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Modeling acid - base properties of montmorillonite-water Interface

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Montmorillonite is a member of smectite group, i.e. 2:1 layer silicate, with two silicate tetrahedral sheets joined to a central octahedral sheet. The clay exhibits variable and permanent charge characteristics. In this work, the interaction mechanisms of protons with montmorillonite were examined using electric double layer theory. In this context, specific surface area was determined by methylene blue (MB) method. The MB replacement point indicates the saturation of surface sites, accordingly the surface area was obtained as 416±5 m^2g^{-1}. When compared to hydrous metal oxides, the proton titration curves of montmorillonite exhibit unusual features, viz. no any common intersection point that corresponds to pH_{pzc}. In montmorillonite there are two site types; amphoteric site (>XOH) along edges and fixed (negative) sites ($>Y^-$) along basal planes. Protons interact with both site types; thus the resultant titration curves exhibit peculiar behavior when compared to in metal hydroxides. Proton interactions on montmorillonite were modeled by 2-pK approach. Proton affinity constants and site density values were estimated by a numerical optimization and found to be: $>Y^- + H^+ \Rightarrow >YH$, K_Y=9.28; $>XOH + H^+ \Rightarrow >XOH_2^+$, log K_1=5.89; $>XOH \Rightarrow >XO^- + H^+$, log K_2=6.12 and >XOH=1.38×10^{-4} mol dm^{-3}, >Y=2.28×10^{-4} mol dm^{-3} respectively. Calculations suggest that pH_{PZC} = ~6 along edge sites. Therefore, montmorillonite surface is dominantly negative when pH > ~6. Surface titration curves of 0.100 and 0.010 mol dm^{-3} $NaNO_3$ are fitted well with 2-pK diffuse layer model whereas the titration curve obtained in 0.001 mol dm^{-3} $NaNO_3$ shows least fitting quality.

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