SELF-SHIELDING OF THE E(1)-X(0) BAND OF CO IN A HOT SOLAR NEBULA. E. T. D. Boney[1], J. R. Lyons[2], R. A. Marcus[1] [1]Noyes Laboratory of Chemical Physics, Caltech, Pasadena, 91125 (boney@caltech.edu) [2]Institute of Geophysics and Planetary Physics, UCLA, Los Angeles, CA 90095-1567

Introduction: CO self-shielding has been put forth as a possible mechanism to explain the slope-1 oxygen 3-isotope plot observed in CAIs [1]. In particular, this theory posits self-shielding takes place at the X-point of an early solar nebula. We are testing this hypothesis in multiple X-point geometries. We have previously confirmed that self-shielding occurs for the E(1) band at very high temperatures, although the presence of H_2 leads to a non-slope-1 isotope enrichment [2]. We take advantage of the computed opacities of McCandliss [3] to explicitly treat the hydrogen absorption spectrum rather than make use of a shielding function, and we make use of Ubachs [4] high resolution data to construct an absorption spectrum of the E(1) band of CO at 1500K. We have also undertaken a comparison of these self-shielding results with the results of Navon and Wasserburg for O_2 [5]. Finally, we are in the process of adding all relevant photochemical reactions to the nebular model to test whether any isotope signature from CO cleavage will be preserved in interstellar water at 1500 K, a necessary condition of the x-point self-shielding hypothesis. We discuss the timescales of reactions expected to play an important role in isotope mixing.

Shielding at X-point, role of H_2 in the E(1) band: With the assistance of precise molecular parameters [4], we are able to calculate accurate absorption spectra for CO at 1500 K assuming Voigt line profiles. Using a standard disk model for the density [6], we calculate the CO self-shielding, and report it here for radiation normal to the nebular midplane. The effect of self-shielding on CO number density and CO and O isotopes can be observed in figures 1 and 2. Work on a geometry with radiation incident along the midplane, which we expect to be dominant at the X-point, is in progress. Further discussion of these details can be found in [2].

Literature data for H_2 transmission [3] enable a mutual-shielding to be estimated for that species. A coincidence of transmission in the McCandliss H_2 spectrum with the E(1) Q-branch absorption in the $C^{17}O$ spectrum leads to a steeply sloped 3-isotope plot (slope ~ 3) (see figure 3 of [2]). One band of a spectrum is not indicative of the total behavior of CO photodissociation. However, van Dishoek and Black [7] have measured that band 31 is responsible for 58% of the overall photodissociation rate of $C^{18}O$ at temperatures ~20 K, about 4x the contribution of the next highest band, suggesting that there could be a non-negligible contribution of this band to the final O 3-isotope plot.

Comparison to Navon and Wasserburg: Navon and Wasserburg showed that self-shielding in O_2 cannot occur at high temperatures due to the overlap of lines in the Schumann-Runge bands [5]. However,.the low energy bands of CO have narrower natural line widths, lessening the problem of overlap. To illustrate the role of line width, we computed an artificial E(1) spectrum with lines ~ the width of O_2 bands. The line-type structure is nearly gone (Fig. 3), and fractionation is greatly reduced (Fig. 4).

Effects of Nebular Mixing and Chemistry: Regardless of the exact isotopic composition of oxygen from CO self-shielding, photodissociation is not the end of the journey for isotopic oxygen. Estimates of the residence timescale of the gas at the X-point are ~2 weeks [8], which is of the same order of magnitude as the dissociation timescale of CO for normally incident radiation (Fig. 1). Thermal ionization of trace constituents of the gas should ensure that MRI-driven turbulent mixing is operative.

At the high temperatures and densities of the X-point, many other reactions must be taken into account. At high temperatures O, liberated by CO photolysis, proceeds to H_2O by rapid reaction with H_2. For a number density $n(H_2) = 3.0 \times 10^{18}$ cm^{-3} representative of the mid-plane of the X-point, the timescales of the forward and backward rate of are 1.3×10^{-7} s and 4.9×10^{-8} s, respectively. The self-shielding derived oxygen isotope signature is rapidly transferred to H_2O. Loss of that signature occurs by the oxygen-exchange reaction with CO On a timescale ~ 2×10^{-4} s. Thus, the incorporation of the isotope into water is 3-4 orders of magnitude faster than isotope scrambling by exchange with CO at the X-point, as one might expect from the abundances of CO and H_2, and the assumption of rapid incorporation of molecular oxygen into water appears justified [1]. Subsequent reactions involve OH, CO_2, and organic species produced from C atoms, and we are working to incorporate ~ 200 reactions into the nebular model to address the fate of O liberated by CO photolysis.

