

AstroChemical Newsletter #82

September 2022

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

Confirmation of Gaseous Methanediol from State-of-the-Art Theoretical Rovibrational Characterization

Megan C. Davis, Noah R. Garrett and Ryan C. Fortenberry

High-level rovibrational characterization of methanediol, the simplest geminal diol, using state-of-the-art, purely ab initio techniques unequivocally confirms previously reported gas phase preparation of this simplest geminal diol in its C₂ conformation. The F12-TZ-cCR and F12-DZ-cCR quartic force fields (QFFs) utilized in this work are among the largest coupled cluster-based anharmonic frequencies computed to date, and they match the experimental band origins of the spectral features in the 980–1100 cm⁻¹ range to within 3 cm⁻¹, representing a significant improvement over previous studies. The simulated spectrum also matches the experimental spectrum in the strong Q branch feature and qualitative shape of the 980–1100 cm⁻¹ region. Additionally, the full set of rotational constants, anharmonic vibrational frequencies, and quartic and sextic distortion constants are provided for both the lowest energy C₂ conformer as well as the slightly higher C_s conformer. Several vibrational modes have intensities of 60 km mol⁻¹ or higher, facilitating potential astronomical or atmospheric detection of methanediol or further identification in laboratory work especially now that gas phase synthesis of this molecule has been established.

Physical Chemistry Chemical Physics, 2022, 24, 18552 - 18558

DOI: [10.1039/D2CP02076A](https://doi.org/10.1039/D2CP02076A)

Full-text URL: <https://pubs.rsc.org/en/content/articlelanding/2022/cp/d2cp02076a/unauth>

Identification and characterization of a new ensemble of cometary organic molecules

N. Hänni, K. Altwegg, M. Combi, S. A. Fuselier, J. De Keyser, M. Rubin, and S. F. Wampfler

In-situ study of comet 1P/Halley during its 1986 apparition revealed a surprising abundance of organic coma species. It remained unclear, whether or not these species originated from polymeric matter. Now, high-resolution mass-spectrometric data collected at comet 67P/Churyumov-Gerasimenko by ESA's Rosetta mission unveil the chemical structure of complex cometary organics. Here, we identify an ensemble of individual molecules with masses up to 140 Da while demonstrating inconsistency of the data with relevant amounts of polymeric matter. The ensemble has an average composition of C₁H_{1.56}O_{0.134}N_{0.046}S_{0.017}, identical to meteoritic soluble organic matter, and includes a plethora of chain-based, cyclic, and aromatic hydrocarbons at an approximate ratio of 6:3:1. Its compositional and structural properties, except for the H/C ratio, resemble those of other Solar System reservoirs of organics—from organic material in the Saturnian ring rain to meteoritic soluble and insoluble organic matter –, which is compatible with a shared prestellar history.

Nature Communications, volume 13, Article number: 3639 (2022)

DOI: [10.1038/s41467-022-31346-9](https://doi.org/10.1038/s41467-022-31346-9)

Full-text URL: <https://www.nature.com/articles/s41467-022-31346-9>

Adsorption of Polycyclic Aromatic Hydrocarbons and C₆₀ onto Forsterite: C–H Bond Activation by the Schottky Vacancy

Dario Campisi, Thanja Lamberts, Nelson Y. Dzade, Rocco Martinazzo, Inge Loes ten Kate, and Alexander G. G. M. Tielens

