Astrochemistry at High Resolution

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Participants and contribution abstracts

in alphabetical order

Isabel Aleman Jodrell Bank Centre for Astrophysics, The University of Manchester

Poster *Molecular Hydrogen in the Ionized Region of Planetary Nebula*
The analysis of the H_2 line emission of planetary nebulae (PNe) have been done in the literature assuming that the molecule survives only in neutral environments, as in photodissociation or shocked regions. However, there is strong evidence that at least part of the H_2 emission is produced inside the ionized region of such objects. In the present work, we calculate and study the infrared line emission of H_2 produced inside the ionized region of PNe using the one-dimensional photoionization code Aangaba. We show that the contribution of the ionized region for the H_2 emission can be significant, particularly in the case of nebulae with high temperature central stars. This result explains why H_2 emission is more frequently observed in bipolar planetary nebulae (Gatley's rule), since this kind of object typically has hotter stars.

Estelle Bayet UCL - London

Talk *Molecules for inferring the influence of the galactic nucleus activity on its star formation activity.*
To better understand how stars are forming in the Universe and get better insights on how galaxies thus form and evolve in it, it is essential to disentangle first the influence of galactic nucleus activity on the star formation activity. By identifying molecular tracers of dense gas ($n_{\rm H} \approx 10^7$ cm^{-3}) and less dense gas ($n_{\rm H} \approx 10^{3-4}$ cm^{-3}) in a wide variety of extragalactic environments (starburst, AGN-dominated, mergers, etc), this study is actually possible now to perform.
In my talk, I will present and explain the modelling approaches we have used to identify the ideal molecular tracers of dense and less dens gas for a large range of galaxy types. Then, I will show the first detections ever obtained in nearby galaxies of these species, validating the modelling predictions. The ISM physical properties derived from these molecular tracers under non-LTE assumption will be also shown in my talk, allowing us to better determine the physical and dynamical conditions required to form stars in nearby extragalactic regions.
I will finally finish my talk by presenting the perspectives of this work, especially at higher-z and emphasizing an ALMA context.

Peter Be00rnath University of York

Talk *Laboratory spectra of astrophysically important molecules*

Peter Botschwina Institute of Physical Chemistry, University Goettingen

Talk *High-level ab initio Calculations for (potential) Interstellar Anions: Structures, Spectroscopic Properties and Energetics*

Jane Buckle University of Cambridge

Talk *A wide-field high-resolution view of NGC2264*
Although filamentary structure is ubiquitous in molecular clouds, little is known about the physical conditions and star forming activity within them. In low-mass clouds, clusters form in high column-density filaments. Towards massive star-forming regions, protoclusters dominate in the data and analysis, and filamentary structure has been less well-studied. Utilizing new, wide-field and high-resolution data, we use a variety of techniques in order to determine the physical and kinematical conditions across the NGC2264 cloud complex. NGC2264 demonstrates large-scale filamentary structure extending in several directions from a ridge containing two mixed-mass protoclusters. We relate the physical conditions to ongoing star formation activity, both in the protoclusters and the more isolated parts of the cloud. We aim to determine whether the the filamentary structures are active sites of fragmentation and core collapse, and the extent of interaction with the massive outflows generated from the protoclusters.

Martin Bureau University of Oxford

Poster *The CO Tully-Fisher relation of early-type galaxies*
The Tully-Fisher relation has been extensively studied in gas rich systems and provides a wealth of kinematic information, as well as being important for the cosmic distance ladder. In gas-poor systems such as early-type galaxies, however, the relation becomes hard to study, requiring detailed modelling of the stellar kinematics. We demonstrate using both single-dish and interferometric observations that CO molecules are an excellent kinematic tracer, even in the highest mass galaxies, allowing us to investigate the Tully-Fisher relation of early-type galaxies relatively easily. We find that the Tully-Fisher relation of early-types is offset from that of spirals by $\sim$1 magnitude at K band, in line with other results. Next generation facilities such as the LMT and ALMA should allow this technique to be extended to high-redshift systems, providing a new simple tool to trace the M/L evolution of galaxies of all masses over

Alessandra Candian University of Nottingham

Poster *Assignment of UIRs bands to specific classes of PAHs*
The Unidentified Infrared Bands (UIRs) are a family of infrared features observed in a variety of astronomical objects. The wavelengths at which they appear are indicative of vibrations from aromatic molecules: neutral or ionised polycyclic aromatic hydrocarbons (PAHs) are widely believed to be the carriers. So far it has not been possible to identify a specific class of PAHs. Using Density Functional Theory (DFT) together with close comparison with experimental data, we assign the 11.0 μm feature to acenes. In addition we are able to model the shape of the 11.2 μm feature in terms of size distribution of large compact PAHs.

