AstroChemical Newsletter #13

November 2016

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

Detection of recurrent fluorescence photons

Yuta Ebara, Takeshi Furukawa, Jun Matsumoto, Hajime Tanuma, Toshiyuki Azuma, Haruo Shiromaru, and Klavs Hansen

We have detected visible photons emitted from the thermally populated electronic excited state, namely recurrent fluorescence (RF), of C6- stored in an electrostatic ion storage ring. Clear evidence is provided to distinguish RF from normal fluorescence, based on the temporal profile of detected photons synchronized with the revolution of C6- in the ring, for which the timescale is far longer than the lifetime of the intact photo-excited state. The relaxation (cooling) process via RF is likely to be commonplace for isolated molecular systems and crucial to the stabilization of molecules in interstellar environments.

Physical Review Letters (2016) 117, 133004
DOI: 10.1103/PhysRevLett.117.133004
Full-text URL: http://gup.ub.gu.se/records/fulltext/242263/242263.pdf

A correlation between chemistry, polarization and dust properties in the Pipe Nebula starless core FeSt 1-457

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Pre-stellar cores within molecular clouds provide the very initial conditions in which stars are formed. We use the IRAM 30m telescope and the PdBI to study the chemical and physical properties of the starless core FeSt 1-457 (Core 109), in the Pipe nebula. We fit the hyperfine structure of the N2H+(1-0) IRAM 30m data. This allow us to measure with high precision the velocity field, line widths and opacity and derive the excitation temperature and column density in the core. We use a modified Bonnor-Ebert sphere model adding a temperature gradient towards the center to fit the 1.2 mm continuum emission and visual extinction maps. Using this model, we estimate the abundances of the N2H+ and the rest of molecular lines detected in the 30 GHz wide line survey performed at 3 mm with IRAM 30m using ARTIST software. The core presents a rich chemistry with emission from early (C3H2, HCN, CS) and late-time molecules (e.g., N2H+), with a clear chemical spatial differentiation for nitrogen, oxygen and sulphurated molecules. For most of the molecules detected (HCN, HCO+, CH3OH, CS, SO, 13CO and C18O), abundances are best fitted with three values, presenting a clear decrease of abundance of at least 1 or 2 orders of magnitude towards the center of the core. The Bonnor-Ebert analysis indicates the core is gravitationally unstable and the magnetic field is not strong enough to avoid the collapse. Depletion of molecules onto the dust grains occurs at the interior of the core, where dust grain growth and dust depolarization also occurs. This suggests that these properties may be related. On the other hand, some molecules exhibit asymmetries in their integrated emission maps, which appear to be correlated with a previously reported submillimeter polarization asymmetry. These asymmetries could be due to a stronger interstellar radiation field in the western side of the core.

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Full-text URL: https://arxiv.org/pdf/1609.09406v1.pdf

Photo-fragmentation behavior of methyl- and methoxy-substituted derivatives of hexa-peri-hexabenzocoronene (HBC) cations

Junfeng Zhen, Pablo Castellanos, Harold Linnartz, Alexander G.G.M. Tielens

A systematic study, using ion trap time-of-flight mass spectrometry, is presented for the photo- fragmentation of methyl- and methoxy-substituted derivatives of HBC cations, (OCH3)6HBC+ and (CH3)4(OCH3)2HBC+. Both substituted HBC cations fragment through sequential loss of CH3CO units upon laser (595nm) irradiation, resulting in a PAH-like derivative C36H12+ and a methyl-substituted PAH derivative C44H24+, respectively. Upon ongoing irradiation, these species further fragment. For lower laser energy C44H24+ dehydrogenates and photo-fragments through CH3 and CHCH2 unit losses; for higher laser energy isomerization takes place, yielding a regular PAH-like configuration, and both stepwise dehydrogenation and C2/C2H2 loss pathways are found. C36H12+ follows largely this latter fragmentation scheme upon irradiation. It is concluded that the photo-dissociation mechanism of the substituted PAH cations studied here is site selective in the substituted subunit. This work also shows experimental evidence that photo-fragmentation of substituted PAHs may contribute to the formation in space of smaller species that are normally considered to form by merging atoms and molecules.

