AstroChemical Newsletter #64

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Abstracts

Lyman-α irradiation of superhydrogenated coronene films: implications for H2 formation

V. Mennella, T. Suhasaria, L. Hornekaer, J. D. Thrower, and G. Mulas

We present the results of an experimental study of the interaction of Ly-α photons with superhydrogenated coronene films. The effects of UV irradiation have been analyzed with infrared spectroscopy. The spectral changes provide evidence for UV photodestruction of the C-D bonds of the superhydrogenated coronene with a cross-section of 8±2x1e-20 cm2. The comparison of our experimental result with the prediction from theoretical modeling suggests an extension of the region inside PDRs where superhydrogenated coronene can survive and contribute to H2 formation. H2 formation through abstraction in superhydrogenated coronene dominates over direct H2 loss induced by UV photodestruction.

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Contrasting Mechanisms for Photodissociation of Methyl Halides Adsorbed on Thin Films of C6H6 and C6F6

E. T. Jensen

The mechanisms for photodissociation of methyl halides (CH3X, X= Cl, Br, I) have been studied for these molecules when adsorbed on thin films of C6H6 or C6F6 on copper single crystals, using time-of-flight spectroscopy with 248nm and 193nm light. For CH3Cl and CH3Br monolayers adsorbed on C6H6, two photodissociation pathways can be identified– neutral photodissociation similar to the gas-phase, and a dissociative electron attachment (DEA) pathway due to photoelectrons from the metal. The same methyl halides adsorbed on a C6F6 thin film display only neutral photodissociation, with the DEA pathway entirely absent due to intermolecular quenching via a LUMO- derived electronic band in the C6F6 thin film. For CH3I adsorbed on a C6F6 thin film, illumination with 248nm light results in CH3 photofragments departing due to neutral photodissociation via the A-band absorption. When CH3I monolayers on C6H6 thin films are illuminated at the same wavelength, additional new photodissociation pathways are observed that are due to absorption in the molecular film with energy transfer leading to dissociation of the CH3I molecules adsorbed on top. The proposed mechanism for this photodissociation is via a charge-transfer complex for the C6H6 layer and adsorbed CH3I.

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The Perseus ALMA Chemistry Survey (PEACHES). I. The Complex Organic Molecules in Perseus Embedded Protostars

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To date, about two dozen low-mass embedded protostars exhibit rich spectra with complex organic molecule (COM) lines. These protostars seem to possess different enrichment in COMs. However, the statistics of COM abundance in low-mass protostars are limited by the scarcity of observations. This study introduces the Perseus ALMA Chemistry Survey (PEACHES), which aims at unbiasedly characterizing the chemistry of COMs toward the embedded (Class 0/I) protostars in the Perseus molecular cloud. Among the 50 embedded protostars surveyed, 58% of them have emission from COMs. A 56%, 32%, and 40% of protostars have CH3OH, CH3OCHO, and N-bearing COMs, respectively. The detectability of COMs depends on neither the averaged continuum brightness temperature, a proxy of the H2 column density, nor the bolometric luminosity and the bolometric temperature. For the protostars with detected COMs, CH3OH has a tight correlation with CH3CN, spanning more than two orders of magnitude in column densities normalized by the continuum brightness temperature, suggesting a chemical relation between CH3OH and CH3CN and large chemical diversity among the PEACHES samples at the same time. A similar trend with more scatter is also found between all identified COMs, hinting at common chemistry for the sources with COMs. The correlation between COMs is insensitive to the protostellar properties, such as the bolometric luminosity and the bolometric temperature. The abundance of larger COMs (CH3OCHO and CH3OCH3) relative to that of smaller COMs (CH3OH and CH3CN) increases with the inferred gas column density, hinting at an efficient production of complex species in denser envelopes.

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Testing Short-term Variability and Sampling of Primary Volatiles in Comet 46P/Wirtanen

