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Far-infrared spectra of synthetic $^{[4]}[(Al_{2-x}Ga_x)(Si_{2-y}Ge_y)](OH,OD,F)_2$-kinoshitalite: Characterization and assignment of interlayer Ba-O_{inner} and Ba-O_{outer} stretching bands

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ABSTRACT

Far-infrared spectroscopy and X-ray diffraction Rietveld structure-refinement of synthetic kinoshitalite (Kn) solid solutions, $BaMg_3[(Al_{2-x}Ga_x)(Si_{2-y}Ge_y)]O_{10}(OH,OD,F)_2$: (x = 0.0–2.0, y = 0.0–2.0), show that there is complete solid solution for all compositions in each (OH/OD)- and F-series: $^{[4]}[Al_2(Si_{2-y}Ge_y)]$-, $^{[4]}[(Al_{2-x}Ga_x)Si_2]$-, $^{[4]}[Ga_2(Si_{2-y}Ge_y)]$-, $^{[4]}[(Al_{2-x}Ga_x)Ge_2]$-Kn, and in OH/OD-for-F substituted $^{[4]}(Al_2Si_2)$-, $^{[4]}(Ga_2Si_2)$-, $^{[4]}(Al_2Ge_2)$-, $^{[4]}(Ga_2Ge_2)$-Kn end-member compositions. In the far-infrared region, 170–40 cm^{-1}, three kind of bands are observed; an in-plane tetrahedral torsional mode, an interlayer Ba-O_{inner} stretching vibration and a Ba-O_{outer} stretching vibration. With increasing tetrahedral $^{[4]}$Al-for-$^{[4]}$Ga and Si-for-Ge substitution, the frequencies and intensities of the tetrahedral in-plane torsional bands decrease in both the (OH/OD)- and F-bearing phases, but in the $^{[4]}(Al_2Si_2)$-, $^{[4]}(Ga_2Si_2)$-, $^{[4]}(Al_2Ge_2)$-, $^{[4]}(Ga_2Ge_2)$-Kn end-member compositions, the frequencies are unaffected by (OH/OD)-for-F substitution. The frequencies of both the Ba-O_{inner} and Ba-O_{outer} stretching bands increase with increasing $^{[4]}$Al-for-$^{[4]}$Ga and Si-for-Ge substitution, but the frequencies of the Ba-O_{inner} stretching bands decrease with increasing (OH/OD)-for-F substitution in the $^{[4]}(Al_2Si_2)$-, $^{[4]}(Ga_2Si_2)$-, $^{[4]}(Al_2Ge_2)$-, $^{[4]}(Ga_2Ge_2)$-Kn end-member compositions. The frequency difference between the Ba-O_{inner} and Ba-O_{outer} stretching bands is linearly related to the tetrahedral rotation angles (α), and these differences are about 10 cm^{-1} larger in the (OH/OD)-bearing phases than in the corresponding F-bearing phases. The ranges of absorption frequencies and their corresponding deformation modes are as follows: (1) in-plane tetrahedral torsional mode, 105–150 cm^{-1}; (2) Ba-O_{inner} stretching vibration, 105–140 cm^{-1}; and (3) Ba-O_{outer} stretching vibration, 75–90 cm^{-1}.

Keywords: Far-infrared spectra, synthetic kinoshitalite, in-plane torsional mode, Ba-O_{inner} stretching band, Ba-O_{outer} stretching band