AstroChemical Newsletter #50

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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

The Sub-millimeter Rotational Spectrum of Ethylene Glycol up to 890 GHz and Application to ALMA Band 10 Spectral Line Data of NGC 6334I

Mattia Melosso, Luca Dore, Filippo Tamassia, Crystal L. Brogan, Todd R. Hunter, Brett A. McGuire

The rotational spectrum of the most stable conformer of ethylene glycol (HO(CH2)2OH) has been recorded between 360-890 GHz using a frequency-modulation sub-millimeter spectrometer. The refinement and extension of the spectroscopic parameters over previous efforts provides predicted catalog frequencies for ethylene glycol with sufficient accuracy for comparison to high-frequency astronomical data. The improvement in the cataloged line positions, and the need for improved accuracy enabled by high-frequency laboratory work, is demonstrated by an analysis of ethylene glycol emission at 890 GHz in the high-mass star-forming region NGC 6334I in ALMA Band 10 observations. The need for accurate rotational spectra at sub-millimeter wavelengths/THz frequencies is discussed.

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HCN/HNC intensity ratio: a new chemical thermometer for the molecular ISM

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Context. The gas kinetic temperature (TK) determines the physical and chemical evolution of the Interestellar Medium (ISM). However, obtaining reliable TK estimates usually requires expensive observations including the combination of multi-line analysis and dedicated radiative transfer calculations. Aims. This work explores the use of HCN and HNC observations, and particularly its I(HCN)/I(HNC) intensity ratio of their J=1-0 lines, as direct probe of the gas kinetic temperature in the molecular ISM. Methods. We obtained a new set of large-scale observations of both HCN and HNC (1-0) lines along the Integral Shape Filament (ISF) in Orion. In combination with ancillary gas and dust temperature measurements, we find a systematic temperature dependence of the observed I(HCN)/I(HNC) intensity ratio across our maps. Additional comparisons with chemical models demonstrate that these observed I(HCN)/I(HNC) variations are driven by the effective destruction and isomerization mechanisms of HNC under low energy barriers. Results. The observed variations of I(HCN)/I(HNC) with TK can be described with a two-part linear function. This empirical calibration is then used to create a temperature map of the entire ISF. Comparisons with similar dust temperature

measurements in this cloud, as well as in other regions and galactic surveys, validate this simple technique to obtain direct estimates of the gas kinetic temperature in a wide range of physical conditions and scales with an optimal working range between 15K<=TK<=40K. Conclusions. Both observations and models demonstrate the strong sensitivity of the I(HCN)/I(HNC) ratio to the gas kinetic temperature. Since these lines are easily obtained in observations of local and extragalactic sources, our results highlight the potential use of this observable as new chemical thermometer for the ISM.

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Full-text URL: https://ui.adsabs.harvard.edu/abs/2019arXiv191013754H/abstract

Rotationally inelastic processes of C2- colliding with He (1 S) at low temperatures: ab initio interaction potential, state changing rates and kinetic modelling

B P Mant, F A Gianturco, L González-Sánchez, E Yurtsever and R Wester

We discuss in detail the quantum rotationally inelastic dynamics of an important anion often discussed as a possible constituent of the interstellar medium (ISM) and in different environments of circumstellar envelopes: the C2- molecular ion. Its interaction forces with one of the most abundant atoms of the ISM, the neutral helium atom, are obtained for the first time using ab initio quantum chemistry methods. The overall angular anisotropy of the potential energy surface is analysed in order to link its features with the efficiency of transferring energy from the abundant He atoms to the internal rotational levels of this molecular anion. Calculations of the corresponding rotational state-to-state inelastic cross sections, for both excitation and de-excitation paths are obtained by using a multichannel quantum method. The corresponding inelastic rates at the temperatures of interest are determined and their role in distributing molecular states over the different populations of the rotational levels at the temperatures of that environment is discussed. These computed rates are also linked to the dynamical behaviour of the title molecule when confined in cold ion traps and made to interact with He as the common buffer gas, in preparation for state-selective photo-detachment experiments.

