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

Introduction: At present CO self-shielding appears to be a possible mechanism for explaining the solar system slope 1 line [1]. Recent oxygen isotope measurements of poorly-characterized phases (PCP) in Acfer matrix support this view [2], and several possible sites for CO self-shielding have been suggested [1,3,4]. On the other hand, the new PCP phases in Acfer matrix have a mass fraction ~ 100 ppm, too small to form the needed oxygen isotope reservoir, and the principal location for CO self-shielding is still uncertain. In addition, a non-statistical surface mechanism during CAI formation has also been proposed [5]. Here we focus on our latest results on self-shielding in the vicinity of the X-point, in order to evaluate Clayton's original suggestion.

Shielding at the X-point: Clayton [1] proposed that CO self-shielding in the vicinity of the X-point produces an H_2O reservoir with a positive oxygen isotope anomaly that was transferred to silicates. The X-point is a difficult environment for which to do self-shielding calculations, with gas temperatures > 1400 K, high disk pressures, and high X-ray fluxes. The X-point is located at the disk corotation radius, where the Keplerian angular velocity of the disk equals the rotational angular velocity of the star. The disk is truncated at the radius at which the disk magnetic pressure balances the ram pressure of the accreting nebular gas. For accretion rates ~ 10^{-8} M_{solar} yr^{-1} and disk fields B_{disk} ~ 100 G, the X-point radius is $R_X \sim 5R_{star}$ AU and the truncation radius is slightly inward of R_x [6].

We have undertaken shielding calculations at 1500 K for the CO E(1)-X(0) band [7] including the effects of H_2 absorption [8]; X-rays are ignored. The temperature dependence of the CO band spectrum is shown in Figure 1 on a relative scale. Figure 2 shows the synthetic spectrum for $C^{17}O$ at 1500 K and the H_2 transmission for a column density of 10^{21} cm^{-2}. The H_2 transmission includes contributions from J=0 to 15 in the Lyman and Werner bands for ground state v=0. The H_2 transmission is reduced considerably from that at low temperatures.

Three-isotope plots for O produced during CO dissociation are shown in Figure 3 at three disk locations. These calculations only include photodissociation of CO and its isotopologues; subsequent formation of H_2O and reformation of CO, and transfer of the isotope anomaly to silicates, are neglected. At 50 K and 300 K this CO band yields anomalies with slope slightly < 1 due to structure in the H_2 spectrum (not shown). At 1500 K the slope is >> 1 due to the coincidence of the $C^{17}O$ Q-branch (at 105.2 nm) with a peak in H_2 transmission (Fig. 2). Both the high slope and the small $\delta^{18}O$ value at 1500 K (Fig. 3) suggest that self-shielding at 1500 K will be inadequate, but the contributions of several other bands will have to be included before a more definitive 3-isotope plot can be constructed. CO reformation during rapid back reactions will reduce the delta values further.

The timescales of X-point processes must also be considered. The gas resides in the vicinity of the X-point for a time t_X, after which transport along flux tubes either accretes the gas onto the protostar or removes it in a disk wind. Once nebular gas reaches the sonic transition, which is at gas densities ~ 10^3 times lower than the peak disk densities at the X-point, the gas accelerates out of the X-region [6]. Figure 4 shows vertical profiles of CO and O (considering only the CO photodissociation reactions) at .035 AU and at various times, and assuming an FUV flux similar to the modern Sun (at .035 AU). The height above the midplane corresponding to the gas density of the sonic transition is shown by the arrow. The time required for the fraction of CO to decrease by a factor of 2, which corresponds to the approximate peak oxygen isotope anomaly, is as short as 4 days (4-400 curve, Fig. 4), and reaches a depth into the disk is within a factor of ~ 3 of the sonic transition gas density. We will compare this timescale to an estimated t_X to determine if CO is dissociated on a timescale comparable to the residence time for the gas in the X-region.

In summary, CO self-shielding in the E(1)-X(0) band does occur at high temperatures in the presence of H_2, but is clearly diminished relative to temperatures lower than ~ 100 K. At high temperatures formation of H_2O from O will be rapid, but back reactions to reform CO will also be rapid. These reactions, and the reactions of H_2O with silicate precursors (e.g., SiO), will be added in future work.

Genesis measurements: It is expected that Genesis oxygen isotope results will be reported at this meeting. A $\Delta^{17}O$ value for solar wind of ~ -20 permil or less will likely validate Clayton's hypothesis that CO self-shielding was a dominant isotopic process in the early solar system. It then remains to sort out the location of the self-shielding [1,3,4]. A $\Delta^{17}O$ value of ~ 0 permil (i.e., terrestrial value) will likely validate the hypothesis of a non-statistical chemical mechanism during CAI formation [5].

