Fractionation of isotopes in space: from the solar system to galaxies

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Book of abstracts

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Invited talks

Maite Beltrán

Osservatorio di Arcetri, OAA-INAF

ALMA Band 2+3 Science Cases

Receiver technology has advanced since the original definition of the ALMA frequency bands and it is now feasible to produce a single receiver which could cover whole frequency range from 67 GHz to 116 GHz, encompassing Band 2 and Band 3 in a single receiver cartridge, in the so called Band 2+3 system. In this presentation, I will discuss the main Galactic and Extragalactic science drivers for ALMA Band 2+3. The science drivers of Band 2 are obviously covered by the Band 2+3 science but the simultaneous frequency coverage allows to perform critical measurements that cannot be done (or can be done in a sub-optimal way) with the two bands separated.

Nicolas Biver

LESIA, Observatoire de Paris

Measurements of isotopic ratios in solar system bodies

Isotopic ratios in small solar system bodies provide keys for the understanding of the physical and chemical conditions in the early Solar Nebula. We will review here measurements on the D/H, 14N/15N, 16O/18O, 12C/13C and 32S/34S ratios in cometary comae, titan and planetary atmospheres, and some samples of cometary grains and meteorites. Remote techniques such as high resolution visible to infrared spectroscopy with 8-m class telescopes to radio spectroscopy (Odin, Herschel, IRAM, ALMA) are powerful tools that have enabled many measurements over the past years.

Sandra Brünken

I. Physikalisches Institut, Universität zu Köln

From gas-phase isotope exchange reactions to isotopomer spectroscopy (and back)

Laboratory experiments provide crucial information for the interpretation of observational studies of isotopic fractionation in many different ways. Maybe the most direct one is the provision of accurate transition frequencies and strengths from spectroscopic studies, prerequisite for the identification and quantification of new isotopic molecular species. Equally important are experimental data, under conditions resembling those in space (i.e. low temperatures and number densities), on rate coefficients for relevant gas-phase reactions, e.g. isotope exchange reactions, and for processes on grain surfaces, that can be included in chemical reaction networks.

In this review, I will give an overview of state-of-the-art experimental techniques, with an emphasis on gas-phase ion-molecule isotopic exchange reactions, e.g. primary deuteration reactions involving H3+ and CH3+ studied in cryogenic ion traps, and methods to study neutral-neutral reactions, which might be responsible for, e.g., carbon isotopomer fractionation observed in cold, dense molecular clouds. I will also report on experimental progress in spectroscopic studies of molecular isotopomers, e.g. ionic species and complex organic molecules. An interesting aspect is that on the one hand chemical reactions can be used for spectroscopic studies (e.g. via laser induced reactions), and on the other hand spectroscopy provides means to probe the kinetics and product distribution of chemical reactions.

Ursina Calmonte

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New results on deuteration and fractionation from Rosetta/ROSINA

The European Space Agency´s spacecraft Rosetta accompanied comet 67P/Churyumov-Gerasimenko for more than 2 years going to perihelia and back to round 3.5 AU. On board of is the Rosetta Orbiter Sensor for Ion and Neutral Analysis (ROSINA) that consists of a pressure sensor and two complementary mass spectrometers. Among many results, it measured D/H in water in the early mission phase (Altwegg et al. 2015). Here we will give a summary of the so far published and presented results considering the deuteration of water, the oxygen isotopes, the fractionation seen for 34S and 33S in H2S, SO2, and CS2, and the noble gas isotopic ratio. Furthermore the obtained results will be discussed for their implication on the Solar System formation.

Cecilia Ceccarelli

IPAG, Universitè Grenoble Alpes

Fractionation in protostars: observations

The last decade has seen a flourishing of studies about fractionation of H and also of N in low- to high- mass protostars. In addition to having a powerful diagnostic value in itself, H and N fractionation in molecules provides a link with objects of the Solar System helping to elucidate its past history. In this presentation, I will review the observations and and the information they supply.

Steven Charnley

NASA Goddard Space Flight Center

A Connection Between Interstellar and Solar System Isotopic Fractionation ?

This talk will review the possible connection between the fractionation processes that are thought to occur in molecular clouds, involving carbon, nitrogen and hydrogen, with the isotopic ratios measured in comets and meteorites

Ilsedore Cleeves

Harvard-Smithsonian Center for Astrophysics

Physical and Chemical Drivers of Deuteration in Protoplanetary Disks

A wide variety of solar system bodies exhibit elevated deuterium-to-hydrogen (D/H) ratios compared to the bulk atomic value in both water and organic material. Furthermore, organics are typically more enriched in D/H compared to water and show greater D/H variation. These isotopologue features provide key clues toward determining these reservoirs' initial formation environments. In particular, elevated D/H points to formation in very cold (T < 50-100 K) gas, facilitated by the presence of ionizing agents, i.e., cosmic rays, radionuclide decay, and X-rays. These requirements point to two possibilities: 1) formation within the outer protoplanetary disk or 2) inheritance from the parent molecular cloud. By examining the physical conditions within the disk environment using detailed theoretical models of the key ionizing processes, we put constraints on the active deuterium chemistry in the protoplanetary disk phase. We find that the addition of CH2D+ pathways and the accessibility of volatile carbon relative to oxygen lead to higher D/H ratios in organics compared to water via disk chemistry. We find that while a significant fraction of water ice was likely inherited from the parent molecular cloud, organics (as traced by D/H) have a much more complex and varied history.

Christian Johann Henkel

MPI fuer Radioastronomie, Bonn/King Abdulaziz University, Jeddah

Nucleosynthesis and Molecular Isotope Ratios in Extragalactic Systems

The determination of extragalactic CNO-S-Si isotope ratios requires observations with extreme sensitivity. As a consequence of limited signal-to-noise ratios and isotope ratios often exceeding an order of magnitude, very little could been done so far. However, this is now changing, thanks to the construction of ALMA and the expansion of the Plateau de Bure Interferometer into NOEMA. This talk provides a brief summary of extragalactic work so far done on CNO-S-Si isotope ratios, mentioning the main underlying processes of nucleosynthesis. Also introduced are cases, where fractionation can be neglected, and others, where fractionation might influence the resulting ratios, even though it is not yet possible to quantify such effects.