B P Mant et al 2020 J. Phys. B: At. Mol. Opt. Phys. 53 025201
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Evaporative cooling of icy interstellar grains. I

J. Kalvans, J. R. Kalnin

Context. While radiative cooling of interstellar grains is a well-known process, little detail is known about the cooling of grains with an icy mantle that contains volatile adsorbed molecules. Aims. We explore basic details for the cooling process of an icy grain with properties relevant to dark interstellar clouds. Methods. Grain cooling was described with a numerical code considering a grain with an icy mantle that is structured in monolayers and containing several volatile species in proportions consistent with interstellar ice. Evaporation was treated as first-order decay. Diffusion and subsequent thermal desorption of bulk-ice species was included. Temperature decrease from initial temperatures of 100, 90, 80, 70, 60, 50, 40, 30, and 20K was studied, and we also followed the composition of ice and evaporated matter. Results. We find that grain cooling occurs by partially successive and partially overlapping evaporation of different species. The most volatile molecules (N2) first evaporate at the greatest rate and are most rapidly depleted from the outer ice monolayers. The most important coolant is

CO, but evaporation of more refractory species, such as CH4 and even CO2, is possible when the former volatiles are not available. Cooling of high-temperature grains takes longer because volatile molecules are depleted faster and the grain has to switch to slow radiative cooling at a higher temperature. For grain temperatures above 40K, most of the thermal energy is carried away by evaporation. Evaporation of the nonpolar volatile species induces a complete change of the ice surface, as the refractory polar molecules (H2O) are left behind. Conclusions. The effectiveness of thermal desorption from heated icy grains (e.g., the yield of cosmic-ray-induced desorption) is primarily controlled by the thermal energy content of the grain and the number and availability of volatile molecules.

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Investigation of Chemical Differentiation among the NGC2264 Cluster-Forming Clumps

Kotomi Taniguchi, Adele Plunkett, Eric Herbst, Kazuhito Dobashi, Tomomi Shimoikura, Fumitaka Nakamura, Masao Saito

We have carried out mapping observations of molecular emission lines of HC3N and CH3OH toward two massive cluster-forming clumps, NGC2264-C and NGC2264-D, using the Nobeyama 45-m radio telescope. We derive an I(HC3N)/I(CH3OH) integrated intensity ratio map, showing a higher value at clumps including 2MASS point sources at the northern part of NGC2264-D. Possible interpretations of the I(HC3N)/I(CH3OH) ratio are discussed. We have also observed molecular emission lines from CCS and N2H+ toward five positions in each clump. We investigate the N(N2H+)/N(CCS) and N(N2H+)/N(HC3N) column density ratios among the ten positions in order to test whether they can be used as chemical evolutionary indicators in these clumps. The N(N2H+)/N(CCS) ratio shows a very high value toward a bright embedded IR source (IRS1), whereas the N(N2H+)/N(HC3N) ratio at IRS1 is comparable with those at the other positions. These results suggest that UV radiation affects the chemistry around IRS1. We find that there are positive correlations between these column density ratios and the excitation temperatures of N2H+, which implies the chemical evolution of clumps. These chemical evolutionary indicators likely reflect the combination of evolution along the filamentary structure and evolution of each clump.

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ALMA and ROSINA detections of phosphorus-bearing molecules: the interstellar thread between star-forming regions and comets

V. M. Rivilla, M. N. Drozdovskaya, K. Altwegg, P. Caselli, M. T. Beltrán, F. Fontani, F.F.S. van der Tak, R. Cesaroni, A. Vasyunin, M. Rubin, F. Lique, S. Marinakis, L. Testi, the ROSINA team

