AstroChemical Newsletter #36

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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

Protonated CO2 in massive star-forming clumps

F. Fontani, A. Vagnoli, M. Padovani, L. Colzi, P. Caselli, V.M. Rivilla

Interstellar CO2 is an important reservoir of carbon and oxygen, and one of the major constituents of the icy mantles of dust grains, but it is not observable directly in the cold gas because has no permanent dipole moment. Its protonated form, HOCO+, is believed to be a good proxy for gaseous CO2. However, it has been detected in only a few star-forming regions so far, so that its interstellar chemistry is not well understood. We present new detections of HOCO+ lines in 11 high-mass star-forming clumps. Our observations increase by more than three times the number of detections in star-forming regions so far. We have derived beam-averaged abundances relative to H2 in between 0.3 and 3.8 x 1e-11. We have compared these values with the abundances of H13CO+, a possible gas-phase precursor of HOCO+, and CH3OH, a product of surface chemistry. We have found a positive correlation with H13CO+, while with CH3OH there is no correlation. We suggest that the gas-phase formation route starting from HCO+ plays an important role in the formation of HOCO+, perhaps more relevant than protonation of CO2 (upon evaporation of this latter from icy dust mantles).

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The first detection of H2S in a protoplanetary disk: The dense GG Tau A ring

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Studying molecular species in protoplanetary disks is very useful to characterize the properties of these objects which are the site of planet formation. We attempted to constrain the chemistry of S-bearing molecules in the cold parts of circumstellar disk of GG Tau A by searching for H2S, CS, SO and SO2 in the dense disk with the NOEMA interferometer. We detected H2S emission from the dense and cold ring orbiting around GG Tau A. This is the first detection of H2S in a protoplanetary disk. We also detected HCO+, H13CO+, DCO+ in the disk. Upper limits for other molecules, CCS, SO2, SO, HC3N and c-C3H2 are also obtained. The observed DCO+/HCO+ ratio is similar to those in other disks. The observed column densities derived using our radiative transfer code DiskFit, are then compared with those from our chemical code Nautilus. The column densities are in reasonable agreement for DCO+, CS, CCS, and SO2. For H2S and SO, our predicted vertical integrated column densities are more than a factor of 10 higher than the measured values. Our results reinforce the hypothesis

that only a strong Sulfur depletion may explain the low observed H2S column density in the disk. The H2S detection in GG Tau A is most likely linked to the much larger mass of this disk compared to that in other T Tauri systems.

2018 A&A, 616L,5P
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Methanol and its relation to the water snowline in the disk around the young outbursting star V883 Ori

Merel L.R. van 't Hoff, John J. Tobin, Leon Trapman, Daniel Harsono, Patrick D. Sheehan, William J. Fischer, S. Thomas Megeath, and Ewine F. van Dishoeck

We report the detection of methanol in the disk around the young outbursting star V883 Ori with the Atacama Large Millimeter/submillimeter Array (ALMA). Four transitions are observed with upper level energies ranging between 115 and 459 K. The emission is spatially resolved with the 0.14" beam and follows the Keplerian rotation previously observed for C18O. Using a rotational diagram analysis, we find a disk-averaged column density of ~1e17 cm-2 and a rotational temperature of ~90-100 K, suggesting that the methanol has thermally desorbed from the dust grains. We derive outer radii between 120 and 140 AU for the different transitions, compared to the 360 AU outer radius for C18O. Depending on the exact physical structure of the disk, the methanol emission could originate in the surface layers beyond the water snowline. Alternatively, the bulk of the methanol emission originates inside the water snowline, which can then be as far out as ~100 AU, instead of 42 AU as was previously inferred from the continuum opacity. In addition, these results show that outbursting young stars like V883 Ori are good sources to study the ice composition of planet forming material through thermally desorbed complex molecules, which have proven to be hard to observe in more evolved protoplanetary disks.

