Isotopes in the ISM and Solar System Materials

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Why Study Isotopes?

- Measurements of elemental abundances and isotopic ratios allow to trace the history of nucleosynthesis in the Universe.
- Big Bang—primordial abundances of light elements (D, $^3$He, $^4$He, $^7$Li).
- Subsequent stellar processing alters abundances of light elements and produces heavy elements (C, N, O—"metals").
- D always destroyed; $^3$He, $^7$Li may be net produced; $^4$He certainly net produced (see reviews by Wilson & Rood 1994; Wilson 1999).
- Nucleosynthesis products expelled into the ISM, incorporated into planet forming bodies in disks.
- Separate aspect: astrochemistry and fractionation—complication for understanding the nucleosynthesis but of great interest for ISM studies.

http://www.space.com
Measurement and Interpretation Challenges

- **Solar System:** in situ measurements with space probes, solar wind measurements, meteorites, solar photosphere (spectroscopy)
- **ISM:** spectroscopic measurements of *gas-phase* species
- *Gas-phase* abundances affected by *freeze-out* of molecules onto dust grains, but such processes do not affect isotopic ratios
- UV/visible wavelengths strongly affected by *dust extinction* → submm/radio wavelengths key for exploring abundance gradients in the disk
- *Beam averaging:* ~1pc in radio vs. 10^-4 pc in UV/visible; the larger the sampled region the more representative the result
- *Optical depth* effects—photon trapping; use rare isotopologues, e.g. $^{12}\text{C}^{18}\text{O}/^{13}\text{C}^{18}\text{O}$, or line wings; weak lines, need very high sensitivity
- *Chemical fractionation*—caused by small differences in molecular binding energies, e.g.
  \[
  (^{13}\text{CO}/^{12}\text{CO})_{\text{measured}} = (^{13}\text{CO}/^{12}\text{CO})_{\text{actual}} \times \exp(35K/T)
  \]
  CH⁺ produced at high T, fractionation not important
- *Selective photodissociation*—more abundant isotopologue can self shield—dominant effect in diffuse clouds (UV measurements)
- Need to measure isotopic ratios in many species to check for systematics
Talk Outline

• Multiple aspects of isotopic studies:
  • Nucleosynthesis—isotopic gradients and anomalies
  • Astrochemistry—fractionation, molecular formation pathways...
  • ISM structure—isotopic species as tracers of star formation

• High-density, low-temperature conditions typical for prestellar cores lead to depletion of abundant gas-phase species onto grain mantles
• Which species are optimum tracers of cold dense gas at the onset of star formation (temperature, density, velocity field)?
• Focus on:
  • Deuterium fractionation and the role of deuterated molecules as tracers of H₂ (isotopologues of H₃⁺, N₂H⁺ and ammonia)
  • Nitrogen fractionation ratios
• Comparison between the ISM and Solar System materials (Solar System isotopic ratios frozen in time over 4.6 bln years—time evolution)
• Prospects for isotopic studies with ALMA
• Will only cover gas-phase measurements, not ices
Galactic Gradients

- Gradients in isotopic ratios with galactocentric distance have been reported; in particular for $^{16}\text{O}/^{18}\text{O}$
- $^{16}\text{O}$ primary, $^{18}\text{O}$ secondary—support for standard Galactic chemical evolution
- Recent data do not exhibit a significant trend (Polehampton et al. 2005; OH)

- Local ISM: Orion A at 500 pc has O/H, N/H a factor of 2 lower than Solar System
- N and O abundances expected to increase with time due to chemical evolution of the Galaxy—Orion A should have higher abundances than solar
- O atoms on grains? No O/H gradients with the distance from the Trapezium
- Solar System abundances may not be representative of the local ISM 4.6 Gyr ago

