AstroChemical Newsletter #40

March 2019

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Abstracts

Protoplanetary discs: sensitivity of the chemical composition to various model parameters

Wakelam, V.; Chapillon, E.; Dutrey, A.; Guilloteau, S.; Iqbal, W.; Coutens, A.; Majumdar, L.

Protoplanetary discs are challenging objects for astrochemical models due to strong density and temperature gradients and due to the UV photons 2D propagation. In this paper, we have studied the importance of several model parameters on the predicted column densities of observed species. We considered: (1) two-phase (gas and homogeneous grains) or three-phase (gas, surface, and bulk of grains) models, (2) several initial compositions, (3) grain growth and dust settling, and (4) several cosmic-ray ionization rates. Our main result is that dust settling is the most crucial parameter. Including this effect renders the computed column densities sensitive to all the other model parameters, except cosmic-ray ionization rate. In fact, we found almost no effect of this parameter for radii larger than 10 au (the minimum radius studied here) except for N2H+. We also compared all our models with all the column densities observed in the protoplanetary disc around DM Tau and were not able to reproduce all the observations despite the studied parameters. N2H+ seems to be the most sensitive species. Its observation in protoplanetary discs at large radius could indicate enough N2 in the gas phase (inhibited by the three-phase model, but boosted by the settling) and a low electron abundance (favoured by low C and S elemental abundances).

MNRAS, Volume 484, Issue 2, p.1563-1573
DOI: 10.1093/mnras/stz068
Full-text URL: https://arxiv.org/abs/1901.10191

Molecular tracers of radiative feedback in Orion (OMC-1). Widespread CH+ (J=1-0), CO (10-9), HCN (6-5), and HCO+ (6-5) emission

J. R. Goicoechea, M. G. Santa-Maria, E. Bron, D. Teyssier, N. Marcelino, J. Cernicharo, S. Cuadrado

Young massive stars regulate the physical conditions, ionization, and fate of their natal molecular cloud. It is important to find tracers that help quantifying the stellar feedback processes that take place at different spatial scales. We present ~85 arcmin^2 velocity-resolved maps of several submm molecular lines toward the closest high-mass star-forming region, OMC-1. The observed rotational lines include probes of warm and dense molecular gas that are difficult to detect from ground-based telescopes: CH+ (1-0), CO (10-9), HCO+ (6-5), and HCN (6-5). These lines trace a thin but very extended layer of molecular gas at high thermal pressure, P_th ~ 1e7-1e9 K/cm3, associated with the FUV-irradiated surface of OMC-1. The intense FUV field - emerging from massive stars in the Trapezium cluster - heats, compresses and photoevaporates the cloud edge. It also triggers the formation of reactive molecules such as CH+. The CH+ (1-0) emission spatially correlates with the flux of FUV photons impinging the cloud: G_0 from 1e3 to 1e5. This correlation is supported by isobaric PDR models in the parameter space P_th/G_0 ~ [5e3-8e4] K/cm3 where many PDRs seem to lie. The CH+ (1-0) emission correlates with the extended emission from vibrationally excited H2, and with that of [CII]158um and CO 10-9, all emerging from FUV-irradiated gas. These correlations link the presence of CH+ to the availability of C+ ions and of FUV-pumped H2(v>0) molecules. The parsec-scale CH+ emission and narrow-line (dv ~ 3 km/s) mid-J CO emission arises from extended PDRs and not from fast shocks. PDR line tracers are the smoking gun of the stellar feedback from young massive stars. The PDR component in OMC-1 represents 5 to 10% of the total gas mass, however, it dominates the emitted line luminosity. These results provide insights into the source of submm CH+ and mid-J CO emission from distant star-forming galaxies.