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The exceptionally favorable close approach of Jupiter-family comet 46P/Wirtanen in 2018 December enabled characterization of its primary volatile composition with exceptionally high spatial resolution and sensitivities using the iSHELL spectrograph at the NASA Infrared Telescope Facility on Maunakea, HI. We sampled emissions from H2O, HCN, C2H2, NH3, C2H6, and CH3OH on UT 2018 December 21 using two instrumental settings that spanned the 2.9–3.6 µm spectral region. We also obtained a sensitive 3σ upper limit for H2CO and for the rarely studied molecule HC3N. We report rotational temperatures, production rates, and mixing ratios (relative to H2O as well as to C2H6). We place our results in context by comparing them with other comets observed at near-IR wavelengths. We also compare our results with those obtained using the NIRSPEC-2 spectrograph on Keck II on UT December 17 and 18 and with results obtained from iSHELL on other dates during the same apparition. Within 1–2σ uncertainty, production rates obtained for all molecules in this work were consistent with those obtained using NIRSPEC-2 except H2O, indicating low-level variability on a timescale of days. Mixing ratios with respect to H2O in 46P/Wirtanen were consistent with corresponding values from NIRSPEC-2 within the uncertainty with the exception of CH3OH, which yielded a higher ratio on December 21. Our measurements afforded a high temporal resolution that spanned ~2/3 of the rotational period of 46P/Wirtanen, enabling us to test short-term variability in the production rates of H2O and HCN due to rotational effects. Both H2O and HCN production rates showed similar temporal variability, resulting in nearly constant HCN/H2O.

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Space and laboratory discovery of HC3S+

J. Cernicharo, C. Cabezas, Y. Endo, N. Marcelino, M. Agundez, B. Tercero, J. D. Gallego, P. de Vicente

We report the detection in TMC-1 of the protonated form of C3S. The discovery of the cation HC3S+ was carried through the observation of four harmonically related lines in the Q band using the Yebes 40m radiotelescope, and is supported by accurate ab initio calculations and laboratory measurements of its rotational spectrum. We derive a column density N(HC3S+) = (2.0 +/- 0.5)e11 cm-2, which translates to an abundance ratio C3S/HC3S+ of 65 +/- 20. This ratio is comparable to the CS/HCS+ ratio (35 +/- 8) and is a factor of about ten larger than the C3O/HC3O+ ratio previously found in the same source. However, the abundance ratio HC3O+/HC3S+ is 1.0 +/- 0.5, while C3O/C3S is just 0.11. We also searched for protonated C2S in TMC-1, based on ab initio calculations of its spectroscopic parameters, and derive a 3sigma upper limit of N(HC2S+) < 9e11 cm-2 and a C2S/HC2S+ > 60. The observational results are compared with a state-of-the-art gas-phase chemical model and conclude that HC3S+ is mostly formed through several pathways: proton transfer to C3S, reaction of S+ with c-C3H2, and reaction between neutral atomic sulfur and the ion C3H3+.

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Discovery of the acetyl cation, CH3CO+, in space and in the laboratory

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Using the Yebes 40m and IRAM 30m radiotelescopes, we detected two series of harmonically related lines in space that can be fitted to a symmetric rotor. The lines have been seen towards the cold dense cores TMC-1, L483, L1527, and L1544. High level of theory ab initio calculations indicate that the best possible candidate is the acetyl cation, CH3CO+, which is the most stable product resulting from the protonation of ketene. We have produced this species in the laboratory and observed its rotational transitions Ju = 10 up to Ju = 27. Hence, we report the discovery of CH3CO+ in space based on our observations, theoretical calculations, and laboratory experiments. The derived rotational and distortion constants allow us to predict the spectrum of CH3CO+ with high accuracy up to 500 GHz. We derive an abundance ratio N(H2CCO)/N(CH3CO+) = 44. The high abundance of the protonated form of H2CCO is due to the high proton affinity of the neutral species. The other isomer, H2CCOH+, is found to be 178.9 kJ/mol above CH3CO+. The observed intensity ratio between the K=0 and K=1 lines, 2.2, strongly suggests that the A and E symmetry states have suffered interconversion processes due to collisions with H and/or H2, or during their formation through the reaction of H3+ with H2CCO.

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Space and laboratory observation of the deuterated cyanomethyl radical HDCCN

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Our observations of TMC-1 with the Yebes 40 m radio telescope in the 31.0-50.3 GHz range allowed us to detect a group of unidentified lines, showing a complex line pattern indicative of an open-shell species. The observed frequencies of these lines and the similarity of the spectral pattern with that of the 2,0,2-1,0,1 rotational transition of H2CCN indicate that the lines arise from the deuterated cyanomethyl radical, HDCCN. Using Fourier transform microwave spectroscopy experiments combined with electric discharges, we succeeded in producing the radical HDCCN in the laboratory and observed its 1,0,1-0,0,0 and 2,0,2-1,0,1 rotational transitions. From our observations and assuming a rotational temperature of 5 K, we derive an abundance ratio H2CCN/HDCCN=20 +/- 4. The high abundance of the deuterated form of H2CCN is well accounted for by a standard gas-phase model, in which deuteration is driven by deuteron transfer from the H2D+ molecular ion.

