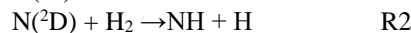


SIMULTANEOUS CO AND N₂ SELF-SHIELDING IN A VERTICALLY MIXED SOLAR NEBULA. J. R. Lyons¹, ¹School of Earth & Space Exploration, Arizona State University, Tempe, AZ, 85287, USA; jim.lyons@asu.edu

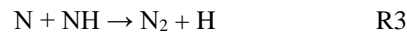
Introduction: Photodissociation of CO in the solar nebula (or parent cloud) may be responsible for the distribution of O isotopes observed in the Sun and in planetary and meteoritic materials. The similarity between the isotopically lightest CAIs [1] and the solar wind [2] and photosphere [3] suggests that the bulk material from which the solar system formed was roughly 60‰ lighter in ¹⁷O and ¹⁸O than modern Earth mean ocean water. N isotopes are even more dramatically fractionated between the Sun and Earth atmosphere, with the former about 400‰ lighter than the latter [4]. N₂ photodissociation may be responsible for this difference also, but the key mass-independent signature is not available because N only has 2 stable isotopes. A recent analysis of the C isotope ratio of the solar photosphere suggests a Sun depleted in ¹³C relative to planetesimal and planet-forming materials [3]. Because both CO and N₂ have high vapor pressures in the solar nebula (or parent cloud), photodissociation and self-shielding of these molecules may explain all 3 of these observed isotope distributions. Here, I evaluate N and O isotopes due to CO and N₂ self-shielding in a vertically-mixed solar nebula.

CO and N₂ photodissociation: CO photodissociation in H-rich astrochemical environments occurs from 91.1 to 108 nm. H atoms limit the minimum photodissociation wavelength to 91.1 nm, the onset of the H ionization continuum. The products of CO photodissociation are mostly C(³P) and O(³P), the electronic ground states of the two atoms. At wavelengths < about 95 nm, either O(¹D) or C(¹D) are produced in small fractions [5]. Electronically excited species are important because they react at a collisional rate (i.e. fast) with H₂ to make OH and CH radicals, both of which may be important intermediaries in the sequestration of CO self-shielding isotope signatures in reservoir species (e.g., H₂O and C grains) in the solar nebula.

N₂ is photodissociated from 91.1 to 100 nm in H-rich environments. The product N atoms are roughly equally divided between N(⁴S), the ground state, and N(²D), the first excited state. As with the excited state C and O, N(²D) reacts collisionally with H₂, producing the radical NH. The rate coefficient difference in the two reactions



is about a several orders of magnitude at 50 K [6]. The formation of NH allows the reformation of N₂ by the reaction



Rapid reformation of N₂ from the products of N₂ self-shielding means that the enrichment of ¹⁵N in N and depletion of ¹⁵N in the remaining N₂ are both reduced in magnitude.

Results: Shielding functions are used for CO and N₂ self and mutual-shielding as in [7], [8]. Isotopic photodissociation rate coefficients were computed as a function of height in the disk at 30 AU (Fig. 1a, 1b), and clearly exhibit self-shielding. Delta-values for CO and H₂O ice produced from dissociated CO (H₂O_{gr}), and for N₂ and HCN ice produced from dissociated N₂ (HCN_{gr}) are shown in Fig. 2a and 2b. Fig. 3 shows the time evolution of midplane total H₂O and total HCN.

Conclusions: CO self-shielding yields enough isotope fractionation to explain the Sun-planetary difference, but N₂ self-shielding does not. Possible reasons for this include: 1) N(²D) formation (not in [9]) during N₂ dissociation is leading to rapid NH formation and N₂ reformation; 2) an NH₃ reservoir (not included here, but in [9]) sequesters a large proportion of δ¹⁵N material; 3) N₂ self-shielding in the solar nebula is not responsible for the ~400‰ difference between the Sun/Jupiter and inner solar system materials. The first two possibilities are under further evaluation.

References: [1] Clayton R. N. et al. (1973) *Science*, 182, 485. [2] McKeegan K. et al. (2011) *Science*, 332, 1528. [3] Lyons J. R. et al. (2018) *Nat. Comm.*, 9, art. 908. [4] Marty B. et al. (2011) *Science*, 332, 1533. [5] Gao H et al. (2013) *J. Phys. Chem A*, 117, 6185. [6] kinetics.nist.gov [7] Lyons JR and Young ED (2005) *Nature* 435, 317. [8] Heays A et al. (2014) *A&A* 562, A61. [9] Visser R et al. (2018) *A&A*, 615, A75.

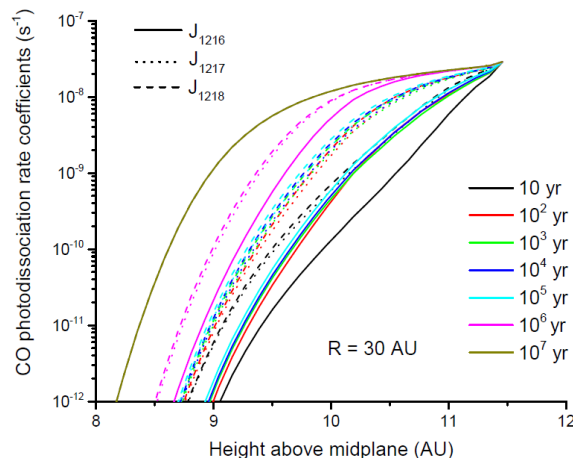


Fig 1a Photodissociation rate coefficients for CO isotopologues in the UV surface region of the solar nebula at a heliocentric distance of 30 AU. The lower rate coefficient for $^{12}\text{C}^{16}\text{O}$ is due to self-shielding. By 10^7 years (upper limit to nebular lifetime) CO abundance is too low for self-shielding to occur.

