

# AstroChemical Newsletter #83

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## Abstracts

### The formation of CO<sub>2</sub> through consumption of gas-phase CO on vacuum-UV irradiated water ice

**J. Terwisscha van Scheltinga, N.F.W. Ligterink, A.D. Bosman, M.R. Hogerheijde, H. Linnartz**

[Abridged] Observations of protoplanetary disks suggest that they are depleted in gas-phase CO. It has been posed that gas-phase CO is chemically consumed and converted into less volatile species through gas-grain processes. Observations of interstellar ices reveal a CO<sub>2</sub> component within H<sub>2</sub>O ice suggesting co-formation. The aim of this work is to experimentally verify the interaction of gas-phase CO with solid-state OH radicals above the sublimation temperature of CO. Amorphous solid water (ASW) is deposited at 15 K and followed by vacuum-UV (VUV) irradiation to dissociate H<sub>2</sub>O and create OH radicals. Gas-phase CO is simultaneously admitted and only adsorbs with a short residence time on the ASW. Products in the solid state are studied with infrared spectroscopy and once released into the gas phase with mass spectrometry. Results show that gas-phase CO is converted into CO<sub>2</sub>, with an efficiency of 7-27%, when interacting with VUV irradiated ASW. Between 40 and 90 K, CO<sub>2</sub> production is constant, above 90 K, O<sub>2</sub> production takes over. In the temperature range of 40-60 K, the CO<sub>2</sub> remains in the solid state, while at temperatures  $\geq 70$  K the formed CO<sub>2</sub> is released into the gas phase. We conclude that gas-phase CO reacts with solid-state OH radicals above its sublimation temperature. This gas-phase CO and solid-state OH radical interaction could explain the observed CO<sub>2</sub> embedded in water-rich ices. It may also contribute to the observed lack of gas-phase CO in planet-forming disks, as previously suggested. Our experiments indicate a lower water ice dissociation efficiency than originally adopted in model descriptions of planet-forming disks and molecular clouds. Incorporation of the reduced water ice dissociation and increased binding energy of CO on a water ice surfaces in these models would allow investigation of this gas-grain interaction to its full extend.

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### The ALMA Survey of 70 $\mu$ m Dark High-mass Clumps in Early Stages (ASHES). VI. The Core-scale CO Depletion

**G. Sabatini, S. Bovino, P. Sanhueza, K. Morii, S. Li, E. Redaelli, Q. Zhang, X. Lu, S. Feng, D. Tafuya, N. Izumi, T. Sakai, K. Tatematsu and D. Allingham**

Studying the physical and chemical properties of cold and dense molecular clouds is crucial for the understanding of how stars form. Under the typical conditions of infrared dark clouds, CO is removed from the gas phase and trapped onto the surface

of dust grains by the so-called depletion process. This suggests that the CO-depletion factor ( $f_D$ ) can be a useful chemical indicator for identifying cold and dense regions (i.e., prestellar cores). We have used the 1.3 mm continuum and C18O (2-1) data observed at the resolution of  $\sim 5000$  au in the ALMA Survey of 70  $\mu\text{m}$  Dark High-mass Clumps in Early Stages (ASHES) to construct averaged maps of  $f_D$  in 12 clumps to characterize the earliest stages of the high-mass star formation process. The average  $f_D$  determined for 277 of the 294 ASHES cores follows an unexpected increase from the prestellar to the protostellar stage. If we exclude the temperature effect due to the slight variations in the  $\text{NH}_3$  kinetic temperature among different cores, we explain this result as a dependence primarily on the average gas density, which increases in cores where protostellar conditions prevail. This shows that  $f_D$  determined in high-mass star-forming regions at the core scale is insufficient to distinguish among prestellar and protostellar conditions for the individual cores and should be complemented by information provided by additional tracers. However, we confirm that the clump-averaged  $f_D$  values correlate with the luminosity-to-mass ratio of each source, which is known to trace the evolution of the star formation process.

