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High-pressure synthesis, crystal and electronic structures of a new scandium tungstate $Sc_{0.67}WO_4$ JOHN MITCHELL, Argonne National Laboratory, TAMAS VARGA, Pacific Northwest National Laboratory, CHRISTO MALLIAKAS, Northwestern University, BRIAN TOBY, JUN WANG, LINDSAY ARNOLD, Argonne National Laboratory — Negative thermal expansion (NTE) materials possess a low-density, open structure that can respond to high pressure conditions, with potential for new compounds with unusual physical properties. Here we report that one such NTE material—white, insulating, orthorhombic $Sc_2W_3O_{12}$—transforms into a black, electrically conducting compound when treated at 4 GPa and 1400 °C. The high pressure phase, $Sc_{0.67}WO_4$, crystallizes in a defect-rich wolframite-type structure, a dense, monoclinic structure (space group $P12/c1$) containing 1-D chains of edge-sharing WO_6 octahedra.. The chemical bonding of $Sc_{0.67}WO_4$ vis-à-vis the ambient pressure $Sc_2W_3O_{12}$ phase can be understood on the basis of the Sc defect structure. Magnetic susceptibility, electrical conductivity, and thermoelectric power measurements reveal that $Sc_{0.67}WO_4$ is a metallic paramagnet. Conductivity varies linearly with temperature from 3-300 K, which may be understood in terms of weak localization and electron-electron interactions in this poor metal. Oxygen vacancies are suggested as a potential mechanism for generating the carriers in this defective wolframite.

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