2019, A&A., 622, 91
DOI: [10.1051/0004-6361/201834409](10.1051/0004-6361/201834409)
Full-text URL: https://arxiv.org/abs/1812.00821

An ALMA view of CS and SiS around oxygen-rich AGB stars

T. Danilovich, A. M. S. Richards, A. I. Karakas, M. Van de Sande, L. Decin and F. De Ceuster

We aim to determine the distributions of molecular SiS and CS in the circumstellar envelopes of oxygen-rich asymptotic giant branch stars and how these distributions differ between stars that lose mass at different rates. In this study, we analyse ALMA observations of SiS and CS emission lines for three oxygen-rich galactic AGB stars: IK Tau, with a moderately high mass-loss rate of 5e−6 M⊙/yr, and W Hya and R Dor with low mass-loss rates of ∼1e−7 M⊙/yr. These molecules are usually more abundant in carbon stars but the high sensitivity of ALMA allows us to detect their faint emission in the low mass-loss rate AGB stars. The high spatial resolution of ALMA also allows us to precisely determine the spatial distribution of these molecules in the circumstellar envelopes. We run radiative transfer models to calculate the molecular abundances and abundance distributions for each star. We find a spread of peak SiS abundances with ∼1e−8 for R Dor,

∼1e−7 for W Hya, and ∼3e−6 for IK Tau relative to H2. We find lower peak CS abundances of ∼7e−9 for R Dor, ∼7e−8 for W Hya, and ∼4e−7 for IK Tau, with some stratifications in the abundance distributions. For IK Tau, we also calculate abundances for the detected isotopologues: C34S, 29SiS, 30SiS, Si33S, Si34S, 29Si34S, and 30Si34S. Overall, the isotopic ratios we derive for IK Tau suggest a lower metallicity than solar.

MNRAS 484, 494–509 (2019)
DOI: 10.1093/mnras/stz002
Full-text URL: https://arxiv.org/abs/1901.00070

Methyl cyanide (CH3CN) and propyne (CH3CCH) in the low-mass protostar IRAS 16293-2422

Andron, Inès; Gratier, Pierre; Majumdar, Liton; Vidal, Thomas H. G.; Coutens, Audrey; Loison, Jean-Christophe; Wakelam, Valentine

Methyl cyanide (CH3CN) and propyne (CH3CCH) are two molecules commonly used as gas thermometers for interstellar gas. They are detected in several astrophysical environments and in particular towards protostars. Using data of the low-mass protostar IRAS 16293-2422 obtained with the IRAM 30-m single-dish telescope, we constrained the origin of these two molecules in the envelope of the source. The line shape comparison and the results of a radiative transfer analysis both indicate that the emission of CH3CN arises from a warmer and inner region of the envelope than the CH3CCH emission. We compare the observational results with the predictions of a gas-grain chemical model. Our model predicts a peak abundance of CH3CCH in the gas-phase in the outer part of the envelope, at around 2000 au from the central star, which is relatively close to the emission size derived from the observations. The predicted CH3CN abundance only rises at the radius where the grain mantle ices evaporate, with an abundance similar to the one derived from the observations.

MNRAS, Volume 481, Issue 4, p.5651-5659
DOI: 10.1093/mnras/sty2680
Full-text URL: https://arxiv.org/abs/1812.05416

Survey Observations to Study Chemical Evolution from High-Mass Starless Cores to High-Mass Protostellar Objects II. HC3N and N2H+

Kotomi Taniguchi, Masao Saito, T. K. Sridharan, Tetsuhiro Minamidani

We have carried out survey observations of molecular emission lines from HC3N, N2H+, CCS, and cyclic-C3H2 in the 81−94 GHz band toward 17 high-mass starless cores (HMSCs) and 28 high-mass protostellar objects (HMPOs) with the Nobeyama 45-m radio telescope. We have detected N2H+ in all of the target sources except one and HC3N in 14 HMSCs and in 26 HMPOs. We investigate the N(N2H+)/N(HC3N) column density ratio as a chemical evolutionary indicator of massive cores. Using the Kolmogorov-Smirnov (K-S) test and Welch's t test, we confirm that the N(N2H+)/N(HC3N) ratio decreases from HMSCs to HMPOs. This tendency in high-mass star-forming regions is opposite to that in low-mass star-forming regions. Furthermore, we found that the detection rates of carbon-chain species (HC3N, HC5N, and CCS) in HMPOs are different from those in low-mass protostars. The detection rates of cyanopolyynes (HC3N and HC5N) are higher and that of CCS is lower in high-mass protostars, compared to low-mass protostars. We discuss a possible interpretation for these differences.