Understanding how to catalytically break the C–H bond of aromatic molecules, such as polycyclic aromatic hydrocarbons (PAHs), is currently a big challenge and a subject of study in catalysis, astrochemistry, and planetary science. In the latter, the study of the breakdown reaction of PAHs on mineral surfaces is important to understand if PAHs are linked to prebiotic molecules in regions of star and planet formation. In this work, we employed a periodic density functional theory along with Grimme's D4 (DFT-D4) approach for studying the adsorption of a sample of PAHs (naphthalene, anthracene, fluoranthene, pyrene, coronene, and benzocoronene) and fullerene on the [010] forsterite surface and its defective surfaces (Fe-doped and Ni-doped surfaces and a MgO-Schottky vacancy) for their implications in catalysis and astrochemistry. On the basis of structural and binding energy analysis, large PAHs and fullerene present stronger adsorption on the pristine, Fe-doped, and Ni-doped forsterite surfaces than small PAHs. On a MgO-Schottky vacancy, parallel adsorption of the PAH leads to the chemisorption process (C–Si and/or C–O bonds), whereas perpendicular orientation of the PAH leads to the catalytic breaking of the aromatic C–H bond via a barrierless reaction. Spin density and charge analysis show that C–H dissociation is promoted by electron donation from the vacancy to the PAH. As a result of the undercoordinated Si and O atoms, the vacancy acts as a Frustrated Lewis Pair (FLP) catalyst. Therefore, a MgO-Schottky vacancy [010] forsterite surface proved to have potential catalytic activity for the activation of C–H bond in aromatic molecules.

Reconciling spectroscopy with dynamics in global potential energy surfaces: the case of the astrophysically relevant SiC₂

C. M. R. Rocha, H. Linnartz, and A. J. C. Varandas

SiC₂ is a fascinating molecule due to its unusual bonding and astrophysical importance. In this work, we report the first global potential energy surface (PES) for ground-state SiC₂ using the combined-hyperbolic-inverse-power-representation (CHIPR) method and accurate ab initio energies. The calibration grid data is obtained via a general dual-level protocol developed afresh herein that entails both coupled-cluster and multireference configuration interaction energies jointly extrapolated to the complete basis set limit. Such an approach is specially devised to recover much of the spectroscopy from the PES, while still permitting a proper fragmentation of the system to allow for reaction dynamics studies. Bound vibrational state calculations have been carried out, unveiling an excellent match of the available experimental data on c-SiC₂. To further exploit the global nature of the PES, exploratory quasi-classical trajectory calculations for the endothermic C₂+Si → SiC+C reaction are also performed, yielding thermalized rate coefficients for temperatures up to 5000 K. The results hint for the prominence of this reaction in the innermost layers of the circumstellar envelopes around carbon-rich stars, thence conceivably playing therein a key contribution to the gas-phase formation of SiC, and eventually, solid SiC dust.

2022 Journal of Chemical Physics, in press

DOI: [10.1063/5.0096364](https://doi.org/10.1063/5.0096364)

Full-text URL: <https://arxiv.org/abs/2208.05203>

Methanol deuteration in high-mass protostars

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The deuteration of molecules forming in the ices such as methanol (CH₃OH) is sensitive to the physical conditions during their formation in dense cold clouds and can be probed through observations of deuterated methanol in hot cores. Observations with ALMA containing transitions of CH₃OH, CH₂DOH, CHD₂OH, 13CH₃OH, and CH₁₈₃OH are investigated. The column densities of CH₂DOH, CHD₂OH, and CH₃OH are determined for all sources, where the column density of CH₃OH is derived from optically thin 13C and 18O isotopologues. Consequently, the D/H ratio of methanol is derived taking statistical effects into account. Singly deuterated methanol (CH₂DOH) is detected toward 25 of the 99 sources in our sample of the high-mass protostars. Including upper limits, the (D/H)_{CH₃OH} ratio inferred from N_{CH₂DOH}/N_{CH₃OH} was derived for 38 of the 99 sources and varies between ~1e⁻³–1e⁻². Including other high-mass hot cores from the literature, the mean methanol D/H ratio is (1.1±0.7)e⁻³. This is more than one order of magnitude lower than what is seen for low-mass protostellar systems ((2.2±1.2)e⁻²). Doubly deuterated methanol (CHD₂OH) is detected toward 11 of the 99 sources. Including upper limits for 15 sources, the (D/H)_{CH₂DOH} ratios derived from N_{CHD₂OH}/N_{CH₂DOH} are more than two orders of magnitude higher than (D/H)_{CH₃OH} with an average of (2.0±0.8)e⁻¹ which is similar to what is found for low-mass sources. Comparison with literature GRAINOBLE models suggests that the high-mass prestellar phases are either warm (>20 K) or live shorter than the free-fall timescale. In contrast, for low-mass protostars, both a low temperature of <15 K and a prestellar phase timescale longer than the free-fall timescale are necessary.