Alison Craigon University of Strathclyde

Talk *Observational evidence for photoelectric heating in Barnard 35A*
I will present observational evidence for a correlation between the intensity of polyaromatic hydrocarbon (PAH) emission near 8 μm and gas excitation temperature across a (1.1 $\times$ 1.6) pc region of Barnard 35A (B35A). This relationship is consistent with photoelectric heating, where the absorption of UV photons by PAHs results in either infrared emission or the ejection of energetic photoelectrons that heat the gas. B35A is a bright-rimmed cloud with a photodissociation region (PDR) along its western edge, which faces the O8 III star lambda Orionis. The gas excitation temperature of B35A was obtained from CO (J = 3 - 2 (JCMT) and J = 2 -1 (IRAM 30m)) observations and the PAH emission was taken from archival Spitzer InfraRed Array Camera (IRAC) 8 μm data.

Timothy Davis University of Oxford

Talk *On the origin of molecular gas in early-type galaxies*
Recently, early-type galaxies have shed their "red-and-dead" moniker, thanks to the discovery that many host residual star formation. As part of the ATLAS-3D project, we are conducting a complete, volume-limited survey of the molecular gas in 263 local early-type galaxies with the IRAM-30m telescope and the CARMA interferometer, in an attempt to understand the fuel powering this star formation. We find that around 23% of early-type galaxies in the local volume host large gas reservoirs, with molecular central discs, polar structures and rings being common. We present results showing that galaxies in clusters always feature molecular gas aligned with the stellar kinematics, consistent with material cooling from recycled stellar mass loss. In the field, however, nearly random kinematic misalignments between the stellar and gaseous components imply that the molecular gas is primarily supplied by external sources. We also touch on results from a pathfinder project exploring denser gas tracers such as 13CO, HCN and HCO+, which suggest that 13CO is enhanced, and HCO+ possibly suppressed in early-types compared to other galaxy types.

Dieter Engels Hamburger Sternwarte, Germany

Talk *AKARI observations of the dust around AGB and early post-AGB stars*
We observed about a dozen extremely red IRAS sources with the Japanese infrared satellite AKARI between 5 and 18 μm. The sources observed are carbon- or oxygen-rich AGB and post-AGB stars, where the optically thick dust shell obscures the star in the optical and near-infrared wavelength region. The AKARI observations confirm the presence of extremely red carbon stars in the IRAS color-color region populated by hidden post-AGB stars. Some O-rich post-AGB stars exhibit a near-infrared excess at $\lambda < 3$ μm. The modelling of the spectral energy distributions require the presence of C-rich dust close to the stars seen through a screen of silicate-rich dust, which also hosts the still detectable OH masers. The short-wavelength excess emission is probably coming from bipolar lobes, seen by HST in at least one of the observed sources.

Sandra Etoka The University of Manchester

Talk *Late-type star evolution as seen through OH maser emission*
Maser emission is a powerful tool to study both the geometrical and kinematic structure of the circumstellar envelope surrounding evolved stars. High spectral resolution monitoring allow you to trace any changes as they propagate while high spectral and spatial resolution imaging allow you to study the geometrical structure of an object at a given time in its evolution. I shall present late-type star evolution as seen through OH maser emission. Not only OH maser allow us to probe in great detail the kinematic and geometrical structure of the outer part of the circumstellar shell, but they also allow us to retrieve the polarimetric information associated with the maser spots and consequently gain information about the magnetic field structure and strength in these regions.

Luca Fossati The Open University

Talk *HST observations of the hot transiting extrasolar planet WASP-12b: atmospheric blow-off and peculiar stellar evolution?*
WASP-12 is a 2 Gyr old solar type star, hosting WASP-12b, one of the most irradiated transiting planets currently known. Previous observations of HD 209458 b, the prototype 'hot Jupiter' transiting exoplanet found a 15% deep transit in Lyman alpha, suggesting the planet atmosphere is being evaproated by the stellar flux. We observed WASP-12 in the UV with the Cosmic Origin Spectrograph (COS) on HST. We report here on our first visit to the target. The observations cover three distinct wavelength ranges in the near UV, the reddest region is centered on the MgII UV resonance lines at 280 nm. The stellar spectrum is a rich forest of photospheric absorption lines. We compare the spectrum in transit with the out of transit spectrum to search for absorption line features in the planetary atmosphere and exosphere. The stellar spectrum indicates the host star evolution is unusual.