Olja Panić

University of Leeds, UK

CO isotopologues in protoplanetary discs

Low temperatures and high optical depth mean that only tenuous emission escapes the actual planet forming regions of discs – the disc midplanes. We have just begun to map midplane gas with ALMA in the recent years. I will present the first results of our ALMA survey of CO isotopologues, targeting warm and bright discs around Herbig Ae stars. These observations place constraints on the amount of gas available for planet formation and, combined with the dust continuum observations, may constrain the gas to dust mass ratio – one of the key inputs in planet formation models.

Chunhua Qi

Harvard-Smithsonian CfA

Observations of isotopic fractionation in circumstellar disks

Isotopic fractionation can be used to probe the physical and chemical structures in circumstellar disks and investigate the origin of molecules in our solar system. I will review the observations of molecular trace species focusing on resolving deuterium and nitrogen isotopic fractionation in disks, and show how the isotopic radios of the molecular content are affected by the temperature structure, radiation field and ionization fraction in disks.

Vianney Taquet

Leiden Observatory

Theoretical review on fractionation in protostellar YSOs

Sub-millimetric observations of embedded protostars have showed that the early stages of star formation are accompanied by an increase of the molecular isotopic fractionation, and in particular of the D/H and the 15N/14N ratios, with their respect to their cosmic value. In this talk, I will review the physical and chemical processes important for the chemical fractionation by emphasising how we can use the molecular fractionation as a tool to constrain the mechanisms and moments of formation of the molecules observed towards protostars.

Leonardo Testi

ESO

Review on ALMA Band 2+3 capabilities

Charlotte Vastel

IRAP

Deuteration and fractionation in prestellar cores and IRDCs: the observational point of view

A tremendous advance in instrumentation for spectroscopy of the interstellar medium took place during the last decade. Major facilities such as ALMA, SOFIA and Herschel have been constructed and commissioned, so that science opportunities in the field of astrochemistry have increased by a huge factor. Major discoveries have occurred because of the greater sensitivities of existing telescopes such as IRAM (30 meters and NOEMA), and also because new spectral ranges, so far hidden by the Earth's atmosphere, were finally revealed. The high sensitivity as well as the spectral resolution of the instruments led to the discovery of many species, and the spatial resolution was the key point to uncover the spatial distribution of these species.

I will present the recent advances made in the earliest phase of star formation in particular, and will acknowledge the links made between molecular physics and chemistry and the beautiful observations performed with nowadays instruments.

Serena Viti

University College London

Deuteration and fractionation in extragalactic sources: a theoretical view.

Deuteration and fractionation in galactic low-mass and high-mass star-forming regions in our own Galaxy is now routinely studied. In recent years efforts have been made to understand the fractionation of in particular carbon and oxygen in other galaxies, where the physical conditions can be drastically different from what we see in our own Galaxy. Deuteration in extragalactic star-forming environments, is, on the other hand, an almost completely unexplored territory. In this talk I will review the modelling efforts undergone to understand and predict fractionation of the main elements and the differences in the D-fractionation and the D/H ratios in regions of star formation in various types of galaxies.

Eva Wirström

Department of Earth and Space Sciences, Chalmers University of Technology

Fractionation in dark pre-stellar clouds

Isotope ratios of stable elements are considered an important tool in tracing the chemical heritage of material through the process of star and planetary system formation. In order to draw conclusions on heritage, environment, or chemistry from observed isotopologue line ratios one really has to consider these as the combined result of local elemental abundance ratios, fractionation processes, excitation, and radiative transfer effects. In this talk I will focus on the theory of isotope fractionation taking place at the very first stages of star formation - driven by disequilibrium chemistry in cold, dense gas. Low-temperature effects on fractionation, such as the role of a varying H2 ortho-to-para ratio, will be discussed. In particular, the current theoretical understanding of 15N fractionation will be reviewed and compared to observations of molecular 14N/15N ratios in pre-stellar cores and young stellar objects.

Contributed talks

Rebeca Aladro

Chalmers University

Author(s): Rebeca Aladro

Chemistry and isotopologues in nearby active galaxies

I will present the results of a molecular line survey done with the IRAM 30m telescope towards eight nearby active galaxies (M83, NGC253, M82, M51, NGC1068, NGC7469, Arp220 and Mrk231). 27 molecules and 10 carbon, sulphur and oxygen isotopologues were detected. I will discuss the chemical complexity of the sample depending on the nuclear activity and evolutionary stage, and the results of isotopic line ratios.

Eleonora Bianchi

Osservatorio Astrofisico di Arcetri

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How H2CO and CH3OH deuteration changes during the formation of a Sun-like star? The SVS13-A case

The deuterium fractionation at the different evolutionary stages of a Sun-like protostar provides us a unique tool to investigate the origin and the evolution of our Solar System. However, while deuterated molecules have been detected towards the early stages of the Sun-like star formation (i.e. prestellar cores and Class 0 objects) as well as directly in the Solar System, no clear result has been obtained for intermediate evolutionary phases (Class I and II objects). In the context of the ASAI IRAM 30-m large program, we report the observation of deuterated formaldehyde and methanol in the Class I object, SVS13-A, located in Perseus. In particular, we detected several lines of H213CO, HDCO and D2CO as well as 13CH3OH and CH2DOH covering a wide range of excitation (up to 270 K). We measure a D/H ~ 10-2 and 10-3 for HDCO and D2CO, respectively, towards SVS13-A. A similar D/H has been measured in the wings of the formaldehyde lines associated with the molecular outflow driven by SVS13-A. On the other hand, the SVS13-A methanol single deuteration is ~10-3 . These findings bridge the gap between protostars and more evolved sources associated with protoplanetary disks. In fact our analysis suggests that the CH3OH and H2CO deuteration decreases as the protostar moves from the Class 0 stage (where the D/H is ~ 0.1-0.2) to the more evolved Class I phase up to the very low values in the Solar System (D/H~ 10-4).