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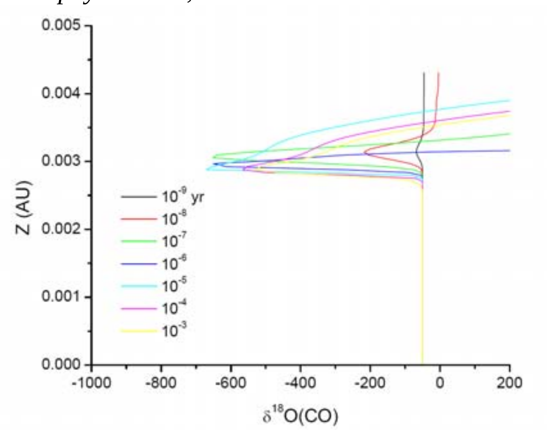
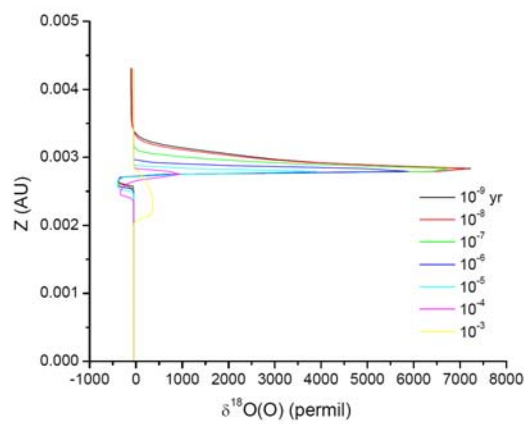
Chem. Phys. 113, 547-560 [5] O. Navon and G. J. Wasserburg, (1985) *Earth Planet. Sci. Lett* 73, 1. [6] Y. Aikawa and E. Herbst (2001) *Astron. Astrophys* 371, 1107. [7] E. F. v. Dishoeck and J. H. Black, (1988) *Astrophys. J.* 334, 77. [8] F. Shu, et. al. (1994). *Astrophys. J.* 429, 781.





Figures 2a & b. Isotope plots showing distribution of δ^{18}O(CO) (top, 1a) and δ^{18}O(O) (bottom, 1b) as a function of Z at R=.035 AU (1500 K) and disk α = .01. The negative delta values in CO and large positive delta values for O are due to CO self-shielding.

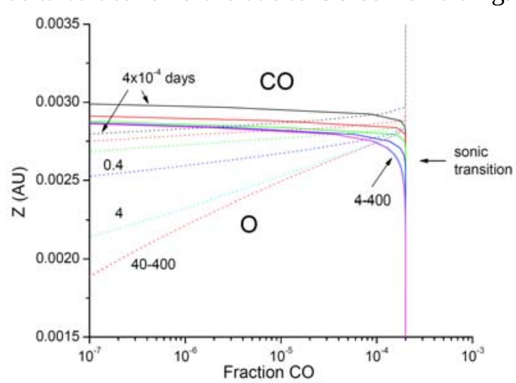


Figure 1. Vertical profiles of CO (solid lines) and O (dotted lines) at R=.035 AU at several times (in days). The gas transport timescale near the X-point is ~ days. The 'sonic transition' is the approximate height from which gas is entrained in accretionary flux tubes.

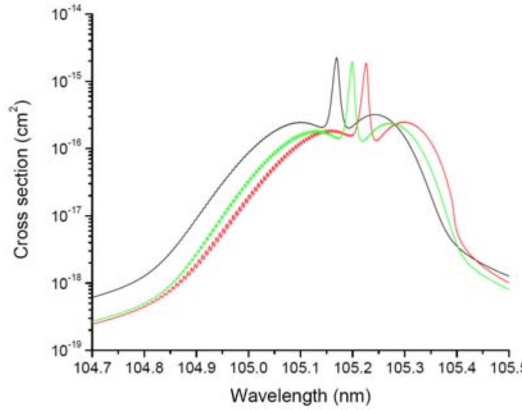


Figure 3. The three isotopomers of ^{12}CO at 1500 K with a natural linewidth in band 31 increased by a factor of 100.

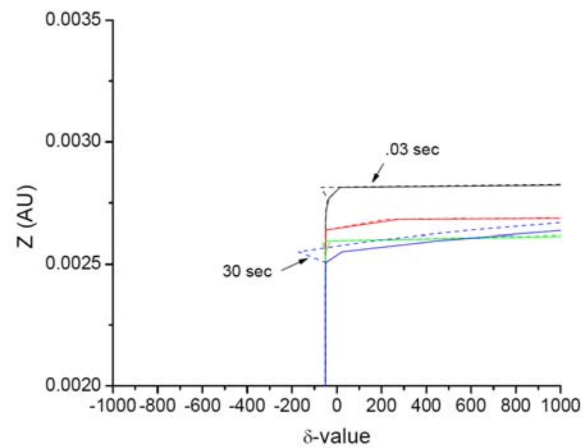


Figure 4. δ^{18}O(CO) as a function of Z at R=.035 AU (1500 K) for CA band 31 with linewidths increased 100 times and disk α = .01. The lack of negative delta values indicates that CO self-shielding is not significant. The positive delta values are a numerical artifact present in CO at very low abundances.