Wilson 1999

Polehampton et al. 2005 (ISO)
Solar System Oxygen Isotopic Anomalies

- $^{17}\text{O}$ and $^{18}\text{O}$ are secondary isotopes, ejected by Type II supernovae; $^{17}\text{O}$ also produced in the intermediate mass progenitors of AGB stars
- Galactic chemical evolution: younger objects should be $^{16}\text{O}$ poor ($^{17}\text{O}$ and $^{18}\text{O}$ rich); $^{17}\text{O}/^{16}\text{O}$ vs. $^{18}\text{O}/^{16}\text{O}$ should show a slope of 1
- $^{18}\text{O}/^{17}\text{O}$ in the Solar system is ~5.2, compared to ~4 in the Galactic disk (e.g., Woouterloot et al. 2008)
- Solar System formed from material polluted in $^{18}\text{O}$ (e.g. Young et al. 2010; 1% enrichment by ejecta from Type II supernovae)
- Enrichment of ISM by $^{17}\text{O}$-rich winds of AGB stars; sequestration of $^{18}\text{O}$-rich ISM gas into long lived low-mass stars (Gaidos et al. 2009)
- At any galactocentric radius, younger objects (ISM, newly formed stars) will be $^{17}\text{O}$-richer than older objects (Solar System)
- Isotopic selective photodissociation in the outer regions of the solar nebula can also affect O isotopic ratios—Sun born in a stellar cluster in the presence of a massive star (Lee et al. 2006)
- Genesis: Sun is $^{16}\text{O}$-rich relative to SMOW (McKeegan et al. 2009, 2010)
- Coexistence of $^{16}\text{O}$-rich and $^{16}\text{O}$-poor reservoirs since the earliest stages of Solar System evolution (Krot et al. 2010)
Atomic $^{12}\text{C}/^{13}\text{C}$

- $^{13}\text{CII}$ fine structure line at 158 $\mu$m first detected in Orion using KAO (Stacey et al. 1991)
- Boreiko & Betz (1996): $^{12}\text{C}/^{13}\text{C}=58(\pm 6, -5)$; $^{12}\text{CII}$ optically thick ($\tau\approx 1.0-1.4$; additional uncertainty)
- Slightly lower than the value obtained for Orion from CO (67±3; Langer & Penzias 1990)
- New Herschel/HIFI data currently being analyzed (HEXOS KP; V. Ossenkopf; also SOFIA)
- $^{13}\text{CI}$ $^3\text{P}_1-^3\text{P}_0$ at 492 GHz completely blended with $^{12}\text{CI}$
- $^{13}\text{CI}$ $^3\text{P}_2-^3\text{P}_1$ at 809 GHz first detected in Orion Bar using CSO
- $^{12}\text{C}/^{13}\text{C}=58\pm 12$; from CO 75±9
- Effect of chemical fractionation small, or compensated by the isotopic-selective photodissociation of $^{13}\text{CO}$
- Difficult measurements; great potential for ALMA!
13C Abundance Anomalies

- Takano et al. (1998): HC$_3$N isotopologues in TMC-1
  - H$_{13}$CCCH/HC$_{13}$CCH/HCC$_{13}$CH = 1.0:1.0:1.4
  - Isotopic fractionation during the formation of HC$_3$N, rather than subsequent isotope exchange reactions
- Sakai et al. (2010): CCH isotopologues in TMC-1 and L1527
  - C$_{13}$CH/13CCH = 1.6
  - Two carbon atoms not equivalent in the formation pathways
- Both 13C species underabundant in comparison with the interstellar 12C/13C
D/H Ratio and Baryon Density

- Abundances of $^3\text{He}$ and, in particular, D are sensitive functions of the baryon-to-photon ratio, $\eta$
- Measurements of HI and DI in quasar absorption line systems indicate D/H $\approx 2.8 \times 10^{-5}$, in agreement with CMB measurements
- Likely the primordial value

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Wilson & Rood 1994

Linsky et al. 2006
D/H in Diffuse Local ISM

• The D/H ratio in the local ISM has been a subject of controversy
• UV/visual absorption spectroscopy measurements toward stars in the vicinity of the Sun indicate D/H \( \sim 1.5 \times 10^{-5} \)
• Significant scatter in the measured D/H ratios is observed beyond the Local Bubble
• Local Bubble measurements may not be representative of the D abundance in the local Galactic disk
• Suggested explanations:
  • Depletion of D atoms onto dust grains (Draine; Linsky et al. 2006)
  • Turbulent diffusion (Bell et al. 2011)
Giant Planets—HD

- ISO/LWS R(2) and R(3) lines of HD at 38 and 29 µm detected (Lellouch et al. 2001)
  - Jupiter D/H = (2.25 ± 0.35) x 10^{-5}
  - Saturn D/H = (1.7 ± 0.75 - 0.45) x 10^{-5}
  - Protosolar value (2.1 ± 0.4) x 10^{-5}
- Minor decrease of the D/H ratio over 4.6 Gyrs (?)
- Herschel/PACS R(0) and R(1) lines of HD at 112 and 56 µm (Lellouch et al. 2010)
  - Neptune D/H = (4.5 ± 1) x 10^{-5}
- Clear D enhancement in Neptune compared to the protosolar value
Comets are among the most primitive bodies left from the planetesimal building stage of the Solar Nebula.