Molecular Astrophysics, Volume 5, November 2016, Pages 1–8
DOI: 10.1016/j.molap.2016.08.001
Full-text URL: http://www.sciencedirect.com/science/article/pii/S240567581630001X

Ion-neutral reaction of C2H2N+ with CH4: An experimental and theoretical study

P. Fathi, W.D. Geppert, F. Lindén, A. Cernuto, D. Ascenzi

The current study was undertaken to probe the ionic products of the ion-neutral reaction of C2H2N+ with CH4 using guided ion beam mass spectrometry (GIB-MS) in which the , CH3+, C2H3+, HCNH+, C2H5+, C2H3N+, and C3H4N+ ions are identified as products. Theoretical calculations were performed to suggest reaction pathways leading to the detected products. These processes might be of relevance for the generation of long chain carbon-nitrogen bearing compounds in Titan’s atmosphere, the interstellar medium or circumstellar envelopes.

Molecular Astrophysics, Volume 5, November 2016, Pages 9–22
DOI: 10.1016/j.molap.2016.07.001
Full-text URL: http://www.sciencedirect.com/science/article/pii/S2405675815300099

Formation of the prebiotic molecule NH2CHO on astronomical amorphous solid water surfaces: accurate tunneling rate calculations

Lei Song, Johannes Kästner

Investigating how formamide forms in the interstellar medium is a hot topic in astrochemistry, which can contribute to our understanding of the origin of life on Earth. We have constructed a QM/MM model to simulate the hydrogenation of isocyanic acid on amorphous solid water surfaces to form formamide. The binding energy of HNCO on the ASW surface varies significantly between different binding sites, we found values between ∼0 and 100 kJ mol−1. The barrier for the hydrogenation reaction is almost independent of the binding energy, though. We calculated tunneling rate constants of H + HNCO → NH2CO at temperatures down to 103 K combining QM/MM with instanton theory. Tunneling dominates the reaction at such low temperatures. The tunneling reaction is hardly accelerated by the amorphous solid water surface compared to the gas phase for this system, even though the activation energy of the surface reaction is lower than the one of the gas-phase reaction. Both the height and width of the barrier affect the tunneling rate in practice. Strong kinetic isotope effects were observed by comparing to rate constants of D + HNCO → NHDCO. At 103 K we found a KIE of 231 on the surface and 146 in the gas phase. Furthermore, we investigated the gas-phase reaction NH2 + H2CO → NH2CHO + H and found it unlikely to occur at cryogenic temperatures. The data of our tunneling rate constants are expected to significantly influence astrochemical models.

2016 Phys. Chem. Chem. Phys. (accepted)
DOI: 10.1039/c6cp05727f
Full-text URL: http://pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp05727f#!divAbstract

Quantum Chemical Analysis of the CO–HNN+ Proton-Bound Complex

Ryan C. Fortenberry, Timothy J. Lee, and Joseph S. Francisco

Proton-bound complexes produce exceptionally bright vibrational modes for stretches involving the hydrogen atom. Binding a proton between various arrangements of N2 and carbon monoxide molecules is known to produce such behavior, and there are four distinct structures involving N2, CO, and a proton. The problem arises in that all four have the same mass and are, consequently, extremely difficult, if not impossible, to resolve experimentally. Fortunately, quantum chemical predictions have produced accurate descriptions of this bright mode and other spectral features for OCHCO+, NNHNN+, and NN–HCO+. The last of this family to be analyzed is CO–HNN+, which is done here. Utilizing high-level coupled cluster computations and quartic force fields, the bright vibrational mode of CO–HNN+ is shown to shift to the red, and the C–O bond is destabilized in this arrangement as opposed to the lower-energy NN–HCO+ isomer studied previously. Furthermore, the 1.87 D center-of-mass dipole moment, spectroscopic constants, and other anharmonic fundamental frequencies and intensities are produced for CO–HNN+ to assist in definitive experimental and even astrochemical classification of this and the other three related mass-57 proton-bound complexes.

J. Phys. Chem. A, 2016, 120 (39), pp 7745–7752
DOI: 10.1021/acs.jpca.6b07515
Full-text URL: http://pubs.acs.org/doi/abs/10.1021/acs.jpca.6b07515

Nitrile versus isonitrile adsorption at interstellar grains surfaces: I - Hydroxylated surfaces