2019, The Astrophysical Journal, Volume 872, Number 2
DOI: 10.3847/1538-4357/ab001e
Full-text URL: https://arxiv.org/abs/1901.06446

Electronic Transitions Responsible for C60+ Diffuse Interstellar Bands

A. O. Lykhin , S. Ahmadvand , S. A. Varganov

Despite the fact that C60+ recently became the first confirmed carrier of several diffuse interstellar bands (DIBs), the nature of the corresponding transitions is not understood. Using electronic structure methods, we show that the two strong C60+ DIBs cannot be explained by electronic transitions to the two different excited 2E1g states or the two spin–orbit components of the lowest 2E1g state, as suggested before. We argue that the strong DIBs at 9632 and 9577 Å correspond to the cold excitations from the non-Franck–Condon region of the ground electronic state to the two components of the lowest 2E1g state split by Jahn–Teller distortion. The weak DIBs at 9428 and 9365 Å are assigned to the first vibronic transitions involving the low-energy vibrational modes and components of the lowest 2E1g electronic state.

J. Phys. Chem. Lett., 2019, 10 (1), pp 115–120
DOI: 10.1021/acs.jpclett.8b03534
Full-text URL: https://pubs.acs.org/doi/full/10.1021/acs.jpclett.8b03534

Organic molecules in the protoplanetary disk of DG Tau revealed by ALMA

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Planets form in protoplanetary disks and inherit their chemical compositions. It is thus crucial to map the distribution and investigate the formation of simple organics, such as formaldehyde and methanol, in protoplanetary disks. We analyze ALMA observations of the nearby disk-jet system around the T Tauri star DG Tau in the o-H2CO 3(1,2)-2(1,1) and CH3OH

3(-2,2)-4(-1,4) E, 5(0,5)-4(0,4) A transitions at an unprecedented resolution of ~0.15", i.e., ~18 au at a distance of 121 pc. The H2CO emission originates from a rotating ring extending from ~40 au with a peak at ~62 au, i.e., at the edge of the 1.3 mm dust continuum. CH3OH emission is not detected down to an r.m.s. of 3 mJy/beam in the 0.162 km/s channel. Assuming an ortho-to-para ratio of 1.8-2.8 the ring- and disk-height-averaged H2CO column density is ~0.3-4e14 cm-2, while that of CH3OH is <0.04-0.7e14 cm-2. In the inner 40 au no o-H2CO emission is detected with an upper limit on its beam-averaged column density of ~0.5-6e13 cm-2. The H2CO ring in the disk of DG Tau is located beyond the CO iceline (R(CO)~30 au). This suggests that the H2CO abundance is enhanced in the outer disk due to formation on grain surfaces by the hydrogenation of CO ice. The emission peak at the edge of the mm dust continuum may be due to enhanced desorption of H2CO in the gas phase caused by increased UV penetration and/or temperature inversion. The CH3OH/H2CO abundance ratio is < 1, in agreement with disk chemistry models. The inner edge of the H2CO ring coincides with the radius where the polarization of the dust continuum changes orientation, hinting at a tight link between the H2CO chemistry and the dust properties in the outer disk and at the possible presence of substructures in the dust distribution.

8 pages, accepted on A&A Letters
DOI: 10.1051/0004-6361/201834475
Full-text URL: https://arxiv.org/abs/1902.02720

Statistical study of uncertainties in the diffusion rate of species on interstellar ice and its impact on chemical model predictions