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## Physical properties of accretion shocks toward the Class I protostellar system Oph-IRS44

**E. Artur de la Villarmois, V. V. Guzmán, J. K. Jørgensen, L. E. Kristensen, E. A. Bergin, D. Harsono, N. Sakai, E. F. van Dishoeck, and S. Yamamoto**

(Abridged) Physical processes such as accretion shocks are thought to be common in the protostellar phase, where the envelope component is still present, and they can release molecules from the dust to the gas phase, altering the original chemical composition of the disk. Consequently, the study of accretion shocks is essential for a better understanding of the physical processes at disk scales and their chemical output. The purpose of this work is to assess the characteristics of accretion shocks traced by sulfur-related species. We present ALMA high angular resolution observations ( $0.1''$ ) of the Class I protostar Oph-IRS 44. The continuum emission at 0.87 mm is observed, together with sulfur-related species such as SO, SO<sub>2</sub>, and <sup>34</sup>SO<sub>2</sub>. Six lines of SO<sub>2</sub>, two lines of <sup>34</sup>SO<sub>2</sub>, and one line of SO are detected toward IRS 44. The emission of all the detected lines peaks at  $\sim 0.1''$  ( $\sim 14$  au) from the continuum peak and we find infalling-rotating motions inside 30 au. However, only redshifted emission is seen between 50 and 30 au. Colder and more quiescent material is seen toward an offset region located at a distance of  $\sim 400$  au from the protostar, and we do not find evidence of a Keplerian profile in these data. Accretion shocks are the most plausible explanation for the high temperatures, high densities, and velocities found for the SO<sub>2</sub> emission. When material enters the disk--envelope system, it generates accretion shocks that increase the dust temperature and desorb SO<sub>2</sub> molecules from dust grains. High-energy SO<sub>2</sub> transitions ( $\sim 200$  K) seem to be the best tracers of accretion shocks that can be followed up by future higher angular resolution ALMA observations and compared to other species to assess their importance in releasing molecules from the dust to the gas phase.

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## The quasi-bound spectrum of H<sub>2</sub>

**E. Roueff & H. Abgrall**

We compute the radiative ro-vibrational emission spectrum of H<sub>2</sub> involving quasi-bound states via a simple numerical method of resolution of the Schrödinger equation by introducing a modified effective molecular potential. The comparison of the eigenvalues obtained with our approximation and other theoretical methods based on scattering resonance properties is excellent. Electric quadrupole and magnetic dipole contributions are calculated and we confirm the previous computations of Forrey of the electric quadrupole transition probabilities. The astrophysical relevance of such quasi-bound levels is emphasized.

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## Binding Energies of Interstellar Relevant S-bearing Species on Water Ice Mantles: A Quantum Mechanical Investigation

**J. Perrero, J. Enrique-Romero, S. Ferrero, C. Ceccarelli, L. Podio, C. Codella, A. Rimola, P. Ugliengo**

Binding energies (BEs) are one of the most important parameters for astrochemical modeling determining, because they govern whether a species stays in the gas-phase or is frozen on the grain surfaces. It is currently known that, in the denser and colder regions of the interstellar medium, sulphur is severely depleted in the gas phase. It has been suggested that it may be locked into the grain icy mantles. However, which are the main sulphur carriers is still a matter of debate. This work aims at establishing accurate BEs of 17 sulphur-containing species on two validated water ice structural models, the proton-ordered crystalline (010) surface and an amorphous water ice surface. We adopted Density Functional Theory (DFT)-based methods (the hybrid B3LYP-D3(BJ) and the hybrid meta-GGA M06-2X functionals) to predict structures and energetics of the adsorption complexes. London's dispersion interactions are shown to be crucial for an accurate estimate of the BEs due to the presence of the high polarizable sulphur element. While on the crystalline model the adsorption is restricted to a very limited number of binding sites with single valued BEs, on the amorphous model several adsorption structures are predicted, giving a BE distribution for each species. With the exception of few cases, both experimental and other computational data are in agreement with our calculated BE values. A final discussion on how useful the computed BEs are with respect to the snow lines of the same species in protoplanetary disks is provided