Helen Fraser University of Strathclyde

Talk *Understanding the Role of Ice in Star and Planet Formation*
Recently we have been able for the first time to map ice abundances towards background stars, using VLT in single pointings, and more recently AKARI, and then to compare ice abundances with gases and dust, to really probe our understanding of ice formation mechanisms. This holds great promise for using ice-mapping as a technique in future missions such as JWST and SPICA. Not only are icy grains the nanofactories of chemical production in star formation, but in out disk regions, their aggregation leads we think, to the formation of planetessimals and cometary nuceli, which subsequently can form or bombard the early terrestrial planets. using recent results from parabolic flight experiments on dust and ice, I will also show how our planet formation models are tested, and what questions remain in linking dust in star formation with the evolution of planetary systems.

Gary Fuller JBCA

Rob Hargreaves University of York

Poster *FeH and NH_3 Observations*
Laboratory spectra of molecules have recently become important in relation to cool astronomical objects, including extrasolar planets and brown dwarfs. Current interest has focussed on ammonia (NH_3) and methane (CH_4) for identifying brown dwarfs and extrasolar planets. At present, iron hydride (FeH) is used to distinguish between M and L dwarfs.
New Fe_H molecular opacities and observations of M and L dwarfs are presented for the 1.6 μm region. In addition, we are in the process of producing a comprehensive NH_3 line list from new laboratory observations to be utilised in brown dwarf and extrasolar planet atmospheric models.

Charlotte Holmes Imperial College London

Poster *Laboratory measurements of neutral vanadium for the study of stellar and sub-stellar objects*
Most of the information for stellar and sub-stellar objects is obtained from the light radiated, absorbed or reflected by them. The ability to correctly interpret spectra from remote sources such as the sun or planetary bodies relies on the accurate measurement of molecular, atomic and solid state spectra in the laboratory. However, the current laboratory database for the neutral vanadium lacks important parameters such as accurate wavelengths (particularly in the UV and IR), intensity measurements (oscillator strengths) and line broadening parameters such as hyperfine structure. The lack of fundamental laboratory determined parameters is one of the major sources of uncertainty in the interpretation of expensively acquired stellar and sub-stellar spectra. We discuss the current measurements of neutral vanadium spectra with applications to galactic chronometry and the study of metal-poor and cool dwarf stars.

Malcolm Gray JBCA

Talk *Masers at ultra-high resolution*
A new generation of radio telescopes, such as *e*-MERLIN and EVLA will be equipped with correlators which have thousands, or even tens of thousands of channels. These devices also have much greater flexibility in their configuration than their predecessors. This offers the possibility of making observations with spectral resolution in the 1 mHz to 1 Hz range. Whilst most sources would have an undetectable flux in such a bandwidth, bright maser lines are still visible, and I will discuss possible experiments which exploit this combination of high brightness and narrow spectral resolution.

Mark Hammonds University of Nottingham

Kerry Hebden Jodrell Bank Centre for Astrophysics, University of Manchester

Liz Humphreys ESO

Talk *The Nature Of An AGN Accretion Disk Within The Central Parsec: Strengthened Evidence For Spiral Structure*
A major issue for understanding the accretion process of active galactic nuclei (AGN) is determining the inner accretion disk structure. The only way to map the disk at distances ¡ 1 pc from the central supermassive black hole is using radio Very Long Baseline Interferometry (VLBI) observations of nuclear water masers. In a new VLBI maser study of AGN NGC 4258, we have imaged a sub-parsec portion of the disk at 18 epochs. This has enabled measurement of the maser medium thickness of 5 microarcseconds or 0.0002 pc (1 sigma). Assuming this corresponds to disk thickness, hydrostatic equilibrium requires a gas temperature of 600 K, consistent with conditions for maser pumping. We confirm the warped disk could obscure the central engine, and find a characteristic scale of 0.03 pc for masers along the disk midline, consistent with a model of spiral density waves.

Nadya Kunawicz Jodrell Bank Centre for Astrophysics

June McCombie University of Nottingham

Daniel McElroy Queen's University Belfast

Andrew Markwick University of Manchester

Karl Menten Max-Planck-Institut für Radioastronomie, Bonn

Talk *The transformational effect of ALMA on astrochemistry*
Compared to all existing instruments, the Atacama Large Millimeter Array will have vastly better sensitivity, frequency coverage and instantaneous bandwidth. This, together with the "adaptive resolution" afforded by its movable antennas, will make ALMA the ultimate astrochemistry imager, allowing mapping of the dusty extended molecular envelopes of protostars and evolved stars down to the scales of their photospheres and of the starburst cores of ultraluminous galaxies in the local and the distant Universe. Three (x,y,v) dimensional line surveys will allow thorough chemical and physical characterization of these objects. After giving a general overview of ALMA's capabilities, I shall illustrate its impact on astrochemistry with a few examples.