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Chemical Diversity in Three Massive Young Stellar Objects associated with 6.7 GHz CH3OH Masers

K. Taniguchi, M. Saito, L. Majumdar, T. Shimoikura., K. Dobashi, H. Ozeki, F. Nakamura, T. Hirota, T. Minamidani, Y. Miyamoto, H. Kaneko

We have carried out observations in the 42-46 and 82-103 GHz bands with the Nobeyama 45-m radio telescope, and in the 338.2-339.2 and 348.45-349.45 GHz bands with the ASTE 10-m telescope toward three high-mass star-forming regions containing massive young stellar objects (MYSOs), G12.89+0.49, G16.86-2.16, and G28.28-0.36. We have detected HC3N including its 13C and D isotopologues, CH3OH, CH3CCH, and several complex organic molecules (COMs). Combining our previous results of HC5N in these sources, we compare the N(HC5N)/N(CH3OH) ratios in the three observed sources. The ratio in G28.28-0.36 is derived to be 0.091, which is higher than that in G12.89+0.49 by one order of magnitude, and that in G16.86-2.16 by a factor of ~ 5. We investigate the relationship between the N(HC5N)/N(CH3OH) ratio and the N(CH3CCH)/N(CH3OH) ratio. The relationships of the two column density ratios in G28.28-0.36 and G16.86-2.16 are similar to each other, while HC5N is less abundant when compared to CH3CCH in G12.89+0.49. These results imply a chemical

diversity in the lukewarm (T ~ 20 - 30 K) envelope around MYSOs. Besides, several spectral lines from complex organic molecules, including very-high-excitation energy lines, have been detected toward G12.89+0.49, while the line density is significantly low in G28.28-0.36. These results suggest that organic-poor MYSOs are surrounded by a carbon-chain-rich lukewarm envelope (G28.28-0.36), while organic-rich MYSOs, namely hot cores, are surrounded by a CH3OH-rich lukewarm envelope (G12.89+0.49 and G16.86-2.16).

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Interferometric Observations of Cyanopolyynes toward the G28.28-0.36 High-Mass Star-Forming Region

K. Taniguchi, Y. Miyamoto, M. Saito, P. Sanhueza, T. Shimoikura, K. Dobashi, F. Nakamura, H. Ozeki

We have carried out interferometric observations of cyanopolyynes, HC3N, HC5N, and HC7N, in the 36 GHz band toward the G28.28− 0.36 high-mass star-forming region using the Karl G. Jansky Very Large Array (VLA) Ka-band receiver. The spatial distributions of HC3N and HC5N are obtained. HC5N emission is coincident with a 450 μm dust continuum emission and this clump with a diameter of ~ 0.2 pc is located at the east position from the 6.7 GHz methanol maser by ~ 0.15 pc. HC7N is tentatively detected toward the clump. The HC3N : HC5N : HC7N column density ratios are estimated at 1.0 : ~ 0. 3 : ~ 0. 2 at an HC7N peak position. We discuss possible natures of the 450 μm continuum clump associated with the cyanopolyynes. The 450 μm continuum clump seems to contain deeply embedded low- or intermediate-mass protostellar cores, and the most possible formation mechanism of the cyanopolyynes is the warm carbon chain chemistry (WCCC) mechanism. In addition, HC3N and compact HC5N emission is detected at the edge of the 4.5 μm emission, which possibly implies that such emission is the shock origin.

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First Hot Corino detected around an Isolated Intermediate-Mass Protostar: Cep E-mm.

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Intermediate-mass (I-M) protostars provide a bridge between the low- and high-mass protostars. Despite their relevance, little is known about their chemical diversity. We want to investigate the molecular richness towards the envelope of I-M protostars and to compare their properties with those of low- and high-mass sources. Methods. We have selected the isolated I-M Class 0 protostar Cep E-mm to carry out an unbiased molecular survey with the IRAM 30m telescope between 72 and 350 GHz with an angular resolution in the range 7 – 34 . Our goal is to obtain a census of the chemical content of the protostellar envelope. These data were complemented with NOEMA observations of the spectral bands 85.9 – 89.6 GHz and 216.8 – 220.4 GHz at an angular resolution of 2.3 and 1.4 respectively. The 30m spectra show bright emission of O- and N-bearing complex organic molecules (COMs): CH3OH and its rare isotopologues CH2DOH and 13CH3OH, CH3CHO, CH3OCH3 , CH3COCH3, HCOOH, HCOOCH3, H2CCO, NH2CHO, CH3CN, C2H3CN, C2H5CN, HNCO and H2CO. We identify up to three components in the spectral signature of COMs: an extremely broad