D/H in cometary water is \(~3\times10^{-4}\), a factor of \(~12\) enrichment over the protosolar value and 2 times terrestrial value, SMOW \(1.5\times10^{-4}\).

Typical ISM hot core ratios are an order of magnitude higher; a few \(10^{-4}\) (e.g., Jacq et al. 1990; Gensheimer et al. 1996; with much higher values, of order \(1\%\) reported; e.g. Bergin et al. 2010, based on HD\(^{18}\)O).

Implication: comets incorporated material reprocessed in the inner nebula.

Isotopic ratios provide strong constraints on the turbulent mixing of the Solar Nebula and the origin of terrestrial water.
Molecular Differentiation in Starless Cores

- “Classical” molecular tracers (e.g., CO, CS) depleted at densities above a few $\times 10^4$ cm$^{-3}$
- Depletion competes with desorption — time and density dependence
- Recent work in Taurus (Pineda et al. 2010): total CO (gas+ice) correlates with $A_V$; CO depletion time scale (4.2±2.4)$\times 10^5$ yr
- N-bearing species, such as $N_2H^+$, unaffected by depletion up to a few $10^5 - 10^6$ cm$^{-3}$
- NH$_3$ abundance may actually be enhanced in the central regions (e.g., Tafalla et al. 2002, 2004)

B68: Bergin et al. 2002
“Complete Freeze-out”

- Chemical calculations (e.g., Walmsley et al. 2004) suggest that at densities above ~$10^6$ cm$^{-3}$ even N-bearing species should condense onto dust grains.
- Under such conditions, H$_3^+$ and its deuterated isotopologues (H$_2$D$^+$ and D$_2$H$^+$) become the only tracers of H$_2$.
- Density threshold time and model dependent—good observational constraints needed.
- Recent interferometric observations show persistence of N-bearing molecules at densities ~few $10^6$ cm$^{-3}$ (e.g., Crapsi et al. 2007; NH$_2$D/NH$_3$~0.5).
- Clear observational evidence that deuterated molecules are some of the best tracers of cold, dense gas.
$\text{H}_2\text{D}^+$

- $\text{H}_3^+$ has no dipole moment $\rightarrow \text{H}_2\text{D}^+$
- $o\text{-H}_2\text{D}^+$ 371 GHz: detected in 7 (out of 10) starless cores and 4 (out of 6) protostars
- Extended, brightest emission toward the densest and most centrally concentrated starless cores (L429, L1544, L694-2, L183)
- Variations in the o/p ratio
- $p\text{-H}_2\text{D}^+$ 1370 GHz: SOFIA/CCAT

\[ \text{Caselli et al. 2003, 2008 (CSO)} \]

\[ \text{Vastel et al. 2006} \]
Deuterated Ammonia

- Ammonia lines have simple hyperfine patterns and can be used as a tracer of the velocity field.
- Submm fundamental rotational lines have very high critical densities (>a few $10^7$ cm$^{-3}$, compared to ~2000 cm$^{-3}$ for the 22 GHz inversion lines) and trace the densest central regions in prestellar cores.
- Fundamental line of NH$_3$ at 572 GHz, not accessible from the ground, but deuterated variants accessible (NH$_2$D 470/492 GHz; ND$_2$H 336/389 GHz, ND$_3$ 309 GHz).
- Fractionation ratios (NH$_3$/NH$_2$D, NH$_2$D/ND$_2$H...) of order 10 not $10^5$ (Roueff et al. 2005)—strong lines.
- Herschel OT1 program on NH$_3$/NH$_2$D.
Very high deuteration levels have been measured in saturated molecules and ions (NH$_3$, H$_2$CO, CH$_3$OH, H$_3^+$, N$_2$H$^+$)

Little known about deuteration in radicals—basic building blocks of saturated species

