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Magnetism of $\text{Ba}_4\text{Ru}_3\text{O}_{10}$ revealed by density functional calculations: Structural trimers behaving as coupled magnetic dimers
ANDRES SAUL, CINaM/CNRS, GUILLAUME RADTKE, IM2NP, YANNICK KLEIN, GWENAELLE ROUSSE, IMPMC/CNRS — From a simple ionic picture, the only magnetically active ions in this compound are the three Ru^{4+} atoms which form trimers of faced shared RuO_6 octahedral. The Ru atom in the middle of the trimer (named Ru(1)) is cristallographically inequivalent to the ones at the corners (named Ru(2)). A naïve analysis of the magnetic properties of this compound compatible with the expected low spin magnetic configuration of the Ru ions would predict a complicate magnetic order at low temperature involving the Ru(1) and Ru(2) ions and a high temperature susceptibility corresponding to three $S=1$ ions per unit cell. In spite of that, we demonstrate in this work, from density functional calculations, that under the influence of Ru-Ru covalent bonding, the structural trimers behave in an extended range of temperature from 0 to 600K, as strong ($S = 1$) antiferromagnetic dimers. Our calculations of the effective exchange interactions show a strong intra-dimer interaction and a weaker inter-dimer one which explains the antiferromagnetic order observed below $T_N = 105\text{K}$ and the magnetic susceptibility in the intermediate and high temperature range (from $T_N=105\text{K}$ up to 612 K).

Andres Saul
CINaM/CNRS

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