

Influence of charge location on ^{29}Si NMR chemical shift of 2:1 phyllosilicates

JESÚS SANZ,^{1,*} JEAN-LOUIS ROBERT,² MAGALI DIAZ,² AND ISABEL SOBRADOS¹

¹Instituto de Ciencia de Materiales, CSIC, Cantoblanco, 28049 Madrid, Spain

²ISTO, UMR 6113, CNRS-Université d'Orléans, 1A rue de la Férellerie, 45071 Orléans Cedex 2, France

ABSTRACT

A series of synthetic sodium-rich saponites and trioctahedral Na, K, and Ba mica solid solutions have been investigated by ^{29}Si MAS-NMR spectroscopy. The salient result is the major effect of the interlayer charge on ^{29}Si chemical shift variations detected in NMR components ascribed to tetrahedral Si_3 , Si_2Al , SiAl_2 , and Al_3 environments. In this analysis, the effect of the octahedral charge is considerably lower. The contribution of the interlayer charge is much more important than the previously reported contribution of the ditrigonal distortion of tetrahedral layers, generated by the misfit between tetrahedral and octahedral layers. This observation rests on the peculiar disposition of tetrahedra in phyllosilicates, with three out of four oxygen atoms exposed to the interlamellar space. A similar effect could be operative in other silicates, like zeolites, in which most of tetrahedra interact with charge compensating cations.

Keywords: Phyllosilicates, crystal structure, order-disorder, chemical shift, ^{29}Si NMR spectroscopy