**TEMPERATURE-DEPENDENT CO SELF-SHIELDING IN THE SOLAR NEBULA.** J. R. Lyons[1], E. Boney[2], R. A. Marcus[2]; [1]Institute of Geophysics and Planetary Physics, and Department of Earth and Space Sciences, UCLA, Los Angeles, CA 90095-1567 (jrl@ess.ucla.edu); [2]Noyes Laboratory of Chemical Physics, Caltech, Pasadena, CA 91125.

**Introduction:** Recent quantitative CO self-shielding models for the solar nebula [1] have utilized shielding functions determined by van Dishoeck and Black [2] for low-temperature (10-20 K) molecular clouds. At 30 AU temperatures in the surface region of the nebula in which CO self-shielding occurs [1] are thought to be ~ 50 – 100 K or more, well above molecular cloud temperatures. Clayton's hypothesis [3] of CO self-shielding near the disk X-point requires self-shielding at temperatures ~ 1000 – 1500 K. For a particular CO predissociation band the number of rovibronic lines relevant to self-shielding increases from less than 10 at 10 K to more than 100 at 1000 K. In addition, v>0 vibrational states must be included in the CO ground electronic state at temperatures ~ 1000 K and higher. It is reasonable to expect that the shielding functions derived in [2] will not be applicable at 1000 K.

The importance of temperature to self-shielding in $O_2$ was discussed in detail by Navon and Wasserberg [4]. Using rectangular line shapes and a probabilistic treatment of line overlap they found that self-shielding in the Schumann-Runge bands was greatly diminished above 300 K. Here we use Lorentzian line shapes and a line-by-line integration to determine the temperature dependence of self-shielding in CO.

**Nebular model:** The present calculations use the nebular model of Lyons and Young [1] to compute CO self-shielding in the $E^1\Pi(v=1) - X^1\Sigma(v=0)$ predissociation band (band #31 in [2]; denoted as E(1)-X(0)). Because line-by-line calculations must be performed at very high spectral resolution ($d\lambda = 1x10^{-5}$ nm ~ .01 $cm^{-1}$ for this band), and because our focus here is on the self-shielding process, the chemical model in [1] has been reduced to only the photolysis reactions for the CO isotopologues. Product O is assumed to be fully converted to $H_2O$, and product C is ignored. Vigorous vertical mixing ($\alpha$=.01) and an enhanced radiation field ($\varepsilon$ = 100 in the notation of [1]) is assumed.

**Line-by-line model:** Line positions for the P, Q and R branches of the E(1)-X(0) band were computed using the spectral constants in Ubachs et al. [5]. The linewidths for the CO isotopologues are .018 to .034 $cm^{-1}$. Doppler line widths vary from 0.026 $cm^{-1}$ at 10 K to 0.26 $cm^{-1}$ at 1000 K. Therefore a Voigt line shape must be used for temperatures above ~ 30 K. The calculations presented here assume a linewidth of .05 $cm^{-1}$ and a Lorentzian line shape; calculations with a Voigt profile are in progress.

**Results and discussion:** Figure 1 shows computed spectra for $C^{16}O$, $C^{17}O$ and $C^{18}O$ at 300 K. Comparison of the $C^{16}O$ spectrum with measurements (not shown) by Stark et al. [6] shows fairly good agreement; inclusion of Doppler broadening should improve agreement.

The photolysis rate constants, $J_{CO,}$ as a function of height above the disk midplane are shown in Figure 2. At a given height below 9 AU, $J_{CQ} \sim J_{CP} >> J_{CO}$, illustrating the self-shielding process.

Figure 3 shows the midplane delta values for total nebular $H_2O$ (defined as parent cloud $H_2O$ plus $H_2O$ produced from CO photolysis in the nebula [1]) at several temperatures. The largest positive delta values are obtained at 10 K, as expected. Smaller but still substantial delta values are computed at 100 and 1000 K. At 10 K $\delta^{17}O > \delta^{18}O$, consistent with some self-shielding by $C^{18}O$. At 100 K $\delta^{17}O < \delta^{18}O$ for nebular $H_2O$, with a $\delta^{17}O/\delta^{18}O$ ratio ~ 0.8. At 1000 K $\delta^{17}O > \delta^{18}O$ again, with a ratio $\delta^{17}O/\delta^{18}O \sim 1.2$. Differential absorption of CO isotopologues by $H_2$ (not included here) may also affect $\delta^{17}O/\delta^{18}O$ [1]. Figure 4 shows the $\Delta^{17}O$ values for nebular $H_2O$ corresponding to Fig. 3.

Our results suggest significant temperature dependence in the isotope selectivity of CO photolysis, which could be a useful diagnostic tool. We also see reduced but still significant self-shielding at 1000 K. Other effects must be included at high temperatures including additional sets of CO vibrational bands, the possibility of overlap with adjacent electronic states, and enhanced absorption by $H_2$.

