AstroChemical Newsletter #46

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Abstracts

Infrared spectrum of hydrogenated corannulene rim-HC20H10 isolated in solid para-hydrogen

Pavithraa Sundararajan, Masashi Tsuge, Masaaki Baba, and Yuan-Pern Lee

Hydrogenated polycyclic aromatic hydrocarbons have been proposed to be carriers of the interstellar unidentified infrared (UIR) emission bands and the catalysts for formation of H2; spectral characterizations of these species are hence important. We report the infrared (IR) spectrum of mono-hydrogenated corannulene (HC20H10) in solid para-hydrogen (p-H2). In experiments of electron bombardment of a mixture of corannulene and p-H2 during deposition of a matrix at 3.2 K, two groups of spectral lines increased with time during maintenance of the matrix in darkness after deposition. Lines in one group were assigned to the most stable isomer of hydrogenated corannulene, rim-HC20H10, according to the expected chemistry and a comparison with scaled harmonic vibrational wavenumbers and IR intensities predicted with the B3PW91/6-311++G(2d,2p) method. The lines in the other group do not agree with predicted spectra of other HC20H10 isomers and remain unassigned. Alternative hydrogenation was achieved with H atoms produced photochemically in the infrared-induced reaction Cl + H2 (v = 1) → H + HCl in a Cl2/C20H10/p-H2 matrix. With this method, only lines attributable to rim-HC20H10 were observed, indicating that hydrogenation via a quantum-mechanical tunneling mechanism produces preferably the least-energy rim-HC20H10 regardless of similar barrier heights and widths for the formation of rim-HC20H10 and hub-HC20H10. The mechanisms of formation in both experiments are discussed. The bands near 3.3 and 3.4 μm of rim-HC20H10 agree with the UIR emission bands in position and relative intensity, but other bands do not match satisfactorily with the UIR bands.

JCP (2019) 151(4): 044304
DOI: 10.1063/1.5111169
Full-text URL: https://aip.scitation.org/doi/10.1063/1.5111169#suppl

Theoretical investigation of methanol formation from methane water-ice cluster following ionization

Sankhabrata Chandra

In this article, I have presented quantum mechanical treatment of methanol formation reaction from methane water-ice cluster after ionization with high energy photons. To mimic water ice structure, six water molecules are arranged in hexagonal form. This is the most stable structure formed by six water molecules. Theoretical Photodesorption study has been performed on this structure. I have investigated a unique reaction mechanism of methanol formation from methane water ice cluster. I have shown that

methanol forms after ionization via two transition states. Hydrogen molecule forms as one of the side product. Initiation of the reaction occurs by dissociation of O H bond in the water cluster followed by C H bond dissociation and formation of C O bond. The timescale of the initial step, which is dissociation of O H bond, has been computed as 50 femtosecond in this article.

Molecular Astrophysics (2019) Volume 16, 100045
DOI: 10.1016/j.molap.2019.100045
Full-text URL: https://www.sciencedirect.com/science/article/pii/S2405675819300120

H2 ortho-para spin conversion on inhomogeneous grain surfaces

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We investigate the evolution of the ortho-to-para ratio of overall (gas + ice) H2 via the nuclear spin conversion on grain surfaces coated with water ice under physical conditions that are relevant to star- and planet-forming regions. We utilize the rate equation model that considers adsorption of gaseous H2 on grain surfaces which have a variety of binding sites with a different potential energy depth, thermal hopping, desorption, and the nuclear spin conversion of adsorbed H2. It is found that the spin conversion efficiency depends on the H2 gas density and the surface temperature. As a general trend, enhanced H2 gas density reduces the efficiency, while the temperature dependence is not monotonic; there is a critical surface temperature at which the efficiency is the maximum. At low temperatures, the exchange of gaseous and icy H2 is inefficient (i.e., adsorbed H2 does not desorb and hinders another gaseous H2 to be adsorbed), while at warm temperatures, the residence time of H2 on surfaces is too short for the spin conversion. Additionally, the spin conversion becomes more efficient with lowering the activation barriers for thermal hopping. We discuss whether the spin conversion on surfaces can dominate over that in the gas-phase in star- and planet-forming regions. Finally, we establish a simple but accurate way to implement the H2 spin conversion on grain surfaces in existing astrochemical models.

