

## High-pressure phase transitions of Fe-bearing orthopyroxene revealed by Raman spectroscopy

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### ABSTRACT

Orthopyroxene is one of the dominant minerals in the Earth's upper mantle. In this study, we used Raman spectroscopy to investigate the lattice vibration and phase transition of orthopyroxene with four different compositions using diamond-anvil cells up to 34 GPa at 300 K. Our orthopyroxene samples contain 0 (En<sub>100</sub>), 9% (En<sub>91</sub>Fs<sub>9</sub>), 11% (En<sub>86</sub>Fs<sub>11</sub>), and 21% (En<sub>74</sub>Fs<sub>21</sub>) Fe. At ambient conditions, the Raman modes exhibit a negative dependence on the Fe content, with the exception of the modes at ~850 and 930 cm<sup>-1</sup>. In contrast, these two Raman modes increase with increasing the Fe content. The phase transition from metastable  $\alpha$ - to  $\beta$ -phase was observed at 12.9–15 GPa for samples with <21 mol% Fe and varying Fe content has a minor effect on the phase transition pressure. Besides Fe, incorporation of 2–24 mol% Al can cause an increase in the phase transition pressure from 10–13 to 14–16 GPa. At 29–30.1 GPa, we observed the second apparent change in the Raman spectra for all four investigated samples. For Fe-bearing orthopyroxene, this change in the Raman spectra and frequency shift is associated with the phase transition from  $\beta$ - to  $\gamma$ -phase, whereas for En<sub>100</sub>, it should be caused by the change of coordination number of Si from 4 to 6 or the presence of  $\alpha$ -popx phase. Using the obtained Raman frequency shifts, we calculated the Grüneisen parameters at high pressures. These parameters are useful for understanding the thermoelastic properties of orthopyroxene at high pressures.

**Keywords:** Raman spectroscopy, orthopyroxene, Fe content, phase transition, high pressure