line (eBL) component associated with the outflowing gas (FWHM > 7 km s −1), a narrow line (NL) component (FWHM < 3 km s −1) associated with the cold envelope, and a broad line (BL) component (FWHM ∼ 5.5 km s −1) which traces the signature of a hot corino. The eBL and NL components are detected only in molecular transitions of low excitation and dominate the emission of CH3OH. The BL component is detected in highly excited gas (E up > 100 K). The NOEMA observations reveal Cep E-mm as a binary protostellar system, whose components, Cep E-A and Cep E-B, are separated by ≈ 1.7" . Cep E-A dominates the core continuum emission and powers the long studied, well-known, high-velocity jet associated with HH377. The lower flux source Cep E-B powers another high-velocity, molecular jet, reaching velocities of ≈ 80 km s −1 , which propagates in a direction close to perpendicular with respect to the Cep E-A jet. Our interferometric maps show that the emission of COMs arises from a region of ≈ 0.7" size around Cep E-A, and corresponds to the BL component detected with the IRAM 30m telescope. On the contrary, no COM emission is detected towards Cep E-B. We have determined the rotational temperature (T rot) and the molecular gas column densities from a simple population diagram analysis or adopting an excitation temperature. Rotational temperatures of COMs emission were found to lie in the range 20 K – 40 K with column densities ranging from a few 10 (15) cm−2 for O-species bearing, down to a few 10 (14) cm−2 for N-bearing species. Molecular abundances are similar to those measured towards other low- and intermediate-mass protostars. Ketene (H2CCO) appears as an exception, as it is found significantly more abundant towards Cep E-A. High-mass hot cores are significantly less abundant in methanol and N-bearing species are more abundant by 2–3 orders of magnitude. Cep E-mm reveals itself as a binary protostellar system with a strong chemical differentiation between both cores. Only the brightest component of the binary is associated with a hot corino. Its properties are similar to those of hot corinos.

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Chemical Signatures of the FU Ori Outbursts

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The FU Ori-type young stellar objects are characterized by a sudden increase in luminosity by 1−2 orders of magnitude, followed by slow return to the pre-outburst state on timescales of ∼10−100 yr. The outburst strongly affects the entire disk, changing its thermal structure and radiation field. In this paper, using a detailed physical-chemical model we study the impact of the FU Ori outburst on the disk chemical inventory. Our main goal is to identify gas-phase molecular tracers of the outburst activity that could be observed after the outburst with modern telescopes such as ALMA and NOEMA. We find that the majority of molecules experience a considerable increase in the total disk gas-phase abundances due to the outburst, mainly due to the sublimation of their ices. Their return to the pre-outburst chemical state takes different amounts of time, from nearly instantaneous to very long. Among the former ones we identify CO, NH3, C2H6, C3H4, etc. Their abundance evolution tightly follows the luminosity curve. For CO the abundance increase does not exceed an order of magnitude, while for other tracers the abundances increase by 2−5 orders of magnitude. Other molecules like H2CO and NH2OH have longer retention timescales, remaining in the gas phase for ∼10−1000 yr after the end of the outburst. Thus H2CO could be used as an indicator of the previous outbursts in the post-outburst FU Ori systems. We investigate the corresponding time-dependent chemistry in detail and

present the most favorable transitions and ALMA configurations for future observations.

