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Influence of hydration on ^{23}Na, ^{27}Al, and ^{29}Si MAS-NMR spectra of sodium saponites and sodium micas†

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ABSTRACT

Synthetic sodium saponites, $Na_xMg_3(Si_{4-x}Al_x)O_{10}(OH)_2 \cdot nH_2O$, with $0.33 \leq x \leq 1$, and trioctahedral sodium micas series, $Na(Mg_{3-y}Al_y)(Si_{3-y}Al_{1+y})O_{10}(OH)_2 \cdot nH_2O$, with $0 \leq y \leq 1$, have been investigated by MAS-NMR spectroscopy. The presence of anhydrous, one-layer and two-layer hydrates, deduced by X-ray diffraction, has been associated with specific lines detected in ^{23}Na MAS-NMR spectra. In these phyllosilicates, the location of tetra- and octahedral charge has been analyzed by ^{27}Al MAS-NMR spectroscopy. The salient result is the major effect of the interlayer charge on ^{29}Si chemical shift of the four NMR components ascribed to Si_3, Si_2Al, $SiAl_2$, and Al_3 environments. This effect is much more important than the most commonly accepted contribution of the ditrigonal distortion of tetrahedral sheets. In saponites, ^{29}Si MAS-NMR spectra change considerably with the sodium hydration. In dehydrated samples, where Na cations are engaged in two pseudo-hexagonal cavities, ^{29}Si MAS-NMR components split as a consequence of the partial sodium occupancy of three neighboring hexagonal rings that surrounds a particular tetrahedron. In hydrated samples, where Na^+ cations interact with water, chemical shifts of resolved components are averaged as a consequence of interlayer water and cation mobilities.

Keywords: 2:1 phyllosilicates; ^{29}Si, ^{27}Al, and ^{23}Na MAS-NMR spectroscopy; Si-Al distribution; charge location; hydration state