To understand how Phosphorus-bearing molecules are formed in star-forming regions, we have analysed ALMA observations of PN and PO towards the massive star-forming region AFGL 5142, combined with a new analysis of the data of the comet 67P/Churyumov-Gerasimenko taken with the ROSINA instrument onboard Rosetta. The ALMA maps show that the emission of PN and PO arises from several spots associated with low-velocity gas with narrow linewidths in the cavity walls of a bipolar outflow. PO is

more abundant than PN in most of the spots, with the PO/PN ratio increasing as a function of the distance to the protostar. Our data favor a formation scenario in which shocks sputter phosphorus from the surface of dust grains, and gas-phase photochemistry induced by UV photons from the protostar allows efficient formation of the two species in the cavity walls. Our analysis of the ROSINA data has revealed that PO is the main carrier of P in the comet, with PO/PN>10. Since comets may have delivered a significant amount of prebiotic material to the early Earth, this finding suggests that PO could contribute significantly to the phosphorus reservoir during the dawn of our planet. There is evidence that PO was already in the cometary ices prior to the birth of the Sun, so the chemical budget of the comet might be inherited from the natal environment of the Solar System, which is thought to be a stellar cluster including also massive stars.

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Full-text URL: https://arxiv.org/abs/1911.11647

Announcements

COSPAR 2020, F3.5: "Pre-biotic and complex molecules in the universe: Observational, laboratory and computational perspectives on the evolution of molecular complexity."

Sydney, Australia 15-22 August, 2020 https://www.cospar-assembly.org/ https://www.cospar2020.org/ ABSTRACT SUBMISSION DEADLINE: *** FEBRUARY 14, 2020 *** The ALMA telescope has now reached maturity, with major discoveries of gas-phase complex and/or organic molecules in interstellar clouds and in star- and planet-forming regions. The JWST mission will also soon bring a wave of complementary solid-phase data. Meanwhile, laboratory experiments and theory/computational studies are exploring a range of mechanisms that could contribute to the production of molecules in the universe, and the spectroscopic data that can be used to find them. COSPAR Scientific Event F3.5 will bring together a broad range of researchers with an interest in the origins, chemistry, detection and interpretation of complex and/or organic molecules in various astrophysical environments. Topics include: Gas-phase and solid-phase galactic molecular observations; Laboratory ice chemistry; Gas-phase laboratory spectroscopy and chemistry; Chemical theory/computation; Astrochemical modeling; and Extragalactic and circumstellar environments. COSPAR may be able to provide some financial support for younger speakers (under 35 on Jan. 1, 2020) as well as those from developing countries (see assembly web page). Abstracts for speaking and poster presentations should be submitted at the COSPAR assembly webpage above, for Session F3.5. The submission deadline in February 14, 2020. Confirmed Invited Speakers include: Nadia Balucani (U. Perugia, Italy) Jordy Bouwman (Leiden U., Netherlands) Qiang Chang (SDUT, China) Ilsa Cooke (U. Rennes, France) Timea Csengeri (U. Bordeaux, France) Kenji Furuya (U. Tsukuba, Japan) Miwa Goto (Universitaets-Sternwarte Muenchen, Germany) Jiao He (Leiden U., Netherlands) Sergio Ioppolo (Queen Mary U./Open U., UK) Ralf Kaiser (U. Hawaii, USA) Jes Jørgensen (Niels Bohr Institute, U. Copenhagen, Denmark) Tomasz Kaminski (Torun, Poland) Niels Ligterink (U. Bern, Switzerland) Sergio Martín (ESO) Brett McGuire (NRAO, USA) Yasuhiro Oba (Hokkaido U., Japan) Klaus Pontoppidan (STScI, USA) Maxime Ruaud (NASA Ames, USA) Marta Sewiło (NASA Goddard/U. Maryland, USA) Chris Shingledecker (Max Planck inst. for Extraterrestrial physics, Germany) Dahbia Talbi (U. Montpellier, France) Satoshi Yamamoto (U. Tokyo, Japan) Main Scientific Organizer: Rob Garrod (U. Virginia) Deputy Scientific Organizer: Gianfranco Vidali (Syracuse U., USA) SOC: Arnaud Belloche (Max Planck Inst. for Radioastronomy, Germany), Adwin Boogert (IFA/U.