Tom Muxlow JBCA

Tom Millar Queen's University Belfast

James Miller University of Strathclyde

Justin Neill University of Virginia

Poster *Chirped Pulse Fourier Transform Microwave Spectroscopy of Molecules of Astrochemical Interest*
With forthcoming advancements in radio telescope technology, high-throughput laboratory techniques must be developed to detect new transitions of molecules of astrochemical interest. This poster will present examples of the application of a chirped-pulse Fourier transform microwave spectrometer, coupled with a pulsed discharge nozzle, to astrochemical systems. As the spectrometer has a bandwidth of up to 15 GHz in a single valve acquisition cycle, a large number of species can be detected simultaneously and efficiently with respect to measurement time and sample consumption, and because the phase of the molecular emission signal is very stable, time-domain signal averaging can be performed over hours or days so that low-abundance or low-polarity species can be detected. Also, the design and performance of a recently commissioned 25–40 GHz chirped pulse FTMW spectrometer will be discussed.

David Nutter Cardiff University

Cormac Purcell Jodrell Bank Centre for Astrophysics

Talk *Early massive star formation in NGC3576.*
Continuum observations at 1.2-mm wavelengths have shown the giant HII region NGC3576 to be embedded in the heart of an extended filamentary dust cloud. The cloud adjacent to the HII region contains a number of clumps suspected to host massive protostellar objects at a very early stage of evolution. We present here the results of an investigation into the star forming state of these clumps conducted by observing the region for radio continuum emission, H_2O masers and multiple thermal molecular transitions.

Matt Redman National University of Ireland Galway

Anthony Remijan NRAO

Talk *Laboratory and Possible Interstellar Detection of /trans/-Methyl Formate*
The rotational spectrum of the trans conformational isomer of methyl formate has been assigned using pulsed jet spectroscopy. A total of 28 transitions, 19 from the A-symmetry torsional state and 9 from the E-symmetry torsional state, have been detected in the laboratory. This spectrum was expected to have strong internal rotor effects due to a low three-fold barrier to methyl group internal rotation, calculated to be around 20 cm^{-1} . The population of this conformer, which lies approximately 2000 cm^{-1} higher in energy than the previously assigned cis conformer, was enhanced through the use of an electric discharge. Transitions were found by a combination of chirped-pulse Fourier transform microwave spectroscopy, a high-sensitivity Fourier transform microwave spectrometer, and microwave- microwave double resonance spectroscopy to confirm quantum state connections. A total of seven transitions (four from the A-symmetry torsional state and three from the E) have been identified in absorption in Green Bank Telescope survey scans towards Sgr-B2(N) as part of the GBT PRIMOS Project, http://www.cv.nrao.edu/∼aremijan/PRIMOS/index.html ¡https://c.mail.virginia.edu/Redirect/www.cv.nrao.edu/%7Earemijan/PRIMOS/ind ex.html¿, showing an abundance relative to the cis conformer that is much higher than the relative energies would predict. This detection could offer insight into the production mechanism of methyl formate in the interstellar medium.

Anita M. S. Richards Jodrell Bank Centre for Astrophysics, University of Manchester,

Talk *Molecules as physical and kinematic tracers*
Maser emission can be imaged with milli/micro-arcsecond resolution using radio interferometry. This provides unparalleled direct measurements of kinematics on scales of less than an AU at better than 100 m s^{-1} resolution, for example showing the internal cloud turbulence in mass-loss from evolved stars, distinguishing between fractal and shock-like structures in star-forming regions. Sub-pc resolution of AGN discs provides the best evidence for the existence of black holes. Estimates of the temperature, density and volume of the emission regions are more model-dependent but provide, for example, guides to the chronology of cloud collapse in star formation. e-MERLIN, ALMA and next-generation VLBI will provide far better constraints by allowing many more maser lines to be observed contemporaneously. The EVLA and ALMA will give improved images of thermal lines also but only the SKA could provide sensitivity approaching that of current maser observations. Developing techniques for comparing high-sensitivity single-dish monitoring with high-resolution interferometry could bridge this gap.

