars. The fellow will exploit molecular modelling to study how radiation affects the stability and chemistry of complex organic molecules in the ice phase. The fellow will have a PhD (or will have submitted the thesis prior to taking up the appointment) in astrophysics, astrochemistry, or physical chemistry, and will have experience in molecular modelling techniques.

To apply for a PhD position at the University of Leeds, please consult the instructions on the following webpage:
https://www.leeds.ac.uk/research-applying/doc/applying-research-degrees

To apply for either of the Research Fellow positions, please follow the links to the job advertisements given above, or consult the instructions on the following webpage: https://jobs.leeds.ac.uk/display.aspx?id=1253&pid=0

COSPAR2022 B1.3 "Astrochemistry and Composition as Ariadne's Threads for Planet Formation"

The abstract submission is open for the 44th COSPAR Scientific Assembly (16-24 July 2022, Athens, Greece in hybrid mode) and we wish to invite you to participate in the scientific event

B1.3 "Astrochemistry and Composition as Ariadne's Threads for Planet Formation"

Event Description: Understanding how planetary systems form is becoming an increasingly interdisciplinary field of study that is approaching the limits of insight being gained from individual disciplines. The composition of planetary bodies and the astrochemical processes that shape it represent the common thread helping us to navigate the multifaceted problem of planetary formation. Future studies will become even more interdependent and will require combining the information supplied by meteorites and polluted white dwarfs, the interstellar medium and protoplanetary disks, comets and asteroids, planetary surfaces and exoplanetary atmospheres, and more. This event aims to offer an interdisciplinary venue to bring together researchers studying the Solar System, exoplanets, star formation, protoplanetary disks, main sequence and evolved stars to combine the insights provided by their theoretical and experimental perspectives, as well as by observations from ground-based and space-borne facilities.

Confirmed Invited Speakers: Alex Cridland (MPE, Germany), Izaskun Jiménez-Serra (CSIC/INTA, Spain), Nami Sakai (RIKEN, Japan), Myriam Telus (UCSC, USA)

Scientific Organizing Committee: Paola Caselli (MPE, Germany), Stavro Lambrov Ivanovski (INAF-OATs, Italy), Dimitris Stamatellos (University of Central Lancashire, UK), Neal Turner (NASA/JPL, USA), Stephanie Werner (University of Oslo, Norway), Ke Zhang (University of Wisconsin-Madison, USA)

Main Scientific Organizers: Diego Turrini (INAF, Italy) & Maria Drozdovskaya (CSH, Switzerland)

Deadlines and Information
Abstract submission deadline: 11 February 2022
More information about scientific event B1.3 can be found at: https://cospar-assembly.org/admin/session_cospar.php?session=1009
More information about COSPAR 2022 and its many other events can be found at: https://www.cosparathens2022.org and https://www.cospar-assembly.org/admin/congress.php?congress=10

AbSciCon 2022 Session: Titan as a Prebiotic Laboratory

Please consider submitting to our Titan focused AbSciCon 2022 session, “Titan as a Prebiotic Laboratory.”

https://agu.confex.com/agu/abscicon21/prelim.cgi/Session/112042

Submission deadline: January 19

From the ionosphere to its rocky core, Titan offers a unique opportunity to explore pathways for prebiotic chemistry. In its N2-CH4-based atmosphere, photolytic and radiolytic chemistry creates a plethora of organic compounds, including large, complex haze particles. These compounds eventually make their way to the surface where geological processes rework and redistribute Titan’s prebiotic manna. Primordial organic material in the interior may be dissolved in the subsurface ocean and serve as the ultimate source of Titan’s atmospheric methane. Whether either of these realms —atmosphere, surface, interior — interacts with the other through the icy crust remains unknown. As the most organic-rich ocean world in the solar system beyond Earth, Titan represents a compelling world to investigate prebiotic chemistry. This session explores how investigating Titan’s different realms provides new insight into our understanding of the limits of prebiotic evolution. Results from remote sensing data, laboratory experiments, modeling, ground-based observations are all welcome.