

Competition between ferromagnetic and antiferromagnetic ground states in CeCrB_4

M. Werwiński,¹ A. Szajek,¹ and A. Kowalczyk¹

¹*Institute of Molecular Physics, Polish Academy of Sciences,
M. Smoluchowskiego 17, 60-179 Poznań, Poland*

Cerium chromium tetraboride (CeCrB_4) was first synthesized in the 1970s [1,2]. However, its magnetic properties have only been discussed in general terms in the context of broader sets of materials in recently published one experimental and one theoretical study [3,4]. In the range above 100 K, magnetic susceptibility of CeCrB_4 was fitted to a modified Curie law and susceptibility measurements down to 1.8 K showed no phase transition [3]. The determined magnetic susceptibility of χ_0 is $+56 \times 10^{-5} \text{ emu mol}^{-1}$ [3]. Moreover, high energy resolution fluorescence detected X-ray absorption spectroscopy (HERFD-XAS) indicates that Ce occurs mainly in the non-magnetic state Ce^{+4} [3]. Filipo *et al.* also suggest that the small effective magnetic moment ($0.6 \mu_B$) determined from magnetic susceptibility comes from the Ce^{+3} contributions. The above outline of the basic magnetic properties is complemented by the aforementioned DFT calculations, which classifies the ground state of CeCrB_4 as conventional antiferromagnetic, in opposition to quantum spin dimers observed for many other MTB_4 compounds [4]. However, the difference in total energy between these two states (of the order of 1 meV f.u.^{-1}) was minuscule. In this work, we have studied in detail the properties of the magnetic ground state of CeCrB_4 using density functional theory calculations as implemented in the full-potential local-orbital (FPLO) code [5]. Fully relativistic calculations using the PBE+U method and optimization of atomic positions indicate for the CeCrB_4 a ferromagnetic ground state. However, the energy of the antiferromagnetic state is similarly close, as in previous studies [4]. The calculated spin magnetic moments on Ce and Cr are approximately 0.03 and $0.40 \mu_B \text{ atom}^{-1}$, respectively, and the orbital magnetic moments are negligible.

References:

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MW acknowledges the financial support of the National Science Centre Poland under the decision DEC-2021/41/B/ST5/02894 (OPUS 21).