We emphasize that these are preliminary results that could change substantially when thermal broadening is included. Thermal broadening will increase the likelihood of line overlap near line center, and should diminish the isotope selectivity by raising the 'pseudo-continuum' level between lines [4]. Calculations at 1500 K are also in progress.

**References:** [1] Lyons J. R. and E. D. Young (2005) *Nature* 435, 317-320. [2] van Dishoeck E. and J. Black, *ApJ* 334, 771-802. [3] Clayton, R. N. (2002) *Nature* 415, 860-861. [4] Navon O. and G. J. Wasserberg (1985) *EPSL* 73,1-16. [5] Ubachs W., I. Velchev,

P. Cacciani (2000) *J. Chem. Phys.* 113, 547-560.
[6] Stark G. et al. (1992) *Astrophys. J.* 395, 705-709.

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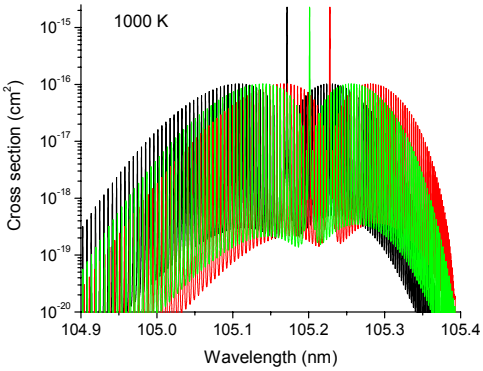


Fig. 1b. Logarithmic plot of Fig. 1a.

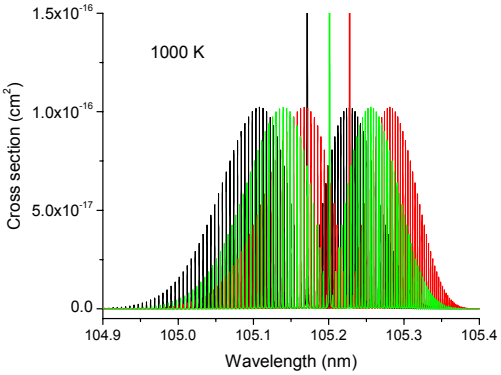


Fig. 1a. Computed spectra for $C^{16}O$ (black), $C^{17}O$ (green), and $C^{18}O$ (red) for the E(1)-X(0) band at 1000 K.

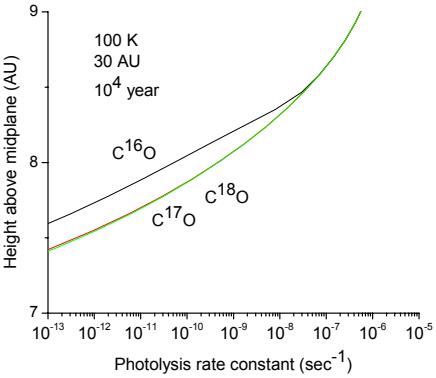


Fig. 2. Illustration of CO self-shielding at 100 K computed by a line-by-line calculation. Same colors as in Fig. 1.

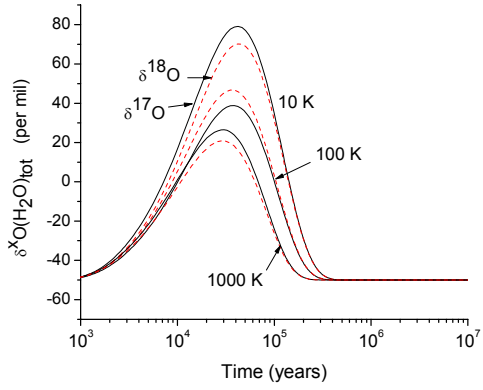


Fig. 3. Computed $\delta^{17}O$ (black solid) and $\delta^{18}O$ (red dashed) values for total nebula water at various CO gas temperatures. Only CO isotopologue photolysis is included in this calculation; all product O is assumed to form $H_2O$. The validity of this assumption must be tested with the full chemical model for temperatures > 100 K.

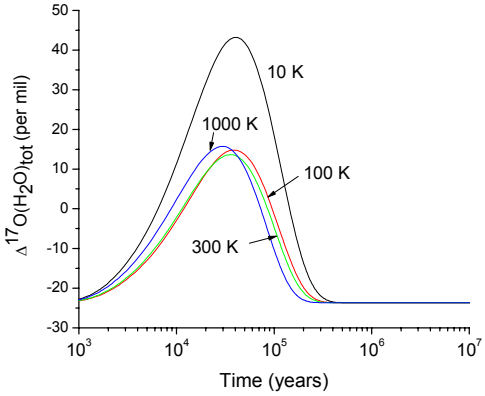


Fig. 4. Computed $\Delta^{17}O$ values for total nebula water.