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A study of C4H3N isomers in TMC-1: line by line detection of HCCCH2CN

N. Marcelino, B. Tercero, M. Agundez, J. Cernicharo

We present Yebes 40m telescope observations of the three most stable C4H3N isomers towards the cyanopolyyne peak of TMC-1. We have detected 13 transitions from CH3C3N (A and E species), 16 lines from CH2CCHCN, and 27 lines (a-type and b-type) from HCCCH2CN. We thus provide a robust confirmation of the detection of HCCCH2CN and CH2CCHCN in space. We have constructed rotational diagrams for the three species, and obtained rotational temperatures between 4-8 K and similar column densities for the three isomers, in the range (1.5-3)e12 cm-2. Our chemical model provides abundances of the order of the observed ones, although it overestimates the abundance of CH3CCCN and underestimates that of HCCCH2CN. The similarity of the observed abundances of the three isomers suggests a common origin, most probably involving reactions of the radical CN with the unsaturated hydrocarbons methyl acetylene and allene. Studies of reaction kinetics at low temperature and further observations of these molecules in different astronomical sources are needed to draw a clear picture of the chemistry of C4H3N isomers in space.

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The connection between warm carbon chain chemistry and interstellar irradiation of star-forming cores

Juris Kalvans

Some observations of warm carbon chain chemistry (WCCC) cores indicate that they are often located near the edges of molecular clouds. This finding may suggest that WCCC is promoted in star-forming cores exposed to radiation from the interstellar medium. We aim to investigate the chemistry of carbon chains in such a core. A chemical simulation of a gas parcel in a low-mass star-forming core with a full level of irradiation by interstellar photons and cosmic rays was compared to a simulation of a core receiving only one-tenth of such irradiation. In the full irradiation model, the abundances of carbon chains were found to be higher by a factor of few to few hundred, compared to the model with low irradiation. Higher carbon-chain abundances in the prestellar stage and, presumably, in the extended circumstellar envelope, arise because of irradiation of gas and dust by interstellar photons and cosmic rays. A full standard rate of cosmic-ray induced ionization is essential for a high carbon-chain abundance peak to occur in the circumstellar envelope, which is heated by the protostar (the "true" WCCC phenomenon). The full irradiation model has lower abundances of complex organic molecules than the low-irradiation model. We conclude that WCCC can be caused by exposure of a star-forming core to interstellar radiation, or even just to cosmic rays. The Appendix describes an updated accurate approach for calculating the rate of cosmic-ray induced desorption.

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Rotational spectroscopy of isotopic cyclopropenone, c-H2C3O, and determination of its equilibrium structure

Holger S. P. Müller, Ananya Brahmi M., Jean-Claude Guillemin, Frank Lewen, Stephan Schlemmer

Cyclopropenone was first detected in the cold and less dense envelope of Sagittarius B2(N). It was found later in several cold dark clouds and it may be possible to detect its minor isotopic species in these environments. In addition, the main species may well be identified in warmer environments. We aim to extend existing line lists of isotopologs of c-H2C3O from the microwave to the millimeter region and create one for the singly deuterated isotopolog to facilitate their detections in space. Furthermore, we aim to extend the line list of the main isotopic species to the submillimeter region and to evaluate an equilibrium structure of the molecule. We employed a cyclopropenone sample in natural isotopic composition to investigate the rotational spectra of the main and 18O-containing isotopologs as well as the two isotopomers containing one 13C atom. Spectral recordings of the singly and doubly deuterated isotopic species were obtained using a cyclopropenone sample highly enriched in deuterium. We recorded rotational transitions in the 70-126 GHz and 160-245 GHz regions for all isotopologs and also in the 342-505 GHz range for the main species. Quantum-chemical calculations were carried out to evaluate initial spectroscopic parameters and the differences between ground-state and equilibrium rotational parameters in order to derive semi-empirical equilibrium structural parameters. We determined new or improved spectroscopic parameters for six isotopologs and structural parameters according to different structure models. The spectroscopic parameters are accurate enough to identify minor isotopic species at centimeter and millimeter wavelengths while those of the main species are deemed to be reliable up to 1 THz. Our structural parameters differ from earlier ones. The deviations are attributed to misassignments in the earlier spectrum of one isotopic species.

