



## Modeling MIF during CO photolysis using line-by-line spectra: Implications for the early solar system

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During the past several years CO self-shielding has been investigated as the source of the  $^{16}\text{O}$ -poor endmember of the CAI mixing line [1-4]. A key assumption in most of the models is that the  $\delta^{17}\text{O}/\delta^{18}\text{O}$  ratio (i.e., 'slope') associated with CO photodissociation under self-shielding conditions (when  $\text{C}^{16}\text{O}$  is optically thick) is unity or very close to unity. Laboratory CO photodissociation experiments by Chakraborty et al. [5] found slopes ranging from  $\sim 1.8$  at 107 nm to  $\sim 0.6$  at 94 nm. Such a strong dependence of slope on wavelength appears to be inconsistent with the CO self-shielding hypothesis.

Here I present simulations of these CO experiments, and also of the solar nebula, using complete line-by-line spectra for the oxygen isotopologues of CO. The questions I address are 1) What is the origin of the wavelength dependence in  $\delta^{17}\text{O}/\delta^{18}\text{O}$  ratio of photoproduct O (as  $\text{CO}_2$ )?; 2) Can a line-by-line spectrum capture the wavelength dependence or is a more complete spectral model necessary?; 3) What are the implications for the self-shielding theory for the solar nebula?

I computed line-by-line spectra for 37 bands of  $^{12}\text{C}^{16}\text{O}$ ,  $^{12}\text{C}^{17}\text{O}$  and  $^{12}\text{C}^{18}\text{O}$  at 300 K from published collections on CO molecular constant data [6,7]. Bands 31-33 have a resolution of  $1 \times 10^{-5}$  nm, and all other bands have a resolution of  $3 \times 10^{-5}$  nm. Simulations of photolysis experiments yield slopes for atomic O of 0.7 to 0.8 at 92.6, 94.1 and 97.0 nm. Measured values [5] were between 0.6 and 1.0, and the calculations agree with the measurements that slopes are  $< 1$  at 92 and 94 nm. Computed and measured slopes at 107 nm are  $> 1$ , as is also found in previous simulations [8], which results from an optically thick column of  $\text{C}^{18}\text{O}$ .

Solar nebula modeling was performed with the computed spectra added to the disk model of [3]. Calculations were done at 30 AU and 50 K, and also at 10 K and 1500 K to explore the temperature dependence of the slope. A slope of  $\sim 0.9$  is found for 50 K (and 1500 K), and  $\sim 1.2$  for 10 K. Thus, temperature dependence is predicted for the slope, which may be useful in eliminating some versions (i.e., locations) of the self-shielding theory. The large range of slopes seen by Chakraborty et al. [5] is not evident in disk models, nor in cloud models [7].

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