

Supporting information for:

## **Effect of iron and trivalent cations on OH-defects in olivine**

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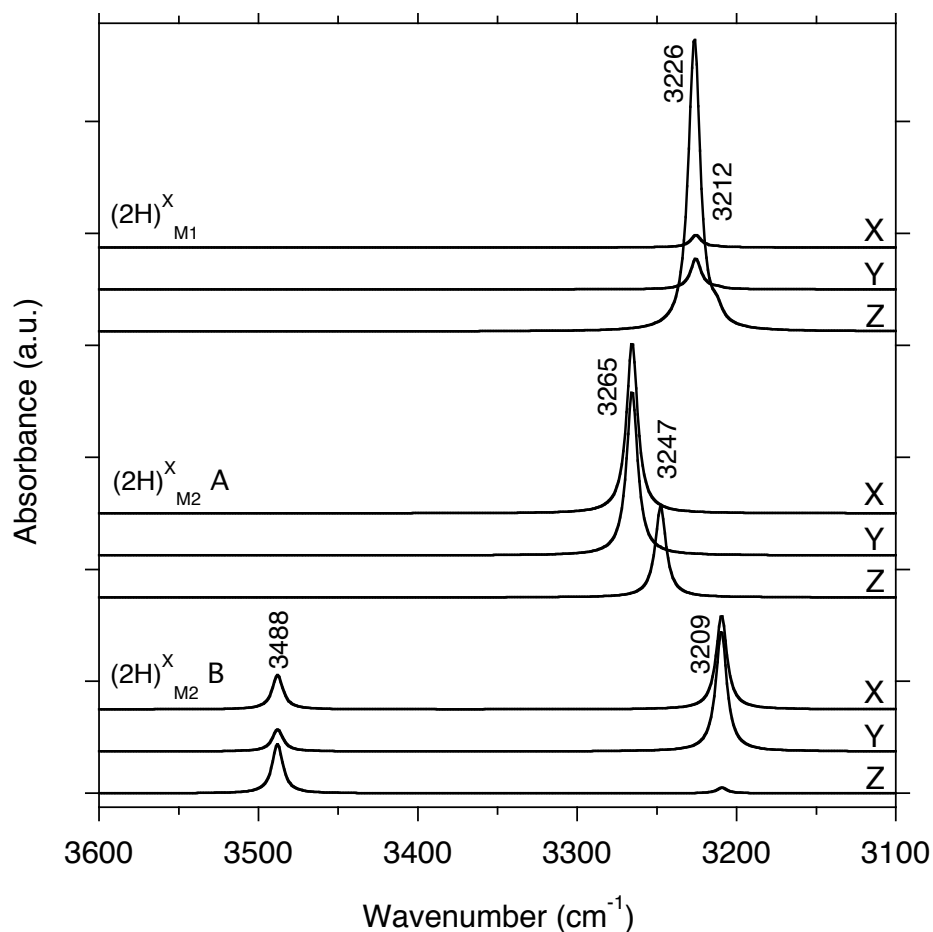
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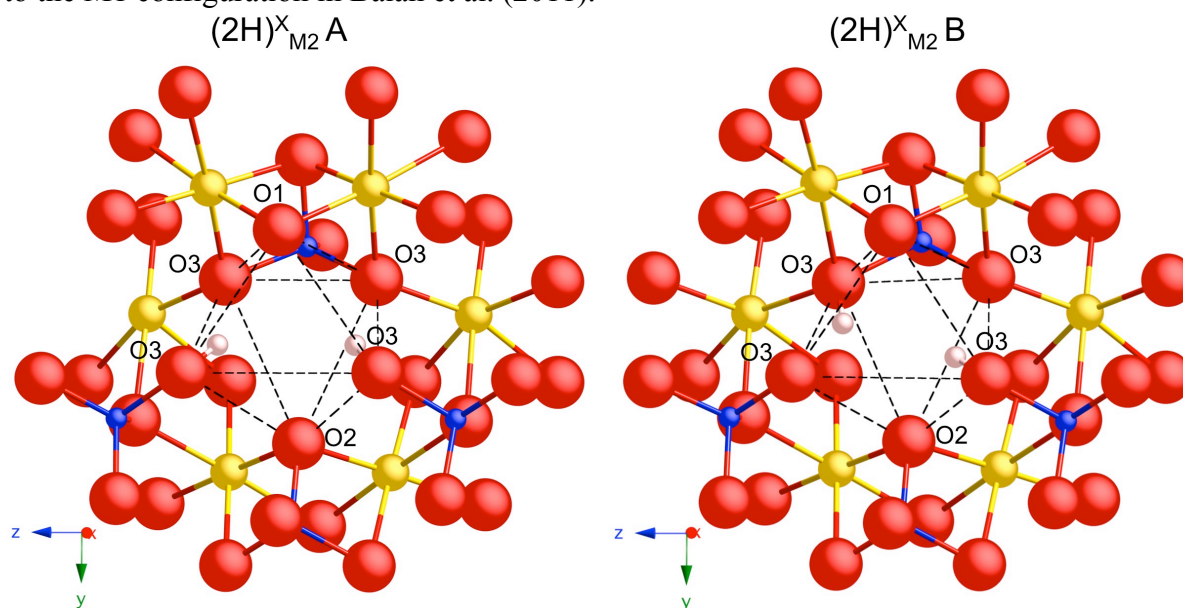
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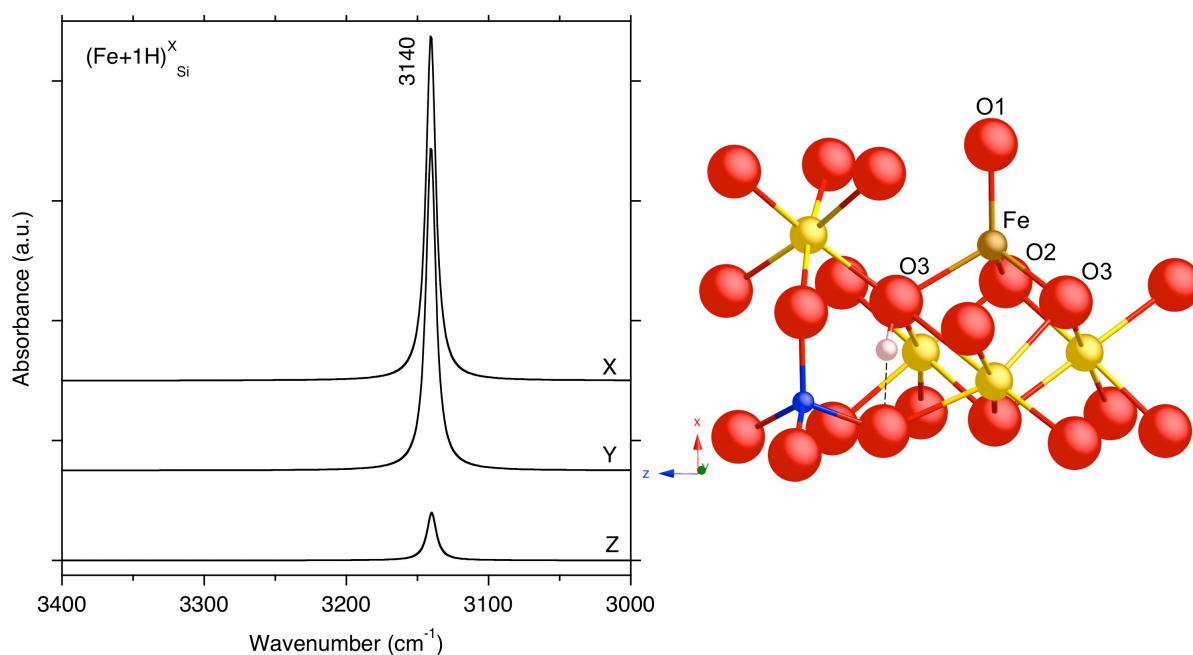
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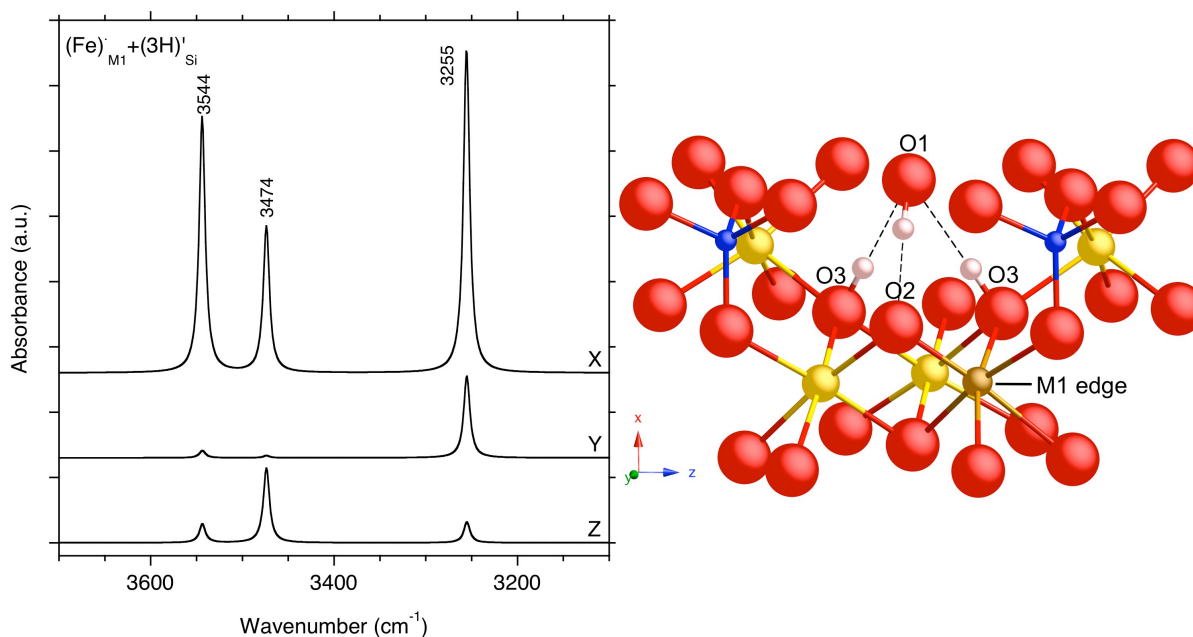
**FIGURE S1.** Theoretical polarized infrared spectra of  $(2H)_M^x$  defects.  $(2H)_{M1}^x$  corresponds to the M1 configuration in Balan et al. (2011).



**FIGURE S2.** Structural models of  $(2H)_{M2}^x$  defects, with Mg in yellow, Si in blue, O in red and H in white (color online).



**FIGURE S3.** Theoretical polarized infrared spectra of  $(\text{Fe}+1\text{H})_{\text{Si}}^x$  defect (left) and the corresponding structural model (right).



**FIGURE S4.** Theoretical polarized infrared spectra of  $[(\text{Fe})_{\text{M1}}^{\bullet}(3\text{H})_{\text{Si}}']^x$  defect (left) and the corresponding structural model (right).