Iqbal, Wasim; Wakelam, Valentine; Gratier, Pierre

Context. Diffusion of species on the dust surface is a key process for determining the chemical composition of interstellar ices. On the dust surface, adsorbed species diffuse from one potential well to another and react with other adsorbed reactants, resulting in the formation of simple and complex molecules. Aims: We study the impact on the abundances of the species simulated by the chemical codes by considering the uncertainties in the diffusion energy of adsorbed species. We aim to limit the uncertainties in the abundances as calculated by chemical codes by identifying the surface species that result in a larger error because of the uncertainties in their diffusion energy. Methods: We ran various cases with 2000-10 000 simulations in each case and varied the diffusion energies of some or all surface species randomly. We calculated Pearson correlation coefficients between the abundances and the ratio of diffusion to binding energy of adsorbed species. We identified the species that introduce maximum uncertainty in the ice and gas-phase abundances. With these species we ran three sets, with 2000 simulations in each, to quantify the uncertainties they introduce. Results: We present the abundances of various molecules in the gas phase and also on the dust surface at different time intervals during the simulation. We show which species produce a large uncertainty in the abundances. We sorted species into different groups in accordance with their importance in propagating uncertainty in the chemical network. Conclusions: We show that CO, H2, O, N, and CH3 are the key species for uncertainties in the abundances, while CH2, HCO, S and O2 come next, followed by NO, HS, and CH. We also show that by limiting the uncertainties in the ratio of diffusion to binding energy of these species, we can eliminate the uncertainties in the gas-phase abundances of almost all the species.

A&A, Volume 620, December 2018
DOI: 10.1051/0004-6361/201833804
Full-text URL: https://arxiv.org/abs/1811.03488

ALMA Autocorrelation Spectroscopy of Comets: The HCN/H13CN Ratio in C/2012 S1 (ISON)

M. A. Cordiner, M. Y. Palmer, M. de Val-Borro, S. B. Charnley, L. Paganini, G. Villanueva, D. Bockelée-Morvan, N. Biver, A. Remijan, Y.-J Kuan, S. N. Milam, J. Crovisier, D. C. Lis, M. J. Mumma

The Atacama Large Millimeter/submillimeter Array (ALMA) is a powerful tool for high-resolution mapping of comets, but the main interferometer (comprised of 50 × 12 m antennas) is insensitive to the largest coma scales due to a lack of very short baselines. In this Letter, we present a new technique employing ALMA autocorrelation data (obtained simultaneously with the interferometric observations), effectively treating the entire 12 m array as a collection of single-dish telescopes. Using combined autocorrelation spectra from 28 active antennas, we recovered extended HCN coma emission from comet C/2012 S1 (ISON), resulting in a fourteen-fold increase in detected line brightness compared with the interferometer. This resulted in the first detection of rotational emission from H13CN in this comet. Using a detailed coma radiative transfer model accounting for optical depth and non-local thermodynamic equilibrium excitation effects, we obtained an H12CN/H13CN ratio of 88 ± 18, which matches the terrestrial value of 89. This is consistent with a lack of isotopic fractionation in HCN during comet formation in the protosolar accretion disk. The possibility of future discoveries in extended sources using autocorrelation spectroscopy from the main ALMA array is thus demonstrated.

2019, ApJ, 870, L26
DOI: 10.3847/2041-8213/aafb05
Full-text URL: https://arxiv.org/abs/1901.08676

Announcements

Celebrating the First 40 Years of Alexander Tielens’ Contribution to Science: the Physics and Chemistry of the ISM

