Structure and electrical conductivity relationship as a function of pressure

The relationship between electrical properties and the structure of $[Mo_{18}As_2O_{62}]^{4-}$ clusters is explored. Piperazinium cations sit between the clusters for charge neutrality. The structure crystallizes in the space group *F*ddd, and each ellipsoidal cluster is built from 18 $Mo^{VI}O_6$ octahedra. Two $As^{V}O_4$ tetrahedral units sit within the cluster and are corner sharing with four MO_6 octahedra. Two partially occupied trigonal pyramidal $As^{III}O_3$ units are on the surface of the cluster. At ambient pressure, the closest distance between clusters is ~ 2.9 Å. Variable temperature electrical conductivity measurements indicate activated behavior, and the short distance between clusters is postulated as a potential pathway for charge hopping. The clusters behave as ridge objects, and this is borne out when the material is compressed under hydrostatic conditions to 4.2 GPa. The material exhibits a reversible phase transition from *F*ddd to *C*2/*m* symmetry at ~0.8 GPa, with a concomitant decrease in the shortest distance between clusters. We correlate the structural change as a function of pressure with the electrical conductivity as a function of pressure.

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