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Assignment of infrared OH-stretching bands in calcic amphiboles through deuteration and heat treatment

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ABSTRACT

Infrared OH-stretching bands of calcic amphiboles in the magnesiohornblende-tschermakite/ferrotschermakite and edenite-pargasite/hastingsite series have been assigned by deuteration and heat treatment in air. Mössbauer spectra indicate that with increasing temperature for heat-treatment in air, Fe^{2+} at the M1 and M3 sites is first converted to Fe^{3+} through dehydrogenation, and then Fe^{2+} at the M2 site is oxidized at higher temperature. The quadrupole-splitting parameters of (oxidized) Fe^{3+} at the M1 and M3 sites and Fe^{3+} at the M2 site are much larger than in natural (= non-dehydrogenated) amphiboles, indicating that dehydrogenation of O3H causes large electric-field-gradients at the M1-3 sites. The intensity of absorption of Fe^{3+} at M2 decreases with heating temperature, which is consistent with the migration of Fe^{3+} at M2 to the M1 and/or M3 sites. The (MgMgAl)-OH band, designated K^*_T, occurs at ~3678 cm^{-1} in Fe^{2+}-poor pargasitic amphiboles, and is assigned to the configuration (MgMgAl)-OH-^{A}(Na,K): $^{T1}Si^{T1}Al$. Three (2–4) of the following four types of band systems occur with decreasing band frequency: (1) A*–D* bands at 3730–3675 cm^{-1}, associated with (M1M1M3)-OH-^{A}(Na,K):$^{T1}Si^{T1}Si$ configurations; (2) A^*_T–D^*_T bands at 3725–3650 cm^{-1}, associated with (M1M1M3)-OH-^{A}(Na,K): $^{T1}Si^{T1}Al$ configurations; (3) A–D bands at 3680–3620 cm^{-1} , associated with (M1M1M3)-OH-$^{A}\square$: $^{T1}Si^{T1}Si$ ($\square$ = vacancy) configurations; and (4) A_T–D_T bands at 3650–3580 cm^{-1} , associated with (M1M1M3)-OH-$^{A}\square$: $^{T1}Si^{T1}Al$ configurations. In addition, A^{**}_T, E^*_T, and K^{**}_T bands ascribed to the configurations (MgMgMg)-OH-^{A}(Na,K)-$^{O3}O^{2-}$:$^{T1}Si^{T1}Al$, (MgMgFe^{3+})-OH-^{A}(Na,K)-$^{O3}O^{2-}$:$^{T1}Si^{T1}Al$, and (MgMgAl)-OH-^{A}(Na,K)-$^{O3}O^{2-}$:$^{T1}Si^{T1}Al$ are important constituents of the spectra of oxidized magnesiohornblende and pargasite. The high frequency bands, A*–D*, are particularly weak, indicating short-range order involving local association of the $^{T1}Si^{T1}Al$ configuration with a locally occupied A-site.

Keywords: Infrared OH-stretching spectra, tetrahedral Al, calcic amphibole, pargasite, deuteration, heat-treatment