

# AstroChemical Newsletter #3

January 2016

Happy New Year and best wishes for 2016. You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter

## Abstracts

### Cyanide Photochemistry and Nitrogen Fractionation in the MWC 480 Disk

V.V. Guzmán, K.I. Öberg, R. Loomis, C. Qi

HCN is a commonly observed molecule in Solar System bodies and in interstellar environments. Its abundance with respect to CN is a proposed tracer of UV exposure. HCN is also frequently used to probe the thermal history of objects, by measuring its degree of nitrogen fractionation. To address the utility of HCN as a probe of disks, we present Atacama Large (sub-) Millimeter Array observations of CN, HCN, H<sup>13</sup>CN, and HC<sup>15</sup>N toward the protoplanetary disk around Herbig Ae star MWC 480, and of CN and HCN toward the disk around T Tauri star DM Tau. Emission from all molecules is clearly detected and spatially resolved, including the first detection of HC<sup>15</sup>N in a disk. Toward MWC 480, CN emission extends radially more than 1" exterior to the observed cut-off of HCN emission. Quantitative modeling further reveals very different radial abundance profiles for CN and HCN, with best-fit outer cut-off radii of >300 AU and 110 ± 10 AU, respectively. This result is in agreement with model predictions of efficient HCN photodissociation into CN in the outer-part of the disk where the vertical gas and dust column densities are low. No such difference in CN and HCN emission profiles are observed toward DM Tau, suggestive of different photochemical structures in Herbig Ae and T Tauri disks. We use the HCN isotopologue data toward the MWC 480 disk to provide the first measurement of the <sup>14</sup>N/<sup>15</sup>N ratio in a disk. We find a low disk averaged <sup>14</sup>N/<sup>15</sup>N ratio of 200 ± 100, comparable to what is observed in cloud cores and comets, demonstrating interstellar inheritance and/or efficient nitrogen fractionation in this disk.

The Astrophysical Journal, Volume 814, Issue 1, article id. 53, 7 pp. (2015)

DOI: [10.1088/0004-637X/814/1/53](https://doi.org/10.1088/0004-637X/814/1/53)

Full-text URL: <http://iopscience.iop.org/article/10.1088/0004-637X/814/1/53/meta>

### Synthesis of formamide and isocyanic acid after ion irradiation of frozen gas mixtures

Z. Kanuchova, R.G. Urso, G.A. Baratta, J.R. Brucato, M.E. Palumbo and G. Strazzulla

Formamide (NH<sub>2</sub>HCO) and isocyanic acid (HNCO) have been observed as gaseous species in several astronomical environments such as cometary comae and pre- and protostellar objects. A debate is open on the formation route of those molecules, in particular if they are formed by chemical reactions in the gas phase and/or on grains. In this latter case it is relevant to understand if the formation occurs through surface reactions or is induced by energetic processing. We present arguments that support the formation of formamide in the solid phase by cosmic-ion-induced energetic processing of ices present as mantles of interstellar grains and on comets. Formamides, along with other molecules, are expelled in the gas phase when the physical parameters are appropriate to induce the desorption of ices. We have performed several laboratory experiments in which ice mixtures (H<sub>2</sub>O:CH<sub>4</sub>:N<sub>2</sub>, H<sub>2</sub>O:CH<sub>4</sub>:NH<sub>3</sub>, and CH<sub>3</sub>OH:N<sub>2</sub>) were bombarded with energetic (30–200 keV) ions (H<sup>+</sup> or He<sup>+</sup>). FTIR spectroscopy was performed before, during, and after ion bombardment. In particular, the formation of HNCO and NH<sub>2</sub>HCO was measured quantitatively. Energetic processing of ice can quantitatively reproduce the amount of NH<sub>2</sub>HCO observed in cometary comae and in many circumstellar regions. HNCO is also formed, but additional formation mechanisms are requested to quantitatively account for the astronomical observations. We suggest that energetic processing of ices in the pre- and proto-stellar regions and in comets is the main mechanism to produce formamide, which, once it is released in the gas phase because of desorption of ices, is observed in the gas phase in these astrophysical environments.