NH$_3$ is an intermediate species in the gas-phase synthesis of ammonia

ND detected by Herschel in IRAS16293

Solar type protostar IRAS16293 displays high deuteration levels: [HDCO/H$_2$CO]=15%, [NH$_2$D]/[NH$_3$] = 10% (van Dishoeck et al. 1995); [CH$_2$DOH]/[CH$_3$OH]=30% (Parise et al. 2004)

Measured ND/NH ratio in the IRAS16293 envelope is ~30–100%!
Deuterated Molecules in Disks

- Difficult observations for current single-dish telescopes and interferometers
- $\text{H}_2\text{D}^+$ detected in TW Hya and DM Tau (Ceccarelli et al. 2004)—measurement of the midplane degree of ionization
- HDO detection (Ceccarelli et al. 2005) disputed by Guilloteau et al. (2006)
- Interferometry: DCO$^+$ and DCN in TW Hya; limits for HDO and $\text{H}_2\text{D}^+$ (Qi et al. 2008)
- Rapid falloff of DCO$^+$ abundance at $R>90\text{AU}$

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Qi et al. 2008
SMA DCO$^+$ TW Hya

Ceccarelli et al. 2004 (CSO)
Nitrogen displays the largest stable isotopic variations in the Solar System, after hydrogen.

Usually explained by mixing between various solar, or possibly pre-solar reservoirs.

Earth, Mars interior, Venus and most primitive meteorites have bulk nitrogen isotopic ratios within 5% of the terrestrial atmospheric ratio, $^{14}\text{N}/^{15}\text{N}=272$

However, the proto-solar nebula was poorer in $^{15}\text{N}$ compared to the terrestrial value, $^{14}\text{N}/^{15}\text{N} \sim 450$ (e.g., Jupiter measurements; solar wind Genesis measurements, Marty et al. 2009; same as local ISM, $450 \pm 22$)
Nitrogen Isotopes in Comets

- Very low $^{14}\text{N}/^{15}\text{N}$ isotopic ratios, $148\pm6$, have been measured in CN in some 23 comets (Manfroid et al. 2009)
- A much higher, roughly terrestrial ratio in HCN, the presumed parent of the CN radical in cometary atmospheres, reported in comet Hale-Bopp (Jewitt et al. 1997, Ziurys et al. 1999)
- However, observations of comet 17P/Holmes (Bockelée-Morvan et al. 2008) suggest similar $^{14}\text{N}/^{15}\text{N}$ isotopic ratios in CN ($139\pm26$) and HCN ($165\pm40$)
- Re-analysis of the archival data suggests that the HC$^{14}\text{N}/\text{HC}^{15}\text{N}$ ratio in Hale-Bopp may in fact have been consistent with the CN measurements
- $^{15}\text{N}$ enhancements often associated with D enhancements

Marty et al. 2009
Multiple Origins of N Isotopic Anomalies

- Meteoritic and cometary organic matter contains three components of different origin (Aléon et al. 2010)
  - **Group 1** (major component of carbonaceous chondrites, IDPs, comet Hale-Bopp): shows linear correlation between H and N fractionation; formed by low-T ion-molecule reactions at the prestellar core stage or in outer regions of the protosolar disk
  - **Group 2** (e.g. Tagish Lake meteorite, comet Wild 2): shows significant $^{15}\text{N}$ excesses above the correlation; late origin in protosolar disk, high-T
  - **Group 3** (unequilibrated ordinary chondrites): shows large D excesses not associated with $^{15}\text{N}$ excesses; interstellar origin
- Isotopic anomalies do not fingerprint interstellar origin
Nitrogen “Super-fractionation” in the ISM

- In cold, dense, CO depleted ISM material, large $^{15}$N enhancements have been suggested to be present in ammonia ices (Rodgers & Charnley 2002, 2008).
- At 10 K, the gas-phase N fractionation in ammonia may reach a factor of ~7-10.
- Enhancement factor time dependent; time at which the maximum fractionation is reached depends strongly on the initial fraction of N in molecular form.
- This process might explain $^{15}$N excesses in primitive refractory organics, if they are synthesized from ammonia.