Hawaii, USA) Nanase Harada (ASIAA, Taiwan), Eric Herbst (U. Virginia, USA), Mike McCarthy (Harvard Smithsonian Center for Astrophysics, USA), Tom Millar (Queen's U., Belfast, UK), Dmitry Semenov (Max Planck Inst. for Astronomy, Germany), Ian Sims (U. Rennes, France)

2 PHD positions in LERMA-Cergy

Two PhD grants in astrochemitry (paid according to French contract standards >1758 euros gross monthly) are available in the LERMA-Cergy group. One of them will be co-directed by Prof. Paola Caselli of the MEP in Garching (D). More information: https://www.u-cergy.fr/fr/laboratoires/lerma-cergy.html

PhD position at QMUL

Applications are invited for a full PhD Studentship starting in 2020 to undertake research in the interdisciplinary area of Laboratory Astrochemistry. All interested candidates with background in Engineering, Physics, Chemistry and Astronomy are encouraged to apply. The studentship will include applied research within the Antennas & Electromagnetic Research Group at Queen Mary University of London and field work at leading European research facilities such as the free-electron laser FELIX Laboratory in the Netherlands (www.ru.nl/felix), the synchrotron ISA-ASTRID2 at the Centre for Storage Ring facility in Denmark (www.isa.au.dk) and the ion accelerator ATOMKI at the Institute of Nuclear Research in Hungary (www.atomki.hu), where ultra-high vacuum end-stations dedicated to the study of interstellar and Solar System ice analogues are developed and led by Dr. Ioppolo and collaborators.

This PhD will investigate the physics and chemistry at play in space related ice surfaces by applying innovative laboratory techniques such as selective IR/THz radiation spectroscopy at FELIX to study the nature of IR/THz modes in solids as well as dynamics and energy relaxation in ices; VUV-UV-Vis spectroscopy in support of space missions, e.g. JUICE - https://sci.esa.int/web/juice, at ASTRID2; 1 – 5 keV electron exposure of ices in laboratories and 200 keV – 1 MeV ion bombardment of ices at ATOMKI to induce molecular synthesis in astrochemical ices. The project will ultimately help answering questions such as: is there a limit to molecular complexity in the Universe? What physics and chemistry drive molecule formation in space? Is there a link between simple species formed in space and life on Earth? Field work at large facilities will be supported by the EPSRC FLUENCE grant (https://www.liverpool.ac.uk/~siggel/FLUENCE/FLUENCE.html), CALIPSOplus (http://www.calipsoplus.eu), Laserlab Europe (https://www.laserlab-europe.eu), and Europlanet Research Infrastructure (http://www.europlanet-2020-ri.eu).

The student will be based in the School of Electronic Engineering and Computer Science (www.eecs.qmul.ac.uk) at Queen Mary University of London, and will be a member of the Antennas & Electromagnetic Research Group (https://antennas.eecs.qmul.ac.uk). Informal enquiries can be made by email to Dr Sergio Ioppolo (s.ioppolo@qmul.ac.uk).

This studentship is available to UK and EU students. It is fully funded by QMUL for three and a half years, it will cover student fees and a tax-free stipend starting at £17,009 per annum.

To apply, please follow the online process https://www.qmul.ac.uk/postgraduate/howtoapply/ by selecting 'Electronic Engineering' in the 'A-Z list of research opportunities' and following the instructions on the right-hand side of the web page.

Please note we request a 'Statement of Research Interests'. Your statement should answer three questions: (i) Why are you interested in the topic? (ii) What relevant experience do you have? and (iii) a research proposal. Your statement should be brief: no more than 750 words or one side of A4 paper. In addition we would also like you to send a sample of your written work. This might be a chapter of your final year

dissertation, or a published conference or journal paper. More details can be found at: http://www.eecs.qmul.ac.uk/phd/apply.php
The closing date for the applications is Friday 21st February 2020. Interviews are expected to take place the week commencing 2nd March 2020.