https://tielens2019.sciencesconf.org/
Venue
The symposium will be held 2—6 September 2019 in the historical Congres du Palais des Papes, Avignon, France (http://www.avignon-congres.com/).
Rational
Xander Tielens has been driving research in the fields of interstellar physics and chemistry and the cosmic cycle of matter with outstanding contributions for 40 years. With this meeting, we wish to celebrate his scientific achievements and discuss future research directions opened up by his contributions.
The meeting will focus on the fields strongly influenced by Xander involving the physical and chemical processes that control the interstellar medium and its life cycle: PDRs, interstellar and circumstellar dust, PAHs, ices and astrochemistry. We will especially emphasize future opportunities offered by the powerful telescopes at our disposal such as, for example, ALMA, SOFIA, and JWST.
The meeting will consist of invited reviews, invited and contributed talks, and posters.
Key dates
February 11: Opening of the registration and abstract submission on the symposium website
June 1: Deadline of Abstract submission for oral contributions
June 15: Announcement of the selected oral contributions
June 20: Deadline of registration
Please note that the symposium participation is restricted to 120 persons, based on first-signed first-selected, so do not delay your registration!
Confirmed invited speakers
L. Allamandola, N. Balucani, A. Boogert, F. Boulanger, S. Cazaux, J. Cernicharo, L. d'Hendecourt, T. de Graauw, J. Goicoechea, H. Habing, D. Hollenbach, C. Joblin, B. Lefloch, M. Kaufman, C. Kemper, M. Meixner, T. Millar, T. Onaka, M-E. Palumbo, E. Roueff, K. Schuster, E. van Dishoeck, R. Waters
Scientific Organizing Committee
C. Ceccarelli (chair), A. Candian (co-chair), J. Cami, C. Dominik, L. Hornekaer, K. Justtanont, E. Peeters, M. Wolfire
Local Organizing Committee
B. Lefloch (chair), E. Bianchi, C. Borye, M. Bouvier, M. De Simone, M-H Sztefek
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Symposium "The Periodic Table Through Space and Time'' September 9-13 of 2019, Saint-Petersburg (Russia)

The 2019 year is claimed as the International Year of the Periodic Table of Chemical Elements. This initiative was supported by many international organizations, including the International Astronomical Union (IAU). In September 9-13 of 2019, Saint-Petersburg (Russia) hosts the XXI Jubilee Mendeleev Congress on General and Applied Chemistry (http://mendeleev2019.ru/index.php/en/). During this Congress, in Sept. 10-13 of 2019, we hold the Symposium "The Periodic Table Through Space and Time''.

Main topics of the Symposium are:
- Big Bang and stellar nucleosynthesis
- Chemical evolution of the Universe: observations and models
- Astrochemistry
- Elemental abundances: a key to stellar physics

Invited speakers: to be confirmed.

Scientific Organizing Committee:
Ewine van DISHOECK (The Netherlands, Co-Chair), Boris SHUSTOV (Co-Chair, Russia), Lyudmila MASHONKINA (Russia, Scientific Secretary), Sergey BLINNIKOV(Russia), John COWAN (USA), Charles Cowley (USA), Alexander DOLGOV (Russia), Nicolas GREVESSE (Belgium), John LANDSTREET (Canada), Alexander LUTOVINOV (Russia), Ken'ichi NOMOTO (Japan), Nikos PRANTZOS (France), Friedrich-Karl THIELEMANN (Switzerland), Dmitry WIEBE (Russia), Gang ZHAO (China).

On behalf of the Organizing Committee of Congress and the SOC of the Symposium we are pleased to invite academic and university researchers, postgraduate students, and students to participate in the Symposium "The Periodic Table Through Space and Time''.

The online registration and abstracts submission is now opened!
The guidelines and abstract template can be found on the Congress website page
http://mendeleev2019.ru/index.php/en/about-the-event-3/abstracts

Please note that timely registration is essential to ensure that visa formalities can be completed in due time.

For questions related to the Symposium, you may contact us via e-mail: mendeleev150@inasan.ru

Postdoc position available for Doctors in Chemistry or Physics

A Postdoc Position is available at University of Castilla-La Mancha (UCLM). Department of Physical Chemistry. Ciudad Real

(Spain).
The postdoc is funded by the European project: Gas and Dust from the Stars to the Laboratory: Exploring the NANOCOSMOS (ERC-2013-SyG Grant Agreement nº 610256).
http://www.icmm.csic.es/nanocosmos/

The main objective is: Measurement of Rate Coefficients of Radical-Molecule Reactions in the Gas-phase At Ultra-low Temperatures Using A Pulsed CRESU (Uniform Supersonic Flow) System Coupled to Pulsed Laser Photolysis and Laser Induced Fluorescence.

Duration is up to July 2020.
Preferred experience: spectroscopy, gases, lasers, programming.
Send your CV and two reference letters to Dr. E. Jiménez (Elena.Jimenez@uclm.es).