An Improved Model for Structural Transformations of Heat-Treated Aluminous Dioctahedral 2:1 Layer Silicates

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Abstract: An improved model for the interpretation of thermal effects during dehydroxylation in aluminous dioctahedral 2:1 layer phyllosilicates considers *trans*-vacant (tv) and *cis*-vacant (cv) 2:1 layers and leads to very different temperatures of dehydroxylation for these tv and cv vacant modifications. In particular, smectites and illites consisting of cv 2:1 layers are characterized by dehydroxylated temperatures which are higher by 150 ° C to 200 ° C than those for the same minerals consisting of the tv 2:1 layers. A considerable lengthening of the OH-OH edges in cv 2:1 layers in comparison with the OH-OH edges in the tv 2:1 layers is postulated as the reason for the higher dehydroxylation.

Dehydroxylation in aluminous cv 2:1 layer silicates should occur in two stages. Initially, each two adjacent OH groups are replaced by a residual oxygen atom and the Al cations, which originally occupied *cis* -and *trans*-sites, become 5- and 6-coordinated, respectively. The structure of 2:1 layers corresponding to this stage of the dehydroxylation is unstable. Thus the Al cations migrate from the former *trans*-sites to vacant pentagonal prisms. The resulting dehydroxylated structure of the original cv 2:1 layers is similar to that of the former tv 2:1 layers.

Diffraction and structural features of the cv dehydroxylates predicted by the model are in agreement with X-ray diffraction effects observed for cv illite, illite-smectite and montmorillonite samples heated to different temperatures. In particular, the diffusion of Al cations to empty five-fold prisms during dehydroxylation of the tv 2:1 layers explains why dehydroxylation of reheated cv montmorillonites occurs at temperatures lower by 150 ° C to 200 ° C than samples that were not recycled.

Key Words: Beidelites • *Cis*-vacant octahedra • Dehydroxylation • Illites • Montmorillonites • *Trans*-vacant octahedra

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