Astronomy & Astrophysics, in press

DOI: [10.1051/0004-6361/201527138](https://doi.org/10.1051/0004-6361/201527138)

Full-text URL: <http://dx.doi.org/10.1051/0004-6361/201527138>

### Deuterium Fractionation in the Ophiuchus Molecular Cloud

A. Punanova, P. Caselli, A. Pon, A. Belloche, Ph. Andre

**Aims.** We measure the deuterium fraction, RD, and the CO-depletion factor, fd, toward a number of starless and protostellar cores in the L1688 region of the Ophiuchus molecular cloud complex and search for variations based upon environmental differences across L1688. The kinematic properties of the dense gas traced by the N<sub>2</sub>H<sup>+</sup> and N<sub>2</sub>D<sup>+</sup> (1-0) lines are also discussed. **Methods.** RD has been measured via observations of the J=1-0 transition of N<sub>2</sub>H<sup>+</sup> and N<sub>2</sub>D<sup>+</sup> toward 33 dense cores in different regions of L1688. fd estimates have been done using C<sup>17</sup>O(1-0) and 850 micron dust continuum emission from the SCUBA survey. All line observations were carried out with the IRAM 30 meter antenna. **Results.** The dense cores show large (2-40%) deuterium fractions, with significant variations between the sub-regions of L1688. The CO-depletion factor also varies from one region to another (1-7). Two different correlations are found between deuterium fraction and CO-

depletion factor: cores in regions A, B2 and I show increasing RD with increasing fd, similar to previous studies of deuterium fraction in pre-stellar cores; cores in regions B1, B1B2, C, E, F and H show a steeper RD-fd correlation, with large deuterium fractions occurring in fairly quiescent gas with relatively low CO freeze-out factors. These are probably recently formed, centrally concentrated starless cores which have not yet started the contraction phase toward protostellar formation. We also find that the deuterium fraction is affected by the amount of turbulence, dust temperature and distance from heating sources in all regions of L1688, although no clear trend is found.

Accepted for publication in A&A

Full-text URL: <http://arxiv.org/abs/1512.02986>

## Reconstructing the history of water ice formation from HDO/H<sub>2</sub>O and D<sub>2</sub>O/HDO ratios in protostellar cores

K. Furuya, E. F. van Dishoeck, Y. Aikawa

Recent interferometer observations have found that the D<sub>2</sub>O/HDO abundance ratio is higher than that of HDO/H<sub>2</sub>O by about one order of magnitude in the vicinity of low-mass protostar NGC 1333-IRAS 2A, where water ice has sublimated. Previous laboratory and theoretical studies show that the D<sub>2</sub>O/HDO ice ratio should be lower than the HDO/H<sub>2</sub>O ice ratio, if HDO and D<sub>2</sub>O ices are formed simultaneously with H<sub>2</sub>O ice. In this work, we propose that the observed feature, D<sub>2</sub>O/HDO > HDO/H<sub>2</sub>O, is a natural consequence of chemical evolution in the early cold stages of low-mass star formation: 1) majority of oxygen is locked up in water ice and other molecules in molecular clouds, where water deuteration is not efficient, and 2) water ice formation continues with much reduced efficiency in cold prestellar/protostellar cores, where deuteration processes are highly enhanced due to the drop of the ortho-para ratio of H<sub>2</sub>, the weaker UV radiation field, etc. Using a simple analytical model and gas-ice astrochemical simulations tracing the evolution from the formation of molecular clouds to protostellar cores, we show that the proposed scenario can quantitatively explain the observed HDO/H<sub>2</sub>O and D<sub>2</sub>O/HDO ratios. We also find that the majority of HDO and D<sub>2</sub>O ices are likely formed in cold prestellar/protostellar cores rather than in molecular clouds, where the majority of H<sub>2</sub>O ice is formed. This work demonstrates the power of the combination of the HDO/H<sub>2</sub>O and D<sub>2</sub>O/HDO ratios as a tool to reveal the past history of water ice formation in the early cold stages of star formation and when the enrichment of deuterium in the bulk of water occurred. Further observations are needed to explore if the relation, D<sub>2</sub>O/HDO > HDO/H<sub>2</sub>O, is common in low-mass protostellar sources.

Accepted by A&A

Full-text URL: <http://arxiv.org/abs/1512.04291>

## Exploring molecular complexity with ALMA (EMoCA): Alkanethiols and alkanols in Sagittarius B2(N<sub>2</sub>)

H. S. P. Müller, A. Belloche, L.-H. Xu, R. M. Lees, R. T. Garrod, A. Walters, J. van Wijngaarden, F. Lewen, S. Schlemmer, K. M. Menten