Gemma Busquet

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The L1157-B1 astrochemical laboratory: testing the origin of DCN

Associated with a low-mass class 0 protostar, L1157-B1 is a protostellar chemically rich bow-shock considered one of the best astrochemical laboratories. As part of the high sensitivity IRAM 30m/ASAI and Herschel/CHESS spectral surveys, L1157-B1 is the first shock where several deuterated molecules have been detected: HDCO, HDO, CH_2DOH, NH_2D, and DCN.

Based on our up-to-date chemical models, we suggested that most of these (e.g. HDCO and CH2DOH) are formed on grain mantles and then realized into the gas phase by the passage of the shock, while DCN is a product of chemical reactions occurred in warm gas.

In this talk, we present high angular resolution (~2”) observations of DCN(2-1) and H13CN(2-1) carried out with NOEMA toward L1157-B1. DCN arises from the region of interface between the jet and the ambient material, traced mainly by HDCO in which we find the fresh material evaporated from the grain mantles (Fontani et al. 2014), but also from another region undetected in HDCO, in which chemistry is likely dominated by warm gas processes. These findings are consistent with the chemical routes that claim that DCN is made in significant quantities in warm gas.

The gas-phase versus mantle production of DCN will be discussed by the light of the present images. We will discuss and compare the different origin of DCN and HDCO with the prediction of chemical models: warm chemistry versus surface chemistry.

Paola Caselli

Max-Planck-Institute for Extraterrestrial Physics

Author(s): Paola Caselli

D and ^{15}N fractionation in pre-stellar cores

Stars like our Sun form within pre-stellar cores. These dense (n(H2)>10^4 cm-3) and cold (T~10 K) clouds contain all the ingredients out of which future stellar systems are made. In this talk, I'll focus the attention on the fractionation of D and 15N within pre-stellar cores and link this to the D and 15N fractions measured in pristine objects within our Solar System. Our astrochemical history will be discussed.

Claudio Codella

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Hot and dense water in the inner 25 AU of SVS13-A

In the context of the ASAI (Astrochemistry Studies At IRAM) project, we carried out an unbiased spectral survey in the millimeter window (0.8-3mm) towards the well known low-mass Class I object SVS13-A.The high sensitivity reached (3-12 mK) allowed us to detect 7 HDO broad emission lines covering a wide spread in excitation, up to Eu = 837 K, indeed the highest excitation HDO line ever observed towards a low-mass young stellar object. A non-LTE LVG analysis implies the presence of very hot (150-260 K) and dense (> 3 10^7 cm-3) gas inside a small radius (25 AU) around the star, supporting the occurrence of a hot corino inside SVS13-A. The temperature is larger than the usual ~ 100 K, i.e. the expected temperature when water molecules are sublimated from the icy dust mantles. Although we cannot exclude we are observing the effects of shocks and/or winds at such small scales, these findings could imply that the observed HDO emission is tracing the water abundance jump expected at temperatures ~ 220-250 K, when the activation barrier of the gas phase reactions leading to water can be overcome. We derived X(HDO) ~ 3 10^{-6}, while the H_2O deuteration is estimated to be larger than 0.015, suggesting that water deuteration does not decrease as the protostellar system evolves from the Class 0 (~ 10^4 yr) to the Class I stage (~ 10^5 yr).

Claudia Comito

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A three-dimensional model of the distribution and deuteration of water in SgrB2(M)

One of the main science rationales behind blasting off a submm/far-infrared, high-resolution spectrometer to space (see the HIFI instrument on board Herschel) is the unique capability of studying the emission and absorption of water molecules in the gas phase towards astronomical objects, without the water vapour in our own Earth atmosphere acting as a screen in between. This was also one of the goals of the HEXOS Key Project, or Herschel observations of EXtraordinary Sources, which included the high-mass star-forming region Sgr B2.

In this work we have concentrated on Sgr B2(M). The HIFI unbiased line survey of this source contains tens of spectral lines from H2O, its 18O and 17O isotopologues, and its deuterated counterpart HDO, plus self-consistent information on the strong dust emission from ~500 GHz to ~2 THz. At the same time, HDO observations carried out with ALMA at 1-mm wavelength provide an insight into the small-scale, hot-core emission of the cloud.

Schmiedeke et al. (2016) have developed a 3D full radiative transfer model of the continuum emission towards the Sgr B2 cloud. We build on this extensive description of the source to include a 3D modeling of the distribution of H2O and HDO (see Comito et al. 2003, 2010), towards the Sgr B2(M) core.

Audrey Coutens

UCL

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Isotopic fractionation of complex organic molecules: Results from the ALMA-PILS survey

Numerous complex organic molecules are detected towards low-mass star-forming regions. Their formation mechanisms are however debated. Measurements of isotopic fractionation (especially deuteration) can be helpful to constrain how these species form. The detection of the isotopologues can however be difficult. With the Atacama Large (Sub-)Millimeter Array (ALMA), it is now possible to detect them. The Protostellar Interferometric Line Survey (PILS) is an ALMA large spectral survey of the solar-type protostar IRAS16293-2422. The sensitivity of the data is sufficiently high to detect the deuterated and 13C isotopologues of several molecules. In particular, we recently detected the three singly deuterated forms of formamide (NH2CHO) as well as DNCO towards the component B (Coutens et al. 2016, A&A Letters). The deuteration is found to be similar for the three different forms of formamide with a value of about 2%. The DNCO/HNCO ratio is also comparable. Based on these results, we will discuss the possible routes for the formation of formamide in low-mass protostars. Other results from the PILS survey will be presented.

Victor de Souza Magalhães

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A study of HF anomalies and carbon fractionation in HCN

The heritage of interstellar materials in planetary systems is a central problem in astrochemistry, cosmochemistry and astrobiology. How much of this material is preserved during the formation of planetary systems is still unknown. Isotopic ratios are the main tool to trace the different reservoirs of interstellar materials (Cleves et al. 2014). In the case of nitrogen, the 14N/15N ratio demonstrates that Jupiter and the Sun trace very similar reservoirs (14N/15N = 441, Fury & Marty 2015). There is however evidence that this is not the case for the rest of the Solar system, in which comets have a mean ratio of 150 in various molecular carriers. This value is similar to the measurements of HCN in the ISM (Hily-Blant et al. 2013), but there is no obvious link between the two.