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Reaction mechanisms of C(3PJ) and C+(2PJ) with benzene in the interstellar medium from quantum mechanical molecular dynamics simulations

M. E. Izadi, K. M. Bal, A. Maghari, E. C. Neyts

We investigate the chemical reaction mechanisms of C(3PJ) + C6H6 and C+(2P) + C6H6 systems using quantum-mechanical molecular dynamics (QMMD) at the PBE0-D3(BJ) level of theory, mimicking a CMB experiment. Both the dynamics of the reactions as well as the electronic structure for the purpose of the reaction network are evaluated. The method is validated for the first reaction by comparison to the available experimental data. The chemistry of the C+(2PJ) + C6H6 system is found to be much richer, due to more exothermic reactions in this system in comparison to those in the C(3PJ) + C6H6 system. Using the QMMD simulation, a number of reaction paths have been revealed that produce three distinct classes of reaction products with different ring sizes. It is also revealed that the collision orientation has a dominant effect on the reaction products in both systems, while the collision energy mostly affects the charged system.

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Complex organic molecules in protoplanetary disks: X-ray photodesorption from methanol-containing ices. Part II - Mixed methanol-CO and methanol-H2O ices

R. Basalgète, R. Dupuy, G. Féraud, C. Romanzin, L. Philippe, X. Michaut, J. Michoud, L. Amiaud, A. Lafosse, J.-H. Fillion, M. Bertin

Astrophysical observations show complex organic molecules (COMs) in the gas phase of protoplanetary disks. X-rays emitted from the central young stellar object (YSO) that irradiate interstellar ices in the disk, followed by the ejection of molecules in the gas phase, are a possible route to explain the abundances observed in the cold regions. This process, known as X-ray photodesorption, needs to be quantified for methanol-containing ices. We aim at experimentally measuring X-ray photodesorption yields of methanol and its photo-products from binary mixed ices: 13CO:CH3OH ice and H2O:CH3OH ice. We irradiated these ices at 15 K with X-rays in the 525 - 570 eV range. The release of species in the gas phase was monitored by quadrupole mass spectrometry, and photodesorption yields were derived. For 13CO:CH3OH ice, CH3OH X-ray photodesorption yield is estimated to be 1e−2 molecule/photon at 564 eV. X-ray photodesorption of larger COMs, which can be attributed to either ethanol, dimethyl ether, and/or formic acid, is detected with a yield of 1e−3 molecule/photon. When methanol is mixed with water, X-ray photodesorption of methanol and of the previous COMs is not detected. X-ray induced chemistry, dominated by low-energy secondary electrons, is found to be the main mechanism that explains these results. We also provide desorption yields that are applicable to protoplanetary disk environments for astrochemical models. The X-ray emission from YSOs should participate in the enrichment of the protoplanetary disk gas phase with COMs such as methanol in the cold and X-ray dominated regions because of X-ray photodesorption from methanol-containing ices.

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Complex Organic Matter Synthesis on Siloxyl Radicals in the Presence of CO

Marco Fioroni, Nathan J. DeYonker

Heterogeneous phase astrochemistry plays an important role in the synthesis of complex organic matter (COM) as found on comets and rocky body surfaces like asteroids, planetoids, moons and planets. The proposed catalytic model is based on two assumptions: (a) siliceous rocks in both crystalline or amorphous states show surface-exposed defective centers such as siloxyl (Si-O•) radicals; (b) the second phase is represented by gas phase CO molecules, an abundant C1 building block found in space. By means of quantum chemistry; (DFT, PW6B95/def2-TZVPP); the surface of a siliceous rock in presence of CO is modeled by a simple POSS (polyhedral silsesquioxane) where a siloxyl (Si-O•) radical is present. Four CO molecules have been consecutively added to the Si-O• radical and to the nascent polymeric CO (pCO) chain. The first CO insertion shows no activation free energy with ΔG200K = −21.7 kcal/mol forming the SiO-CO• radical. The second and third CO insertions show ΔG‡200K ≤ 10.5 kcal/mol. Ring closure of the SiO-CO-CO• (oxalic anhydride) moiety as well as of the SiO-CO-CO-CO• system (di-cheto form of oxetane) are thermodynamically disfavored. The last CO insertion shows no free energy of activation resulting in the stable five member pCO ring, precursor to 1,4-epoxy-1,2,3-butanone. Hydrogenation

reactions of the pCO have been considered on the SiO oxygen or on the carbons and oxygens of the pCO chains. The formation of the reactive aldehyde SiO-CHO on the siliceous surface is possible. In principle, the complete hydrogenation of the (CO)1−4 series results in the formation of methanol and polyols. Furthermore, all the SiO-pCO intermediates and the lactone 1,4-epoxy-1,2,3-butanone product in its radical form can be important building blocks in further polymerization reactions and/or open ring reactions with H (aldehydes, polyols) or CN (chetonitriles), resulting in highly reactive multi-functional compounds contributing to COM synthesis.