Rodgers & Charnley 2008
ISM: $^{14}\text{N}/^{15}\text{N}$ in $\text{NH}_2\text{D}$

- Is there observational evidence for high $^{15}\text{N}$ enhancements in ammonia?
- $^{15}\text{NH}_2\text{D}$ detected in several dense cores (Gerin et al. 2009)
- $^{14}\text{N}/^{15}\text{N}$ isotopic ratios measured in deuterated ammonia are comparable to the protosolar value and higher than the terrestrial ratio, but the error bars are large

Gerin et al. 2009
(IRAM 30-m)
ISM: $^{14}\text{N}/^{15}\text{N}$ in $\text{N}_2\text{H}^+$

- $^{15}\text{NNH}^+$ recently detected in L1544 (Bizzocchi et al. 2010)
- The $^{14}\text{N}/^{15}\text{N}$ ratio is $446\pm71$, close to the protosolar value of $\sim450$ and much higher than the terrestrial ratio

*Bizzocchi et al. 2010 (IRAM 30-m)*
ISM: $^{14}\text{N}/^{15}\text{N}$ in NH$_3$

- **GBT**: NH$_3$ (1,1)—(3,3) and $^{15}$NH$_3$ (1,1) lines observed simultaneously
- **Barnard 1b**: NH$_3$ (1,1) and (2,2) lines are narrow (~0.8 km s$^{-1}$), but the (3,3) line has broad (~3.5 km s$^{-1}$) pedestal—outflow?
- From the rotation diagram analysis we can derive accurate temperature, $T_{rot}=10.9$ K
- From dust continuum maps, beam filling factor ~46%; peak line temperature ~5.7 K, in good agreement with observations
- The NH$_3$/$^{15}$NH$_3$ ratio is 334±50 (3σ), as compared to 470 (+170, −100) in NH$_2$D

*Lis et al. 2010 (GBT)*
New GBT Observations

- Ongoing work using the GBT (Wootten et al., in prep)
- Six more sources observed last Fall
- Preliminary analysis indicates very low $^{14}\text{N}/^{15}\text{N}$ ratios
Chlorine-Bearing Molecules in the ISM

- Prior to Herschel, H$^{35}$Cl and H$^{37}$Cl were the only Cl-bearing molecules detected in the ISM (both lines can be observed simultaneously)
- HCl 1—0 at 625 GHz detected by Blake et al. (1985; KAO)
- Ground based observations, CSO: Schilke et al. (1995), Salez et al. (1996)—strong gas-phase Cl depletion in dense regions
- Chloronium, H$_2$Cl$^+$, predicted to be abundant in UV illuminated regions (Neufeld & Wolfire 2009)
Ground-Based Observations

- Comprehensive survey of HCl in the Galaxy by Peng et al. (2010)
- Fourteen sources observed in both $^{35}$Cl and $^{37}$Cl
- Cl depletion factors up to ~400
- $^{35}$Cl/$^{37}$Cl isotopic ratio varies from unity to ~5, mostly lower than the terrestrial ratio of 3.1
- Nucleosynthesis models in supernovae predict large $^{35}$Cl/$^{37}$Cl variations
- Menten et al. (2011), $^{35}$Cl/$^{37}$Cl~4 toward Sgr B2 (APEX)
- Large errorbars, difficult measurements, low atmospheric transmission, need better SNR

Peng et al. 2010 (CSO)
Herschel Observations

- W3 A: $\text{H}^{35}\text{Cl}/\text{H}^{37}\text{Cl}=2.1\pm0.5$, consistent with the solar ratio
- Chloronium, $\text{H}_2\text{Cl}^+$, detected for the first time in the ISM using HIFI; isotopic ratio $\sim3$
- HIFI has excellent sensitivity and calibration, but “HCl can be done from the ground” → ALMA
Summary and Prospects for ALMA

- Measurements of isotopic ratios are difficult and require excellent sensitivity and calibration—ALMA offers both
- Very good progress can be made for $\text{H}_2\text{D}^+$, CI, HCl, fundamental lines of ammonia isotopologues
- Most of these lines are affected by poor atmospheric transmission
- ALMA will allow measurements of isotopes in more distance sources, e.g. IRDCs (beam dilution for GBT)—improved understanding of Galactic isotopic gradients, leading to non-axisymmetric models
- A combination of high sensitivity and large bandwidth will allow observations of isotopic ratios in heavy organics in hot cores (e.g. tentative detection of DCOOCH$_3$ based on observations of 100 transitions with low blending; D/H 2-6%; Margules et al. 2010)
- Studies of isotopes in disks will be an important program for ALMA
- All these measurements will lead to a quantitative improvement in our understanding of the Galactic nucleosynthesis, astrochemistry and star formation over the next decade