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References: [1] Clayton, R. N. (2002) *Nature* 415, 860-861. [2] Sakamoto N. et al. (2007) *Science* 317, 231-233. [3] Yurimoto H. and Kuramoto K. (2004) *Science* 305, 1763-1766. [4] Lyons J. R. and E. D. Young (2005) *Nature* 435, 317-320. [5] Marcus R. A. (2004), *J. Chem. Phys.* 121, 8201-8211. [6] Shu, F. et al. (1994) *Ap. J.* 429, 781-796. [7] Ubachs W., I. Velchev, P. Cacciani (2000) *J. Chem. Phys.* 113, 547-560. [8] Lyons J. R., Boney E., Marcus R. A., (in prep.)

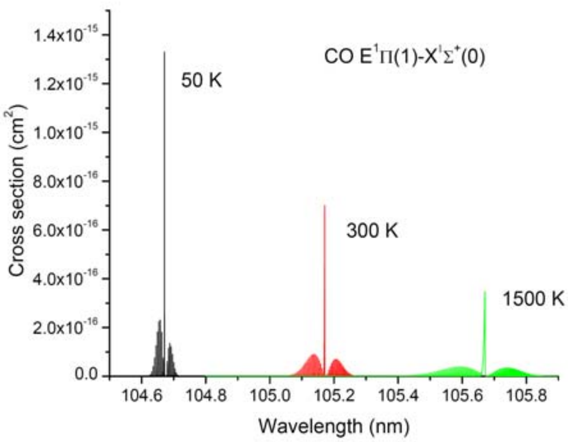

Fig. 1. Synthetic spectrum for CO $E^1\Pi(1)$-X(0) band at several temperatures. The spectra at 50 K and 1500 K are offset in wavelength for clarity.

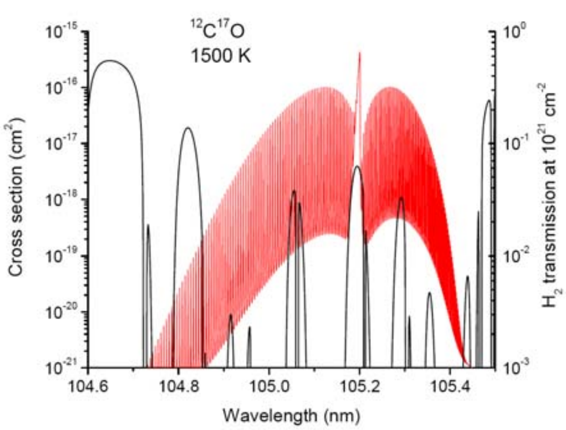

Fig. 2. Synthetic spectrum for $C^{17}O$ at 1500 K, with overlay of H_2 transmission. At high temperatures structure in the H_2 spectrum can produce slopes on the 3-isotope diagram that differ significantly from unity.

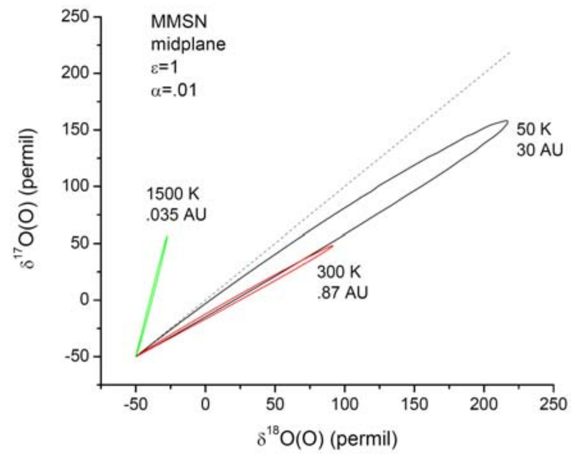

Fig. 3. Three-isotope plot for O atoms produced during CO dissociation at three disk locations. Reactions converting O to water and also reforming CO are not included here. The dotted line has slope 1.

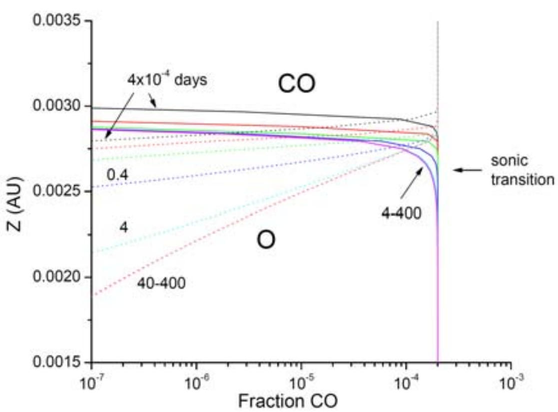

Fig. 4. Vertical profiles of CO (solid lines) and O (dotted lines) at R=.035 AU at several times (in days). The gas transport timescale near the X-point is ~ days. The 'sonic transition' is the approximate height from which gas is entrained in accretionary flux tubes [Shu et al. 1994].