Crystal structures and high-temperature vibrational spectra for synthetic boron and aluminum doped hydrous coesite

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Coesite, a high-pressure SiO₂ polymorph, has drawn extensive interest from the mineralogical community for a long time. In this study, we synthesized hydrous coesite samples with different B and Al concentrations at 5 and 7.5 GPa (1273 K). The B concentration could be more than 400 B/10⁶Si with about 300 ppmw. H₂O, while the Al content can be as much as 1200 ~ 1300 Al/10⁶Si with CH₂O restrained to be less than 10 ppmw. Hence, B-substitution may prefer the mechanism of Si⁴⁺ = B³⁺ + H⁺, whereas Al-substitution could be dominated by 2Si⁴⁺ = 2Al³⁺ + Oᵥ. The doped B³⁺ and Al³⁺ cations may be concentrated in the Si₁ and Si₂ tetrahedra, respectively, and make noticeable changes in the Si-O₄ and Si-O₅ bond lengths. In-situ high-temperature Raman and Fourier Transformation Infrared (FTIR) spectra were collected at ambient pressure. The single crystals of coesite were observed to be stable up to 1500 K. The isobaric Grüneisen parameters (ϒᵢＰ) of the external modes (< 350 cm⁻¹) are systematically smaller in the Al-doped samples, as compared with those for the Al-free ones, while most of the OH-stretching bands shift to higher frequencies in the high temperature range up to ~ 1100 K