In this talk, I present a study of the hyperfine anomalies of HCN, a long standing problem in the determination of HCN column densities. Solving this problem is a prerequisite to elucidate the carbon fractionation of HCN proposed by Roueff et al 2015. The isotopic ratio of carbon in HCN is of crucial importance for the study of nitrogen fractionation because it is the main unknown in the derivation of the isotopic ratio of nitrogen in HCN through the double isotopologue method. To solve this problem we are using a state of the art 1D radiative transfer code that takes into account each hyperfine component independently. The products of this code are then compared to IRAM-30m observations.

Sara Faggi

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First spectrally complete survey of cometary water emission at near IR wavelengths (0.9-2.5 μm): C/2

Comets are the most pristine bodies of Solar System and water is the most abundant constituent of cometary ice its production rate is used to quantify cometary activity and the measurements of ortho-para ratio can clarify the nature and meaning of the spin temperature in the cosmic context. Last February 2015, we acquired the first comprehensive high resolution spectral survey of comet C/2014 Q2 Lovejoy in the 0.9-2.5 μm range, by observing with GIANO - the near-IR spectrograph on TNG (the Italian Telescopio Nazionale Galileo in La Palma, Canary Islands, ES). We detected emissions of radical CN, water (H2O), and many undefined emission features. We quantified the water production rate by comparing the calibrated line fluxes with the NASA Goddard full non resonance fluorescence cascade model for H2O. The production rate of ortho and para water provide an estimation of ortho to para ratio consistent with statistical equilibrium (3.0), but the confidence limits are not small enough to enable a critical test of the nuclear spin temperature in this comet.

Until now, high-resolution spectroscopy in the infrared (2.7 - 5μm) has been a powerful tool to quantify molecular abundances in cometary comae. Today the expansion to the near-IR region (0.9-2.5 μm) will extend this capability to new band systems.

Our observations open a new pathway for cometary science in the near-infrared spectral range (0.9-2.5 μm) and establish the feasibility of astrobiology-related scientific invest.

Alexandre Faure

CNRS / IPAG

Author(s): A. Faure, M. Faure, P. Theulé, E. Quirico, B. Schmitt

D/H equilibrium fractionation in ices

The deuterium fractionation of gas-phase molecules in hot cores and cometary comae is believed to reflect the composition of the primitive ices. The deuteration of protostellar methanol is, however, a major puzzle because the isotopologue ratio [CH2DOH]/[CH3OD] is about a factor of 10 larger in low mass hot-corinos than in high-mass hot cores. In this talk, we will report a new rate equation model of deuterium surface chemistry applied to the hot-core phase of protostellar sources, during which amorphous water ice is heated, crystallizes and eventually sublimates. According to recent experimental data, crystallization is accompanied in its very initial phase by H/D exchanges between water and molecules able to form hydrogen bonds, such as methanol and ammonia. The D/H ratios of such species are thus expected to equilibrate with the D/H ratio of water. As a result, the [CH2DOH]/[CH3OD] ratio is predicted to scale inversely with [HDO]/[H2O]. We will show that our model is able to reproduce the [CH2DOH]/[CH3OD] ratios observed in the hot-corino of IRAS 16293-2422 and in the hot-cores of Orion KL and Sgr B2(N2), provided that the primitive fractionation of water ice [HDO]/[H2O] in these sources is ~2%, ~0.6% and <0.1%, respectively. We conclude that gas-phase molecular D/H ratios measured in hot cores, protoplanetary disks or comets may not be representative of the original ices in the case of molecules with exchangeable deuterium atoms.

Pierre Hily-Blant

IPAG

Author(s): Hily-Blant, Magalhães de Souza, Kastner, Faure, Forveille

The origin of nitrogen in planetary systems

The extent to which interstellar chemical reservoirs are preserved during the formation of planetary systems is central to understanding the origin of the volatile reservoirs in planets. A long-standing problem is the origin of nitrogen in the solar system. The dominant carriers of nitrogen remain poorly known in the prestellar and protosolar phases, but the large variations of the 14N/15N isotopic ratio measured with high accuracy in the solar system indicate that several reservoirs of volatile nitrogen were present in the protosolar nebula (PSN) 4.6 billion years ago. The dominant reservoir, with an elemental isotopic ratio of 440 as derived from the solar wind and giant planet atmospheres, is not found in present-day observations of comets which instead recorded a minor reservoir characterized by an isotopic ratio of 150. We present ALMA observations which provide the present-day elemental isotopic ratio of nitrogen in the solar neighbourhood and evidence the multiple reservoirs of nitrogen in the comet forming region in a protoplanetary disk. We will also present an observational search for multiple solid and gas reservoirs of nitrogen in the interstellar stage. These observations also provide direct tests to the strongly debated possibility of chemical fractionation at the prestellar stage. Observational, theoretical and modelling perspectives for a comprehensive understanding of the origin of nitrogen will be presented.

Antonio Jiménez-Escobar

INAF-OAPa

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First results of the UHV system “LIFE” (Light Irradiation Facility for Exochemistry)

We present the LIFE system (Light Irradiation Facility for Exochemistry), a novel facility designed for studying solids (including ices) in simulated interstellar and circumstellar environments.

The Ultra High Vacuum (UHV) system LIFE reaches a minimum pressure down to 5 x 10^-11 mbar, with the sample cooled down to 10 K. The sample evolution is monitored by FTIR spectroscopy and QMS spectrometry. The UHV system can be tuned up with UV and soft X-ray sources, which can operate separately or simultaneously.

We also summarise the results of the first experiments simulating UV irradiation of methanol ices deposited onto silicates surfaces, consisting mainly of forsterite (Mg2SiO4). In these experiments we analyze the evolution of the CO2/CO product ratio as compared to that obtained in experiments performed with ices deposited onto standard IR transparent windows.