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Constraining Gas-Phase Carbon, Oxygen, and Nitrogen in the IM Lup Protoplanetary Disk

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We present new constraints on gas-phase C, N, and O abundances in the molecular layer of the IM Lup protoplanetary disk. Building on previous physical and chemical modeling of this disk, we use new ALMA observations of C2H to constrain the C/O ratio in the molecular layer to be ~0.8, i.e., higher than the solar value of ~0.54. We use archival ALMA observations of HCN and H13CN to show that no depletion of N is required (assuming an interstellar abundance of 7.5×10−5 per H). These results suggest that an appreciable fraction of O is sequestered in water ice in large grains settled to the disk mid-plane. Similarly, a fraction of the available C is locked up in less volatile molecules. By contrast, N remains largely unprocessed, likely as N2. This pattern of depletion suggests the presence of true abundance variations in this disk, and not a simple overall depletion of gas mass. If these results hold more generally, then combined CO, C2H, and HCN observations of disks may provide a promising path for constraining gas-phase C/O and N/O during planet-formation. Together, these tracers offer the opportunity to link the volatile compositions of disks to the atmospheres of planets formed from them.

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The formation of astrophysical Mg-rich silicate dust

Christopher M. Mauney, David Lazzati

We present new results for ground-state candidate energies of Mg-rich olivine (MRO) clusters and use the binding energies of these clusters to determine their nucleation rates in stellar outflows, with particular interest in the environments of core-collapse supernovae (CCSNe). Low-lying structures of clusters (Mg2SiO4)n $2 \leq n \leq 13$ are determined from a modified minima hopping algorithm using an empirical silicate potential in the Buckingham form. These configurations are further refined and optimized using the density functional theory code Quantum Espresso. Utilizing atomistic nucleation theory, we determine the critical size and nucleation rates of these clusters. We find that configurations and binding energies in this regime are very dissimilar from those of the bulk lattice. Clusters grow with SiO4–MgO layering and exhibit only global, rather than local, symmetries. When compared to classical nucleation theory we find suppressed nucleation rates at most temperatures and pressures, with enhanced nucleation rates at very large pressures. This implies a slower progression of silicate dust formation in stellar environments than previously assumed.

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Formation of acetamide in interstellar medium

Lois Foo, Attil Surányi, Andre Guljas, Milán Szőri, John Justine Villar, Béla Viskolcz, Imre G. G.Csizmadia, Anita Rágyanszki, Béla Fiser

Acetamide (C2H5NO) is the largest molecule containing a peptide bond, which is an amine (-NH2) group bonded to a carbonyl (C = O) group, that has yet been detected in interstellar medium (ISM). It is also considered to be a precursor for amino acids (the building blocks of proteins). Formation of acetamide in ISM is believed to occur due based on evidence for the existence of the molecule itself and its component smaller species in ISM. A case study of acetamide is presented here, to introduce a new method to determine its possible formation reaction pathways in ISM based on the molecular formula of a species. All possible species with the same molecular formula as acetamide (C2H5NO) but with different connectivity, the so-called constitutional isomers of the molecule (198 structures, 91 unique species), were created and studied under the extreme conditions of dense molecular clouds. Acetamide was found to be the most stable of the C2H5NO isomer family. Based on the stability of the uni- and bimolecular species, eight reactions were proposed which could led to the formation of acetamide in ISM.

Molecular Astrophysics, Volume 13, November 2018, Pages 1-5
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Full-text URL: https://www.sciencedirect.com/science/article/pii/S2405675818300101

Catalytic conversion of methanol to larger organic molecules over crystalline forsterite: laboratory study and astrophysical implications

Q.Li, W. Dai B.S.Liu, P.J.Sarre, M.H.Xie, A.S-C.Cheung

Laboratory catalytic reactions of methanol over heated crystalline silicates (forsterite) lead to the formation of gas-phase olefinic and polycyclic aromatic hydrocarbon (PAH) molecules, and are of potential importance in astrophysical environments including hot molecular cores, protoplanetary disks and shocks. In our experiments the methanol reagent, together with intermediate and product gas-phase molecular species were detected using time-of-flight mass-spectrometry (TOF-MS). A solid deposited on the crystalline forsterite surface was examined subsequently using high-resolution transmission electron microscopy and thermal gravimetric techniques and found to comprise amorphous and graphitic carbon. The chemical players in this work - gas-phase methanol, crystalline silicates and PAHs, have been identified spectroscopically in a range of astrophysical environments including young and evolved stars, protoplanetary disks, comets, captured dust particles and meteorites. It is envisaged that reactions on bare dust grains as studied here both experimentally and theoretically through DFT calculations, can have implications for chemical transformations and conversions, in forming PAH molecules and potentially in the synthesis of prebiotic molecules.