Over the past five decades, radio astronomy has shown that molecular complexity is a natural outcome of interstellar chemistry, in particular in star forming regions. However, the pathways that lead to the formation of complex molecules are not completely understood and the depth of chemical complexity has not been entirely revealed. In addition, the sulfur chemistry in the dense interstellar medium is not well understood. We want to know the relative abundances of alkanethiols and alkanols in the Galactic center source Sagittarius B2(N<sub>2</sub>), the northern hot molecular core in Sgr B2(N), whose relatively small line widths are favorable for studying the molecular complexity in space. We investigated spectroscopic parameter sets that were able to reproduce published laboratory rotational spectra of ethanethiol and studied effects that modify intensities in the predicted rotational spectrum of ethanol. We used the Atacama Large Millimeter Array (ALMA) in its Cycles-0 and 1 for a spectral line survey of Sagittarius B2(N) between 84 and 114.4 GHz. These data were analyzed by assuming local thermodynamic equilibrium (LTE) for each molecule. Our observations are supplemented by astrochemical modeling; a new network is used for the first time that includes reaction pathways for alkanethiols. We detected methanol and ethanol in their parent <sup>12</sup>C species and those with one <sup>12</sup>C atom substituted by <sup>13</sup>C; the latter were detected for the first time unambiguously in the case of ethanol. The <sup>12</sup>C/<sup>13</sup>C ratio is ~25 for both molecules. In addition, we identified CH<sub>3</sub>(<sup>18</sup>O)OH with a <sup>16</sup>O/<sup>18</sup>O ratio of ~180 and a (<sup>13</sup>)CH<sub>3</sub>OH/CH<sub>3</sub>(<sup>18</sup>O)OH ratio of ~7.3. Upper limits were derived for the next larger alkanols normal- and iso-propanol. We observed methanethiol, CH<sub>3</sub>SH, also known as methyl mercaptan, including torsionally excited transitions for the first time. We also identified transitions of ethanethiol (or ethyl mercaptan), though not enough to claim a secure detection in this source. The ratios CH<sub>3</sub>SH to C<sub>2</sub>H<sub>5</sub>SH and C<sub>2</sub>H<sub>5</sub>OH to C<sub>2</sub>H<sub>5</sub>SH are > ~21 and > ~125, respectively. In the process of our study, we noted severe discrepancies in the intensities of observed and predicted ethanol transitions and propose a change in the relative signs of the dipole moment components. In addition, we determined alternative sets of spectroscopic parameters for ethanethiol. The astrochemical models indicate that substantial quantities of both CH<sub>3</sub>SH and C<sub>2</sub>H<sub>5</sub>SH may be produced on the surfaces of dust grains, to be later released into the gas phase. The modeled ratio CH<sub>3</sub>SH/C<sub>2</sub>H<sub>5</sub>SH = 3.1 is lower than the observed value of > ~21; the model value appears to be affected most by the underprediction of CH<sub>3</sub>SH relative to CH<sub>3</sub>OH and C<sub>2</sub>H<sub>5</sub>OH, as judged by a very high CH<sub>3</sub>OH/CH<sub>3</sub>SH ratio. The column density ratios involving methanol, ethanol, and methanethiol in Sgr B2(N<sub>2</sub>) are similar to values reported for Orion KL, but those involving ethanethiol are significantly different and suggest that the detection of ethanethiol reported toward Orion KL is uncertain. Our chemical model presently does not permit the prediction of sufficiently accurate column densities of alkanethiols or their ratios among alkanethiols and alkanols. Therefore, additional observational results are required to establish the level of C<sub>2</sub>H<sub>5</sub>SH in the dense and warm interstellar medium with certainty.

Astron. Astrophys., 2015; accepted

DOI: [10.1051/0004-6361/201527470](https://doi.org/10.1051/0004-6361/201527470)  
Full-text URL: <http://arxiv.org/abs/1512.05301>

## Rotational spectra of isotopic species of methyl cyanide, CH<sub>3</sub>CN, in their v<sub>8</sub> = 1 excited vibrational states

H. S. P. Müller, B. J. Drouin, J. C. Pearson, M. H. Ordu, N. Wehres, F. Lewen

Methyl cyanide is an important trace molecule in space, especially in star-forming regions where it is one of the more common molecules used to derive kinetic temperatures. We want to obtain accurate spectroscopic parameters of minor isotopologs of methyl cyanide in their lowest excited v<sub>8</sub> = 1 vibrational states to support astronomical observations, in particular, with interferometers such as ALMA. The laboratory rotational spectrum of methyl cyanide in natural isotopic composition has been recorded from the millimeter to the terahertz regions. Transitions with good signal-to-noise ratios could be identified for the three isotopic species CH<sub>3</sub>(<sup>13</sup>C)N, (<sup>13</sup>C)CH<sub>3</sub>CN, and CH<sub>3</sub>C(<sup>15</sup>N) up to about 1.2 THz (J" ≤ 66). Accurate spectroscopic parameters were obtained for all three species. The present data were already instrumental in identifying v<sub>8</sub> = 1 lines of methyl cyanide with one (<sup>13</sup>C) in IRAM 30 m and ALMA data toward Sagittarius B2(N).

