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Crystal-field dependence with Co^{2+} - F^- distance in the perovskite KCoF₃ FERNANDO RODRIGUEZ, JOSE BARREDA-ARGÜESO, FERNANDO AGUADO, University of Cantabria, SIMON REDFERN, University of Cambridge, UK, UNIV CANTABRIA COLLABORATION, UNIV CAMBRIDGE COLLABO-RATION — Perovskite crystals are attractive for structural studies at high pressure in a wide multidisciplinary science. Perovskite or distorted-perovskite oxides are relevant as solid state devices as many of them exhibit properties such as colossal magnetoresistance, exotic magnetism, or even high $T_{\rm C}$ superconductivity. In geoscience, the understanding of high-pressure posperovskite phase is noteworthy. In this sense, it must be noted that $NaCoF_3$ transforms to the postperovskite phase at a moderate pressure (P = 15 GPa) in comparison to oxides [1]. However KCoF₃ seems to lack this transition as it remains in the perovskite structure up to higher pressure [2]. This work reports a structural study in $KCoF_3$ as a function of pressure in the 0-60 GPa range. Its large pressure perovskite stability is noteworthy. Therefore, this is a unique system to establish correlations between crystal and electronic structures in a high-symmetry phase, where Co^{2+} ions are located in a perfect octahedral environment. Here we present an x-ray diffraction study in correlation with single-crystal optical absorption spectroscopy. The variation of the crystal-field strength and Racah parameters of Co²⁺ with the crystal volume (and Co-F distance) up to 60 GPa are presented, discussed and compared with available data in other structures involving oxides and chlorides.

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