
A NEXAFS Study of the Orientation of Benzoate Intercalated into a Layer Double Hydroxide

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Abstract: NEXAFS is shown to be an excellent technique, of potentially widespread application, for the determination of the orientation of organic molecules intercalated in preferentially oriented thin films of polycrystalline, layered minerals. A NEXAFS study of $[\text{Mg}_2\text{Al}(\text{OH})_6]^+\text{C}_7\text{H}_5\text{O}_2^- \cdot n\text{H}_2\text{O}$, a layered anionic clay, is described. This material shows a transition from a layer spacing of 15.4 Å to only 9 Å at a remarkably low temperature (below 100° C). This is shown to be accompanied by a change in the angle of the plane of the benzoate molecule to the $00l$ planes from $35^\circ \pm 10^\circ$ to $0^\circ \pm 10^\circ$. The tilt of the benzoate anion in the room temperature structure demonstrates the presence of an interaction between the phenyl ring and the positively charged, brucite-like layers. Furthermore it is suggestive of the importance of hydrogen bonding in determining the interlayer spacing and stability.

Key Words: Double hydroxide • Hydrotalcite • NEXAFS • Organic intercalates • Preferred orientation

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