Astron. Astrophys., 2015, accepted  
Full-text URL: <http://arxiv.org/abs/1512.05271>

## Methyl Acetate and Its Singly Deuterated Isotopomers in the Interstellar Medium

Das, Ankan; Majumdar, Liton; Sahu, Dipen; Gorai, Prasanta; Sivaraman, B.; Chakrabarti, Sandip K.

Methyl acetate (CH<sub>3</sub>COOCH<sub>3</sub>) has been recently observed by the IRAM 30 m radio telescope in Orion, though the presence of its deuterated isotopomers is yet to be confirmed. We therefore study the properties of various forms of methyl acetate, namely, CH<sub>3</sub>COOCH<sub>3</sub>, CH<sub>2</sub>DCOOCH<sub>3</sub>, and CH<sub>3</sub>COOCH<sub>2</sub>D. Our simulation reveals that these species could be produced efficiently in both gas and ice phases. Production of methyl acetate could follow radical-radical reaction between acetyl (CH<sub>3</sub>CO) and methoxy (CH<sub>3</sub>O) radicals. To predict abundances of CH<sub>3</sub>COOCH<sub>3</sub> along with its two singly deuterated isotopomers and its two isomers (ethyl formate and hydroxyacetone), we prepare a gas-grain chemical network to study the chemical evolution of these molecules. Since gas-phase rate coefficients for methyl acetate and its related species are unknown, either we consider similar rate coefficients for similar types of reactions (by following existing databases) or we carry out quantum chemical calculations to estimate the unknown rate coefficients. For the surface reactions, we use adsorption energies of reactants from some earlier studies. Moreover, we perform quantum chemical calculations to obtain spectral properties of methyl acetate in infrared and sub-millimeter regions. We prepare two catalog files for the rotational transitions of CH<sub>2</sub>DCOOCH<sub>3</sub> and CH<sub>3</sub>COOCH<sub>2</sub>D in JPL format, which could be useful for their detection in regions of interstellar media where CH<sub>3</sub>COOCH<sub>3</sub> has already been observed.

2015, ApJ, 808, 21  
DOI: [10.1088/0004-637X/808/1/21](https://doi.org/10.1088/0004-637X/808/1/21)  
Full-text URL: <http://iopscience.iop.org/article/10.1088/0004-637X/808/1/21/meta>

## First evidence of the dramatic enhancement of the reactivity of methyl formate (HC(O)OCH<sub>3</sub>) with OH at temperatures of the interstellar medium: A gas-phase kinetic study between 22 K and 64 K

E. Jiménez, M. Antiñolo, B. Ballesteros, A. Canosa, and J. Albaladejo

Gas-phase chemistry of neutral-neutral reactions of interest in the interstellar medium (ISM) is poorly-understood. The rate coefficients (k<sub>OH</sub>) for the majority of the reactions of hydroxyl (OH) radicals with interstellar oxygenated species are unknown at temperatures of the ISM. In this work, we present the first determination of k<sub>OH</sub> for HC(O)OCH<sub>3</sub> between (22.4±1.4) and (64.2±1.7)K. The CRESU (French acronym for Cinétique de Réaction en Ecoulement Supersonique Uniforme or Reaction Kinetics in a Uniform Supersonic Flow) technique was used to create a chemical reactor with a uniform temperature and gas density and the pulsed laser photolysis/laser induced fluorescence technique was used to generate OH radicals and to monitor their temporal profile. It was observed that k<sub>OH</sub>(T) increases one order of magnitude in only about 40K (k<sub>OH</sub>(T=22K)=(1.19±0.36)×10<sup>-10</sup> cm<sup>3</sup>s<sup>-1</sup> and k<sub>OH</sub>(T=64K)=(1.16±0.12)×10<sup>-11</sup> cm<sup>3</sup>s<sup>-1</sup>), and about 3 orders of magnitude with respect to k<sub>OH</sub>(T=298K). This reaction is a very efficient loss route for HC(O)OCH<sub>3</sub> in the gas phase and may have a great impact on the interpretation by astrophysical models of the HC(O)OCH<sub>3</sub> abundances in cold regions of the ISM.