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Almost 20% of the ~ 200 different species detected in the interstellar and circumstellar media present a carbon atom linked to nitrogen by a triple bond. Among these 37 molecules, 30 are nitrile R-CN compounds, the remaining seven belonging to the isonitrile R-NC family. How these species behave in presence of the grain surfaces is still an open question. In this contribution we investigate whether the difference between nitrile and isonitrile functional groups may induce differences in the adsorption energies of the related isomers at the surfaces of interstellar grains of different nature and morphologies. The question was addressed by means of a concerted experimental and theoretical study of the adsorption energies of CH3CN and CH3NC on the surface water ice and silica. The experimental determination of the molecule - surface interaction energies was carried out using temperature programmed desorption (TPD) under an ultra-high vacuum (UHV) between 70 and 160 K. Theoretically, the question was addressed using first principle periodic density functional theory (DFT) to represent the organized solid support. The most stable isomer (CH3CN) interacts more efficiently with the solid support than the higher energy isomer (CH3NC) for water ice and silica. Comparing with the HCN and HNC pair of isomers, the simulations show an opposite behaviour, in which isonitrile HNC are more strongly adsorbed than nitrile HCN provided that hydrogen bonds are compatible with the nature of the model surface. The present study confirms that the strength of the molecule surface interaction between isomers is not related to their intrinsic stability but instead to their respective ability to generate different types of hydrogen bonds.

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DOI: 10.1051/0004-6361/201629394
Full-text URL: https://arxiv.org/abs/1610.05010

A search for O2 in CO-depleted molecular cloud cores with Herschel

E. S. Wirström, S. B. Charnley, M. A. Cordiner, and C. Ceccarelli

The general lack of molecular oxygen in molecular clouds is an outstanding problem in astrochemistry. Extensive searches with the Submillimeter Astronomical Satellite, Odin, and Herschel have only produced two detections; upper limits to the O2 abundance in the remaining sources observed are about 1000 times lower than predicted by chemical models. Previous atomic oxygen observations and inferences from observations of other molecules indicated that high abundances of O atoms might be present in dense cores exhibiting large amounts of CO depletion. Theoretical arguments concerning the oxygen gas–grain interaction in cold dense cores suggested that, if O atoms could survive in the gas after most of the rest of the heavy molecular material has frozen out onto dust, then O2 could be formed efficiently in the gas. Using Herschel HIFI, we searched a small sample of four depletion cores — L1544, L694-2, L429, and Oph D — for emission in the low excitation O2 N_J = 33–12 line at 487.249 GHz. Molecular oxygen was not detected and we derive upper limits to its abundance in the range of N(O2)/N(H2)=(0.6–1.6)*1e-7. We discuss the absence of O2 in the light of recent laboratory and observational studies.

2016, ApJ 830, 102
DOI: 10.3847/0004-637X/830/2/102
Full-text URL: http://dx.doi.org/10.3847/0004-637X/830/2/102

Exploring a Chemical Route for the Formation of Stable Anions of Polyynes [CnH− (n=2,4)] in Molecular Clouds

F. A. Gianturco, M. Satta, M. Mendolicchio, F. Palazzetti, A. Piserchia, V. Barone, and R. Wester

Using quantum chemical methods, we investigate the possible outcomes of H- reactions with acetylene and diacetylene molecules. We find both reactions to be exothermic reactions without barriers, yielding stable anions of the corresponding polyynes: C2H- and C4H-. We show in this work that the computed chemical rates in the case of the formation of the C4H- anion would be larger than those existing for the direct radiative electron attachment (REA) process, the main mechanism generally suggested for their formation. In the case of the C2H- anion, however, the present chemical rates of formation at low T are even lower than those known for its REA process, both mechanisms being inefficient for its formation under astrochemical conditions. The present results are discussed in view of their consequences on the issue of the possible presence of such anions in the ISM environments. They clearly indicate the present chemical route to C2H- formation to be inefficient at the expected temperatures of a dark molecular cloud, whereas this is found not to be the case for the C4H-, in line with the available experimental findings.

The Astrophysical Journal, Volume 830, Number 1
Full-text URL: http://iopscience.iop.org/article/10.3847/0004-637X/830/1/2/meta

Discovery of a Hot Corino in the Bok Globule B335

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We report the first evidence of a hot corino in a Bok globule. This is based on the ALMA observations in the 1.2 mm band toward the low-mass Class 0 protostar IRAS 19347+0727 in B335. Saturated complex organic molecules (COMs), CH3CHO, HCOOCH3, and NH2CHO, are detected in a compact region within a few 10 au around the protostar. Additionally, CH3OCH3, C2H5OH, C2H5CN, and CH3COCH3 are tentatively detected. Carbon-chain related molecules, CCH and c-C3H2, are also found in this source, whose distributions are extended over a few 100 au scale. On the other hand, sulfur-bearing molecules CS, SO, and SO2, have both compact and extended components. Fractional abundances of the COMs relative to H2 are found to be comparable to those in known hot-corino sources. Though the COMs lines are as broad as 5-8 km/s, they do not show obvious rotation motion in the present observation. Thus, the COMs mainly exist in a structure whose distribution is much smaller than the synthesized beam (0."58 x 0."52).