Accepted to A&A

DOI: [10.1051/0004-6361/202244471](https://doi.org/10.1051/0004-6361/202244471)

Full-text URL: <https://arxiv.org/abs/2208.06515>

Polycyclic aromatic hydrocarbon growth in a benzene discharge explored by IR-UV action spectroscopy

A.K. Lemmens, D.B. Rap, S. Brünken, W.J. Buma, A.M. Rijs

Infrared signatures of polycyclic aromatic hydrocarbons (PAHs) are detected towards many phases of stellar evolution. PAHs are major players in the carbon chemistry of the interstellar medium, forming the connection between small hydrocarbons and large fullerenes. However, as details on the formation of PAHs in these environments are still unclear, modeling their abundance and chemistry has remained far from trivial. By combining molecular beam mass-selective IR spectroscopy and calculated IR spectra, we analyze the discharge of benzene and identify resulting products including larger PAHs, radicals and intermediates that serve as promising candidates for radio astronomical searches. The identification of various reaction products indicates that different gas-phase reaction mechanisms leading to PAH growth must occur under the same conditions to account for all observed PAH-related species, thereby revealing the complex and interconnected network of PAH formation pathways. The results of this study highlight key (exothermic) reactions that need to be included in astrochemical models describing the carbon chemistry in our universe.

Phys. Chem. Chem. Phys. 24 (2022) 14816-14824

DOI: [10.1039/D2CP01631A](https://doi.org/10.1039/D2CP01631A)

Full-text URL: <https://doi.org/10.1039/D2CP01631A>

Spectroscopic characterisation of the isomeric H₂NCH⁺ and H₂CNH⁺ radical cations

D. Sundelin, A.N. Marimuthu, S. Thorwirth, S. Brünken, W. Geppert

The vibrational transitions and the relative abundances of the two isomeric ions H₂CNH⁺ and H₂NCH⁺ generated through electron impact ionisation have been investigated in a noble gas tagging experiment. It could be shown that both species were formed with an abundance of 70 and 30% for H₂NCH⁺ and H₂CNH⁺, respectively. The obtained vibrational bands of the two species have been assigned to vibrational transitions through comparison with the results of ab initio calculations. These computations also predict both species to be moderately polar. The present investigations show that both isomers should be included in chemical model calculations of dark interstellar clouds, protoplanetary disks, star-forming regions as well as planetary atmospheres.

J. Mol. Spectrosc. 387 (2022) 111640

DOI: [10.1016/j.jms.2022.111640](https://doi.org/10.1016/j.jms.2022.111640)

Full-text URL: <https://doi.org/10.1016/j.jms.2022.111640>

Grain-Surface Hydrogen-Addition Reactions as a Chemical Link Between Cold Cores and Hot Corinos: The Case of H₂CCS and CH₃CH₂SH

Christopher N. Shingledecker, Tahamida Banu, Yi Kang, Hongji Wei, Joseph Wandishin, Garrett Nobis, Virginia Jarvis, Faith Quinn, Grace Quinn, Germán Molpeceres, Michael C. McCarthy, Brett A. McGuire, and Johannes Kästner

