

Abstract Submitted
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Magnetostructural properties of $R\text{Co}_2$ ($R = \text{rare earth}$) compounds¹ DURGA PAUDYAL, YA. MUDRYK, Ames Laboratory of the USDOE, Iowa State University, Ames, IA-50011, V. K. PECHARSKY, K. A. GSCHNEIDNER, JR., Ames Laboratory of the USDOE and Department of Materials Science and Engineering, Iowa State University, Ames, IA-50011 — First principles electronic structure calculations show that the cubic Laves phase (C15) is stable for GdCo_2 and TbCo_2 , while the ground state structures of DyCo_2 , HoCo_2 , and ErCo_2 are tetragonal distortions of the cubic C15, orthorhombic, and rhombohedral structures, respectively. The R and Co moments exhibit antiparallel coupling, forming a ferrimagnetic state in every ground state structure of $R\text{Co}_2$. The predicted magnetostructural properties of $R\text{Co}_2$ are in good agreement with x-ray powder diffraction and magnetic measurements. The spin splitting of the conduction electrons due to the indirect R-R exchange plays a crucial role in the magnetostructural transformations in the $R = \text{Dy, Ho, and Er}$ $R\text{Co}_2$ phases, and accounts for its absence in the monomorphic GdCo_2 and TbCo_2 compounds.

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