**PHOTODISSOCIATION OF CO ISOTOPOLOGUES: MODELS OF LABORATORY EXPERIMENTS AND IMPLICATIONS FOR THE SOLAR NEBULA**

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**Introduction:** CO photolysis is presently a leading hypothesis for explaining the CAI oxygen isotope mixing line [1], [2]-[4]. In this mechanism, CO photolysis at wavelengths ~100 nm yields enrichment in $^{17}$O and $^{18}$O products when the column density of C$^{16}$O is high enough to be optically thick, thus reducing the production of $^{16}$O. Laboratory CO photodissociation experiments [5], [6] found slopes ranging from ~ 1.8 at 107 nm to ~ 0.6 at 94 nm. Such a strong dependence of slope on wavelength appears to be inconsistent with the CO self-shielding hypothesis, which for CO yields slopes near unity. Here, I present simulations of CO photolysis experiments, and also of the solar nebula, using computed line-by-line spectra for the oxygen isotopologues of CO.

**Modeling the experiments:** The Chakraborty et al experiments [5], [6] were carried out at the ALS synchrotron using a windowless apparatus. Modeling assumes an ALS beam of FWHM = 2.2 nm incident on a photocell of length 100 cm. Pure CO is photolyzed, and product $CO_2$ is collected and analyzed for isotope composition. The most important reactions are the following:

$$CO + h\nu \rightarrow C + O$$

$$O + CO \xrightarrow{M} CO_2$$

$$O + CO \xrightarrow{wall/trap} CO_2$$

$$O_a + CO_b \rightleftharpoons O_b + CO_a$$

$$CO_2 + h\nu \rightarrow CO + O(^1D)$$

$$CO_2 \xrightarrow{trap} CO_{2,ice}$$

Exchange between O atoms and CO had to be turned off in the model to prevent complete erasure of fractionation signatures.

A line-by-line spectral model was developed for the CO isotopic absorption spectra following Eidlesberg et al. [7], updated to more recent molecular parameters [8]. Results for simulation of the long-wavelength experiments between 105 and 108 nm are shown in Figure 1. For the assumption of equal oscillator strengths and dissociation probabilities for all isotopologues, the slope 1 results are obtained, in disagreement with the lab experiments. The experimental data can be matched by reducing the dissociation probability for C$^{18}$O for the E(0) band, and either the E(1) or C(1) bands. The isotopic dissociation probabilities are unknown for CO at any wavelength. At shorter wavelengths, there is more band overlap, and the resulting model photolysis slope is < unity. There is approximate agreement with experimental values at 92 and 94, and less so at 97 nm (Figure 2).

**Implications for the solar nebula:** Using the line-by-line isotopic spectra for CO, the effect of the radiation source on derived slope is explored in a model for the solar nebula [3]. Results for two cases are shown: HD303308, a massive O4 star, and HD36981, a B5 star. The FUV spectra of both stars have been measured by the Far-Ultraviolet Spectroscopic Explorer satellite (*FUSE*). For HD303308 (Fgiure 3), including the reduced dissociation probabilities inferred from the photolysis experiments modeling (Fig. 1.) increases the nebular model slope to near untiy. The HD 36981 results (Fig. 4) are more sensitive to the choice of dissociation probabilities due to lower blackbody flux at < 100 nm.

**Conclusions:** Pure self-shielding explains the magnitude but not the slopes obtained in CO photlysis experiments. Including reduced C$^{18}$O dissociation probabilities can account for the measured slopes. The reduced dissociation proababilties yields slopes near untiy for a mass ive O4 stellar spectrum. Results for a central protostellar spectrum will also be presented.

**References:**

[1] Clayton R. N. et al. (1973) *Science* 182, 485–488. [2] Clayton R. N. (2002) *Nature* 415, 860-861. [3] Lyons J. R. and Young E. D. (2005) ) *Nature* 435, 317-320. [4] Yurimoto H. and Kuramoto K. (2004) Science 305, 1763-1766. [5] Chakraborty S. et al. (2008) *Science* 321, 1328–1331.[6] Chakraborty et al. (2012) J. Chem. Phys. 137, 024309. [7] Eidelsberg M. et al. (1991) A&A S.S. 90, 231-282. [8] Visser R. et al. (2009) A&A 503, 323-343.

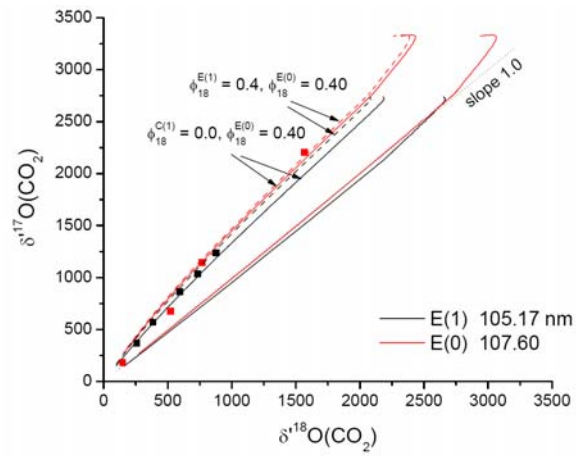


**Fig. 1** Model simulations (solid and dashed lines) of CO photolysis synchrotron experiments (squares) with the beam centered at 105.17 nm (black) and 107.60 nm (red). The model calculation is for an initial CO column density of 7 x $10^{17}$ $cm^{-2}$ in a 100 cm long photocell. The model results that plot close to the slope 1.0 line assume $C^{16}O$ dissociation probabilities for $C^{18}O$ and $C^{17}O$ (i.e., $\phi_{18}^{E(1)}$ = 0.96, $\phi_{18}^{C(1)}$ = 0.56, $\phi_{18}^{E(0)}$ = 0.80). Models with reduced $C^{18}O$ dissociation probabilities for the E(0) band at 107.6 nm and either the E(1) band at 105.17 nm or C(1) band at 106.3 nm match the experimental slopes. Experimental values from [6].

