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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 $CuCr_{1.7}V_{0.3}S_4$ (space group $Fd\overline{3}m$) 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) Å^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