AstroChemical Newsletter #39

February 2019

The AstroChemical Newsletter website is back online. This month's newsletter contains abstracts submitted before the server hosting our website was taken down last November. 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

Deuterated methyl mercaptan (CH3SD): Laboratory rotational spectroscopy and search toward IRAS 16293-2422 B

O. Zakharenko, F. Lewen, V. V. Ilyushin, M. N. Drozdovskaya, J. K. Jørgensen, S. Schlemmer, H. S. P. Müller

Methyl mercaptan (also known as methanethiol), CH3SH, has been found in the warm and dense parts of high- as well as low- mass star-forming regions. The aim of the present study is to obtain accurate spectroscopic parameters of the S-deuterated methyl mercaptan CH3SH to facilitate astronomical observations by radio telescope arrays at (sub)millimeter wavelengths. We have measured the rotational spectrum associated with the large-amplitude internal rotation of the methyl group of methyl mercaptan using an isotopically enriched sample in the 150-510 GHz frequency range using the Köln millimeter wave spectrometer. The analysis of the spectra has been performed up to the second excited torsional state. We present modeling results of these data with the RAM36 program. CH3SH was searched for, but not detected, in data from the Atacama Large Millimeter/submillimeter Array (ALMA) Protostellar Interferometric Line Survey (PILS) of the deeply embedded protostar IRAS 16293-2422. The derived upper limit corresponds to a degree of deuteration of at most ~18%.

A&A Volume 621, A114, January 2019
DOI: 10.1051/0004-6361/201834472
Full-text URL: https://arxiv.org/abs/1812.02454

Laboratory spectroscopic study of isotopic thioformaldehyde, H2CS, and determination of its equilibrium structure

H. S. P. Müller, A. Maeda, S. Thorwirth, F. Lewen, S. Schlemmer, I. R. Medvedev, M. Winnewisser, F. C. De Lucia, E. Herbst

Thioformaldehyde is an abundant molecule in various regions of the interstellar medium. However, available laboratory data limit the accuracies of calculated transition frequencies in the submillimeter region, in particular for minor isotopic species. We aim to determine spectroscopic parameters of isotopologs of H2CS that are accurate enough for predictions well into the submillimeter region. We investigated the laboratory rotational spectra of numerous isotopic species in natural isotopic composition almost continuously between 110 and 377 GHz. Individual lines were studied for most species in two frequency regions between 566 and 930 GHz. Further data were obtained for the three most abundant species in the 1290-1390 GHz region. New or improved spectroscopic parameters were determined for seven isotopic species. Quantum-chemical calculations were carried out to evaluate the differences between ground state and equilibrium rotational parameters to derive semi-empirical equilibrium structural parameters. The spectroscopic parameters are accurate enough for predictions well above 1 THz with the exception of H2(13)C(34)S where the predictions should be reliable to around 700 GHz.

A&A Volume 621, A143 ,January 2019
DOI: 10.1051/0004-6361/201834517
Full-text URL: https://arxiv.org/abs/1812.01554

Rotational Spectroscopy of the two higher energy conformers of 2-Cyanobutane

M. Hermanns, N. Wehres, F. Lewen, H. S. P. Müller, S. Schlemmer

We present high-resolution rotational spectroscopy of the two higher energy conformers of 2-cyanobutane (C4H9CN). We analysed spectra starting from 12-27 GHz using the Cologne chirped-pulse (CP) Fourier transform microwave spectrometer, which we discuss for the first time. Spectra between 36 and 402 GHz were also recorded by means of frequency modulated (FM) absorption spectroscopy. In addition, quantum chemical calculations were performed assisting the assignments. Furthermore ground state energies of the conformers have been calculated and subsequent experimental analysis of line intensities have been performed. This study provides precise spectroscopic constants, relative energies and vibrational frequencies of the three conformers for the search of 2-cyanobutane in star-forming regions. Additionally, this molecule poses an interesting case to test our knowledge of the abundance of chiral molecules in space.

J. Mol. Spectrosc., in press
DOI: 10.1016/j.jms.2018.11.009
Full-text URL: https://doi.org/10.1016/j.jms.2018.11.009

Gas phase detection and rotational spectroscopy of ethynethiol, HCCSH

K.L.K. Lee, M.-A. Martin-Drumel, V. Lattanzi, B. A. McGuire, P. Caselli, M. C. McCarthy

We report the gas-phase detection and spectroscopic characterisation of ethynethiol, a metastable isomer of thioketene using a combination of Fourier-transform microwave and submillimetre-wave spectroscopies. Several a-type transitions of the normal species were initially detected below 40 GHz using a supersonic expansion-electrical discharge source, and subsequent measurement of higher-frequency, b-type lines using double resonance provided accurate predictions in the submillimetre region. With these, searches using a millimetre-wave absorption spectrometer equipped with a radio frequency discharge source were conducted in the range 280–660 GHz, ultimately yielding nearly 100 transitions up to and . From the combined data set, all three rotational constants and centrifugal distortion terms up to the sextic order were determined to high accuracy, providing a reliable set of frequency predictions to the lower end of the THz band. Isotopic substitution has enabled both a determination of the molecular structure of HCCSH and, by inference, its formation pathway in our nozzle discharge source via the bimolecular radical-radical recombination reaction , which is calculated to be highly exothermic (−477 kJ/mol) using the HEAT345(Q) thermochemical scheme.

