

High pressure behavior of stibnite (Sb_2S_3)

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ABSTRACT

High-pressure x-ray diffraction and Raman spectroscopic study of Sb_2S_3 up to 53 GPa reveals two phase transitions at 5 GPa and 15 GPa, respectively. The first transition is evidenced by noticeable compressibility changes in distinct Raman-active modes, in the lattice parameter axial ratios, the unit cell volume, as well as in specific interatomic bond lengths and bond angles. By taking into account relevant results from the literature, we assign these effects to a second-order isostructural transition arising from an electronic topological transition in Sb_2S_3 near 5 GPa. Close comparison between Sb_2S_3 and Sb_2Se_3 up to 10 GPa reveals a slightly diverse structural behavior for these two compounds after the isostructural transition pressure. This structural diversity appears to account for the different pressure-induced electronic behavior of Sb_2S_3 and Sb_2Se_3 up to 10 GPa, i.e. the absence of an insulator-metal transition in Sb_2S_3 up to that pressure. Finally, the second high-pressure modification appearing above 15 GPa appears to trigger a structural disorder at ~ 20 GPa; full decompression from 53 GPa leads to the recovery of an amorphous state.