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Organic Complexity in Protostellar Disk Candidates

Jennifer B. Bergner, Rafael Martín-Doménech, Karin I. Öberg, Jes K. Jørgensen, Elizabeth Artur de la Villarmois, Christian Brinch

We present ALMA observations of organic molecules toward five low-mass Class 0/I protostellar disk candidates in the Serpens cluster. Three sources (Ser-emb 1, Ser-emb 8, and Ser-emb 17) present emission of CH3OH as well as CH3OCH3, CH3OCHO, and CH2CO, while NH2CHO is detected in just Ser-emb 8 and Ser-emb 17. Detecting hot corino-type chemistry in three of five sources represents a high occurrence rate given the relative sparsity of these sources in the literature, and this suggests a possible link between protostellar disk formation and hot corino formation. For sources with CH3OH detections, we derive column densities of 10^17–10^18 cm^–2 and rotational temperatures of ~200–250 K. The CH3OH-normalized column density ratios of large, oxygen-bearing COMs in the Serpens sources and other hot corinos span 2 orders of magnitude, demonstrating a high degree of chemical diversity at the hot corino stage. Resolved observations of a larger sample of objects are needed to understand the origins of chemical diversity in hot corinos, and the relationship between different protostellar structural elements on disk-forming scales.

Earth & Space Chemistry (2019) 38, 1564-1575
DOI: 10.1021/acsearthspacechem.9b00059
Full-text URL: https://arxiv.org/abs/1907.07791

A Survey of C2H, HCN, and C18O in Protoplanetary Disks

Jennifer B. Bergner, Karin I. Öberg, Edwin A. Bergin, Ryan A. Loomis, Jamila Pegues, Chunhua Qi

Molecular lines observed toward protoplanetary disks carry information about physical and chemical processes associated with planet formation. We present ALMA Band 6 observations of C2H, HCN, and C18O in a sample of 14 disks spanning a range of ages, stellar luminosities, and stellar masses. Using C2H and HCN hyperfine structure fitting and HCN/H13CN isotopologue analysis, we extract optical depth, excitation temperature, and column density radial profiles for a subset of disks. C2H is marginally optically thick ($\tau \sim 1$–5) and HCN is quite optically thick ($\tau \sim 5$–10) in the inner 200 au. The extracted temperatures of both molecules are low (10–30 K), indicative of either subthermal emission from the warm disk atmosphere or substantial beam dilution due to chemical substructure. We explore the origins of C2H morphological diversity in our sample using a series of toy disk models and find that disk-dependent overlap between regions with high UV fluxes and high atomic carbon abundances can explain a wide range of C2H emission features (e.g., compact versus extended and ringed versus ringless emission). We explore the chemical relationship between C2H, HCN, and C18O and find a positive correlation between C2H and HCN fluxes but no relationship between C2H or HCN with C18O fluxes. We also see no evidence that C2H and HCN are enhanced with disk age. C2H and HCN seem to share a common driver; however, more work remains to elucidate the chemical relationship between these molecules and the underlying evolution of C, N, and O chemistries in disks.