Physical Chemistry Chemical Physics (PCCP), accepted  
DOI: [10.1039/c5cp06369h](https://doi.org/10.1039/c5cp06369h)  
Full-text URL: <http://pubs.rsc.org/en/content/articlelanding/2015/cp/c5cp06369h#!divAbstract>

## An optical spectrum of a large isolated gas-phase PAH cation: C<sub>78</sub>H<sub>26</sub><sup>+</sup>

Junfeng Zhen, Giacomo Mulas, Anthony Bonnamy, Christine Joblin,

A gas-phase optical spectrum of a large polycyclic aromatic hydrocarbon (PAH) cation C<sub>78</sub>H<sub>26</sub><sup>+</sup> in the 410-610 nm range is presented. This large all-benzenoid PAH should be large enough to be stable with respect to photodissociation in the harsh conditions prevailing in the interstellar medium (ISM). The spectrum is obtained via multi-photon dissociation (MPD) spectroscopy of cationic C<sub>78</sub>H<sub>26</sub> stored in the Fourier Transform Ion Cyclotron Resonance (FT-ICR) cell using the radiation

from a mid-band optical parametric oscillator (OPO) laser. The experimental spectrum shows two main absorption peaks at 431 nm and 516 nm, in good agreement with a theoretical spectrum computed via time-dependent density functional theory (TD-DFT). DFT calculations indicate that the equilibrium geometry, with the absolute minimum energy, is of lowered, nonplanar C<sub>2</sub> symmetry instead of the more symmetric planar D<sub>2h</sub> symmetry that is usually the minimum for similar PAHs of smaller size. This kind of slightly broken symmetry could produce some of the fine structure observed in some diffuse interstellar bands (DIBs). It can also favor the folding of C<sub>78</sub>H<sub>26</sub><sup>+</sup> fragments and ultimately the formation of fullerenes. This study opens up the possibility to identify the most promising candidates for DIBs amongst large cationic PAHs.

Accepted in Molecular Astrophysics

DOI: [10.1016/j.molap.2015.11.001](https://doi.org/10.1016/j.molap.2015.11.001)

Full-text URL: <http://www.sciencedirect.com/science/article/pii/S2405675815300105>

## Implication of Formation Mechanisms of HC<sub>5</sub>N in TMC-1 as Studied by <sup>13</sup>C Isotopic Fractionation

Kotomi Taniguchi, Hiroyuki Ozeki, Masao Saito, Nami Sakai, Fumitaka Nakamura, Seiji Kamenno, Shuro Takano, and Satoshi Yamamoto

We observed the J = 9-8 and 16-15 rotational transitions of the normal species and five <sup>13</sup>C isotopologues of HC<sub>5</sub>N to study its formation mechanisms toward the cyanopolyne peak in Taurus Molecular Cloud-1, with the 45-m radio telescope of Nobeyama Radio Observatory. We detected the five <sup>13</sup>C isotopologues with high signal-to-noise ratios between 12 and 20, as well as the normal species. The abundance ratios of the five <sup>13</sup>C isotopologues of HC<sub>5</sub>N are found to be 1.00:0.97:1.03:1.05:1.16 (0.19) for [H<sup>13</sup>C<sub>5</sub>N]:[HC<sup>13</sup>C<sub>4</sub>N]:[HCC<sup>13</sup>C<sub>3</sub>N]:[HCCC<sup>13</sup>C<sub>2</sub>N]:[HCCCC<sup>13</sup>CN]. We do not find any significant differences among the five <sup>13</sup>C isotopologues. The averaged [HC<sub>5</sub>N]/[<sup>13</sup>C isotopologues] abundance ratio is determined to be 94 (6), which is slightly higher than the local interstellar elemental <sup>12</sup>C/<sup>13</sup>C ratio of 60-70. Possible formation pathways are discussed on the basis of these results.

Accepted for publication in ApJ

Full-text URL: <http://arxiv.org/abs/1512.05783?context=astro-ph.SR>

## Thermal formation of hydroxynitriles, precursors of hydroxyacids in astrophysical ice analogs: Acetone ((CH<sub>3</sub>)<sub>2</sub>CO) and hydrogen cyanide (HCN) reactivity

Aurélien Fresneau, Grégoire Danger, Albert Rimola, Fabrice Duvernay, Patrice Theulé, Thierry Chiavassa

Reactivity in astrophysical environments is still poorly understood. In this contribution, we investigate the thermal reactivity of interstellar ice analogs containing acetone ((CH<sub>3</sub>)<sub>2</sub>CO), ammonia (NH<sub>3</sub>), hydrogen cyanide (HCN) and water (H<sub>2</sub>O) by means of infrared spectroscopy and mass spectrometry techniques, complemented by quantum chemical calculations. We show that no reaction occurs in H<sub>2</sub>O:HCN:(CH<sub>3</sub>)<sub>2</sub>CO ices. Nevertheless, HCN does indeed react with acetone once activated by NH<sub>3</sub> into CN<sup>-</sup> to form 2-hydroxy-2-methylpropanenitrile (HOC(CH<sub>3</sub>)<sub>2</sub>CN), with a calculated activation energy associated with the rate determining step of about 51 kJ mol<sup>-1</sup>. This reaction inhibits the formation of 2-aminopropan-2-ol (HOC(CH<sub>3</sub>)<sub>2</sub>NH<sub>2</sub>) from acetone and NH<sub>3</sub>, even in the presence of water, which is the first step of the Strecker synthesis to form 2-aminoisobutyric acid (NH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>COOH). However, HOC(CH<sub>3</sub>)<sub>2</sub>CN formation could be part of an alternative chemical pathway leading to 2-hydroxy-2-methyl-propanoic acid (HOC(CH<sub>3</sub>)<sub>2</sub>COOH), which could explain the presence of hydroxy acids in some meteorites.