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## Temperature Spectra of Interstellar Dust Grains Heated by Cosmic Rays. III. Mixed Composition Grains

**J. Kalvans, J. R. Kalnin**

Icy grains in the interstellar medium and star-formation regions consist of a variety of materials. Such composite grains interact differently with cosmic-ray (CR) particles compared to simple single-material grains. We aim to calculate the spectra of energies and temperatures of mixed-composition grains undergoing whole-grain heating by CRs. The grains were assumed to consist of a mixture of carbon and olivine, covered by ices

consisting of carbon oxides and water. The energy and temperature spectra for grains with radii 0.05; 0.1, and 0.2 microns impacted by CRs were calculated for eight values of column density, relevant to molecular clouds and star-forming cores. The approach takes into account changes in ice thickness and composition with increasing column density. These detailed data for CR interaction with interstellar grains are intended for applications in astrochemical models. The main finding is that the a more accurate approach on grain heat capacity and other factors prevent a frequent heating of 0.1 micron or larger icy grains to high temperatures.

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## **Inside-Out Planet Formation. VII. Astrochemical Models of Protoplanetary Disks and Implications for Planetary Compositions**

**Arturo Cevallos Soto, Jonathan C. Tan, Xiao Hu, Chia-Jung Hsu, Catherine Walsh**

Inside-Out Planet Formation (IOPF) proposes that the abundant systems of close-in Super-Earths and Mini-Neptunes form in situ at the pressure maximum associated with the Dead Zone Inner Boundary (DZIB). We present a model of physical and chemical evolution of protoplanetary disk midplanes that follows gas advection, radial drift of pebbles and gas-grain chemistry to predict abundances from 300~au down to the DZIB near 0.2 au. We consider typical disk properties relevant for IOPF, i.e., accretion rates  $1E-9 < dM/dt / (M_{\text{sun}}/\text{yr}) < 1E-8$  and viscosity parameter  $\alpha = 1E-4$ , and evolve for fiducial duration of  $t = 1E5$  years. For outer, cool disk regions, we find that C and up to 90% of O nuclei start locked in CO and O<sub>2</sub> ice, which keeps abundances of CO<sub>2</sub> and H<sub>2</sub>O one order of magnitude lower. Radial drift of icy pebbles is influential, with gas-phase abundances of volatiles enhanced up to two orders of magnitude at ice-lines, while the outer disk becomes depleted of dust. Disks with decreasing accretion rates gradually cool, which draws in icelines closer to the star. At  $< \sim 1$  au, advective models yield water-rich gas with C/O ratios  $< \sim 0.1$ , which may be inherited by atmospheres of planets forming here via IOPF. For planetary interiors built by pebble accretion, IOPF predicts volatile-poor compositions. However, advectively-enhanced volatile mass fractions of  $\sim 10\%$  can occur at the water ice line.

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## **CHEMOUT: CHEMical complexity in star-forming regions of the OUTer Galaxy III. Nitrogen isotopic ratios in the outer Galaxy**

**L. Colzi, D. Romano, F. Fontani, V. M. Rivilla, L. Bizzocchi, M. T. Beltrán, P. Caselli, D. Elia, and L. Magrini**

Nitrogen isotopic ratios are a key tool for tracing Galactic stellar nucleosynthesis. We present the first study of the <sup>14</sup>N/<sup>15</sup>N abundance ratio in the outer regions of the Milky Way (namely, for galactocentric distances,  $R_{\text{GC}}$ , from 12 kpc up to 19 kpc), with the aim to study the stellar nucleosynthesis effects in the global Galactic trend. We analysed IRAM 30m observations towards a sample of 35 sources in the context of the CHEMical complexity in star-forming regions of the OUTer Galaxy (CHEMOUT) project. We derived the <sup>14</sup>N/<sup>15</sup>N ratios from HCN and HNC for 14 and 3 sources, respectively, using the  $J = 1-0$  rotational transition of HN<sup>13</sup>C, H<sup>15</sup>NC, H<sup>13</sup>CN, and HC<sup>15</sup>N. The