ApJ 2019, 876:25
DOI: 10.3847/1538-4357/ab141e
Full-text URL: https://arxiv.org/abs/1904.09315

ALMA Detection of Vibrationally Excited (vt = 1, 2) Acetic Acid toward NGC 6334I

C. Xue, A. J. Remijan, C. L. Brogan, T. R. Hunter, E. Herbst, and B. A. McGuire

Vibrationally excited states of detected interstellar molecules have been shown to account for a large portion of unidentified spectral lines in observed interstellar spectra toward chemically rich sources. Here, we present the first interstellar detection of the first and second vibrationally excited torsional states of acetic acid (vt = 1, 2) toward the high-mass star-forming region NGC 6334I. The observations presented were taken with the Atacama Large Millimeter/submillimeter Array in bands 4, 6, and 7 covering a frequency range of 130 – 352 GHz. By comparing a single excitation temperature model to the observations, the best-fit excitation temperature and column density are obtained to be 142(25) K and 1.12(7) × 10^17cm−2 respectively. Based on the intensity maps of the vibrationally excited CH3COOH transitions, we found that the CH3COOH emissions are compact and concentrated toward the MM1 and MM2 regions with a source size smaller than 2″. After locating the emission from different CH3COOH transitions, which cover a large range of excitation energies, we are able to explain the variation of the CH3COOH emission peak within the MM2 core by invoking continuum absorption or outflows.

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Study of CS, SiO, and SiS abundances in carbon star envelopes:Assessing their role as gas-phase precursors of dust

S. Massalkhi, M. Agúndez and J. Cernicharo

Aims: We aim to determine the abundances of CS, SiO, and SiS in a large sample of carbon star envelopes covering a wide range of mass loss rates to investigate the potential role that these molecules could play in the formation of dust in the surroundings of the central AGB star. Methods: We surveyed a sample of 25 carbon-rich AGB stars in the 2 mm band, more concretely in the J = 3-2 line of CS and SiO, and in the J = 7-6 and J = 8-7 lines of SiS, using the IRAM 30 m telescope. We performed excitation and radiative transfer calculations based on the large velocity gradient (LVG) method to model the observed lines of the molecules and to derive their fractional abundances in the observed envelopes. We also assessed the effect of infrared pumping in the excitation of the molecules. Results: We detected CS in all 25 targeted envelopes, SiO in 24 of them, and SiS in 17 sources. Remarkably, SiS is not detected in any envelope with a mass loss rate below 10^-6 solar mass per year while it is detected in all envelopes with mass loss rates above that threshold. We found that CS and SiS have similar abundances in carbon star envelopes, while SiO is present with a lower abundance. We also found a strong correlation in which the denser the envelope, the less abundant are CS and SiO. The trend is however only tentatively seen for SiS in the range of high mass loss rates. Furthermore, we found a relation in which the integrated flux of the MgS dust feature at 30 µm increases as the fractional abundance of CS decreases. Conclusions: The decline in the fractional abundance of CS with increasing density could be due to gas-phase chemistry in the inner envelope or to adsorption onto dust grains. The latter possibility is favored by a correlation between the CS fractional abundance and the 30 micron feature, which suggests that CS is efficiently incorporated onto MgS dust around C-rich AGB stars. In the case of SiO, the observed abundance depletion with increasing density is most likely caused by an efficient incorporation onto dust grains. We conclude that CS, SiO (very likely), and SiS (tentatively) are good candidates to act as gas-phase precursors of dust in C-rich AGB envelopes.

A&A (2019), 628, A62
DOI: 10.1051/0004-6361/201935069
Full-text URL: https://arxiv.org/abs/1906.09461

Structure and Properties of Nanosilicates with Olivine (Mg2SiO4)N and Pyroxene (MgSiO3)N Compositions

Antoni Macià Escatllar, Tomas Lazaukas, Scott M. Woodley, Stefan T. Bromley

Magnesium-rich silicates are ubiquitous both terrestrially and astronomically, where they are often present as small particles. Nanosized Mg-rich silicate particles are likely to be particularly important for understanding the formation, processing, and properties of cosmic dust grains. Although astronomical observations and laboratory studies have revealed much about such silicate dust, our knowledge of this hugely important class of nanosolids largely rests on top-down comparisons with the properties of bulk silicates. Herein, we provide a foundational bottom-up study of the structure and properties of