Molecular Astrophysics, Volume 1, November 2015, Pages 1–12

DOI: [10.1016/j.molap.2015.10.001](https://doi.org/10.1016/j.molap.2015.10.001)

Full-text URL: <http://www.sciencedirect.com/science/article/pii/S240567581530004X>

## Ion-neutral reaction of the C<sub>2</sub>H<sub>2</sub>N<sup>+</sup> cation with C<sub>2</sub>H<sub>2</sub>: an experimental and theoretical study

P. Fathi, W.D. Geppert, A. Kaiser, D. Ascenzi

The ion-neutral reactions of the C<sub>2</sub>H<sub>2</sub>N<sup>+</sup> cation with C<sub>2</sub>H<sub>2</sub> have been investigated using Guided Ion Beam Mass Spectrometer (GIB-MS). The following ionic products were observed: CH<sub>3</sub><sup>+</sup>, C<sub>2</sub>H<sub>2</sub><sup>+</sup>, C<sub>2</sub>H<sub>3</sub><sup>+</sup>, HNC<sup>+</sup>/HCN<sup>+</sup>, HCNH<sup>+</sup>, C<sub>3</sub>H<sup>+</sup>, C<sub>2</sub>N<sup>+</sup>, C<sub>3</sub>H<sub>3</sub><sup>+</sup>, HCCN<sup>+</sup> and C<sub>4</sub>H<sub>2</sub>N<sup>+</sup>. Theoretical calculations have been carried out to propose reaction pathways leading to the observed products. These processes are of relevance for the generation of long chain nitrogen-containing species and they may be of interest for the chemistry of Titan's ionosphere or circumstellar envelopes.

Molecular Astrophysics, Article in Press, accepted manuscript

DOI: [10.1016/j.molap.2015.09.002](https://doi.org/10.1016/j.molap.2015.09.002)

Full-text URL: <http://www.sciencedirect.com/science/article/pii/S2405675815300063>

## Multiple Carbon Monoxide Snow-lines in Disks Sculpted by Radial Drift

L. Ilseidore Cleaves

Observations of protoplanetary disks suggest that the gas and dust follow significantly different radial distributions. This finding can be theoretically explained by a combination of radial drift and gas drag of intermediate-sized dust grains. Using a simple parametric model to approximate the different distributions of the gas and dust components, we calculate and examine the impact of radial drift on the global dust temperature structure. We find that the removal of large grains beyond the "truncation radius" allows this region to become significantly warmer from reprocessed stellar radiation shining down

from the disk upper layers, increasing the outer disk temperature by  $\sim 10\text{--}30\%$ . This change is sufficient to raise the local temperature to a value exceeding the CO desorption temperature. These findings imply that the disk density structures induced by radial drift are able to create multiple CO snow-lines. The inner disk CO is in the gas phase, freezing out near the classical snow-line at  $R \sim 20\text{--}40$  AU. Moving outward, the CO sublimates once again beyond the truncation radius (80 AU in our models) and subsequently re-freezes out at sufficiently large stellar distances, beyond  $R \geq 130\text{--}200$  AU. We find that thermal desorption of CO in the outer disk becomes competitive with external UV photodesorption and that this additional transition from solid state CO to the gas-phase has significant implications for the C/O ratio in the outer disk.