Published 29 November 2018 in Molecular Physics
DOI: 10.1080/00268976.2018.1552028
Full-text URL: https://arxiv.org/abs/1811.12798

Rotational spectroscopy of the HCCO and DCCO radicals in the millimeter and submillimeter range

J. Chantzos, S. Spezzano, C. Endres, L. Bizzocchi, V. Lattanzi, J. Laas, A. Vasyunin, P. Caselli

The ketenyl radical HCCO has recently been detected in the interstellar medium (ISM) for the first time. Further astronomical detections of HCCO will help us understand its gas-grain chemistry, and subsequently revise the oxygen-bearing chemistry towards dark clouds. Moreover, its deuterated counterpart DCCO has never been observed in the ISM. A broad spectroscopic investigation is still lacking for both HCCO and DCCO, although they exhibit a significant astrophysical relevance. In this work we aim to measure the pure rotational spectra of the ground state of HCCO and DCCO in the millimeter and submillimeter region, considerably extending the frequency range covered by previous studies. The spectral acquisition was performed using a frequency-modulation absorption spectrometer between 170 and 650 GHz. The radicals were produced in a low-density plasma generated from a select mixture of gaseous precursors. We were able to detect and assign more than 100 rotational lines for each isotopolog. The new lines have significantly enhanced the previous data set allowing the determination of highly precise rotational and centrifugal distortion parameters. In our analysis we took into account the interaction between the ground electronic state and a low-lying excited state (Renner-Teller pair) which enables the prediction and assignment of rotational transitions with Ka up to 4. The present set of spectroscopic parameters provides highly accurate, millimeter, and submillimeter rest-frequencies of HCCO and DCCO for future astronomical observations. We also show that towards the pre-stellar core L1544, ketenyl peaks in the region where c-C3H2 peaks, suggesting that HCCO follows a predominant hydrocarbon chemistry, as already proposed by recent gas-grain chemical models.

A&A Volume 621, A111, January 2019
DOI: 10.1051/0004-6361/201834419
Full-text URL: https://arxiv.org/abs/1811.11602

Abundant Z-cyanomethanimine in the interstellar medium: paving the way to the synthesis of adenine

V. M. Rivilla, J. Martín-Pintado, I. Jiménez-Serra, S. Zeng, S. Martín, J. Armijos-Abendaño, M. A. Requena-Torres, R. Aladro, D. Riquelme

We report the first detection in the interstellar medium of the Z-isomer of cyanomethanimine (HNCHCN), an HCN dimer proposed as precursor of adenine. We identified six transitions of Z-cyanomethanimine, along with five transitions of E-cyanomethanimine, using IRAM 30m observations towards the Galactic Center quiescent molecular cloud G+0.693. The Z-isomer has a column density of (2.0±0.6)×1e14 cm−2 and an abundance of 1.5×1e−9. The relative abundance ratio between the isomers is [Z/E]∼6. This value cannot be explained by the two chemical formation routes previously proposed (gas-phase and grain surface), which predicts abundances ratios between 0.9 and 1.5. The observed [Z/E] ratio is in good agreement with thermodynamic equilibrium at the gas kinetic temperature (130−210 K). Since isomerization is not possible in the ISM, the two species may be formed at high temperature. New chemical models, including surface chemistry on dust grains and gas-phase reactions, should be explored to explain our findings. Whatever the formation mechanism, the high abundance of Z-HNCHCN shows that precursors of adenine are efficiently formed in the ISM.

Monthly Notices of the Royal Astronomical Society: Letters, Volume 483, Issue 1, 11 February 2019, Pages L114–L119
DOI: 10.1093/mnrasl/sly228
Full-text URL: https://arxiv.org/abs/1811.12862

2018 Census of Interstellar, Circumstellar, Extragalactic, Protoplanetary Disk, and Exoplanetary Molecules

B. McGuire

To date, 204 individual molecular species, comprised of 16 different elements, have been detected in the interstellar and

circumstellar medium by astronomical observations. These molecules range in size from 2 atoms to 70, and have been detected across the electromagnetic spectrum from centimeter wavelengths to the ultraviolet. This census presents a summary of the first detection of each molecular species, including the observational facility, wavelength range, transitions, and enabling laboratory spectroscopic work, as well as listing tentative and disputed detections. Tables of molecules detected in interstellar ices, external galaxies, protoplanetary disks, and exoplanetary atmospheres are provided. A number of visual representations of these aggregate data are presented and briefly discussed in context.