Recently, searches were made for H₂CCS and HCCSH in a variety of interstellar environments—all of them resulted in nondetections of these two species. Recent findings have indicated the importance of destruction pathways, e.g., with atomic hydrogen, in explaining the consistent nondetection of other species, such as the H₂C₃O family of isomers. We have thus performed ab initio calculations looking at reactions of H₂CCS, HCCSH, and related species with atomic hydrogen. Our results show that H₂CCS and HCCSH are both destroyed barrierlessly by atomic hydrogen, thus providing a plausible explanation for the nondetections. We further find that subsequent reactions with atomic hydrogen can barrierlessly lead to CH₃CH₂SH, which has been detected. Astrochemical simulations including these reactions result not only in reproducing the observed abundance of H₂CCS in TMC-1 but also show that CH₃CH₂SH, produced via our H-addition pathways and subsequently trapped on grains, can desorb in warmer sources up to abundances that match previous observations of CH₃CH₂SH in Orion KL. These results, taken together, point to the importance of grain-surface H-atom addition reactions and highlight the chemical links between cold prestellar cores and their subsequent, warmer evolutionary stages.

J. Phys. Chem. A 2022, 126, 32, 5343–5353

DOI: [10.1021/acs.jpca.2c01447](https://doi.org/10.1021/acs.jpca.2c01447)

Full-text URL: <https://pubs.acs.org/doi/10.1021/acs.jpca.2c01447>

Binding Energy Evaluation Platform: A Database of Quantum Chemical Binding Energy Distributions for the Astrochemical Community

G. M. Bovolenta, S. Vogt-Geisse, S. Bovino, T. Grassi

The quality of astrochemical models is highly dependent on reliable binding energy (BE) values that consider the morphological and energetic variety of binding sites on the surface of ice-grain mantles. Here, we present the Binding Energy Evaluation Platform (BEEP) and database that, using quantum chemical methods, produces full BE distributions of molecules bound to an amorphous solid water (ASW) surface model. BEEP is highly automatized and allows one to sample binding sites on a set of water clusters and to compute accurate BEs. Using our protocol, we computed 21 BE distributions of interstellar molecules and radicals on an amorphized set of 15–18 water clusters of 22 molecules each. The distributions contain between 225 and 250 unique binding sites. We apply a Gaussian fit and report the mean and standard deviation for each distribution. We compare with existing experimental results and find that the low- and high-coverage experimental BEs coincide well with the high-BE tail and mean value of our distributions, respectively. Previously reported single BE theoretical values are broadly in line with ours, even though in some cases significant differences can be appreciated. We show how the use of different BE values impacts a typical problem in astrophysics, such as the computation of snow lines in protoplanetary disks. BEEP will be publicly released so that the database can be expanded to other molecules or ice models in a community effort.

The Astrophysical Journal Supplement Series, 262:17 (15pp), 2022 September

DOI: [10.3847/1538-4365/ac7f31](https://doi.org/10.3847/1538-4365/ac7f31)

Full-text URL: <https://arxiv.org/abs/2207.13095>

Infrared H₂O Absorption in Massive Protostars at High Spectral Resolution: Full Spectral Survey Results of AFGL 2591 and AFGL 2136

Barr, A.G., Boogert, A., Li, J., DeWitt, C.-N., Montiel E., Richter, M.J., Lacy, J.H., Indriolo, N., Pendleton, Y., Chiar, J., Tielens, A.G.G.M

We have performed a high-resolution 4–13 μm spectral survey of the hot molecular gas associated with the massive protostars AFGL 2591 and AFGL 2136. Here we present the results of the analysis of the ν₂ band of H₂O, detected with the

Echelon Cross Echelle Spectrograph on board the Stratospheric Observatory for Infrared Astronomy between wavelengths of 5 and 8 μm . All lines are seen in absorption. Rotation diagrams indicate that the gas is optically thick and lines are observed to saturate at 40% and 15% relative to the continuum for AFGL 2136 and AFGL 2591, respectively. We applied two curve of growth analyses to derive the physical conditions, one assuming a foreground origin and one a circumstellar disk origin. We find temperatures of 400–600 K. A foreground origin would require the presence of externally heated clumps that are smaller than the continuum source. The disk analysis is based on stellar atmosphere theory, which takes into consideration the temperature gradient in the disk. We discuss the challenges with each model, taking into consideration the properties of other species detected in the spectral survey, and conclude that further modeling efforts are required to establish whether the absorption has a disk or foreground origin. The main challenge to the foreground model is that molecules are expected to be observed in emission. The main challenges to the disk model are the midplane heating mechanism and the presence of narrow absorption lines shifted from the systemic velocity.

