

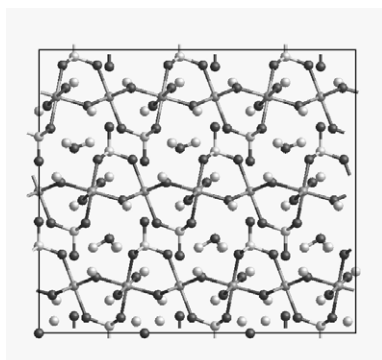
## The structure of hydronium alunite: A first principles study

K. WRIGHT<sup>1\*</sup>, J.D. GALE<sup>1</sup> AND K. HUDSON-EDWARDS<sup>2</sup>

<sup>1</sup>Nanochemistry Research Institute, Department of Chemistry,  
Curtin University of Technology, PO Box U1987, Perth,  
WA 6845, Australia (\*correspondence: kate@ivec.org)

<sup>2</sup>Department of Earth and Planetary Sciences, Birkbeck,  
University of London, Malet St, London WC1E 7HX, UK

Minerals of the alunite supergroup are widely distributed and play significant roles in the storage and release of water, acidity and toxic elements. Although alunite can contain many different cations, a particularly interesting case is that where the A site is occupied by hydronium. Despite many different experimental studies, a recent paper concluded that the existence of hydronium immediately adjacent to several hydroxyl anions remains in question [1]. To date it has proved impossible to locate the positions of the hydrogen atoms and one paper has concluded that the problem may only be resolved by 'rigorous numerical simulation' [2].



**Figure 1:** One possible ordered structure for H<sub>3</sub>O<sup>+</sup>-alunite.

In order to probe the existence or otherwise of hydronium in alunite we have performed quantum mechanical simulations based on density functional theory [3].

Current proposals for the structure of H<sub>3</sub>O<sup>+</sup>-alunite suggest that the hydronium ions are arranged about an axis of rotational symmetry with the hydrogens pointing either up or down relative to the *c* axis of the hexagonal structure. Our research demonstrates that the hydrogens are actually distributed in a different manner to any of the experimental models and explain why it is unlikely that the protons will ever be accurately resolved using diffraction methods.

[1] Nielson *et al.* (2007) *Am. Miner.* **92**, 587–597. [2] Lager *et al.* (2001) *Can. Miner.* **39**, 1131–1138. [3] Soler *et al.* (2002) *J. Phys. Cond. Matter* **14**, 2745–2780.

## Metabolic diversity and identification of soil microbial communities in mercury contaminated soil of Oak Ridge, TN

KENDRA L. WRIGHT<sup>1</sup>, KAREN S. MCNEAL<sup>2</sup>  
AND FENGXIANG X. HAN<sup>3</sup>

<sup>1</sup>(klw404@msstate.edu)

<sup>2</sup>(ksm163@msstate.edu)

<sup>3</sup>(han@icet.msstate.edu)

In the 1950s, the Department of Energy Y-12 Plant in Oak Ridge, TN used mercury in the production of nuclear weapons. Through the production process, mercury was released into the Oak Ridge environment. Mercury is known to cause serious health problems, and remediation efforts are on the forefront of the scientific research done in the area.

To provide a better understanding of mercury's effects on microbial communities, the metabolic diversity of Oak Ridge grassland and woodland soil microbial communities were compared using Biolog Ecoplates and Anaerobic plates. Samples were taken from the field locations and analyzed in the laboratory. Also, the potential for mercury phytoremediation was examined in laboratory plants (*Brassica juncea*). Soil samples were taken from the rhizosphere and outermost potting soil, and metabolic diversity was measured. Microbial identification was completed for all sample types using Biolog GEN III MicroLog-M software.

Preliminary data suggests laboratory soil treated with HgS<sub>2</sub> or HgCl<sub>2</sub> had significantly less metabolic diversity than the control samples. Furthermore, as mercury concentrations increase, field samples taken directly from the Oak Ridge site show variations in microbial diversity and community composition.