An experimental and *ab initio* study of water in $CaSiO_3$-walstromite

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Walstromite-structured $CaSiO_3$ is found in super-deep diamond inclusions where it is thought to represent a retrograde transformation product from the dominant calcium bearing lower mantle phase $CaSiO_3$-perovskite [1]. Estimates of water solubility in $CaSiO_3$-perovskite are contradictory and range from 0.4wt.% [2] to near zero [3]. In contrast, other calcium silicate phases including larnite (β-Ca2SiO4; stable at 9-11 GPa) and post-hatrurite (Ca_3SiO_5; stable at ~17 GPa) can contain 4.06wt.% and 5.84 wt.% H_2O, respectively [4]. In contrast little is known about the solubility of water and its substitution mechanism in $CaSiO_3$-walstromite (stable from 3-9 GPa). This information is necessary to determine whether the measured water contents in naturally occuring $CaSiO_3$-walstromite inclusions in super-deep diamonds represent a solubility limit imposed by the walstromite structure during retrogression or the original water content of the $CaSiO_3$-perovskite within the diamond forming region of the lower mantle.

Using high-pressure/temperature experiments, we report that $CaSiO_3$-walstromite has a limited water capacity (<100 ppm) based on Fourier transform infrared (FTIR) spectroscopy which shows a narrow hydroxyl (OH-) absorption band at ~3560 cm^{-1}. In adidtion, using *ab initio* simulations, we calculate the thermodynamic stability of various hydrous defects in $CaSiO_3$-wasltromite at a range of P-T conditions and water contents. These calculations indicate that substitution of 4H for Si on the A site is the most favourable incorporation mechanism in $CaSiO_3$-walstromite. We will also present experimental and computational results on the influence of Ti content on both the water solubility and incorporation mechanism.

[1] Gasparik T et al. (1994) Am. Mineral. **79**, 1219–1222 [2] Murakami M et al. (2002) Science **295**, 1885-1887 [3] Ross N et al. (2003) Am. Mineral. **88**, 1452–1459 [4] Németh P. et al. (2017) Earth Planet. Sci. Lett. **469**, 148-155