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# Orientation of Trimethylphenylammonium (TMPA) on Wyoming Montmorillonite: Implications for Sorption of Aromatic Compounds

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**Abstract:** The orientation of TMPA cations on montmorillonite affects the adsorbate-accessible siloxane surface area and determines whether the TMPA phenyl ring can interact with other aromatic adsorbates by  $\pi$ - $\pi$  interactions. The purpose of this study was to determine the orientation of TMPA ions in the interlayer of normal-charge and reduced-charge Wyoming montmorillonite. The orientation of TMPA's phenyl group was investigated using infrared dichroism of selected aromatic ring vibrations. X-ray diffraction (XRD) and MacEwan Fourier transforms were used to determine interlayer spacings and to ascertain whether reduced-charge Wyoming montmorillonite is a randomly interstratified mixture of layers with two different d-spacings. For normal-charge montmorillonite, the infrared results showed that the C-N bond axis is neither perpendicular nor parallel to the surface, yet X-ray data suggested that the TMPA phenyl ring is perpendicular or nearly perpendicular to the siloxane surface. In this orientation, the average adsorbate-accessible space between adjacent TMPA ions is  $24 \text{ \AA}^2$ , or about 1/3 of the total surface. When the phenyl ring of TMPA is perpendicular to the clay surface, aromatic compounds should be able to interact with TMPA's aromatic ring by  $\pi$ - $\pi$  interactions, while polar compounds such as water can interact with positively charged nitrogen atom. The reduced-charge montmorillonite used in this study is a randomly interstratified mixture of about 25% collapsed layers with no adsorbed cations and 75% expanded layers that are propped open by TMPA's methyl groups, not by the aromatic ring. The adsorbate-accessible surface area on expanded layers of reduced-charge montmorillonite is 1.5 to 2 times that on normal-charge TMPA-clay, depending on the orientation of TMPA's aromatic ring.

**Key Words:** Adsorbate • Infrared dichroism • Montmorillonite • Trimethylphenylammonium (TMPA)

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