Mg-rich nanosilicates based on carefully procured atomistic models. Specifically, we employ state-of-the-art global optimization methods to search for the most stable structures of silicate nanoclusters with olivine (Mg2SiO4)N and pyroxene (MgSiO3)N compositions with N = 1–10. To ensure the reliability of our searches, we develop a new interatomic potential that has been especially tuned for nanosilicates. Subsequently, we refine these searches and calculate a range of physicochemical properties of the most stable nanoclusters using accurate density functional theory based electronic structure calculations. We report a detailed analysis of structural and energy properties, charge distributions, and infrared vibrational spectra, where in all cases we compare our finding for nanosilicates with those of the corresponding bulk silicate crystals. For most properties considered, we find large differences with respect to the bulk limit, underlining the limitations of a top-down approach for describing these species. Overall, our work provides a new platform for an accurate and detailed understanding of nanoscale silicates.

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Full-text URL: https://pubs.acs.org/doi/full/10.1021/acsearthspacechem.9b00139

Dissociative recombination of CH+ molecular ion induced by very low energy electrons.

J. Zs. Mezei, M. D. Epée Epée, O. Motapon, I. F. Schneider.

We used the multichannel quantum defect theory to compute cross sections and rate coefficients for the dissociative recombination of CH+ initially in its lowest vibrational level vi+ = 0 with electrons of incident energy below 0.2 eV. We have focused on the contribution of the 2 2Π state which is the main dissociative recombination route at low collision energies. The final cross section is obtained by averaging the relevant initial rotational states (Ni+ = 0, . . . , 10) with a 300 K Boltzmann distribution. The Maxwell isotropic rate coefficients for dissociative recombination are also calculated for different initial rotational states and for electronic temperatures up to a few hundred Kelvins. Our results are compared to storage-ring measurements.

Atoms 7, 82 (2019)
DOI: 10.3390/atoms7030082
Full-text URL: https://www.mdpi.com/2218-2004/7/3/82

Announcements

Postdoctoral research position: The NASA Ames PAH IR Spectroscopic Database

The NASA Ames PAH IR Spectroscopic Database (PAHdb) Team is offering a 1-2 year postdoctoral research position. The PAHdb Team is part of the Astrophysics & Astrochemistry Laboratory group at NASA Ames Research Center (ARC), in the Space Science and Astrobiology Division. Located in the heart of Silicon Valley, ARC lies at the southern tip of the San Francisco Bay, bordering the city of Mountain View. This highly interdisciplinary research group consists of chemists, physicists, and astronomers. The successful applicant is expected to work on applying the data and tools that are part of PAHdb to analyze and interpret the emission attributed to polycyclic aromatic hydrocarbons in astronomical observations, as well as further develop and expand the (software) tools in preparation for the James Webb Space Telescope (JWST). JWST will measure the PAH features with spectral coverage and sensitivity that far exceeds

earlier observations and with a reach that is far deeper than previously possible. Work is expected to be published in peer-reviewed journals and there is strong encouragement to present your research at (international) conferences, both oral and in posters. Some recent relevant publications (DOIs) are given below and the development of the (software) tools is done on GitHub.
10.3847/1538-4357/aaf562
10.3847/1538-4365/aaa019
10.3847/1538-4357/aabcbe
10.25080/majora-4af1f417-00f
Applicants must be highly qualified, self-motivated, fluent in English, have a solid background in infrared astronomy, and knowledgeable with infrared spectroscopy. Being able to use Python is a must. Some exposure to IDL and experience with software development would be highly beneficial. The application package should be send to Christiaan.Boersma@nasa.gov and include:
1. Cover letter
2. CV/Résumé
3. List of publications
4. Statement of qualifications relevant to the position (e.g., coding experience/examples)
5. Research interests
6. Names and contact information of two references