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Complex organic molecules in protoplanetary disks: X-ray photodesorption from methanol-containing ices. Part I - Pure methanol ices

R. Basalgète, R. Dupuy, G. Féraud, C. Romanzin, L. Philippe, X. Michaut, J. Michoud, L. Amiaud, A. Lafosse, J.-H. Fillion, M. Bertin

Astrophysical observations show complex organic molecules (COMs) in the gas phase of protoplanetary disks. X-rays emitted from the central young stellar object (YSO) that irradiate interstellar ices in the disk, followed by the ejection of molecules in the gas phase, are a possible route to explain the abundances observed in the cold regions. This process, known as X-ray photodesorption, needs to be quantified for methanol-containing ices. This paper I focuses on the case of X-ray photodesorption from pure methanol ices. We aim at experimentally measuring X-ray photodesorption yields of methanol and its photo-products from pure CH3OH ices, and to shed light on the mechanisms responsible for the desorption process. We irradiated methanol ices at 15 K with X-rays in the 525 - 570 eV range. The release of species in the gas phase was monitored by quadrupole mass spectrometry, and photodesorption yields were derived. Under our experimental conditions, the CH3OH X-ray photodesorption yield from pure methanol ice is 1e−2 molecule/photon at 564 eV. Photo-products such as CH4, H2CO, H2O, CO2 , and CO also desorb at increasing efficiency. X-ray photodesorption of larger COMs, which can be attributed to either ethanol, dimethyl ether, and/or formic acid, is also detected. The physical mechanisms at play are discussed and must likely involve the thermalization of Auger electrons in the ice, thus indicating that its composition plays an important role. Finally, we provide desorption yields applicable to protoplanetary disk environments for astrochemical models. The X-rays are shown to be a potential candidate to explain gas-phase abundances of methanol in disks. However, more relevant desorption yields derived from experiments on mixed ices are mandatory to properly support the role played by X-rays in nonthermal desorption of methanol (see paper II).

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The warm-up phase in massive star-forming cores around RCW 120

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We study molecular emission in a massive condensation at the border of the HII region RCW 120, paying particular attention to the Core 1 and Core 2 objects, the most massive fragments of the condensation found previously by ALMA. The latter fragment was previously suggested to host a high-mass analogue of Class 0 young stellar object. We present spectra of molecular emission in the 1 mm range made with the APEX telescope. We detect CH3OH and C34S lines in Core 1 and Core 2. The CH3CN series and the SO2 lines are only found in Core 2. We estimate gas physical parameters using methanol lines and obtain gas temperature less than 100 K in both regions. Molecular hydrogen number density in Core 2 is in the range of 10(5)−10(7) cm(−3) and is more uncertain in Core 1. However, the detection of the CH3CN lines corresponding to highly excited transitions (Eu >400 K) in Core 2 indicates that the region contains hot gas, while the abundances of CH3OH, CS, SO2 and CH3CN are quite low for a hot core stage. We propose that Core 2 is in the warm-up phase prior to the establishing of the hot gas chemistry. We suggest that Core 2 is in the beginning of the hot core stage. There are no detected CH3CN lines in Core 1, therefore, it might be on an even less evolved evolutionary stage.

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Complex structure of a proto-brown dwarf

B. Riaz, M. N. Machida

We present ALMA 12CO (2-1), 13CO (2-1), C18O (2-1) molecular line observations of a very young proto-brown dwarf system, ISO-OPH 200. We have conducted physical+chemical modelling of the complex internal structure for this system using the core collapse simulations for brown dwarf formation. The model at an age of ∼6000 yr can provide a good fit to the observed kinematics, spectra, and reproduce the complex structures seen in the moment maps. Results from modelling indicate that 12CO emission is tracing an extended (∼1000 au) molecular outflow and a bright shock knot, 13CO is tracing the outer (∼1000 au) envelope/pseudo-disc, and C18O is tracing the inner (∼500 au) pseudo-disc. The source size of ∼8.6 au measured in the 873 mu image is comparable to the inner Keplerian disc size predicted by the model. A 3D model structure of ISO-OPH 200 suggests that this system is viewed partially through a wide outflow cavity resulting in a direct view of the outflow and a partial view of the envelope/pseudo-disc. We have argued that ISO-OPH 200 has been mis-classified as

a Class Flat object due to the unusual orientation. The various signatures of this system, notably, the young ~616 yr outflow dynamical age and high outflow rate (~1e-7 Msun/yr), silicate absorption in the 10 mu mid-infrared spectrum, pristine ISM-like dust in the envelope/disc, comparable sizes of the extended envelope and outflow, indicate that ISO-OPH 200 is an early Class 0 stage system formed in a star-like mechanism via gravitational collapse of a very low-mass core.

