AB INITIO CALCULATION ON PHOTO-DISSOCIATION OF CO MOLECULES TO TEST THE SELF-SHIELDING MODEL

A. Yamada[1], S. Nanbu[2], and M. Ozima[1]. [1]Department of Earth and Planetary Science, University of Tokyo, Tokyo 113-0033, Japan. E-mail: yamada@eps.s.u-tokyo.ac.jp. [2]Sophia University.

The mass-independently fractionated oxygen isotope in CAI of primitive meteorites is commonly attributed to self-shielding effect of CO [e.g.,1]. Besides its unusual implication that CAI oxygen must be the same as the solar oxygen, the self-shielding hypothesis is based on several dubious premises including no isotopic effect of photo-dissociation of CO. Here, we show from a quantum mechanical calculation that photo-dissociation of CO seems to give rise to yield substantial isotopic effect on the photo-dissociation.

Ab initio reaction dynamics simulations were performed to compute the photolysis rate for the $E^1\angle \bullet X^1\Sigma^+$ electronic transition with non-adiabatic transition to $k^3\Pi$ and dissociative channel. This transition is considered one of the important transition for a CO self-shielding model. We used the Born-Oppenheimer approximation; in the first step the time independent Schrödinger equation was solved only for the electron-motion, and in the second step we performed the time dependent wave-packet dynamics for the nuclei-motion in the potential energy curves. The theoretical photo-dissociation cross section as a function of wavelength of excitation light was estimated by the Fourier transform of the autocorrelation function, $\langle\varphi(0)|\varphi(t)\rangle$ [2]. Assuming the Boltzmann distribution for vibrational and rotational state, we summed up to get the total cross section. Using photo-dissociation cross secions calculated for respective isotopes (i = 16, 17, 18), we will disscuss photo-dissociation rate $J_i = \int I(z,\lambda)\phi_i(\lambda)\sigma_i(\lambda)\mathrm{d}\lambda$, where i is for an isotope, I is light intensity, φ is the quantum yield assumed unity, σ is the cross secion.

References: [1] Lyons et al. (2009) *GCA* 73, 4998-5017. [2] Heller (1978) *J. Chem. Phys* 68, 2066-2075.