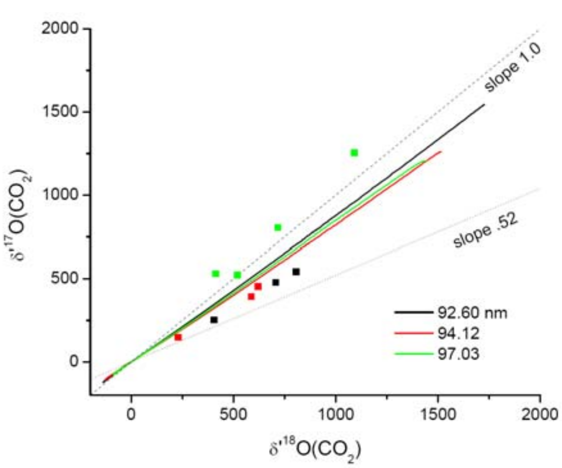


**Fig. 2** Model simulations (solid lines) of CO photolysis synchrotron experiments (squares) with the beam centered at 92.60 nm (black), 94.12 nm (red) and 97.03 nm (green). The model calculation is for an initial CO column density of 7 x $10^{17}$ $cm^{-2}$ in a 100 cm long photocell. In all 3 cases the model slope is ~ 0.8, which shows fair agreement with data from Chakraborty et al. (2012) which have slope ~ 0.7 at 92.6 and 94.1 nm, and slope ~ 1.1 at 97.0 nm. The model slopes are < 1 because there are more diffuse bands, and therefore some MDF, present at higher energies.

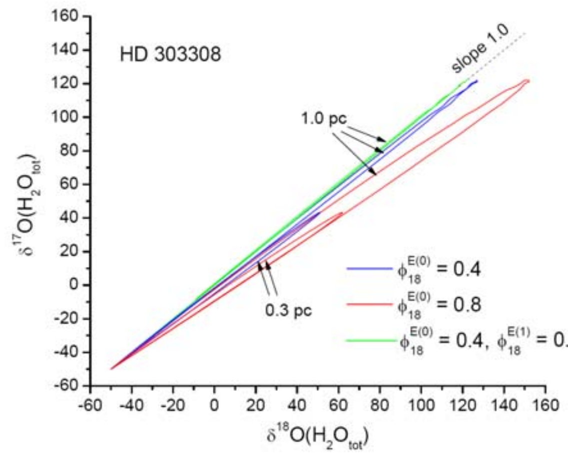


**Fig. 3** Three-isotope plot of total nebular $H_2O$ for a disk illuminated by HD 303308 at distances of 1 and 0.3 pc. Results are shown at 30 AU and the midplane. Wavelength-dependent $H_2$ absorption is included. Assuming all dissociation probabilities have the $C^{16}O$ values yields slopes well below unity (red curves). A reduction of the E(0) dissociation probability for $C^{18}O$ increases the slope (blue curves). Decreasing the $C^{18}O$ dissociation probabilities for both the E(0) and E(1) bands increases the slope further to near unity. Model results are independent of changes in the C(1) dissociation probability ($\phi_{18}^{C(1)}$) due to absorption by disk $H_2$.

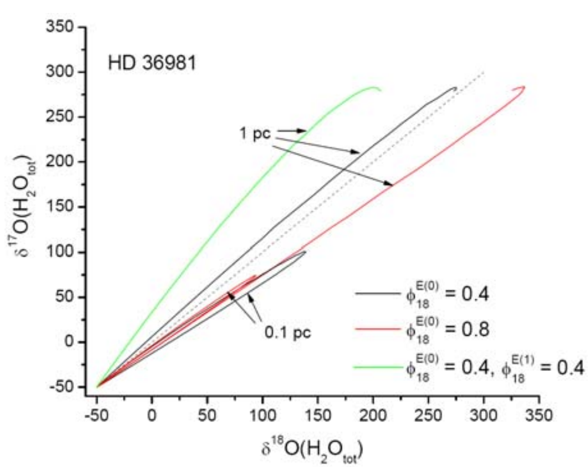


**Fig 4** Three-isotope plot of nebular $H_2O$ for a disk illuminated by HD 36981 at distances of 1 and 0.1 pc, and for a gas temperature of 50 K. The stellar intensity falls off at wavelengths shortward of ~ 100 nm compared to HD 303308, causing a greater sensitivity of the computed slope to the assumed dissociation probabilities of the long-wavelength CO bands. The slope is also dependent in intensity, as evidenced by the 0.1 pc curves.