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Electronically Excited States of Closed-Shell, Cyano-Functionalized Polycyclic Aromatic Hydrocarbon Anions

Taylor J. Santaloci and Ryan C. Fortenberry

Few anions exhibit electronically excited states, and, if they do, the one or two possible excitations typically transpire beyond the visible spectrum into the near-infrared. These few, red-shifted electronic absorption features make anions tantalizing candidates as carriers of the diffuse interstellar bands (DIBs), a series of mostly unknown, astronomically ubiquitous absorption features documented for over a century. The recent interstellar detection of benzonitrile implies that cyano-functionalized polycyclic aromatic hydrocarbon (PAH) anions may be present in space. The presently reported quantum chemical work explores the electronic properties of deprotonated benzene, naphthalene, and anthracene anions functionalized with a single cyano group. Both the absorption and emission properties of the electronically excited states are explored. The findings show that the larger anions absorption and emission energies possess both valence and dipole bound excitations in the 450-900 nm range with oscillator strengths for both types of >1e-4. The valence and dipole bound excited state transitions will produce slightly altered substructure from one another making them appear to originate with different molecules. The known interstellar presence of related molecules, the two differing natures of the excited states for each, and the wavelength range of peaks for these cyano-functionalized PAH anions are coincident with DIB properties. Finally, the methods utilized appear to be able to predict the presence of dipole-bound excited states to within a 1.0 meV window relative to the electron binding energy.

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Carbon-Chain Chemistry vs. Complex-Organic-Molecule Chemistry in Envelopes around Three Low-Mass Young Stellar Objects in the Perseus Region

Kotomi Taniguchi, Liton Majumdar, Shigehisa Takakuwa, Masao Saito, Dariusz C. Lis, Paul F. Goldsmith, Eric Herbst

We have analyzed ALMA Cycle 5 data in Band 4 toward three low-mass young stellar objects (YSOs), IRAS 03235+3004 (hereafter IRAS 03235), IRAS 03245+3002 (IRAS 03245), and IRAS 03271+3013 (IRAS 03271), in the Perseus region. The HC3N (J=16−15; Eup/k=59.4 K) line has been detected in all of the target sources, while four CH3OH lines (Eup/k=15.4−36.3 K) have been detected only in IRAS 03245. Sizes of the HC3N distributions (~2930−3230 au) in IRAS 03235 and IRAS 03245 are similar to those of the carbon-chain species in the warm carbon chain chemistry (WCCC) source L1527. The size of the CH3OH emission in IRAS 03245 is ~1760 au, which is slightly smaller than that of HC3N in this source. We compare the CH3OH/HC3N abundance ratios observed in these sources with predictions of chemical models. We confirm that the observed ratio in IRAS 03245 agrees with the modeled values at temperatures around 30--35 K, which supports the HC3N formation by the WCCC mechanism. In this temperature range, CH3OH does not thermally desorb from dust grains. Non-thermal desorption mechanisms or gas-phase formation of CH3OH seem to work efficiently around IRAS 03245. The fact that IRAS 03245 has the highest bolometric luminosity among the target sources seems to support these mechanisms, in particular the non-thermal desorption mechanisms.

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Sulfur Molecules in Space by X-rays: A Computational Study

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X-ray astronomy lacks high resolution spectra of interstellar dust analogues and molecules, severely hampering interstellar medium studies based on upcoming X-ray missions. Various theoretical approaches may be used to address this problem, but they must first be shown to reproduce reliable spectra compared to the experiment. In this work, we calculate the sulfur K edge X-ray absorption spectra of H2S, SO2, and OCS, whose spectra are already known from X-ray experiments and predict the X-ray spectrum of CS, which as far as we are aware has not been measured, thereby hampering its detection by X-ray telescopes. We chose these four molecules as the astrochemistry of sulfur is an unsolved problem and as the four molecules are already known to exist in space. We consider three types of methods for modeling the X-ray spectra: more accurate calculations with the algebraic-diagrammatic construction (ADC) and the CC2, CCSD, and CC3 coupled cluster (CC) approaches as well as more affordable ones with transition potential density functional theory (TP-DFT). A comparison of our computational results to previously reported experimental spectra shows that the core–valence separation (CVS) approaches CVS-ADC(2)-x and CVS-CC3 generally yield a good qualitative level of agreement with the experiment,

suggesting that they can be used for interpreting measured spectra, while the TP-DFT method is not reliable for these molecules. However, quantitative agreement with the experiment is still outside the reach of the computational methods studied in this work.

