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## Structural instability in BiVO<sub>4</sub> under compression

Wednesday, 6 November 2024 10:00 (20 minutes)

Bismuth Vanadate displays rich polymorphism, resulting in a complex structural phase diagram. Owing to its potential as a photocatalyst for hydrogen production understanding the factors that influence its structure are important. This presentation focus on variable pressure neutron diffraction studies that reveal BiVO<sub>4</sub> undergoes an unusual increase in symmetry, from monoclinic to tetragonal, upon application of modest pressure. This correlates with a significant reduction in both the volume and distortion of the BiO<sub>8</sub> polyhedra, consistent with pressure induced melting of the Bi 6s<sup>2</sup> lone pair electrons. Conversely the VO<sub>4</sub> tetrahedra are relatively incompressible. The behaviour of BiVO<sub>4</sub> is compared to that of the isostructural oxide LaNbO<sub>4</sub> that lacks lone pair electrons.

### Topics

Chemistry and Crystallography

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