

SPINELS RENAISSANCE: THE PAST, PRESENT, AND FUTURE OF THOSE UBIQUITOUS MINERALS AND MATERIALS

High-pressure behavior of thiospinel CuCr_2S_4 †

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ABSTRACT

This study reports for the first time the lattice parameters and the complete crystal structure evolution with increasing pressure for a thiospinel with composition $\text{CuCr}_{1.7}\text{V}_{0.3}\text{S}_4$ (space group $Fd\bar{3}m$) measured by single-crystal X-ray diffraction as a function of pressure up to 7 GPa. The P - V data are adequately described to a fourth-order Birch-Murnaghan equation of state with the following coefficients: $V_0 = 947.86(6) \text{ \AA}^3$, $K_{T0} = 88(1)$, and $K' = 6.3(9)$, $K'' = -1.1(4)$. This is the first time that the compressibility behavior of a spinel structure has been described by a fourth-order Birch-Murnaghan equation of state. The unit-cell volume shows a compression of about 6.3% over the entire pressure range investigated. The crystal structure evolution clearly indicates that the main compression mechanism is related to the compression of the CuS_4 tetrahedron, which is significantly greater than the CrS_6 octahedron. The tetrahedral volume decreases by 7.8% over the pressure range studied while the octahedral volume decreases by 5.5%. The change in the octahedral volume is accompanied by a decrease in the angular distortion of the CrS_6 octahedra.

Keywords: Thiospinel, high pressure, single-crystal X-ray diffraction