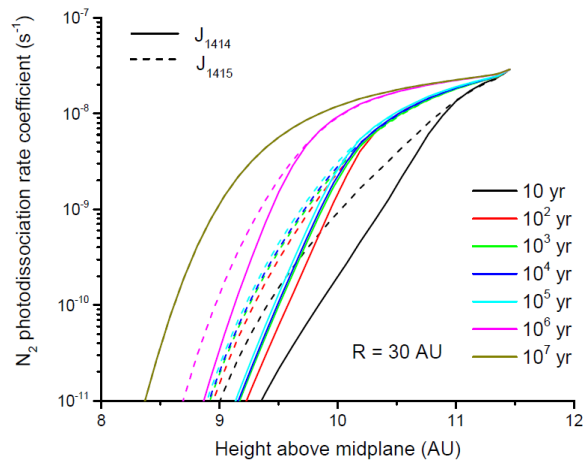


Fig. 1b Same as Fig. 1a but for N_2 isotopologues. In this case the rate coefficient for N_2 (1414) dissociation is lowered by self-shielding, except again at 10^7 years.

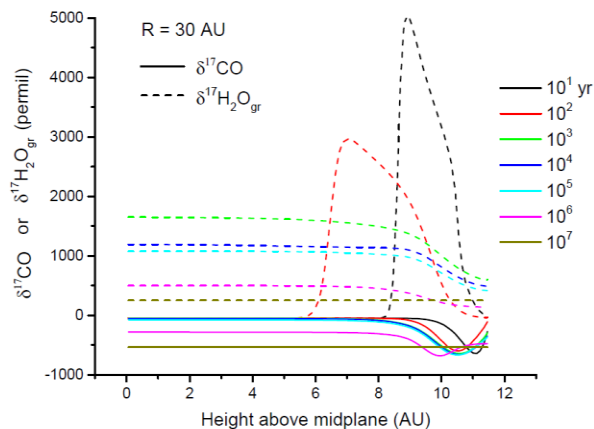


Fig 2a Delta-values ($\delta^{17}\text{O}$ only) for CO gas and H_2O condensed onto grain surfaces ($\text{H}_2\text{O}_{\text{gr}}$). $\text{H}_2\text{O}_{\text{gr}}$ is defined as ice condensate on grains formed only from O liberated by CO dissociation. The massive early enrichments are mixed vertically through the disk assuming a turbulent viscosity coefficient of $\alpha = .01$. Delta-values are relative to SMOW.

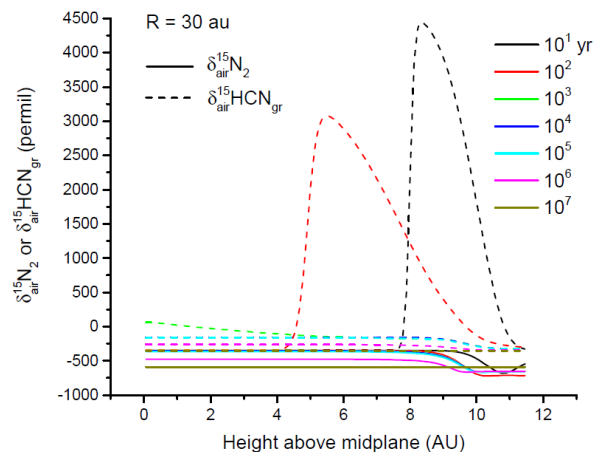


Fig. 2b $\delta^{15}\text{N}$ values (relative to air) for N_2 and HCN condensed onto grain surface. HCN_{gr} is formed only from N atoms derived from N_2 dissociation.

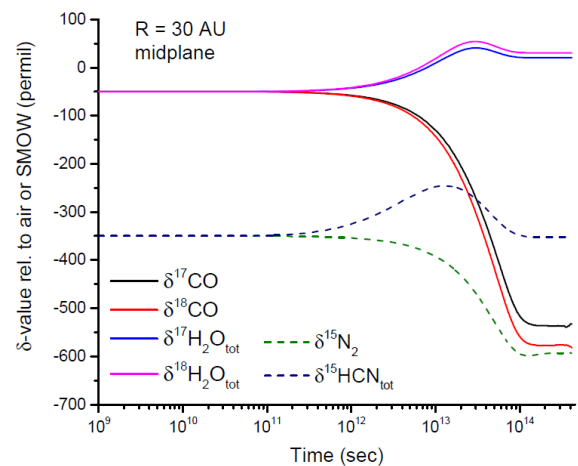


Fig. 3 Delta-values at the midplane vs. time for O and N isotopes. For O isotopes total nebular water rises by ~ 100 ‰ to values required by the CAI mixing line, assuming dilution by parent cloud water at -50 ‰. By contrast, total nebular HCN is far below the ~ 0 ‰ Earth atmosphere. Several possible reasons for this difference are discussed in the text.