2018 Astrophysical Journal Supplements 239, 17
DOI: 10.3847/1538-4365/aae5d2
Full-text URL: https://arxiv.org/abs/1809.09132

Announcements

Astrochemistry symposium in honor of John H. Black

to be held in Gothenburg Sweden 24-28 June, 2019.
Abstract deadline: 1 April
Registration deadline: 17 May
Register at: https://admin.chalmers.se/en/conference/JHBlacksymp2019/Pages/Registration-Abstract-Submission.aspx

The scientific purpose of this symposium is to highlight the fundamental connection between the theory of microscopic processes studied on Earth and the understanding of phenomena in a wide range of space environments.
The symposium is organised in honour of Prof. John H. Black, who throughout his career has demonstrated an outstanding ability to grasp, apply, and explain these connections - always maintaining a cosmic perspective regardless of scales or wavelengths.

Confirmed invited speakers:
Nathalie Carrasco
Paola Caselli
Ilsedore Cleeves
Carla Coppola
Elvire de Beck
Edith Falgarone
Javier Goicoechea
Isabelle Grenier
Nanase Harada
Eric Herbst
Liv Hornekaer
Brett McGuire
Sebastien Muller
David Neufeld
Fereshteh Rajabi
Evelyne Roueff
Stephan Schlemmer
Linda Tacconi
Floris van der Tak
Ewine van Dishoeck
Geronimo Villanueva
Naoki Watanabe

SOC
Eva Wirström, Chalmers University of Technology (chair)
Susanne Aalto, Chalmers University of Technology
Ewine van Dishoeck, Leiden Observatory
Maryvonne Gerin, LERMA-LRA
Eric Herbst, University of Virginia
Gunnar Nyman, Gothenburg University
Amiel Sternberg, Tel Aviv University
Naoki Watanabe, Hokkaido University

LOC
Susanne Aalto
Per Bjerkeli
Sabine König
Boy Lankhaar
Gunnar Nyman
Sandra Treviño-Morales
Eva Wirström

For more information browse the symposium webpages at:
http://www.chalmers.se/en/conference/JHBlacksymp2019/Pages/default.aspx

Announcement ACS Symposium on Water in the Universe

258th ACS National Meeting
ACS Symposium on Water in the Universe
25-29 August 2019 - San Diego, California – USA
https://callforpapers.acs.org/sandiego2019/PHYS

Symposium organizers:
Geoffrey A. Blake (California Institute of Technology),
Sergio Ioppolo (Queen Mary University of London)

Summary
Formed from two of the most abundant elements in the universe, the special chemical and physical properties of water make it a uniquely important molecule in the quest to understand our origins. Dramatic advances in observational capabilities from millimeter-wave to infrared wavelengths and in our ability to study water vapor, liquid water, and water ice from first principles calculations and with ever more capable laboratory methods now enables astronomers, planetary scientists and chemists to follow the 'water trail' from the interstellar medium to mature (exo)planetary systems. The timing of the meeting is particularly relevant to this topic, as by summer 2019 the Atacama Large Millimeter Array (ALMA) will have completed two observing cycles with its full suite of imaging and high frequency capabilities that are particularly critical to studies of water, and the Transiting Exoplanet Survey Satellite (TESS) will have over a year of scientific results in hand. Thus, exoplanet science will have fully entered the phase that explores the nature of potentially habitable terrestrial planets. This symposium will highlight the cosmic history of water, its critical role in the formation and early evolution of planetary systems, and the means by which habitable environments are created across the universe. With a strong focus on the chemistry of, and enabled by, water, and the interplay between studies of our own and exoplanetary systems, we aim to create a program that will draw in a wide range of chemists and (planetary) astronomers to the San Diego meeting.
Symposium Structure
Over the course of the symposium (following previous meetings there will be seven half-day topical sessions), we anticipate hosting approximately 28 invited talks (30 minute talks followed by 5 minutes of discussion) and 14 contributed talks (of 15 minute duration, with 5 minutes for discussion). The invited speakers will feature a mix of senior and junior scientists from the United States and from many countries whose scientists are actively engaged in astrochemistry. The envisioned program will be both gender-balanced and inclusive, and include a balance of perspectives from astronomical observations to theory/modeling to chemical synthesis. In many meetings of this type, the theory and laboratory sessions are often 'isolated' to their own half-day. We feel this discourages dialog between different communities, and so we aim to dovetail observations, theory, and key laboratory work within themes that are science-focused.

Proposed Session Topics (not necessarily in this order)
1. Water at cosmic distances.
2. Water in the interstellar medium (from diffuse to dense molecular clouds).
3. Water and associated volatiles in protoplanetary disks (snow lines, planetesimal and planet formation).
4. Water and associated volatiles in the solar system and debris disks (comets, icy satellites, meteorites).
5. Water in exoplanetary systems.
6. Water and associated volatile delivery to young, rocky planets.
7. Spread throughout all sessions – Ab initio theory, chemical modeling, and laboratory astrophysics studies of the water molecule and water-rich ices.