# Synchrotron X-ray powder diffraction investigation of the crystal structure of HoCo12B6-xCx

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Rare earth-transition metal borides are of significant interest due to their diverse structural and magnetic properties, which make them promising candidates for advanced functional materials [1]. Within this class, the HoCo12B6 compound was selected for detailed investigation due to its structural stability and unusually low magnetic ordering temperature [2-6]. This compound exhibits a rhombohedral structure, based on the hexagonal SrNi12B6-type structure, with a space group R-3m. Since carbon is chemically similar to boron and has a comparable atomic radius, it is a logical candidate for partial substitution without drastically altering the crystal framework [7]. In this study, we focus on the structural evolution of the HoCo12B6-xCx series with increasing carbon content, aiming to determine the solubility limit of carbon and evaluate the effects of substitution on lattice parameters and magnetic behaviour.

X-ray diffraction measurements using synchrotron radiation were performed at room temperature at the ROBL beamline (BM20) of the European Synchrotron Radiation Facility (ESRF). These high-resolution data enabled precise determination of lattice parameters and phase composition. The results demonstrate a linear decrease in the lattice constants and unit cell volume with increasing carbon content up to x = 0.8, after which a stabilization is observed. Rietveld refinement confirms the trends observed by both XRD methods, while SEM-EDX analysis verifies the elemental composition and homogeneity of the samples.

The synchrotron data reveal a near-isotropic lattice contraction, with the a and c parameters decreasing at similar rates. The contraction rate of the unit cell volume is approximately 0.5% per C/f.u. up to x = 0.8. Importantly, the c/a ratio remains nearly constant throughout the substitution range, indicating uniform shrinkage of the unit cell. Comparison with laboratory XRD shows more pronounced variation in the c parameter, while synchrotron XRD provides enhanced accuracy and signal-to-noise ratio. These findings offer insight into the structural effects of carbon incorporation in HoCo12B6 and lay the groundwork for further magnetic property investigations.

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