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Physical and chemical structure of the Serpens filament: Fast formation and gravity-driven accretion

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The Serpens filament, a prominent elongated structure in a relatively nearby molecular cloud, is believed to be at an early evolutionary stage, so studying its physical and chemical properties can shed light on filament formation and early evolution. The main goal is to address the physical and chemical properties as well as the dynamical state of the Serpens filament at a spatial resolution of ∼0.07 pc and a spectral resolution of 0.1 km/s. We performed 13CO (1-0), C18O (1-0), C17O (1-0), 13CO (2-1), C18O (2-1), and C17O (2-1) imaging observations toward the Serpens filament with the Institut de Radioastronomie Millim{é}trique 30-m (IRAM-30 m) and Atacama Pathfinder EXperiment (APEX) telescopes. Widespread narrow 13CO (2-1) self-absorption is observed in this filament, causing the 13CO morphology to be different from the filamentary structure traced by C18O and C17O. Our excitation analysis suggests that the opacities of C18O transitions become higher than unity in most regions, and this analysis confirms the presence of widespread CO depletion. Further we show that the local velocity gradients have a tendency to be perpendicular to the filament's long axis in the outskirts and parallel to the large-scale magnetic field direction. The magnitudes of the local velocity gradients decrease toward the filament's crest. The observed velocity structure can be a result of gravity-driven accretion flows. The isochronic evolutionary track of the C18O freeze-out process indicates the filament is young with an age of $\lesssim$2 Myr. We propose that the Serpens filament is a newly-formed slightly-supercritical structure which appears to be actively accreting material from its ambient gas.

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High-resolution infrared spectroscopy of DC3N in the stretching region

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The perspectives opened by modern ground-based infrared facilities and the forthcoming James Webb Telescope mission have brought a great attention to the ro-vibrational spectra of simple interstellar molecules. In this view, and because of the lack of accurate spectroscopic data, we have investigated the infrared spectrum of deuterated cyanoacetylene (DC3N), a relevant astrochemical species. The nu1, nu2, and nu3 fundamentals as well as their hot-bands were observed in the stretching region (1 500–3 500 cm−1) by means of a Fourier transform infrared spectrometer. Supplementary measurements were performed at millimeter-wavelengths (243–295 GHz) with a frequency-modulation spectrometer equipped with a furnace, that allowed to probe pure rotational transitions in the investigated stretching states. Furthermore, since HC3N is observed as by-product in our spectra and suffers from the same deficiency of accurate infrared data, its ro-vibrational features have been analyzed as well. The combined analysis of both rotational and ro-vibrational data allowed us to determine precise spectroscopic constants that can be used to model the infrared spectra of DC3N and HC3N. The importance of accurate molecular data for the correct modeling of proto-planetary disks and exoplanetary atmospheres is then discussed.

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Carbonyl Sulfide (OCS): Detections in comets C/2002 T7 (LINEAR), C/2015 ER61 (PanSTARRS), and 21P/Giacobini–Zinner and stringent upper-limits in 46P/Wirtanen.

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Carbonyl sulfide (OCS) is one of the sulfur-bearing molecules detected in different astronomical environments, including comets. The present-day sulfur chemistry in comets may reveal much about the origin of these ices and their subsequent processing history. Cometary sulfur molecules such as H2S, H2CS, SO2, SO, CS, CS2, S2, and NS have been detected in many comets. However, OCS, the only sulfur-bearing species with fluorescence emission lines at infrared wavelengths, is under-represented in comet volatile studies, having been reported in only six comets so far. We targeted OCS with the NASA Infrared Telescope Facility in comets 46P/Wirtanen, 21P/Giacobini–Zinner, and C/2015 ER61 (PanSTARRS) in 2017–2018 using the high-resolution iSHELL spectrograph, and in C/2002 T7 (LINEAR) in 2004 using the heritage CSHELL spectrograph. In comet C/2015 ER61, the OCS abundance was similar to those measured in bright comets such as comets C/2012 S1 (ISON) and C/1996 B2 (Hyakutake), whereas in C/2002 T7 it was relatively depleted. Our OCS measurement in 21P/Giacobini–Zinner is the first definitive detection of this molecule in a Jupiter-family comet from a ground based facility

and is close to the average OCS abundance determined in comet 67P/Churyumov–Gerasimenko by the Rosetta mission. Our 3σ upper limit for comet 46P/Wirtanen is the lowest reported OCS abundance in any comet. We present production rates and mixing ratios (with respect to H2O) for these comets and place our results in the context of comets measured to date.

