

THE $\delta^{17}\text{O}/\delta^{18}\text{O}$ RATIO ASSOCIATED WITH CO PHOTODISSOCIATION IN THE SOLAR NEBULA. J.

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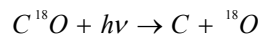
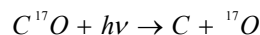
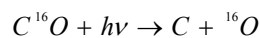
Introduction: The photodissociation of CO offers a quantitative and potentially self-consistent explanation for the origin of the mass-independent fractionation observed in CAIs [1]. Self-shielding due to the line-type absorption spectrum of CO yields product O with large, positive $\delta^{17}\text{O}$ and $\delta^{18}\text{O}$ values. Conversion of this O to H_2O forms the ^{16}O -depleted end member of a two-component mixing model for primitive materials in the solar system [2]. Model results for CO self-shielding in the parent molecular cloud [3] and in the surface region of the solar nebula [4] indicate that CO self-shielding is a viable mechanism, given a flux of far-ultraviolet (FUV) radiation significantly enhanced ($\sim 10^3$ times) above local interstellar medium (ISM) values, consistent with a star-forming region.

If CO self-shielding is, in fact, the mechanism by which the slope-1 line (where 'slope' = $\delta^{17}\text{O}/\delta^{18}\text{O}$) in CAIs formed, then the measured CAI slope should be obtained during the primary photolysis step. Measured slopes in CAIs range from 0.95 [5] to 1.00 [6]. Most CAIs fall on a line of slope 0.95 \pm 0.01, referred to as the CCAM (carbonaceous chondrite anhydrous minerals) line [5]. One particular CAI (USNM 3576-1) in the Allende meteorite has several unaltered phases with slopes = 1.00 \pm .03 [6], suggesting that the primitive oxygen isotope reservoir of the solar nebula may have had a slope close to 1.00. Photodissociation of pure CO is expected to yield a slope > 1 , analogous to self-shielding in pure O_2 [8], due to greater self-shielding in C^{18}O versus C^{17}O . Model results for pure CO in the solar nebula predict a slope ~ 1.10 [7], well outside the range of measured slopes in CAIs.

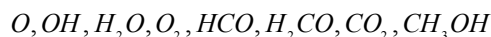
In an interstellar or nebular environment CO photodissociation occurs in the presence of abundant H_2 . Here I investigate the effect of H_2 absorption on isotope-selective CO self-shielding.

Photochemical model of nebula:

The photochemical model is a 2-D axisymmetric nebula with 1-D (vertical) radiative transfer and mixing [7]. The model has been substantially updated [4] and now includes ion-molecule, gas phase, and gas-grain chemistry, using rate coefficients from the astrochemistry literature, e.g. [9,10]. H_2O production is now explicitly computed, and is found to occur primarily on grain surfaces. Non-mass dependent fractionation occurs during photolysis of CO isotopologues [7]:



where photodissociation occurs in the wavelength range 91.2 to 110 nm in the presence of abundant hydrogen [11]. The gas-phase species in the model are



and the ion species are

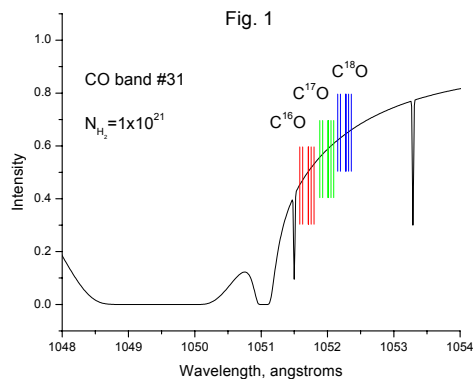


All gas-phase species also exist as molecules bound to grain surfaces. Molecular binding energies for adsorption to ice-coated grain surfaces are taken from previously published disk models [10]. The anomalous fractionation produced during CO photolysis is passed to other oxygen-containing molecular species during chemical reactions. At present the model has 96 species and 375 reactions.

Shielding by H_2 during CO photodissociation:

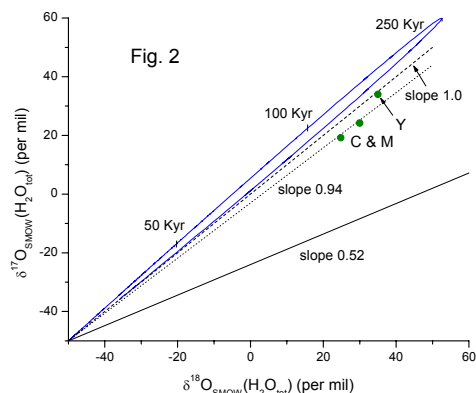
Assuming cosmic abundances of the elements, $\text{CO}/\text{H}_2 \sim 2 \times 10^{-4}$ in the solar nebula. Unity optical depth in CO thus occurs in the presence of highly saturated and broadened H_2 absorption lines. CO photodissociation occurs in ~ 30 bands, and about 8 of the bands undergo a large wavelength shift upon isotope substitution. H_2 and CO absorption spectra for a diffuse molecular cloud are given by van Dishoeck and Black [11]. Line-by-line calculations [11] showed that $\sim 60\%$ of C^{18}O photodissociation occurred in just one band, labeled as band #31, centered at 1051.70 Å.

