120d Roles of Steric and Acid-Base Factors in CO2 Adsorption in Alkali-Metal Cation Exchanged Y and X Zeolites

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The ability to tune the adsorption properties of Y and X zeolites by ion exchange has led to many studies of these materials for use in adsorptive separation and purification processes. The type of cation influences the electric field inside the pores, as well as the available pore volume. The extent or strength of adsorption of molecules in zeolitic pores can be dominated by interactions of the adsorbate with the electric field induced by the cations, but the acid-base properties of the zeolite framework can also play an important role in determining adsorption properties. The exchangeable cation is an acid site and the framework oxygen nearest to the cation provides a basic site. This basicity increases with an increase in framework aluminum content (so X should be more basic than Y) and also increases as the cation electronegativity decreases. CO2 is an acidic molecule that also possesses a quadrupole moment, so adsorption has the potential to be dominated by acid-base effects or interaction of the quadrupole moment with the electric field. However, strong interactions of an adsorbate with the framework or with cations at low coverage do not necessarily translate to high capacities. In this paper, a systematic investigation of CO2 adsorption in Y and X zeolites exchanged with Li, Na, K, Rb, and Cs cations of the family of alkali metals will be presented. Emphasis will be on the roles of steric and acid-base factors on capacities and isotherm shape.