Finally, we present the results of an experiment performed at the National Synchrotron Radiation Research Center in Taiwan exploiting soft X-rays in the range 0.25 - 1.2 keV in the irradiation of silicate analogues of protoplanetary disk dust. Our results may be interpreted in terms of amorphization induced by the irradiation.

Leslie Hunt

INAF-Osservatorio di Arcetri

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CO fractionation in a low metallicity starburst

The extreme environment around low-metallicity super-star clusters (SSCs) can give rise to physical conditions that are very different from those in our Galaxy and the Local Group. In a metal-poor dwarf starburst galaxy hosting 6 SSCs, at 20 Mpc distance, with radiative transfer model fitting of six 12CO and 13CO transitions, we have found extremely low ratios of 12CO/13CO (8-14) between 2 and 3 times lower than the Galactic center. Because of the young age of the starburst in this galaxy, it is virtually impossible to explain this low ratio in terms of 13C enhancement from nucleosynthesis and dredge-up in evolved stars. Rather, the physical conditions found by our model fits correspond to the maximum efficiency of the 13CO fractionation process. More data are needed to determine whether this is a common phenomenon in low metallicity environments, and to better assess its effect on cloud structure in the interstellar medium.

Yoshida Kento

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Author(s): Kento Yoshida, Satoshi, Yamamoto, Nami Sakai, and ASAI team members

Molecular isotopic ratios in the low-mass protostar L1527

We present our recent works on the isotope anomalies found in the low-mass protostar L1527. In the last decade, we have been reporting significant anomalies of the 12C/13C ratio in various carbon-chain molecules in cold starless cores; dilution of 12C/13C ratios in molecules and different 13C abundances among different 13C atoms in a single molecular species. Recently, we have found these two anomalies for c-C3H2 in the low-mass star-forming region, L1527. The abundances of the two 13C isotopic species are found to be different, giving a stringent constraint on the production mechanism of this molecule.

The isotope anomaly in molecules can vary along the evolution from starless cores to protostars. From ALMA observations, we have recently found that the CCD/CCH ratio is lower in the vicinity of the protostar than in the outer envelope. This seems to originate from the contribution of Warm Carbon-Chain Chemistry (WCCC) near the protostar, where the lower CCD/CCH ratio is expected. If so, 12C/13C ratio of CCH could also be changed near the protostar, which will be detected with ALMA. Detailed comparisons of the 12C/13C ratios between L1527 and TMC-1 would also be useful for understanding the molecular formation in star-forming region. Furthermore, observations of the 13C anomalies can be extended to disk-forming regions with ALMA, which will provide us with rich information bridging the interstellar chemistry and the planetary chemistry.

Sabine König

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Deep ALMA imaging of the merger NGC 1614 - Is CO tracing a massive inflow of non-star~-forming gas?

Observations of the molecular gas over scales of a few 100 pc to several kpc provide crucial information on how molecular gas moves through galaxies, especially in mergers and interacting systems, where it ultimately reaches the galaxy center, accumulates and feeds nuclear activity. We used 12CO, 13CO and C18O 1-0 ALMA observations to assess the properties of the large-scale molecular gas reservoir and its connection to the circumnuclear molecular ring in the merger NGC 1614. We find that the 12CO-to-13CO 1-0 line ratio in NGC 1614 changes from >45 in the 2 kpc dust lane to ~30 in the starburst nucleus. This drop in ratio with decreasing radius is consistent with the molecular gas in the dust lane being kept in a diffuse, unbound state while it is being funneled towards the nucleus. We find a high 16O-to-18O abundance ratio in the starburst region (900), typical of quiescent disk gas. This is surprising since, by now, the starburst is expected to have enriched the nuclear ISM in 18O relative to 16O. We suggest that the massive inflow of gas may be partially responsible for the low 18O/16O abundance since it will dilute the starburst enrichment with unprocessed gas from greater radial distances. The 12CO-to-13CO abundance of >90 we infer from the line ratio is consistent with this scenario. It suggests that the nucleus of NGC 1614 is in a transient phase of its evolution where starburst and nuclear growth are still being fuelled by returning gas from the minor merger event.

Thanja Lamberts

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Importance of tunneling in H-abstraction reactions by OH radicals: The case of CH4 + OH

We present a combined experimental and theoretical study on the importance of quantum tunneling of atoms in the reaction between CH_4 and OH and isotope-substited analogs. Although this reaction has been studied previously both on the surface and in the gas phase, quantification of the reaction rates at low temperature is not trivial in either case. Quantitative rates, however, are needed for astrochemical models. Here, we are mainly concerned with two reactions: CH_4 +OD --> CH_3 +HDO and CD_4 +OH --> CD_3 +HDO.

From the signal-to-noise ratio in the ultra-high vacuum surface experiments we can draw the conclusion that the reaction rates are related via $R_{CH4 + OD} > 4.5\ R_{CD4 + OH}$ at 15 K. This is further quantified by gas-phase calculations of the corresponding uni- and bimolecular reaction rate constants using instanton theory. Unimolecular reactions correspond to the Langmuir-Hinshelwood process and can as such be compared to the experimental findings. The ratio between the rate constants is then $k_{CH4 + OD} \approx 7\ k_{CD4 + OH}$ at 60 K. The unimolecular rate constants presented here can be used by the modeling community as a first approach to describe OH-mediated abstraction reactions in the solid phase. Finally, the bimolecular rate constants can be used for the description of low-temperature gas-phase reactions as well as for the Eley-Rideal mechanisms.

Jean-Christophe Loison

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The photochemical fractionation of oxygen isotopes in Titan's atmosphere

The atmosphere of Titan is the place of a complex photochemistry producing hydrocarbons, nitriles, imines and oxygen compounds. Carbon monoxide is one of the most abundant molecule. It has been observed by many authors. However, its origin is still a matter of debate. Different scenarii have been proposed to explain its abundance but there are no definitive arguments to discriminate between an external origin of oxygen (micrometeorites, Enceladus' plumes) and an internal origin (outgassing of primordial CO from the surface). The study of isotopic ratios can give valuable constrained on the formation and evolution of planetary atmospheres. In particular, it could help to discriminate between different physical and chemical processes that have been or are presently preponderant. In this context, the study of oxygen isotopologues seems to be a promising step toward a better understanding of the origin and evolution of TitanÂs origin and atmospheric composition. Several observations (on C18O and OC18O) give some constraints on the 16O/18O ratio in Titan's atmosphere.

