

TOWARDS AN EVALUATION OF SELF-SHIELDING AT THE X-POINT AS THE ORIGIN OF THE OXYGEN ISOTOPE ANOMALY IN CAIs. J. R. Lyons¹ and E. D. Young², ¹IGPP Center for Astrobiology, UCLA, Los Angeles, CA 90095-1567, jrl@ess.ucla.edu, ²Department of Earth and Space Sciences, UCLA, Los Angeles, CA 90095-1567, eyoung@ess.ucla.edu.

Introduction:

Self-shielding during photodissociation of CO is a well-established process for producing depletions in $C^{17}O$ and $C^{18}O$ relative to $C^{16}O$ at the edges of molecular clouds (e.g., van Dishoeck and Black [1]; Warin et al. [2]). Recent observations of $C^{17}O$ and $C^{18}O$ are consistent within errors with an approximately mass-independent fractionation of the mass 17 and 18 isotopes [3]. Recently Clayton [4] suggested that self-shielding of CO also occurred in the very inner solar nebula (near the X point), and produced a mass-independent excess of ^{17}O and ^{18}O atoms in the vicinity of the X-point. Incorporation of the excess ^{17}O and ^{18}O (which together we will refer to as ‘Q’ atoms) into silicates, followed by entrainment of the Q-enriched silicates into the X-wind, delivered silicate material to the inner solar system ($\sim 1 - 3$ AU) with $\Delta^{17}O$ comparable to bulk meteorite silicate. In Clayton’s hypothesis CAI’s and other highly refractory grains resisted isotope exchange, and retained their original $\Delta^{17}O$ of ~ -20 ‰. The implications of this hypothesis are extraordinary: 1) the entire inner solar system, excluding CAI’s, condensed from material that passed through the X-point and experienced self-shielding, and 2) solar oxygen isotopes should be similar to the lightest CAI’s. Our goal here is to perform a plausibility test of Clayton’s hypothesis by estimating the total mass of Q produced by self-shielding.

Self-shielding at the X-point:

To make quantitative estimates of timescales and chemical production rates in the vicinity of the X-point, we utilize the 2-D α -disk model results of Huré [5]. Huré’s model does not include an X-point or any reconnection physics, so the calculations presented here are incomplete in this sense. For an X-point at ~ 0.1 AU, Huré’s model predicts $T \sim 2000$ K and $P \sim 10$ mbar at the midplane for $\alpha = 10^{-3}$ and an accretion rate $dM/dt = 10^{-7} M_{\text{solar}} \text{ yr}^{-1}$. We assume a 1000-fold enhancement in EUV flux from the protosun, consistent with observations of T Tauri stars [6]. CO photolysis occurs for wavelengths < 1100 Å, but because of shielding by H_2 , CO photodissociation occurs only at four lines (923.1, 933.4, 949.7, and 977.0 Å). The flux-weighted cross section for CO dissociation is $\sigma_{CO} = 1.1 \text{ E-}17 \text{ cm}^2$, and the vacuum photodissociation rate coefficient at 0.1 AU is $J_{CO} \sim 8.5 \text{ E-}3 \text{ s}^{-1}$. The fate of O (and Q) atoms liberated by CO photolysis at X-point-

like conditions is to react with H_2 to form OH, followed by reaction of OH with H_2 to form H_2O . For temperatures > 1000 K, the timescale for loss of O to H_2 is $\sim 10^{-2}$ times the timescale for loss of O to exchange with CO, assuming $CO/H_2 = 7 \text{ E-}4$. This ensures that an enrichment in Q produced in the self-shielding zone implies a nearly equal enrichment in H_2Q .

We next consider the fate of H_2Q . Reactions between CO and QH, such as $CQ + OH \rightarrow COQ + H$, followed by $COQ + H \rightarrow CQ + OH$, are capable of re-equilibrating CO and H_2O . The timescale for such re-equilibration is ~ 30 seconds at 0.1 AU. (For comparison, Huré’s model at 1 AU (1000 K and 0.1 mbar) yields a timescale $\sim 10^3$ years.) Competing with CO- H_2O equilibration are reactions that can transfer the Q-enrichment in water to silicate precursors. One such reaction (brought to our attention by R. Marcus, pers. comm., 2002) is $SiO + H_2Q \rightarrow SiOQH_2$. We are in the process of estimating a rate coefficient for this reaction, and therefore do not give the timescale for SiO loss, but given that the reaction occurs with one of the principal constituents of the nebular gas (i.e., H_2O), it is likely to be faster than CO- H_2O equilibration. If CO and H_2O can exchange O directly, rather than via an OH intermediate, then reaction of SiO with water may not serve to sequester Q in silicate. Additionally, exchange between CO and SiO could also inhibit enrichment of silicate, depending on the timescale for SiO condensation. For now, we assume that the $SiO + H_2O$ reaction represents a viable pathway for transfer of Q to silicates.

We now consider the size of the self-shielding zone. For the conditions of Huré [5] at 0.1 AU (2000 K, 10 mbar), unity optical depth for $C^{16}O$ occurs at $\sim (n_{CO}\sigma_{CO})^{-1} \sim 4000$ cm. Thus, $C^{16}O$ becomes self-shielding at the very inner edge of the solar nebula. (Needless to say, we know very little about conditions at the X-point, so the specific value of 40 meters should not be taken seriously. The point, however, is that $C^{16}O$ very rapidly becomes self-shielding as photons impinge upon the nebula. Additionally, we have not considered the temperature dependence of σ_{CO} .) CO photodissociates by a predissociation mechanism, meaning that EUV photons first promote bound-bound transitions before curve-crossing to an unbound state. This produces a line absorption spectrum for CO, with

different line occurrences for the various CO isotopomers. $C^{18}O$ becomes optically thick at a distance ~ 500 times that for $C^{16}O$, because $^{16}O/^{18}O \sim 500$, which suggests that the size of the self-shielding zone is ~ 20 km. However, H_2O is a strong absorber at the dissociation wavelengths of CO ($\sigma_{H_2O} \sim 2 \text{ E-17 cm}^2$), which reduces the size of the self-shielding zone back to ~ 20 to 40 meters in thickness.