Accepted for publication in ApJL

Full-text URL: <http://arxiv.org/abs/1512.05836>

## The Effects of Grain Size and Temperature Distributions on the Formation of Interstellar Ice Mantles

Tyler Pauly, Robin T. Garrod

Computational models of interstellar gas-grain chemistry have historically adopted a single dust-grain size of 0.1 micron, assumed to be representative of the size distribution present in the interstellar medium. Here, we investigate the effects of a broad grain-size distribution on the chemistry on dust-grain surfaces and the subsequent build-up of molecular ices on the grains, using a three-phase gas-grain chemical model of a quiescent dark cloud. We include an explicit treatment of the grain temperatures, governed both by the visual extinction of the cloud and the size of each individual grain-size population. We find that the temperature difference plays a significant role in determining the total bulk ice composition across the grain-size distribution, while the effects of geometrical differences between size populations appear marginal. We also consider collapse from a diffuse to a dark cloud, allowing dust temperatures to fall. Under the initial diffuse conditions, small grains are too warm to promote grain-mantle build-up, with most ices forming on the mid-sized grains. As collapse proceeds, the more abundant, smallest grains cool and become the dominant ice carriers; the large population of small grains means that this ice is distributed across many grains, with perhaps no more than 40 monolayers of ice each (versus several hundred assuming a single grain size). This effect may be important for the subsequent processing and desorption of the ice during the hot-core phase of star-formation, exposing a significant proportion of the ice to the gas phase, increasing the importance of ice-surface chemistry and surface-gas interactions.

Accepted for publication in ApJ; 22 pages, 10 figures

Full-text URL: <http://arxiv.org/abs/1512.06714>

## Spectroscopic variability of IRAS22272+5435

L.Zacs, F.Musaev, B.Kaminsky, Y.Pavlenko, A.Grankina, J.Sperauskas, B.Hrivnak

A time series of high-resolution spectra was observed in the optical wavelength region for the bright proto-planetary nebula IRAS22272+5435 (HD235858), along with a simultaneous monitoring of its radial velocity and BVR magnitudes. The object is known to vary in light, color, and velocity due to pulsation with a period of 132 days. The light and color variations are accompanied by significant changes in spectral features, most of which are identified as lines of carbon-bearing molecules. According to the observations, the C<sub>2</sub> Swan system and CN Red system lines are stronger near the light minimum. A photospheric spectrum of the central star was calculated using new self-consistent atmospheric models. The observed intensity variations in the C<sub>2</sub> Swan system and CN Red system lines were found to be much larger than expected if due solely to the temperature variation in the atmosphere of the pulsating star. In addition, the molecular lines are blueshifted relative to the photospheric velocity. The site of formation of the strong molecular features appears to be a cool outflow triggered by the pulsation. The variability in atomic lines seems to be mostly due variations of the effective temperature during the pulsation cycle. The profiles of strong atomic lines are split, and some of them are variable in a time scale of a week or so, probably because of shock waves in the outer atmosphere.

ApJ, vol.816, 3(14pp), 2016

DOI: [10.3847/0004-637X/816/1/3](https://doi.org/10.3847/0004-637X/816/1/3)

Full-text URL: <http://arxiv.org/abs/1511.03450>

## Announcements

### Postdoctoral Positions Reaction Dynamics, University of Hawaii at Manoa, USA

The Reaction Dynamics Group, Department of Chemistry, University of Hawai'i at Manoa, invites applications for four postdoctoral positions. The appointment period is initially for one year, but can be renewed annually based on availability of funds and satisfactory progress. The salary is competitive and commensurate with experience. Successful applicants should have a strong background in one or more of the following: experimental reaction dynamics, molecular beams, combustion chemistry, low temperature condensed phase, UHV technology, pulsed laser systems. 2 Positions: Reaction Dynamics & Combustion Chemistry (Gas Phase). The prime directive of the experiments is to investigate the formation of carbonaceous molecules (PAHs) in combustion systems exploiting crossed molecular beams along with mass spectrometry and ion imaging (Hawaii) and a pyrolytic micro reactor (Advanced Light Source, Lawrence Berkeley Laboratory). 2 Positions: Planetary Chemistry & Astrobiology (Condensed Phase). The goal of these experiments is to probe the formation of alkylphosphonic acids via interaction of ionizing radiation with low temperature interstellar and cometary analog ices. Reaction products will be probed via tunable vacuum ultraviolet photoionization of the subliming molecules. Solid

communication skills in English (written, oral), a publication record in internationally circulated, peer-reviewed journals, and willingness to work in a team are mandatory. Only self-motivated and energetic candidates are encouraged to apply. Please send a letter of interest, three letters of recommendation, CV, and publication list to Prof. Ralf I. Kaiser, Department of Chemistry, University of Hawai'i at Manoa, Honolulu, HI 96822-2275, USA [ralfk@hawaii.edu]. Applicants must demonstrate their capability to prepare manuscripts for publications independently. The review of applications will start December 15, 2015, and continues until the position is filled. A description of our current research group can be found at <http://www.chem.hawaii.edu/Bil301/welcome.html>. Examples of recent publications can be seen at *Int. Rev. Phys. Chem.* 34, 461-514 (2015). *Annu. Rev. Physical Chemistry* 66, 43-67 (2015). *The Astrophysical Journal* 814, 45 (2015). *Chemical Communications* 51, 11305-11308 (2015). *Angewandte Chemie – International Edition* 54, 5421-5424 (2015). *Angewandte Chemie – International Edition* 54, 195-200 (2015). *Angewandte Chemie – International Edition* 53, 4608-4613 (2014). *Angewandte Chemie – International Edition* 53, 7440-7444 (2014). *The Journal of the American Chemical Society* (2014). *Chem. Soc. Rev.* 43, 2701-2713 (2014).