We present a new photochemical model to study isotopic distribution between the various oxygen species to search for some additional constraints on the origin of oxygen in the atmosphere of Titan. It also gives new information about the formation of Titan and Enceladus (which is an important Oxygen source of Titan atmosphere).

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Rare-Earth Element Fractionation Evidence in the Solar Nebula From the Study of Primitive Chondrites

Undifferentiated meteorites so-called chondrites are direct evidence of physico-chemical processes occurred in the protoplanetary disk at the time of its formation ~ 4.5 Gyr ago. During the solar nebula condensation, chemical fractionations of elements occurred among chondritic meteorites [1,2]. Rare-Earth elements (REEs) were some of the first elements that condensed along with Ca, Al, Ti-rich oxides and silicates. In fact, refractory inclusions are of special interest because they contain short-lived chronometers showing that they are the oldest materials in the solar system [3].

In general, undifferentiated meteorites have unfractionated refractory element patterns when normalized to CI chondrites, the group that have solar abundances [1,4]. However, from the study of primitive carbonaceous chondrites by ICP-MS analyses of REEs, some of them for the first time, we have found some anomalies that indeed depict fractionations in the early solar nebula. Some of them are already described in previous works [5,6], but some patterns are new and they could offer new insights into the chemical environment from which the primordial building blocks of planets formed.

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13C fractionation in photon-dominated regions

The high spectral sensitivity of the HIFI instrument onboard Herschel allowed us to address the lines of the 13C isotopologues of many species and compare their abundance with those of their 12C counterparts.

Simulations of chemical fractionation show that carbon fractionation can be significant even in relatively warm photon-dominated regions (PDRs). It occurs mainly through the reaction 13C+ + CO -> C+ + 13CO. A direct search for the increased C+/13C+ or 13CO/CO ratios is, however, hindered by the significant optical depth of the main isotopic lines.

An observational confirmation of chemical fractionation thus has to rely on proxies. CH turns out to be the most sensitive tracer. The CH/13CH ratio can be enhanced by large factors compared to the elemental abundance. We confirmed this for the first time by direct observations.

To finally quantify the role of the fractionation reactions in PDRs, we have to carefully calibrate the 13C/12C elemental abundance in the models. It turns out, however, that the measurements of the 13C18O/C18O ratio, used so far to obtain the elemental abundances, are affected as well by chemical fractionation. This asks for a revision of our current picture.

Thushara Pillai

MPIfR

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Primordial Deuterium Astration in the Galactic Center

The detection of DCN in SgrB2 in the 1970s was unexpected: galactic chemical evolution models predict that deuterium should be absent in regions with significant star formation (SF) like the Galactic Center. Further observations not only confirmed the presence of D in the GC, but also determined that the elemental [D]/[H] ratio was larger than predicted by the models. This implied enrichment via primordial gas infall. However, these observations were towards two active SF regions where physical and excitation conditions were estimated crudely and fractionation reactions play a very dominant role. Using APEX and IRAM 30m observations on diverse molecular clouds with and without SF as well as regions where there is other evidence of interaction with primordial gas, we report on improved estimates of the [D]/[H] ratio as a function of distance from SgrA*.

Linda Podio

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The L1157-B1 protostellar shock: Si fractionation and chemistry

The gravitational infall from which a new star is formed is accompanied by the ejection of highly supersonic jets. The shocks produced when the ejected material impacts on the high-density surrounding medium rapidly heat and compress the gas, triggering several microscopic processes, such as molecular dissociation, gas ionisation, endothermic chemical reactions, ice sublimation, and dust grain disruption. It is well known that these processes produce a strong enhancement of the abundance of some molecules, which are evaporated or sputtered from dust grains.

I will present a study of molecular complexity in the protostellar shock L1157-B1 developed in the context of the Large Programme ASAI (Astrochemical Surveys At IRAM). The shock presents a very rich chemistry, showing emission lines of molecular ions, S and Si bearing molecules, and complex organic molecules. In particular, the fractionation and abundance of Si-bearing molecules are compared with the predictions of chemical models. This allow us to constrain the chemistry of the shock and the relative importance of the gas phase processes as compared to a direct formation of molecules on the dust grain surfaces. This kind of studies are key to understand the processes which allow building up the chemical complexity up to the formation of pre-biotic molecules in the interstellar medium.

Anna Punanova

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Deuterium fractionation in the Taurus molecular cloud

In this work we measure the deuterium fraction towards dense cores along the filamentary structure L1495 in Taurus. We compare deuterium fractionation in two molecular ions, HCO+ and N2H+, and study the gas traced by different species. Because of the CO freeze-out, the HCO+ abundance decreases toward the centres of dense cores, while N2H+ stays in the gas phase there; N2H+ is vanishingly rare in the less dense surroundings of the cores as nitrogen is probably still in atomic form there. The same scenario works for their deuterated isotopologues. Therefore HCO+/DCO+ traces the less dense periphery of the cores and N2H+/N2D+ traces more dense centres of the cores. For this study, N2H+(1-0), N2D+(2-1), H13CO+(1-0) and DCO+(2-1) on-the-fly maps of 13 cores were completed to measure the deuterium fraction and reveal the kinematics of the cores. Observations were performed with the IRAM 30-meter telescope. Most of the cores have moderate deuterium fractions (10-25%). A velocity gradient of 0.3-0.6 km s-1 was found across most of the cores, which shows the possible presence of rotation with rotation axis aligned with the filament. The effects of different physical conditions (temperature, density, mass, amount of CO freeze-out) on the deuterium fraction will be discussed. The results will be compared to those of a similar study toward dense cores in L1688 in Ophiuchus, to gain understanding on the chemical evolution of pre-stellar cores embedded in different environments.