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Ro-vibrational analysis of SiO in UV-irradiated environments

Ziwei E. Zhang, R.S. Cumbee, P.C. Stancil, G.J.Ferland

SiO emission lines are important probes of chemical processes in diverse astrophysical

environments, commonly observed in shocks associated with the outflows of young stellar objects, both low- and high-mass, and in the envelopes of evolved stars. Modelling SiO emission for conditions of non-local thermodynamic equilibrium (NLTE) requires collisional rate coefficients due to H2, H, and He impact, with the first of these of limited availability. Unknown collisional rate coefficients are often estimated from known systems. For the case of SiO-H2, rate coefficients have previously been adapted from a different collider, He, based on a reduced-mass scaling approach. Here, we construct comprehensive SiO collisional rate coefficients data with multiple colliders (H2, He and H) and rovibrational transitions up to v=5 and J=39 . A reduced-potential scaling approach is used to estimate unknown collisional data. Using RADEX and Cloudy, we investigate the rotational and rovibrational SiO emission in various astrophysical environments, including photodissociation regions (PDR) and the envelope of VY Canis Majoris.

Molecular Astrophysics, Volume 13, November 2018, Pages 6-21
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Developing a self-consistent AGB wind model: I. Chemical, thermal, and dynamical coupling

J. Boulangier, N. Clementel, A. J. van Marle, L. Decin, A. de Koter

The material lost through stellar winds of Asymptotic Giant Branch (AGB) stars is one of the main contributors to the chemical enrichment of galaxies. The general hypothesis of the mass loss mechanism of AGB winds is a combination of stellar pulsations and radiative pressure on dust grains, yet current models still suffer from limitations. Among others, they assume chemical equilibrium of the gas, which may not be justified due to rapid local dynamical changes in the wind. This is important as it is the chemical composition that regulates the thermal structure of the wind, the creation of dust grains in the wind, and ultimately the mass loss by the wind. Using a self-consistent hydrochemical model, we investigated how non-equilibrium chemistry affects the dynamics of the wind. This paper compares a hydrodynamical and a hydrochemical dust-free wind, with focus on the chemical heating and cooling processes. No sustainable wind arises in a purely hydrodynamical model with physically reasonable pulsations. Moreover, temperatures are too high for dust formation to happen, rendering radiative pressure on grains impossible. A hydrochemical wind is even harder to initiate due to efficient chemical cooling. However, temperatures are sufficiently low in dense regions for dust formation to take place. These regions occur close to the star, which is needed for radiation pressure on dust to sufficiently aid in creating a wind. Extending this model self-consistently with dust formation and evolution, and including radiation pressure, will help to understand the mass loss by AGB winds.

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Bayesian Inference of Reaction Rates in Icy Mantles

J. Holdship, N. Jeffrey, A. Makrymallis, S. Viti, J. Yates

Grain surface chemistry and its treatment in gas-grain chemical models is an area of large uncertainty. Whilst laboratory experiments are making progress, there is still much that is unknown about grain surface chemistry. Further, the results and parameters produced by experiment are often not easily translated to the rate equation

approach most commonly used in astrochemical modelling. It is possible that statistical methods can reduce the uncertainty in grain surface chemical networks. In this work, a simple model of grain surface chemistry in a molecular cloud is developed and a Bayesian inference of the reactions rates is performed through MCMC sampling. Using observational data of the solid state abundances of major chemical species in molecular clouds, the posterior distributions for the rates of seven reactions producing CO, CO2, CH3OH and H2O are calculated, in a form that is suitable for rate equation models. This represents a vital first step in the development of a method to infer reaction rates from observations of chemical abundances in astrophysical environments.