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Vibrationally resolved NO dissociative excitation cross sections by electron impact

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A theoretical investigation of the dissociative excitation by electron impact on the NO molecule is presented, aiming to make up for the lack of data for this process in the literature. A full set of vibrationally-resolved cross sections and corresponding rate coefficients are calculated using the local-complex-potential approach and five resonant states of NO− .

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Announcements

Ph. D position at the Laboratoire d'Astrophysique de Bordeaux (France). A study of the winds of evolved cold stars

Applications are invited for a Ph.D. student position in Astrophysics at the Laboratoire d'Astrophysique de Bordeaux, Bordeaux University, France. Project description: Evolved cool stars are major cosmic engines, providing strong mechanical, chemical, and radiative feedback to their host environments. Through strong stellar winds, still poorly understood, they enrich their environment with chemical elements, which are the building blocks of planets and life. A complete understanding of their evolution in the near and distant Universe can only be achieved with detailed knowledge of wind physics over the life cycle of these stars as well as in relation to their circumstellar environment. A complete picture of all the physical processes that simultaneously trigger and shape the strong winds of evolved cold stars is still missing. This thesis is part of Project PEPPER (https://lagrange.oca.eu/fr/welcome-to-anr-pepper), funded by the French Agence Nationale pour la Recherche, aiming to build a coherent and comprehensive description of the mass-loss mechanism, in close collaboration with the ATOMIUM project (https://fys.kuleuven.be/ster/research-projects/aerosol/atomium/atomium). The main questions we endeavour to tackle in this project are: How are the winds launched and which physical processes determine their properties? How do the mass-loss rate and other wind properties depend on fundamental stellar parameters? What is the origin of the detected magnetic field on the stellar surface? What chemical processes dominate in the winds? Where does the interaction between dynamics and chemical phenomena lie? The core of our approach is the synergy between theory and observation in order to obtain a global, coherent vision of the evolved cool stars, from the bottom of the atmosphere up to the circumstellar environment. We will use high-angular resolution observations with SPHERE and MATISSE and observations made quasi-simultaneously with ALMA (all already in hand). For the interpretation, the student will actively participate in the modeling using various codes.
The Ph.D. student will work together with Fabrice Herpin and other PEPPER team members, in close collaboration with the ATOMIUM team. More information on the Laboratoire d'Astrophysique de Bordeaux can be found at https://astrophy.u-bordeaux.fr
The position is a 3-year appointment and requires a University degree in Astronomy or Physics at an advanced level (e.g., a M.Sc. degree), completed by the time of employment. The earliest starting date is 1 October 2021. Applications should include a brief description of research interests and relevant experience, CV, copies of Master's University grades, certificates and diplomas, B.Sc./M.Sc. thesis/internship (or draft thereof), and contact details for the Master director and internship supervisors. Practical experience with python, numerical simulations of gas dynamics, or with observational data on AGB and RSG stars, will be considered a merit.
The complete announcement is posted at https://lagrange.oca.eu/fr/welcome-to-anr-pepper and the application deadline is 1 June 2021. Applications should be sent to Fabrice Herpin (fabrice.herpin@u-bordeaux.fr).
For further information, please contact Fabrice Herpin (fabrice.herpin@u-bordeaux.fr).

Postdoctoral Research Position in Massive Star and Star Cluster Formation (Astrobiology Center, Madrid)

The ISM group at the Astrobiology Centre in Madrid, invites applicants to pursue an observational study on the dynamics and chemistry of the molecular gas toward a sample of Infrared-Dark Clouds in the Galactic Disk and of Giant Molecular Clouds in the Galactic Centre. The successful applicant will work with Dr. Izaskun Jimenez-Serra, Dr. Victor Rivilla and Prof. Jesus Martin-Pintado, experts on star formation and astrochemistry.
The Astrobiology Centre (CAB) provides a lively and stimulating research environment, which includes over 100 staff members, postdocs, and PhD students, and which covers research topics as diverse as prebiotic chemistry, biochemistry, planetology, and the discovery of biosignatures in planets in our Solar System.
The position is to be filled as soon as possible and no later than 1 September 2021. For questions, contact Dr. Izaskun Jimenez-Serra (ijimenez@cab.inta-csic.es) or Dr. Victor Rivilla (vrivilla@cab.inta-csic.es). The candidate should be in

possession of a PhD.
This is a 2-year position with the possibility of an extension for a third year depending on funding availability.
Applications should include a motivation letter, a CV, a publication list, and a summary of past research (max 2 pages).
These documents must be sent via email to I. Jimenez-Serra (ijimenez@cab.inta-csic.es) and V. Rivilla (vrivilla@cab.inta-csic.es). Review starts on 10 March 2021.