ApJL, 2016, 830, L37
DOI: 10.3847/2041-8205/830/2/L37

Full-text URL: https://arxiv.org/abs/1610.03942

Tracing water vapor and ice during dust growth

S. Krijt, F. J. Ciesla, E. A. Bergin

The processes that govern the evolution of dust and water (in the form of vapor or ice) in protoplanetary disks are intimately connected. We have developed a model that simulates dust coagulation, dust dynamics (settling, turbulent mixing), vapor diffusion, and condensation/sublimation of volatiles onto grains in a vertical column of a protoplanetary disk. We employ the model to study how dust growth and dynamics influence the vertical distribution of water vapor and water ice in the region just outside the radial snowline. Our main finding is that coagulation (boosted by the enhanced stickiness of icy grains) and the ensuing vertical settling of solids results in water vapor being depleted, but not totally removed, from the region above the snowline on a timescale commensurate with the vertical turbulent mixing timescale. Depending on the strength of the turbulence and the temperature, the depletion can reach factors of up to ~50 in the disk atmosphere. In our isothermal column, this vapor depletion results in the vertical snowline moving closer to the midplane (by up to 2 gas scale heights) and the gas-phase C/O ratio above the vertical snowline increasing. Our findings illustrate the importance of dynamical effects and the need for understanding coevolutionary dynamics of gas and solids in planet-forming environments.

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Water delivery from cores to disks: deuteration as a probe of the prestellar inheritance of H2O

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We investigate the delivery of regular and deuterated forms of water from prestellar cores to circumstellar disks. We adopt a semi-analytical axisymmetric two-dimensional collapsing core model with post-processing gas-ice astrochemical simulations, in which a layered ice structure is considered. The physical and chemical evolutions are followed until the end of the main accretion phase. When mass averaged over the whole disk, a forming disk has a similar H2O abundance and HDO/H2O abundance ratio as their precollapse values (within a factor of 2), regardless of time in our models. Consistent with previous studies, our models suggest that interstellar water ice is delivered to forming disks without significant alteration. On the other hand, the local vertically averaged H2O ice abundance and HDO/H2O ice ratio can differ more, by up to a factor of several, depending on time and distance from a central star. Key parameters for the local variations are the fluence of stellar UV photons en route into the disk and the ice layered structure, the latter of which is mostly established in the prestellar stages. We also find that even if interstellar water ice is destroyed by stellar UV and (partly) reformed prior to disk entry, the HDO/H2O ratio in reformed water ice is similar to the original value. This finding indicates that some caution is needed in discussions on the prestellar inheritance of H2O based on comparisons between the observationally derived HDO/H2O ratio in clouds/cores and that in disks/comets. Alternatively, we propose that the ratio of D2O/HDO to HDO/H2O better probes the prestellar inheritance of H2O. It is also found that icy organics are more enriched in deuterium than water ice in forming disks. The differential deuterium fractionation in water and organics is inherited from the prestellar stages.

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Announcements

RAS/RSC Astrophysical Chemistry Group Annual Meeting and AstroSurf 2017 as part of the Faraday Joint Interest Group Conference

It is our pleasure to announce that this year’s RAS/RSC Astrophysical Chemistry Group (ApChem) meeting and the AstroSurf 2017 meeting will take place 11-13 April 2017 at the University of Warwick, UK. AstroSurf 2017 is the fifth in a series of meetings established by the UK AstroSurf Network then integrated in the European LASSIE Network and now part of the scientific activities of the EuroPAH Network. The meeting will be part of the Faraday Joint Interest Group Conference, which brings together a number of the RSC’s Faraday Division special interest groups in one location with plenary and parallel sessions. ApChem and EuroPAH will be running one parallel session and the programme is open for contributions from postgraduate students and postdoctoral researchers either as contributed talks or as posters. The list of confirmed invited speakers for these sessions are: Xander Tielens (Leiden University and Observatory); Sandra Brünken (University of Cologne); Ian Sims (University of Rennes); Anthony Meijer (University of Sheffield). Note that registration is already open and further details of the conference can be found on the website: http://www2.warwick.ac.uk/fac/sci/chemistry/news/events/faraday2017/. The deadline for registration is March 14th for those seeking to give oral presentations and March 28th for others. Abstracts for consideration by the organisers must be submitted on the template found here (http://www2.warwick.ac.uk/fac/sci/chemistry/news/events/faraday2017/preregistration/abstract_template.doc). The deadlines for abstract submission are; Abstracts for oral presentation must be received by 4:00 pm on March 14th, 2017; Abstracts for poster presentations must be received by 4:00 pm on March 28th, 2017. Submission of abstracts can be done through the conference website when you register. Late submissions will not be considered so please stick to the deadline. Put the date in your diary and we look forward to seeing you there! Best wishes, Wendy Brown Martin McCoustra (University of Sussex) (Heriot- Watt University)

