

## Split H-site model in synthetic Al-for-Ga substituted germanate-muscovites: FTIR and neutron powder diffraction studies

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FTIR and powder neutron diffraction studies of synthetic deuterated aluminogallogermanate muscovites have been made at ambient temperature. More than three infrared OD-stretching bands were analyzed in the OD-form's micas. A neutron powder diffraction Rietveld analyses for two germanate-micas of the compositions  $\text{KAl}_{1.5}\text{Ga}_{1.5}\text{Ge}_3\text{O}_{10}(\text{OD})_2$  and  $\text{KGa}_3\text{Ge}_3\text{O}_{10}(\text{OD})_2$ , up to three hydrogen sites were derived, reflecting a crescent or horseshoe-like D distribution sitting on the (1-10) plane with various angles from the (001) plane (= O6-O6-D angles); their site occupancies and the angles (degree) from the (001) plane are 0.36(-3.9), 0.45(29.2), and 0.18(80.8) in the former mica, 0.28(-18.7), 0.45(15.4), and 0.26(62.4) in the latter, respectively. The higher frequency infrared OH/OD-stretching bands ascribed to the higher angle H/D from the (001) plane. These split H/D-sites are derived mainly by the local negative charges which occur by the short range order of the tetrahedral tetravalent and trivalent cations.