I have computed a synthetic H_2 absorption spectrum for the region of CO band #31 (Fig. 1, black curve) [12]. The calculation is for an H_2 column density of $1 \times 10^{21} \text{ cm}^{-2}$. Band #31 line locations for C^{16}O , C^{17}O and C^{18}O are shown in color. Five lines are shown for each isotopologue, corresponding to transitions from the $J'' = 1$ and 2 rotational states of the



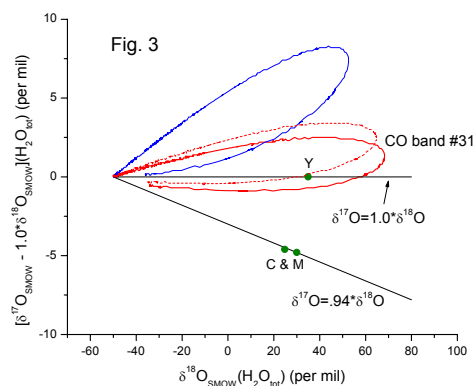
electronic ground state $\text{CO}(X^1\Sigma)$ to the $J' = 0 - 3$ rotational states of the electronic excited state $\text{CO}(E^1\Pi)$. These lines correspond to the most populated rotational ground states at 20 K, and so are particularly relevant to molecular cloud conditions. At temperatures $\sim 50 - 100$ K, typical disk surface temperatures, more rotational states will be occupied, and the isotopologue transitions will overlap. Line positions were calculated using published molecular constants for CO and its isotopologues [13]. By computing H_2 absorption spectra as a function of H_2 column density, I was able to compute a shielding function that accounts for the differential effects of H_2 absorption during photodissociation of CO isotopologues in band #31 [4].

Results: Model results for total nebular water at the midplane, $\text{H}_2\text{O}_{\text{tot}}$, which includes H_2O produced from O liberated during CO dissociation and (unfractionated) H_2O inherited from the parent cloud, are shown in Figure 2. The calculations are for a heliocentric distance $R = 30$ AU (midplane temperature = 51 K) and a viscosity parameter $\alpha = 10^{-2}$. The effects of H_2 absorption (i.e., band #31) are not included here. Figure 2 demonstrates that on timescales of 10^5 years, midplane $\text{H}_2\text{O}_{\text{tot}}$



reaches δ -values comparable to nebular water values inferred from carbonaceous chondrites [2,14]. However, as discussed above, when differential shielding due to H_2 is neglected, the predicted slope of $\text{H}_2\text{O}_{\text{tot}}$ is > 1 .

Figure 3 shows the effect of including band #31. In order to more easily see the slope change, I've re-plotted the standard 3-isotope plot as $\delta^{18}\text{O}$ versus $\delta^{17}\text{O} - 1.0 \cdot \delta^{18}\text{O}$. The blue curve is the same as that shown in Fig. 2. The red curve shows the result obtained by applying the band #31 shielding function (which has a power law dependence on N_{H_2} , the H_2 column density) at all N_{H_2} . The dotted red curve shows the result when the maximum N_{H_2} is limited to $1.5 \times 10^{21} \text{ cm}^{-2}$, and demonstrates that the bulk of the differential shielding occurs for H_2 column densities $< 1.5 \times 10^{21} \text{ cm}^{-2}$.



Conclusions: H_2 absorption effects on CO band #31 yield a predicted model slope for total nebular water that is within the measured range for CAIs. Additional calculations are needed to evaluate H_2 absorption effects on other CO bands.

References: [1] Clayton R. N. (2002) *LPSC XXXIII*, abstract #1326. [2] Clayton R. N. and Mayeda T. K. (1984) *Earth Planet. Sci. Lett.*, 67, 151-161. [3] Yurimoto, H. and Kuramoto, K. (2004) *Science* 305, 1763-1766. [4] Lyons J. R. and Young E. D. (2004), *submitted*. [5] Clayton, R. N. (1993), *Ann. Rev. Earth Space Sci.* 21, 115-149. [6] Young, E. D. and Russell, S. S. (1998) *Science* 282, 452-455. [7] Lyons, J. R. and Young, E. D. (2004), *LPSC XXXV*, abs. #1970. [8] Navon O. and Wasserburg G. J. (1985), *Earth Planet. Sci. Lett.* 73, 1-16. [9] Hasegawa T. et al. (1992) *Astrophys. J.* 82, 167-195. [10] Willacy K. et al. (1998) *Astron. Astrophys.* 338, 995-1005. [11] van Dishoeck E. and Black J. (1988) *Astrophys. J.* 334, 771-802. [12] McCandliss S. R. (2003) *Pub. Astron. Soc. Pacific* 115, 651-661. [13] Ubachs W. et al. (2000) *J. Chem. Phys.* 113, 547-560. [14] Young E. D. (2000) *Phil. Trans. Roy. Soc. Lond.* 359, 2095-2110.