Nami Sakai

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Tracing the production pathways of molecules by 12C/13C ratio

Toward some starless cores, we measured the 12C/13C ratios of various carbon-chain molecules (CCH, CCS, C3S, C4H), and discovered large anomalies of the 13C abundance within a single species. For instance, the C13CS/13CCS ratio was found to be as large as 4.2. Furthermore, most of the 12C/13C ratios in carbon-chain molecules are found to be significantly higher (>250 for the highest case) than the elemental 12C/13C ratio of 60-70. The dilution of the 13C species is theoretically predicted by Langer et al. (1984). In molecular clouds, the main reservoir of 13C is 13CO. C+ and 13C+ is formed from CO and 13CO by the reaction with He+. However, only 13C+ goes back to 13CO by the isotope exchange reaction with CO in cold clouds. Thus, 12C+/ 13C+ ratio becomes higher than 60-70, and consequently, the 12C/13C ratio in various molecules formed from C+ becomes higher. This effect is observationally confirmed by our studies. The abundance anomaly within a single species and the dilution degree both reflect the formation processes of molecules. By use of such an Âisotope tracerÂ, the main production pathways of the molecules could be constrained in a microscopic way not only for the carbon chain molecules but also for other C-bearing species. I will present how it can be applied for some of the important species.

Jonathan Tan

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Deuteration Studies of Massive Star Formation

I review our work using N2D+ and other deuterated species to identify the initial conditions of massive stars, including both theoretical models/simulations and observational studies, primarily with ALMA.

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Deuteration around the ultracompact HII region Mon R2

MonR2 is the most active star formation site in the Monoceros molecular cloud. It contains a cluster of recently formed high-mass stars driving an HII region that is surrounded by a series of photon-dominated regions (PDRs). On basis of IRAM-30m observations, we have studied the chemistry of the deuterated molecules toward two positions (namely IF and MP2) in MonR2. We find a rich chemistry of deuterated species towards MonR2, including C2D, DCN, DNC, DCO+, D2CO, HDCO, NH2D, and N2D+. Our high spectral resolution observations allow to resolve three velocity components associated with different PDRs exposed to different UV radiation fields. We calculate the deuterium fraction (Dfrac=[XD]/[XH]) of the different species to be about 0.01, except for HCO+ and N2H+ with values 10 times lower. The Dfrac values found in MonR2 are similar to those measured in the Orion Bar, and are well explained with a pseudo-time dependent gas-phase model for an object with an age of 0.1 Myr. The deuterium chemistry is used to study the evolutionary stage of different low-mass and high-mass star forming regions. However, while for low mass regimes it seems to be enough to determine Dfrac for molecules like N2H+ and HCO+, a more complete modelling is required to date high-mass star forming regions.

Riccardo Giovanni Urso

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A laboratory study of the OD stretching mode band in H2O:HDO ice mixtures

The infrared spectrum of solid HDO shows three fundamental absorption bands due to the OH and OD stretching modes and the bending mode. The OH stretching mode occur at about 3300 cm^-1 (3.03 um) while the OD stretching mode shifts to about 2425 cm^-1 (4.1 um). This latter band is not observable from ground-based telescope because of the strong telluric absorption.

In space, molecules in the solid phase have been detected in the line of sight of quiescent molecular clouds and star forming regions as icy mantles on dust grains. Some of the observed species (such as CO) freeze out from the gas phase while others (such as water) are formed on grains after surface reactions. It is generally accepted that icy grain mantles suffer from energetic processing due to cosmic-ray bombardment and UV photolysis. Most of our knowledge on the chemical composition and physical structure of icy mantles is based on the comparison between astronomical and laboratory spectra.

In dense molecular clouds deuterated species are expected to form on icy mantles. In fact HDO has been detected towards the line of sight of two high mass young stellar objects (namely W33A and NCG7538 IRS9) by the ISO. It is expected that other detections will be available after the launch of the James Webb Space Telescope.

Here we will present some preliminary experimental results on the profile and intensity of the OD band in H2O:HDO mixtures as a function of the temperature of the ice and after ion bombardment.

Malcolm Walmsley

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What happens at high density in cores?

I will discuss briefly recent ALMA results towards the contrasting cores IRAS 1629 and L1544 . In both cases, densities of order 10^7 cm-3 and size scales of order 1000 AU are being sampled and the question arises of what consequences this has for the chemistry in general and fractionation in particular.

Susanne Wampfler

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Spatially resolved measurements of the 14N/15N ratio around protostars

The solar system solids (terrestrial planets, comets, meteorites) are significantly enriched in nitrogen-15 compared to the gas reservoir, represented by the Sun and the gas giants. The origin of this isotopic anomaly puzzles astrochemists and cosmochemists likewise. Two main scenarios have been proposed to explain the observed 14N/15N variations among the solar system bodies: chemical fractionation and isotope-selective photochemistry. Nitrogen isotope fractionation during star formation can be studied by measuring the 14N/15N ratio in prestellar cores, protostellar envelopes, and in protoplanetary disks. However, single-dish measurements of the 14N/15N ratio in star-forming regions have so far remained inconclusive on the dominant process. Interferometric observations are key to probing spatial signatures, which are predicted to be different for the two mechanisms.

We will present a spatially resolved measurement of the 14N/15N ratio around the class 0 protostar NGC 1333 IRAS 2A with the Plateau de Bure Interferometer, where the largest isotopic variations occur along the outflow, hinting at a photochemical origin. First results from the Protostellar Interferometric Line Survey (PILS), a 329-363 GHz full spectral scan of IRAS 16293-2422 with ALMA, will also be presented. To fully exploit the potential of isotopic ratios as tracers for the origin of solar system matter, we will discuss strategies for linking astronomical results to laboratory measurements of meteorites.