Monica Rodriguez Instituto de Astrofisica de Andalucia

Paul Ruffle Queen's University Belfast

Christopher Rushton University of Leeds

Peter Sarre The University of Nottingham

Daan Schram Eindhoven University of Technology

Talk *The influence of the plasma state in astro- and plasma chemistry*
Charged particles, electrons and ions form the essence of a plasma. They make dissipation possible and cause ionization and dissociation of molecules by charge transfer and dissociative recombination. Radical fluxes to surfaces are high, surfaces become passivated and molecule formation on surfaces may become different in a plasma environment. If hot weakly adsorbed fragments are involved, excited molecules are produced, which can lead to negative ions, important for cluster formation. In this contribution analogies will be sought between astro-chemical plasmas and well diagnosed earthly plasmas, realizing the vast differences in densities temperatures and length and time scales. The presence of electrons indicates non-equilibrium and thus a history in ionizing and recombining phases, which has consequences for the relation between emission and composition of the plasma. The influence of the plasma state on emission and molecule formation at the surface will be discussed at the hand of some well diagnosed earthly plasmas.

Trevor Sears Brookhaven National Laboratory, Upton, NY 11973, USA

Ian Sims Institut de Physique de Rennes

Keith Smith The University of Nottingham

Talk *Studies of Interstellar Matter on Scales from 10 AU to 1 pc*
Over the past decade, mounting evidence from high resolution radio and optical observations has indicated that the diffuse interstellar medium (ISM) is structured on scales down to a few AU. Such 'small-scale structure' leads to variations in density, temperature etc. which have important implications for the chemistry in the diffuse ISM; the physical processes responsible are currently unknown. Here, I present optical observations of stars, binary systems and the globular cluster omega Centauri which probe the atoms, molecules and diffuse interstellar band carriers in the diffuse ISM over scales from 10 AU to 1 pc. Implications for the physical and chemical conditions within the small-scale structures are discussed, along with constraints on the 'families' of diffuse interstellar bands.

Azrael von Prochazka Queen's University Belfast

Poster *Modelling Hot Cores in the Interstellar Medium*
The diversity of chemical compounds detected in interstellar molecular clouds has attracted interest from the astronomical community as an essential key towards understanding the evolution of matter as it is processed towards the creation of young stellar objects, protoplanetary disks, planets, and, ultimately, life. Previously, it was thought that complex organic species could form and survive only in the cold outer regions of a collapsing cloud, where molecules would be shielded from dissociation by incoming photons and cosmic ray particles. However, recent detections of large organic species in low-mass protostars have caused a paradigm shift with regard to our understanding of the mechanisms and timescales by which these species are formed and destroyed. At the heart of our analysis is grain surface chemistry – an investigation into the accretion, migration, bonding, and evaporation mechanisms which are expected to occur on interstellar grains to form complex species which would otherwise not be expected to exist in the gas phase. We present two models; the first is of the chemistry of a single point of gas as it evolves in time through the freeze out period of a collapsing cloud, the second is a combined gas phase and grain surface chemistry multipoint representation of the chemistry of the outer envelope as the density and temperature of each point of gas vary with distance from the central core. While grain surface chemistry is in many ways a viable explanation for the existence of low-mass prestellar complex organics, we will address the significant uncertainties in our theories which would do well to be addressed and explored by the experimental solid state and gas-kinetic chemistry communities.

Nicholas Walker University of Bristol

Catherine Walsh Queen's University Belfast

Talk *Molecular Line Emission from Protoplanetary Disks*
We have calculated the chemical structure of a protoplanetary disk surrounding a typical T Tauri star with the disk model of Nomura and Millar, 2005 as our physical basis, using the gas-phase chemical network from the most recent UMIST Database for Astrochemistry and allowing the accretion and thermal desorption of gas phase species onto, and from dust grains. We have investigated the effects on the chemical structure of non-thermal desorption mechanisms including cosmic-ray induced desorption, photo-desorption and X-ray desorption and have added a large grain-surface chemical network to study effects on the synthesis of small organic molecules. We compute the radiative transfer in the disk at various inclination angles and compare our disk integrated molecular line profiles and intensities with existing observations. We also use our calculations as input to the GILDAS ALMA simulator to both study the impact ALMA will have on the observation of molecular line emission from protoplanetary disks and determine optimum observation parameters for several molecular transitions, source distances and disk inclinations.

Derek Ward-Thompson Cardiff University

Talk *Exciting new results from Herschel and SCUBA II*

Jennifer Williams University of Manchester

Talk *Modelling massive protostellar envelopes.*
We are modelling the sub-millimeter dust emission from young massive protostellar cores to determine the properties of the dusty envelopes. We use the 1-D radiative transfer code DUSTY to create models, with an adaptive grid of parameters, which are compared to spatial intensity profiles of the observations from SCUBA to find the model with the best fitting set of parameters. We are also investigating the chemistry in the envelopes for a subset of sources using SCUBA and HARP observations and modelling the dust and molecular emission.

Paul Woods University of Manchester