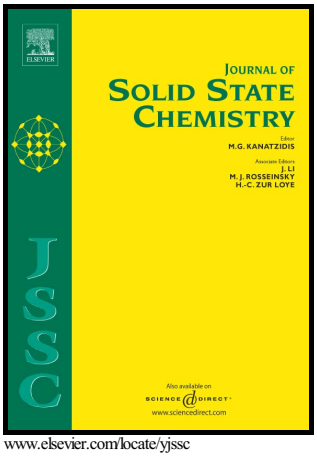

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PII: S0022-4596(18)30312-8
DOI: https://doi.org/10.1016/j.jssc.2018.07.028
Reference: YJSSC20309

To appear in: *Journal of Solid State Chemistry*

Cite this article as: P.A. Smith, S.M. Aksenov, S. Jablonski and P.C. Burns, Structural Unit Charge Density and Molecular Cation Templating Effects on Orientational Geometric Isomerism and Interlayer Spacing in 2-D Uranyl Sulfates, *Journal of Solid State Chemistry,* https://doi.org/10.1016/j.jssc.2018.07.028

Structural Unit Charge Density and Molecular Cation Templating Effects on Orientational Geometric Isomerism and Interlayer Spacing in 2-D Uranyl Sulfates

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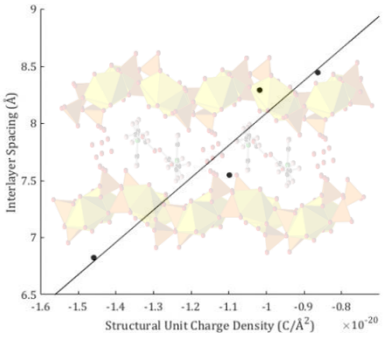
Abstract

The new uranyl aqua sulfate compound $[(\{CH_3\}_3N_2C_3H_3\{CH_2COOH\})(H_3O)][(UO_2)_2(SO_4)_3(H_2O)] \cdot 1.5H_2O$ was synthesized and the crystal structure determined. The two-dimensional uranyl-aqua sulfate compound exhibits a previously reported anionic structural unit topology, but features an interstitial complex incorporating hydronium in the form of a disorder Zundel cation and the cation moiety from the ionic liquid 1-carboxymethyl 3-methylimidazolium bistriflimide [HBetMIm][Tf_2N], which forms hydrogen bonding dimer pairs. An analysis of similar uranyl sulfate complexes from the literature is conducted to explore the relative importance and role of structure directing factors in alkylammonium charge-balanced two-dimensional uranyl sulfates. A correlation is observed between structural unit charge density and interlayer spacing, with a concomitant direction of structural and orientational geometric isomerism of the anionic structural unit. We discuss the role of synthetic conditions and molecular cation properties in directing structural unit formation through charge density matching and hydrogen bonding.

Graphical abstract



1. Introduction

Many uranyl $(UO_2)^{2+}$ compounds have been described over the past two decades, and their structures have underpinned development of hierarchical classifications and tools