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The ALMA-PILS survey: Isotopic composition of oxygen-containing complex organic molecules toward IRAS 16293–2422B

J. K. Jørgensen, H. S. P. Müller, H. Calcutt, A. Coutens, M. N. Drozdovskaya, K. I. Öberg, M. V. Persson, V. Taquet, E. F. van Dishoeck, S. F. Wampfler

This paper presents a systematic survey of the deuterated and 13C isotopologues of a variety of oxygen-bearing complex organic molecules on Solar System scales toward the protostar IRAS 16293-2422B. We use the data from an unbiased molecular line survey between 329 and 363 GHz from the Atacama Large Millimeter/submillimeter Array (ALMA). The observations probe scales of 60 AU where most of the organic molecules have sublimated off dust grains and are present in the gas-phase. The complex organic molecules can be divided into two groups with one group, the simpler species, showing a D/H ratio of approximately 2% and the other, the more complex species, D/H ratios of 4-8%. This division may reflect the formation time of each species in the ices before or during warm-up/infall of material through the protostellar envelope. No significant differences are seen in the deuteration of different functional groups for individual species, possibly a result of the short time-scale for infall through the innermost warm regions where exchange reactions between different species may be taking place. The species show differences in excitation temperatures between 125 K and 300 K. This likely reflects the binding energies/sublimation temperatures of the individual species, in good agreement to what has previously been found for high-mass sources. For dimethyl ether the 12C/13C ratio is found to be lower by up to a factor of 2 compared to typical ISM values similar to what has previously been inferred for glycolaldehyde. The results point to the importance of ice surface chemistry for the formation of these complex organic molecules at different stages in the evolution of embedded protostars and demonstrate the use of accurate isotope measurements for understanding the history of individual species.

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Announcements

Astrochemistry: From nanometers to megaparsecs – A symposium in honour of John H. Black

We welcome all to Gothenburg on 24-28 June, 2019, to attend this meeting in connection to John Black's 70th birthday. Symposium description: Through

astrochemistry, effects on atomic scales are directly linked to the formation and evolution of planets, stars, interstellar clouds, and galaxies across the universe. The scientific purpose of this symposium is to highlight the fundamental connection between the theory of microscopic processes studied on Earth and the understanding of phenomena in a wide range of space environments. In tandem with observations of increasing detail and sensitivity, enabled by technological development, this interplay has been key in advancing the field during the last 30 years, and will become even more important as we move forward into the era of exciting new facilities such as JWST, the Origins Space Telescope, and the SKA. The symposium is organised in honour of Prof. John H. Black, who throughout his career has demonstrated an outstanding ability to grasp, apply, and explain these connections - always maintaining a cosmic perspective regardless of scales or wavelengths. The scientific programme will include both invited and contributed talks as well as a dedicated poster session. A celebratory dinner will be organised on the evening of 27 June. Please visit our website for more information: http://www.chalmers.se/en/conference/JHBlacksymp2019/

First Announcement – Alexander Tielens symposium, Sep 2 – 6, 2019

CELEBRATING 40 YEARS OF ALEXANDER TIELENS' CONTRIBUTION TO SCIENCE: THE PHYSICS AND CHEMISTRY OF THE ISM. September 2 -- 6, 2019 in Avignon, France. Xander Tielens has been driving research in the fields of interstellar physics and chemistry and the cosmic cycle of matter with outstanding contributions for 40 years. With this meeting, we wish to celebrate his scientific achievements and discuss future research directions opened up by his contributions. The meeting will focus on the fields strongly influenced by Xander involving the physical and chemical processes that control the interstellar medium and its life cycle: PDRs, interstellar and circumstellar dust, PAHs, ices and astrochemistry. We will especially emphasize future opportunities offered by the powerful telescopes at our disposal such as, for example, ALMA, SOFIA, and JWST. The meeting will consist of invited reviews, invited and contributed talks, and posters. The second announcement will be made in December 2018. Date: September 2 -- 6, 2019 Location: Centre International de Congres du Palais des Papes, Avignon, France (http://www.avignon-congres.com/) Scientific Organizing Committee: Cecilia Ceccarelli (chair) Alessandra Candian (co-chair) Jan Cami Carsten Dominik Liv Hornekær Kay Justtanont Els Peeters Mark Wolfire Local Organizing Committee: Bertrand Lefloch (chair)