The column production rates (molecules $\text{cm}^{-2} \text{ s}^{-1}$) for Q and O may be evaluated by integrating the photodissociation rate equations radially into the nebula. The ratio of the resulting column rates is given by

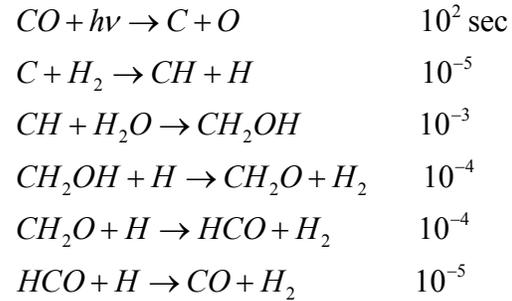
$$\frac{P_Q^{col}}{P_O^{col}} = \frac{n_{CO}}{n_{CO}} \left(1 + \frac{n_{CO}\sigma_{CO}}{n_{H_2O}\sigma_{H_2O}} \right)$$

where n_i is the number density of molecule 'i' and the cross sections are defined above. For $n_{H_2O}/n_{H_2} = 10^{-3}$ the enhancement in Q production over O production is 0.35, meaning that water produced from CO photolysis has a fractionation $\delta^{18}O = \delta^{17}O \sim +350 \text{ ‰}$. The total CO column photodissociation rate is $\sim 2\text{E}+14 \text{ molec cm}^{-2} \text{ s}^{-1}$. If gas and dust are accreting in proportion to their masses in the nebula, then the inward flux of CO is $\sim 1\text{e}+15 \text{ molec cm}^{-2} \text{ s}^{-1}$ at 0.1 AU in Huré's model, and the photodissociation of CO is not mass flux limited. Integrating the CO dissociation flux across the surface area defined by the X-point region (extending ~ 0.01 AU above the midplane) and over 10^5 years yields a total of $3\text{E}+27$ moles of H_2O produced, or 8 Earth masses of oxygen. This is ~ 20 times the mass of oxygen in the inner solar system, and, for a fractionation of 350 ‰, ~ 9 times the fractionation needed to move the entire inner solar system (total mass $\sim 2M_{\text{Earth}}$) $\sim 40\%$ up the slope = 1 line.

Several factors make the calculations presented here an upper limit to what probably occurred in the solar nebula. First, it is not known whether an X-wind was even present; if there was no mechanism to return photoprocessed material to $\sim 1-3$ AU, then self-shielding at the X-point would not have modified oxygen isotopes at $\sim 1-3$ AU. Second, self-shielding of CO may not occur because of increased line overlap at high temperatures. Navon and Wasserburg [7] considered the effects of temperature on self-shielding in O_2 and concluded that mutual shielding by various isotopomer bands reduces the ratio of photodissociation constants from $J_{OQ}/J_{O_2} \sim 10$ at 300 K to ~ 1.5 at 500 K. Applying their results to CO and extrapolating to $\sim 1500-2000$ K suggests that J_{CO}/J_{CO} could be reduced to ~ 1.05 , yielding a maximum Q enhancement of $\sim 50 \text{ ‰}$; absorption by water would further reduce the en-

hancement. Clearly the mutual-shielding effect described by Navon and Wasserburg [7] needs to be considered for CO for plausible X-point conditions.

Another factor to consider is that C produced during CO photolysis may attack water and reform CO. At 2000 K and 10 mbar, the following reaction sequence will occur (loss timescale for left-most reactant is included):



Many other reaction pathways are possible, particularly involving CH_2 , but these mostly cycle CH and CH_2 rapidly between H and H_2 . The above reaction sequence appears to be the fastest route to reformation of CO at high temperatures. The rate limiting step (apart from photodissociation) is the $CH + H_2O$ addition reaction, which occurs on millisecond timescales. Oxygen atoms are lost to reaction with H_2 (to form water) on a timescale $\sim 10^{-5}$ seconds, more rapidly than the above rate limiting step. This sequence of reactions would appear to return O (and Q) to CO well before another Q can be made.

Note that ionization of C to form C^+ , followed by the well-known carbon atom exchange reaction, $C_a^+ + CO \leftrightarrow C^+ + C_aO$, proceeds at a timescale $\sim 10^2$ seconds. **Conclusions:**

For a nebula with an inner edge temperature ~ 2000 K, reformation of CO from H_2O will prevent self-shielding from delivering a Q-enrichment to silicates. Until the physical conditions of the nebula in the vicinity of the X-point are better understood, a more conclusive evaluation of self-shielding at the very inner edge of the nebula is difficult to achieve.

References: [1] van Dishoeck E. F. and Black J. H. (1988) *Astrophys. J.*, 334, 771–802. [2] Warin S. et al. (1996) *Astron. Astrophys.*, 308, 535–564. [3] Sheffer Y. et al. (2002) *Astrophys. J.*, 574, L171–L174. [4] Clayton R. N. (2002) *LPS XXXIII*, Abstract #1326. [5] Huré J.-M. (2000) *Astron. Astrophys.*, 358, 378–394. [6] Imhoff C. L. and Appenzeller I. (1987) in *Scientific Accomplishments of the IUE* (ed. Kondo Y.), Reidel Publishing. [7] Navon O. and Wasserburg G. J. (1985) *Earth Planet. Sci. Lett.*, 73, 1–16.