Laboratory Astrophysics Dissertation Prize

The Laboratory Astrophysics Division (LAD) of the American Astronomical Society (AAS) invites nominations for the 2017 Laboratory astrophysics Dissertation Prize. The field of laboratory astrophysics encompasses all fundamental theoretical and experimental research into the underlying processes that drive the cosmos. The Dissertation Prize is presented, normally on an annual basis, to recognize an outstanding doctoral dissertation (or the equivalent) in laboratory astrophysics. The prize will be awarded to an individual who has completed their Ph.D. or equivalent degree in any of the three calendar years immediately preceding the award year. The prize will include a cash award, a citation, and an invited lecture by the recipient at a meeting of the Division. The recipient for 2017 will be announced in early 2017 and the presentation made at the June 2017 LAD meeting. Any nominee not selected will be automatically considered in the next two consecutive years, or as long as the nominee is eligible, whichever is less. The nomination package for the Dissertation Prize must include: a. A three-page summary of the thesis (not to exceed 5 pages total including figures and bibliography). b. A nomination letter. c. Two additional letters of recommendation. d. A statement from the nominee’s university stating that the Ph.D. or equivalent degree has been awarded. e. A curriculum vitae. f. A publication list. Nominators, letter writers, and candidates need not be AAS or LAD members. Self-nominations are allowed. The deadline for receipt of the nomination package and supporting letters is Saturday 31 December 2016. Attracting and serving a diverse and inclusive membership worldwide is a primary goal for LAD. In calling for nominations, we wish to remind you how important it is to give full consideration to qualified women, members of underrepresented minority groups, and scientists from outside the United States. All nomination material should be sent by the deadline directly to the LAD Secretary (ladsec@aas.org). Additional information can be found at https://lad.aas.org/prizes Daniel Wolf Savin LAD Secretary

Astrochemistry Week (January 16-20, 2017, Faro, Portugal)

SOC: L. Wiesenfeld, J. Brandao, I. Kamp, H. Fraser, J. Joergensen, H. Cuppen, P. Slavicek, C. Vastel Announcement: The main objective of the COST Action "Our Astro-Chemical History" is to bring together chemical and astrophysical laboratories to focus on the molecular evolution towards complexity, from early stages of star formation to the present day Solar System. The Action is supposed to bring deeper understanding of the astrophysical data now being provided by the large European instruments and to deliver innovative experimental and theoretical schemes for physical chemistry at large. This conference aims to focus on the first results of this Action, and in particular on reports from the three Working Group meetings, in Pisa (joint meeting of WG1 and 4, gas phase and isotope chemistry), and in Garching (Theory in gas phase reaction). New collaborations fostered by the Action, driven by the Short Term Scientific Missions will be at the center of the stage. We wish that younger colleagues, postdocs and students come and present their work. In line with the general policies supported by COST in general and this Action in particular, emphasis will be put on results and actions put forward by inclusiveness countries (http://www.cost.eu/about_cost/strategy/excellence-inclusiveness). The meeting will host keynote and invited speakers, about recent experimental, theoretical and observational advances, as well as future observational capabilities. Some highlights on new results will be presented. Other topics will be presented with short talks and extensive poster sessions. See https://astrochem2017.sciencesconf.org/ for more details. The General Meeting is open to the whole community of physical chemistry and astrochemistry, while the two WG2 (Chemistry inside ices) and WG3 (Non thermal desorption) sessions will be specialized working meetings with a limited number of invited participants. Deadline for abstract submission is Friday November 11th, 2016. Deadline for registration is Friday December 9th, 2016.