2022, ApJ, 935, 165

DOI: [10.3847/1538-4357/ac74b8](https://doi.org/10.3847/1538-4357/ac74b8)

Full-text URL: <https://iopscience.iop.org/article/10.3847/1538-4357/ac74b8/pdf>

LIDA - The Leiden Ice Database for Astrochemistry

W. R. M. Rocha, M. G. Rachid, B. Olsthoorn, E. F. van Dishoeck, M. K. McClure, H. Linnartz

High quality vibrational spectra of solid-phase molecules in ice mixtures and for temperatures of astrophysical relevance are needed to interpret infrared observations toward protostars and background stars. Over the last 25 years, the Laboratory for Astrophysics at Leiden Observatory has provided more than 1100 spectra of diverse ice samples. Timely with the recent launch of the James Webb Space Telescope, we have fully upgraded the Leiden Ice Database for Astrochemistry (LIDA) adding recently measured spectra. The goal of this manuscript is to describe what options exist to get access to and work with a large collection of IR spectra, and the UV/vis to mid-infrared refractive index of H₂O ice and astronomy-oriented online tools to support the interpretation of IR ice observations. LIDA uses Flask and Bokeh for generating the web pages and graph visualization, respectively, SQL for searching ice analogues within the database and Jmol for 3D molecule visualization. The infrared data in the database are recorded via transmission spectroscopy of ice films condensed on cryogenic substrates. The real UV/vis refractive indices of H₂O ice are derived from interference fringes created from the simultaneous use of a monochromatic HeNe laser beam and a broadband Xe-arc lamp, whereas the real and imaginary mid-IR values are theoretically calculated. LIDA also offers online tools. The first tool, SPECIFY, used to create a synthetic spectrum of ices towards protostars. The second tool aims at the calculation of mid-infrared refractive index values. LIDA allows to search, download and visualize experimental data of astrophysically relevant molecules in the solid phase, as well as to provide the means to support astronomical observations. As an example, we analyse the spectrum of the protostar AFGL 989 using the resources available in LIDA and derive the column densities of H₂O, CO and CO₂ ices.

A&A, Accepted for publication

Full-text URL: <https://arxiv.org/abs/2208.12211>

Tracking the Ice Mantle History in the Solar-type Protostars of NGC 1333 IRAS 4

Marta De Simone, Cecilia Ceccarelli, Claudio Codella, Brian E. Svoboda, Claire J. Chandler, Mathilde Bouvier, Satoshi Yamamoto, Nami Sakai, Yao-Lun Yang, Paola Caselli, Bertrand Lefloch, Hanyu Baobab Liu, Ana López-Sepulcre, Laurent Loinard, Jaime E. Pineda, Leonardo Testi

To understand the origin of the diversity observed in exoplanetary systems, it is crucial to characterize the early stages of their formation, represented by Solar-type protostars. Likely, the gaseous chemical content of these objects directly depends on the composition of the dust grain mantles formed before the collapse. Directly retrieving the ice mantle composition is challenging, but it can be done indirectly by observing the major components, such as NH₃ and CH₃OH at cm wavelengths, once they are released into the gas-phase during the warm protostellar stage. We observed several CH₃OH and NH₃ lines toward three Class 0 protostars in NGC1333 (IRAS 4A1, IRAS 4A2, and IRAS 4B), at high angular resolution (1"; ~300 au) with the VLA interferometer at 24-26 GHz. Using a non-LTE LVG analysis, we derived a similar NH₃/CH₃OH abundance ratio in the three protostars (<0.5, 0.015-0.5, and 0.003-0.3 for IRAS 4A1, 4A2, and 4B, respectively). Hence, we infer they were born from pre-collapse material with similar physical conditions. Comparing the observed abundance ratios with astrochemical model predictions, we constrained the dust temperature at the time of the mantle formation to be ~17 K, which coincides with the average temperature of the southern NGC 1333 diffuse cloud. We suggest that a brutal event started the collapse that eventually formed IRAS 4A1, 4A2 and 4B, which, therefore, did not experience the usual pre-stellar core phase. This event could be the clash of a bubble with NGC 1333 south, that has previously been evoked in the literature.

