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Electronic and Structural Properties of Reduced-Charge Montmorillonites

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Running title: Electronic and Structural Properties of RCMs

Abstract Solid state silica (^{29}Si) and aluminum (^{27}Al) nuclear magnetic resonance (NMR) spectroscopy was applied to a series of reduced-charge montmorillonites (RCM) to discern changes in electronic and structural properties that are induced by Li fixation. Room temperature ^{29}Si MAS-NMR spectra revealed a consistent chemical shift to more negative values and increased line-width of the main Q^3(0Al) Si resonance with increasing levels of Li-fixation in the RCM series. A decreased line width of the octahedral Al ($Al_{[6]}$) environment was observed and may be attributed to formation of a more uniform electronic environment surrounding $Al_{[6]}$ as charge reduction occurs. No appreciable changes in the tetrahedral Al ($Al_{[4]}$) peak were observed for the series, except for line broadening. Correlations of ^{29}Si NMR chemical shifts with layer charge and infrared-active structural vibrations indicated that distortions in the Si-O-T bond angles (T = tetrahedral Si or Al) occurred following charge reduction, with the mean Si-O-T bond angle increasing.. These results are interpreted as evidence of a redistribution both of layer charge and improvement of the fit between octahedral and tetrahedral sheets following Li-fixation and charge reduction. Our results are consistent with the formation of pyrophyllite-like character in reduced-charge montmorillonite.