

O atom sites in natural kaolinite and muscovite: ^{17}O MAS and 3QMAS NMR study

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ABSTRACT

The layer silicates are among the most common minerals in the Earth's surface environment, play important roles in many geological processes, and have diverse technological applications. While it has been suggested that O isotope exchange and dissolution kinetics in aqueous solutions are controlled by chemical bonding and local atomic structures, the effect of atomic environment around O atom sites in clay minerals on their site-specific reactivities with H_2O are not well known, mainly because direct experimental evidence is lacking.

Here, we present for the first time detailed high-resolution ^{17}O NMR data for ^{17}O -exchanged natural kaolinite [$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$] and muscovite [$\text{KAl}_2(\text{AlSi}_3)\text{O}_{10}(\text{OH})_2$] using ^{17}O triple quantum magic angle spinning (3QMAS) and MAS NMR at high fields. At least two basal O atom sites in kaolinite are resolved: O4, and (O3 + O5). Apical O atoms (^{14}Si -O- ^{26}Al) and hydroxyl groups are also shown in these spectra. The ^{17}O 3QMAS spectrum for muscovite shows improved resolution over the ^{17}O MAS NMR spectrum, allowing us to resolve several basal O atoms, including (^{14}Si -O- ^{14}Al), as well as hydroxyl groups. The fraction of each O atom appears to deviate somewhat from the stoichiometric value, suggesting that each crystallographically distinct site may have a different rate of exchange with the O atom in H_2O .