https://www.astrochemistry.org/pahdb/ NASA Ames PAH IR Spectroscopic Database
https://www.astrochemistry.org Astrophysics & Astrochemistry Laboratory group
https://www.nasa.gov/ames NASA Ames Research Center
https://www.nasa.gov/content/space-science-and-astrobiology-ames Space Science and Astrobiology Division
https://github.com/PAHdb GitHub
https://doi.org/10.3847/1538-4357/aaf562 10.3847/1538-4357/aaf562
https://doi.org/10.3847/1538-4365/aaa019 10.3847/1538-4365/aaa019
https://doi.org/10.3847/1538-4357/aabcbe 10.3847/1538-4357/aabcbe
https://doi.org/10.25080/majora-4af1f417-00f 10.25080/majora-4af1f417-00f

Registration OPEN: 2020 Submillimeter Array Interferometry School

We are happy to announce that registration is now OPEN for the first (2020) SMA Interferometry school at our website: bit.ly/sma-school
The school will be held on January 12-17th 2020 in Hilo, on the Big Island of Hawai'i (conveniently following the Winter AAS Meeting in Honolulu), and is organized by the Center for Astrophysics, in conjunction with the Academia Sinica Institute of Astronomy and Astrophysics and the University of Hawaii. The goals of the school are to provide graduate students, postdocs and scientists outside the field with a broad knowledge of interferometry and data reduction techniques at (sub)millimeter wavelengths.
The workshop will provide a series of lectures on the fundamentals of radio interferometry with a special emphasis on observations at (sub)millimeter wavelengths. The school will extensively utilize the Submillimeter Array (SMA) on Mauna Kea, Hawaii and its new capabilities. We particularly stress the hands-on nature of this School, where participants will be able to experience actively performing observations and data reduction for their own proposed projects. The program of the School can be found at our website and will include lectures and hands-on tutorials, a one-day trip to the Maunakea summit including (but not limited to) the SMA, as well as reduction, analysis and presentation of results from observations obtained during the School.
There will be no registration fee for the school, and support towards ground

transportation, meals and lodging will be provided. Because of the hands-on nature of the school, we will be accepting a limited number of 18 participants, which will be selected based on their application. As part of the application, students will be required to submit a brief proposal for an observation with the SMA to be executed (as conditions allow) during the school.
Registration will close on September 8th, 2019. Admitted and waitlisted students will be notified by October 1st, 2019.
Looking forward to seeing you in Hilo!

Faculty and Postdoctoral Positions in School of Earth and Planetary Sciences (SEPS), National Institute of Science Education and Research (NISER), Bhubaneswar, India

NISER is one of India's premier research-driven academic institutes. SEPS/NISER is a unique center in India that has been established to emerge and excel in high quality and interdisciplinary scientific research works in Planetary Sciences, Earth Sciences, and Atmospheric-Ocean Sciences. NISER provides start-up grant and academic freedom for promising candidates.
SEPS seeks faculty applications from highly motivated and promising candidates for faculty positions at various level. Interested candidates should send their application to fa@niser.ac.in
Current faculty members in SEPS are involved actively in Indian and large international collaborative projects and astronomy/planetary/exoplanetary missions, e.g., SKA, TMT, ALMA, NASA's JWST, SOFIA and Dawn. Interdisciplinary works on astrochemistry & astrobiology, star & planet formation, radio/sub-mm/infrared astronomy, exoplanets, planetary minerology & morphology, small bodies & meteorites, planetary remote sensing, land-atmosphere coupling, boundary layer dynamics, current challenges in climate change, etc., have been initiated already.
Applications and positions are subject to rolling basis as per NISER/DAE norms: https://www.niser.ac.in/notices/2017/recruitments/Faculty-Rolling-Advertisement-2017.pdf
NISER/SEPS also highly welcome candidates who are interested in prestigious independent faculty/fellowship program, for example, Ramanujan Fellowship, DST INSPIRE Faculty, SERB-NPDF etc.