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High Pressure X-ray diffraction study of alpha-As2Te3

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The structural properties of arsenic telluride with monoclinic C2/m structure (alpha-As2Te3) have been studied both experimentally and theoretically under compression at room temperature by means of X-ray powder diffraction measurements up to 23 GPa and total-energy *ab initio* calculations. It has been found experimentally that alpha-As2Te3 remains in its initial monoclinic structure up to 14 GPa. At this pressure, a phase transition is observed in contrast to previous results that reported a phase transition between 6 and 8 GPa to the R-3m phase (beta-As2Te3) [1]. The pressure dependence of the structural parameters and equation of state for the low-pressure phase of As2Te3 have been determined by Rietveld refinement. The reported results are compared with those available in the literature for related *A2X3* compounds.

References

[1] T.J. Scheidelmantel, J.F. Meng and J.V. Badding, J. Phys. Chem. Solids 66, 1744 (2005).

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