### **The Hydride Toolbox. Paris December 12 - 15, 2016**

Hydrides are among the first molecules detected in Astronomy, outside the solar system. Hydrides are defined as molecules, radicals and molecular ions containing only one "heavy atom" (e.g., C, N, O, F, S, Cl, Ar, etc.) bound with hydrogen atoms. Such molecules are therefore relatively chemically simple. They lie at the root of interstellar chemistry, as hydrides are among the first species to form in initially atomic gas, together with molecular hydrogen and its associated ions. Despite this relative simplicity, building chemical models explaining the astronomical data on hydrides has required several decades. Several independent factors contributed to enhancing the difficulty. The relative scarcity of astronomical data due to the limited number of spectral lines accessible from the ground, the specific thermodynamic and chemical properties of hydrides of astrophysical interest, leading to slow formation processes for key species like CH<sup>+</sup> in average interstellar conditions, and the need for advanced modeling approaches combining fluid dynamics, gas phase and solid phase chemistries, and including radiative and chemical formation pumping. Thanks to the development of submillimeter astronomy, especially the Herschel satellite and the SOFIA stratospheric airplane, the knowledge of astronomical hydrides has rapidly progressed. Advances in astronomical observations have been matched by similar progresses in theory and in laboratory data. Several hydrides are now accessible either from space or from the ground, including distant objects at high redshift, as well as protoplanetary disks and exoplanet atmospheres. Hydrides are now detected in a wide range of environments, from the low density diffuse matter with mostly atomic hydrogen, up to the dense FUV illuminated interfaces of molecular gas and HII regions, to cold and dense prestellar cores, and to molecular shocks. Because water is the main ice constituent, hydrides are also important probes of the planet formation process, including the role of the snow line in the growth of planet embryos, and the emergence of planet atmospheres. Hydride spectral lines bear interesting diagnostics of important properties of interstellar medium, be it local or at cosmological distances. This includes the molecular hydrogen content, the ionization rate due to cosmic rays, the dissipation rate of turbulence, the kinetic temperature, the magnetic field intensity, as well as the ice condensation and evaporation processes, and the evolutionary time scale of the matter through for instance the abundance ratio of spin symmetry states of H<sub>2</sub> and hydrides like NH<sub>3</sub>. The goal of this 4-day meeting is to bring together the molecular physics (gas phase and solid phase; theory and experiments) and astrophysical community interested in hydrides, and to benchmark the hydride diagnostic capabilities, to expand the validation domain from the local universe to distant systems. The sessions will be organized with introductory review talks, and ample time for contributed talks and poster presentations. Main Topics: ----- \* Hydrides as probes of the diffuse ISM and of the CO-Dark gas. \* Hydrides as probes of PDRs and star forming regions, from local regions to the high redshift universe. \* Hydrides in shocks, probing the stellar feedback \* Hydrides as probes of the interaction of cosmic rays with matter, and relation with magnetic field structure. \* Hydrides as probes of energetic processes XDRs, and AGN activity diagnostics (across redshift). \* Hydrides as probes of the planet formation process, hydrides in exoplanets. \* Molecular physics of hydrides: formation, excitation, reactivity including the role of the spin symmetries . \* Hydrides in solid phase : physical processes and chemistry. Scientific Organizing Committee: : Yuri Aikawa (Japan), Edwin Bergin (USA), John Black (Sweden), Paola Caselli (Germany), Maryvonne Gerin (France) chair, Javier Goicoechea (Spain) co-chair, Eduardo Gonzalez-Alfonso (Spain), Di Li (China), Xavier Michaut (France) David Neufeld (USA) co-chair, Karin Öberg (USA) Ewine van Dishoeck (The Netherlands). Local Organizing Committee : Mathieu Bertin (LERMA - UPMC), Patrick Boissé (IAP - UPMC) Maryvonne Gerin (LERMA - CNRS), Benjamin Godard (LERMA - Observatoire de Paris), Pascal Jeseck (LERMA - CNRS), Darek Lis (LERMA - Observatoire de Paris), Xavier Michaut (LERMA - UPMC), Laurent Philippe (LERMA - UPMC), Nora Roger (LERMA - CNRS)