Sarolta Zahorecz

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Fractionation in GRB host galaxies

Gamma-ray bursts (GRBs) are the most energetic explosions in the Universe. A massive star undergoes core collapse, or a double neutron star or a neutron star and a black hole binary merges (Woosley et al. 2006, ARA&A, 44, 507). Their hosts are typically metal poor galaxies of intermediate mass (Savaglio, Glazebrook & Le Borgne 2009, ApJ, 691, 182; Castro Ceron et al. 2010, ApJ, 721, 1919; Levesque et al. 2010, AJ, 140, 1557). GRBs prefer host galaxies with active star formation. Fractionation of different atoms are well studied in our Galaxy, but only a few measurements are available toward extragalactic sources. The 12CO/13CO ratio gives us information on the stellar evolution and nucleosynthesis. It is expected to decrease with time and to depend on the star formation history. 12C is directly produced in the triple-alpha process, while 13C is created from 12C as an intermediate product of the carbon-nitrogen-oxygen cycle. The 12CO/13CO ratio in galaxies varies systematically as a function of gas surface density and of the star formation rate surface density (Davis 2014, MNRAS, 445, 237. 12CO/13CO ratios between 5 - 40 were detected by Davis (2014). We estimate the possible 12CO/13CO ratio in GRB host galaxies. Possible observations of fractionation in the host galaxies at different z will be discussed.

Posters

Laura Colzi

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Nitrogen and Hydrogen fractionation in high-mass star forming clumps

The two stable less abundant isotopes of nitrogen and hydrogen, 15N and D, are both enriched in comets and carbonaceous chondrites with respect to the values measured in the proto-solar nebula. This raises the question whether the two enrichments have a common origin, and how both are linked to the past chemical history of the Solar System. To put constraints on chemical models, observations in molecular cores that are similar to the environment in which our Sun was born are required, but up to now only a handful of observational studies has been performed.

I will present new low-angular resolution observations of isotopologues of HCN and HNC toward dense cores that belong to different evolutionary stages of the massive star-formation process: from massive starless cores, to high-mass protostellar objects, to UC HII regions. These cores represent likely environments similar to that in which our Sun was born, as suggested by recent findings.

Marta De Simone

University of Florence

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Glycolaldehyde in Perseus young Solar analogs

Glycolaldehyde (HCOCH2OH) is the simplest of the monosaccharide sugars and it is expected to be a precursor of ribose, an RNA component; it is playing a major role in the prebiotic chemistry in low-mass star forming regions from the astro-biological perspective. As part of the CALYPSO (http://irfu.cea.fr/Projects/Calypso) survey with the IRAM PdBI interferometer, we have obtained high angular resolution (< 1") spectral maps at 1.3 mm and 1.4 mm of 12 Solar-mass Class 0 protostellar systems in L1448 and NGC-1333 regions in Perseus. This deep survey led to the detection of a large number of lines emitted by complex organic molecules in several sources: our analysis was based on the searching of Glycolaldehyde emission. Preliminary results: (i) 4 (33%) of 12 individual sources show HCOCH2OH emission; (ii) detection of several lines covering a large spread in excitation (30 to 370 K); (iii) The line intensities seem to be consistent with a single temperature LTE emission (~100-180 K). Our results suggest that the Glycolaldehyde emission is confined to a limited region of the inner envelope where the gas temperature is sufficiently high to evaporate the ice mantles. Our preliminary analysis shows that the Glycolaldehyde gas phase abundance relative to molecular hydrogen has a spread of a factor of ~10 among the detected sources.

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Deuterated molecules in the Galactic center

We present measurements of deuterated molecules towards selected "quiescent" molecular clouds in the Galactic center. The high kinetic temperatures, the low dust temperatures and the large abundance of complex organic molecules observed in the Galactic center offer the opportunity to use deuterated molecules to differentiate between formation in gas phase and on grains. The observed isotopic ratios will be discussed in the context of molecules formation. A comparison with observations in other galactic nuclei will be also discussed.

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Gas phase vs. dust grain deuterated chemistry: HDCO and D_2CO in massive star-forming regions

Deuterated molecules are formed at low temperatures and high densities. Therefore the deuteration fraction (the relative abundance between a species containing D as compared to the same species containing H) is expected to be enchanced in the cold, dense prestellar cores in molecular clouds and to decrease after the protostellar birth. Previous studies showed that for low-mass and also for high-mass star-forming cores, some species could be an evolutionary indicator. A different evolutionary trend was seen for the species formed exclusively in the gas and the species formed partially or totally on grain mantles (Fontani et al. 2015, A&A, 575, 87).

Formaldehyde can be produced both in the gas phase and on grain surfaces, but the relative importance of the two chemical path is not clear. Comparison of the deuteration properties of formaldehyde with previously studied molecules can help us to understand the formation way.

We have used the APEX SEPIA Band 5 receiver to study the deuteration fraction of formaldehyde. We have detected single deuterated formaldehyde for high-mass star-forming cores from the early to the late evolutionary stages. The deuteration fraction is expected to decrease with the evolutionary stage. In agreement with this, the doubly deuterated formaldehyde line was detected only in the earlier evolutionary stages (Zahorecz et al. in prep). Comparison of the deuteration fraction of different molecules will be discussed.

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Measurements of 15N/14N Fractionation toward Infrared-Dark Clouds

Being the fifth most abundant elements in the Universe, the nitrogen isotopic ratio has the potential to provide key information about the initial environment of the proto-Solar nebula. Recent findings suggest that the Sun may have formed in a high-mass star-forming region. Infrared-Dark Clouds (IRDCs) are believed to be the precursors of the massive star and star cluster formation. Therefore these regions represent a unique opportunity to test the 15N/14N fractionation processes under physical conditions similar to those proposed for the proto-Solar nebula. In this contribution we will present measurements of the J=1-0 rotational transitions of H13CN, HC15N, HN13C and H15NC obtained toward a sample of 22 massive dense cores in four IRDCs, IRDC C, F, G and H with the IRAM-30m telescope. The resulting 14N/15N ratio measured from HCN and HNC found to be 131-599 and 219-630 receptively. For IRDCs C, F and H, results are higher by factors of 2 and 1.5 respectively when compared with measurements toward low-mass pre-stellar and protostellar cores. However for IRDC G, the results are systematically lower by a factor of 2, and comparable to those measured in small cosmomaterials, planets and low-mass star-forming regions. Since IRDC G has the lowest average gas density among the four targeted clouds, we propose that the density of molecular gas could be the important parameter affecting the initial nitrogen isotopic composition in protosolar nebulae.