The Astrophysical Journal Letters, Volume 935, L14

DOI: [10.3847/2041-8213/ac85af](https://doi.org/10.3847/2041-8213/ac85af)

Full-text URL: <https://arxiv.org/abs/2208.00247>

Confirmation of the outflow in L1451-mm: SiO line and CH₃OH maser detections

V. Wakelam, A. Coutens, P. Gratier, T.H G Vidal, N. Vaytet

The observational counterparts of theoretically predicted first hydrostatic cores (FHSC) have been searched for in the interstellar medium for nearly two decades now. Distinguishing them from other types of more evolved but still embedded

objects remains a challenge because these objects have a short lifetime, are small, and embedded in a dense cocoon. One possible lead to finding them is the characterization of the outflows that are launched by these objects. We observed the L1451-mm FHSC candidate with the NOEMA interferometer in order to study the emission of several molecules. A nonlocal thermodynamic equilibrium analysis of the CH₃OH detected lines was performed to retrieve the physical conditions of the emitting region around the central source, together with the CH₃OH, SiO, CS, and H₂CO column densities. Of the targeted molecules, we detected lines of c-C₃H₂, CH₃OH, CS, C₃S, SO, DCN, DCO⁺, H₂CO, HC₃N, HDCO, and SiO. One of the methanol lines appears to be a maser line. The detection of this class I maser and the SiO line in L1451-mm support the presence of a low-velocity and compact outflow. The excitation conditions of the thermal lines of methanol are also compatible with shocks (H₂ density of $\sim 3 \times 10^6 \text{ cm}^{-3}$ and a temperature higher than 40-K). Although these low-velocity outflows are theoretically predicted by some models of FHSC, these models also predict the shock temperature to be below 20-K, that is, not evaporating methanol. In addition, the predicted velocities would not erode the grains and release silicon in the gas phase. We therefore conclude that these new observations favor the hypothesis that L1451-mm would be at a very early protostellar stage, launching an outflow nearly on the plane of the sky with a higher velocity than is observed.

Accepted for publication in A&A.

Full-text URL: <https://arxiv.org/abs/2208.13606>

The gas-phase reaction of NH₂ with formaldehyde (CH₂O) is not a source of formamide (NH₂CHO) in interstellar environments

Kevin M. Douglas, Daniel Lucas, Catherine Walsh, Niclas A. West, Mark A. Blitz, Dwayne E. Heard

The first experimental study of the low-temperature kinetics of the gas-phase reaction of NH₂ with formaldehyde (CH₂O) has been performed. This reaction has previously been suggested as a source of formamide (NH₂CHO) in interstellar environments. A pulsed Laval nozzle equipped with laser-flash photolysis and laser-induced fluorescence spectroscopy was used to create and monitor the temporal decay of NH₂ in the presence of CH₂O. No loss of NH₂ could be observed via reaction with CH₂O and we place an upper-limit on the rate coefficient of $< 6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 34K. Ab initio calculations of the potential energy surface were combined with RRKM calculations to predict a rate coefficient of $6.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 35K, consistent with the experimental results. The presence of a significant barrier, 18 kJ mol⁻¹, for the formation of formamide as a product, means that only the H-abstraction channel producing NH₃ + CHO, in which the transfer of an H-atom can occur by quantum mechanical tunnelling through a 23 kJ mol⁻¹ barrier, is open at low temperatures. These results are in contrast with a recent theoretical study which suggested that the reaction could proceed without a barrier and was therefore a viable route to gas-phase formamide formation. The calculated rate coefficients were used in an astrochemical model which demonstrated that this reaction produces only negligible amounts of gas-phase formamide under interstellar and circumstellar conditions. The reaction of NH₂ with CH₂O is therefore not an important source of formamide at low temperatures in interstellar environments.

