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The crystal structure of barite, $BaSO_4$, at high pressure

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Abstract

The structure of barite, or baryte, $BaSO_4$, has been refined by single-crystal methods at room temperature to a maximum of 21.5 GPa in He medium. Lattice parameters have been obtained at select pressures by powder diffraction and complemented by the collection of Raman specta at the highest attained pressure. The results of all analyses correspond to $BaSO_4$ remaining in the barite-type structure to the highest investigated pressure. Therefore, the search for transitions leading to a post-barite structure, in $BaSO_4$, must be conducted at pressures higher than those investigated here, or, in "lower pressure" analogs.

Keywords: Barite, single crystal, high pressure, diffraction, phase transition, sulfate, synchrotron, compressibility