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Molecular cluster models of aluminum oxide and aluminum hydroxide surfaces

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ABSTRACT

Ab initio, molecular orbital calculations for two different Hartree-Fock basis levels were performed on clusters in the system Al-O-H, and tested by comparing derived vibrational frequencies to the measured values for aluminum oxides and aluminum oxyhydroxide minerals. Models were chosen to reflect surface groups that may be present on aluminous minerals such as α-Al_2O_3 (corundum) and $Al(OH)_3$ (gibbsite). Protonation and deprotonation reactions on bridging and terminal oxygen or hydroxyl sites were modeled to investigate the effects of solution *pH* on the structure of surface groups. Relative deprotonation energies, including solvation effects, were calculated for each site using the self-consistent isodensity polarized continuum model of Keith and Frisch (1994), and then used to predict the order in which each particular surface group protonates.