results found in the outer Galaxy have been combined with previous measurements obtained in the inner Galaxy. We find an overall linear decreasing H13CN/HC15N ratio with increasing  $R_{GC}$ . This translates to a parabolic 14N/15N ratio with a peak at 11 kpc. Updated Galactic chemical evolution models have been taken into account and compared with the observations. The parabolic trend of the 14N/15N ratio with  $R_{GC}$  can be naturally explained (i) by a model that assumes novae as the main 15N producers on long timescales ( $>1$  Gyr) and (ii) by updated stellar yields for low- and intermediate-mass stars.

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## Different degrees of nitrogen and carbon depletion in the warm molecular layers of protoplanetary disks

**K. Furuya, S. Lee, H. Nomura**

Observations have revealed that the elemental abundances of carbon and oxygen in the warm molecular layers of some protoplanetary disks are depleted compared to those in the interstellar medium by a factor of  $\sim 10$ -100. Meanwhile, little is known about nitrogen. To investigate the time evolution of nitrogen, carbon, and oxygen elemental abundances in disks, we develop a one-dimensional model that incorporates dust settling, turbulent diffusion of dust and ices, as well as gas-ice chemistry including the chemistry driven by stellar UV/X-rays and the galactic cosmic rays. We find that gaseous CO in the warm molecular layer is converted to CO<sub>2</sub> ice and locked up near the midplane via the combination of turbulent mixing (i.e., the vertical cold finger effect) and ice chemistry driven by stellar UV photons. On the other hand, gaseous N<sub>2</sub>, the main nitrogen reservoir in the warm molecular layer, is less processed by ice chemistry, and exists as it is. Then the nitrogen depletion occurs solely by the vertical cold finger effect of N<sub>2</sub>. As the binding energy of N<sub>2</sub> is lower than that of CO and CO<sub>2</sub>, the degree of nitrogen depletion is smaller than that of carbon and oxygen depletion, leading to higher elemental abundance of nitrogen than that of carbon and oxygen. This evolution occurs within 1 Myr and proceeds further, when the alpha parameter for the diffusion coefficient is  $\sim 0.001$ . Consequently, the N<sub>2</sub>H<sup>+</sup>/CO column density ratio increases with time. How the vertical transport affects the midplane ice composition is briefly discussed.

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## First detection of methyl formate in the hot molecular core IRAS 18566+0408

**Arijit Manna, Sabyasachi Pal**

The studies of the complex molecular emission lines in the millimeter and submillimeter wavelengths towards the hot molecular cores reveal valuable details about the chemical complexity in the interstellar medium (ISM). We presented the first detection of the rotational emission lines of the complex organic molecule methyl formate (CH<sub>3</sub>OCHO) towards the hot molecular core region IRAS 18566+0408 using the high-resolution Atacama Large Millimeter/Submillimeter Array (ALMA) band 3 observation. The estimated column density of CH<sub>3</sub>OCHO using the rotational diagram analysis was  $(4.1 \pm 0.1) \times 10^{15}$  cm<sup>-2</sup> with a rotational temperature of  $102.8 \pm 1.2$  K. The estimated fractional abundance of CH<sub>3</sub>OCHO relative to hydrogen (H<sub>2</sub>) towards the IRAS

18566+0408 was  $3.90 \times 10^{-9}$ . We noted that the estimated fractional abundance of CH<sub>3</sub>OCHO is fairly consistent with the simulation value predicted by the three-phase warm-up model from Garrod (2013). We also discussed the possible formation mechanism of CH<sub>3</sub>OCHO towards the IRAS 18566+0408.

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