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Structural instability in BiVO4 under compression

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Bismuth Vanadate displays rich polymorphism, resulting in a complex structural phase diagram. Owing to it's 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 BiVO4 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 BiO8 polyhedra, consistent with pressure induced melting of the Bi 6s2 lone pair electrons. Conversely the VO4 tetrahedra are relatively incompressible. The behaviour of BiVO4 is compared to that of the isostructural oxide LaNbO4 that lacks lone pair electrons.

Topics

Chemistry and Crystallography

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