Accepted in ApJ Letters

Full-text URL: <https://arxiv.org/abs/2208.12658>

Announcements

Astrochemistry at High Resolution: Faraday Discussion

Astrochemistry at high resolution: Faraday Discussion

31 May – 2 June 2023

Space Telescope Science Institute

Baltimore, Maryland, United States

We are currently promoting for oral abstract submission. The event will bring together researchers from astronomy, gas-phase, solid state and surface physics, and chemistry communities to address the wide-ranging future of astrochemistry. You can find more about the event and the themes on the website: <https://www.rsc.org/events/detail/72754/>

2023 Kavli-IAU Astrochemistry Symposium. Astrochemistry VIII - From the First Galaxies to the Formation of Habitable Worlds

2023 Kavli-IAU Astrochemistry Symposium

10 – 14 Jul 2023 (Traverse City, MI, USA)

Astrochemistry VIII - From the First Galaxies to the Formation of Habitable Worlds.

<https://events.mpe.mpg.de/event/14/>

Astrochemistry is at the heart of many astrophysical fields, from the early Universe to local galaxies, to star- and planet-formation and evolution in our Milky Way, to exoplanet atmospheres, and to our Solar System. Decades-long concerted efforts of astronomers and theoretical/experimental chemists have provided a solid base for using molecules as powerful diagnostic tools of the physical and chemical structure, dynamics, and history of a multitude of astrophysical objects, allowing connections and glimpses into the life cycle of the interstellar medium, as well as into the growth of chemical complexity in space. The great sensitivity, high angular resolution and frequency coverage of telescopes such as ALMA have allowed unprecedented views of stellar and planet nurseries. JWST with its sensitive near- to mid-infrared spectrometers will soon open a new sensitive and sharp observing window into major molecular ingredients such as water, carbon dioxide as well as other key organic species. JWST will allow us to probe composition of ices on interstellar and

planet-forming scales, enabling studies of the linked-chemistry of exoplanetary atmospheres and protoplanetary disks. It is therefore timely for the eighth IAU Symposium on Astrochemistry that will allow the ever-growing astrochemical community to meet and discuss recent achievements and future progress including the possibilities of new connections to other fields.

Research Fellow in ALMA Observations of Protoplanetary Disks

The University of Leeds (UK) is seeking a research fellow to work on an STFC-funded project with Dr Catherine Walsh in the Astrophysics Group, to investigate the chemistry of complex organic molecules in planet-forming disks around nearby young stars.

The successful candidate will carry out a research program to search for emission from complex organic molecules in nearby protoplanetary disks using observations from the Atacama Large Millimeter/submillimeter Array (ALMA). They will conduct analyses of the data to derive the distribution and abundance of complex organic molecules using molecular line radiative transfer methods, and they will aid interpretation of the data by running astrochemical models to determine the chemical origin of complex organic molecules in protoplanetary disks.

The successful candidate will have a PhD in Astrophysics or a related field (or will have submitted their thesis prior to taking up the appointment), and will have experience in the reduction and analysis of observational data at (sub)millimeter or radio wavelengths and a developing track record of peer-reviewed publications in international journals.

The position is available immediately and thus the starting date will be as soon as possible. This role will be based on the university campus, with scope for it to be undertaken in a hybrid manner. We are also open to discussing flexible working arrangements.

For further details on the post and how to apply please visit: <https://jobs.leeds.ac.uk/Vacancy.aspx?ref=EPSPA1068>