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^{11}B-NMR STUDIES OF WEAKLY FERROMAGNETIC BaB_6*

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BaB_6 is a weakly ferromagnetic material with a Curie temperature T_C well above room temperature. From the results of d.c. magnetization measurements on single crystalline BaB_6, the saturation magnetization at low temperatures is $8\times10^{-4}(\mu_B/\text{f.u.})$, in line with other weak ferromagnets of the hexaboride series. The ^{11}B-NMR spectra measured on a collection of single crystals of BaB_6 yield a quadrupolar frequency of 472 KHz, in good agreement with calculated field gradients for this type of materials. The central ^{11}B-NMR transition consists of two partially resolved signals, where the frequency displacement between them is of the order of 10 KHz. One of the signals exhibits a positive, the other a negative frequency shift, both of the order of 50 ppm. Between 7 K and room temperature these shifts do not vary with temperature. The temperature dependence of the spin-lattice relaxation rate $T_1^{-1}(T)$ at the B sites is similar to that of other alkaline-earth hexaborides.

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Alkaline-earth hexaboride compounds XB_6 (where X=Ca, Sr and Ba) adopt a simple cubic CsCl-type crystal structure containing divalent metal ions and B_6-octahedra. In spite of this simple crystal structure they show very puzzling physical properties. *E.g.*, La-doped $Ca_{1-x}La_xB_6$ with x=0.005 and SrB_6 exhibit weak ferromagnetism with very high Curie temperatures [1, 2] of the order of 600 K or more.

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In figure 1 we show one example of a hysteresis loop of BaB_6, measured at 200 K, using a commercial SQUID magnetometer. From this type of measurements we found that BaB_6 orders ferromagnetically with a Curie temperature T_C well above room temperature. The coercive field H_C at 200 K is of the order of 250 Oe and the saturation magnetization at this temperature is $6.5\times10^{-4}(\mu_B/\text{f.u.})$. In addition to the ferromagnetic part of the magnetization, we also identify paramagnetic and diamagnetic contributions. The temperature dependence of the magnetic susceptibility $\chi\ (T)$, measured at 5 T, exhibits a Curie–Weiss behavior with an effective magnetic moment of $5.6\times10^{-2}(\mu_B/\text{f.u.})$ and a paramagnetic Curie temperature of θ=-6 K. The diamagnetic offset is -2×10^{-6}(emu/mol of f.u.) [3]. Similar results were obtained for other weak ferromagnets in the hexaboride series.

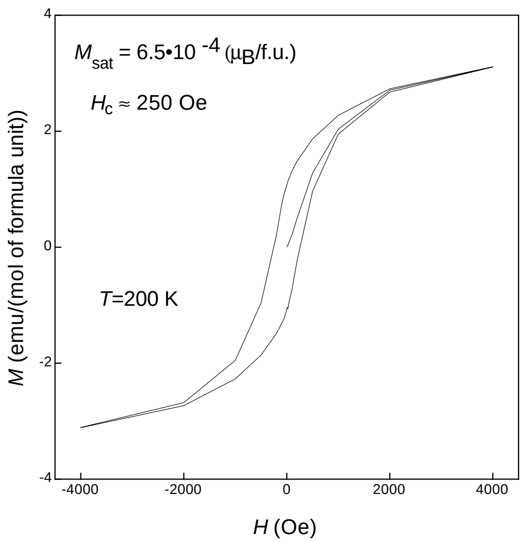

Fig. 1. Hysteresis loop $M(H)$ of BaB_6 at 200K.

In order to obtain additional microscopic information on the magnetic features of BaB_6, we made NMR measurements on ^{11}B nuclei. For these measurements we have used two types of standard spin-echo NMR techniques: sweeping the magnetic field H at a constant frequency ν and sweeping the frequency at a constant magnetic field, respectively, and by recording the spin-echo intensity as a function of H or ν. The wide NMR spectra which include the central line and quadrupolar wings were measured by magnetic field sweeping. High resolution measurements of the central line alone were performed at a fixed magnetic field and changing stepwise the frequency. From our measurements of the wings of the ^{11}B-NMR (data not shown here [3]), we extract a quadrupolar frequency for the ^{11}B nuclei of 472 KHz, which implies an electric field gradient at the B sites of 1.09×10^{21} V/m^2. This value is in good agreement (better than 5 %) with theoretical values predicted for BaB_6 [4].

Figure 2 depicts the central transition ($-1/2 \longleftrightarrow +1/2$) for ^{11}B nuclei taken at 85 K in a field of 7.06 T. The central transition consists of two partially overlapping signals with frequency shifts of +60 ppm and –40 ppm, respectively. The frequency shifts have been measured by comparing the position of the two peaks of the ^{11}B central line in BaB_6 with the resonant frequency of ^{11}B nuclei in liquid $B(OH)_3$. Between 7 K and room temperature the ^{11}B NMR line shifts do not vary with temperature. The width of each of the two individual ^{11}B NMR-signals is 10 KHz and their intensities are approximately equal. One may interpret the results for the ^{11}B NMR central line as an indication that in BaB_6 the B sites experience two magnetically different environments. The appearance of two peaks in the ^{11}B central line seems to be independent of the concentration of conduction electrons, because it has also been observed in hexaborides with very different transport properties, such as CaB_6, La-doped CaB_6 ($Ca_{1-x}La_xB_6$ for $x = 0.005, x = 0.1$ and $x = 0.2$), BaB_6, LaB_6 and YbB_6 [3, 5].

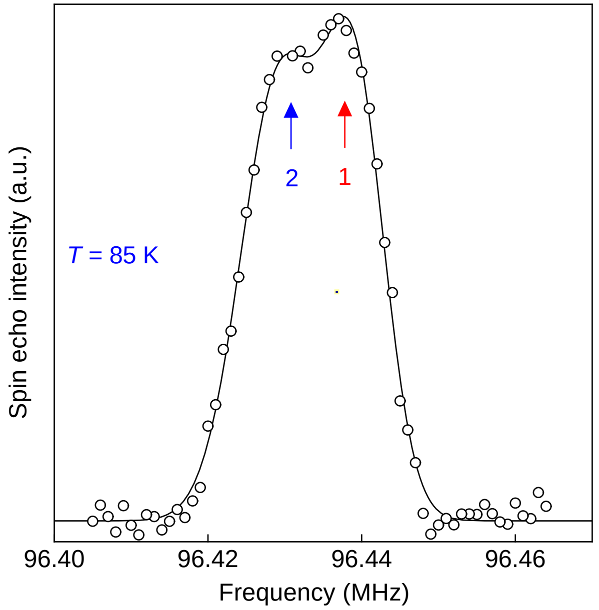

Fig. 2. Central signal of the ^{11}B-NMR Spectrum of BaB_6 at 7.2 T. The solid line represents the best fit to the data at 85 K using the sum of two Gaussian functions.

The temperature dependence of the spin-lattice relaxation rate $T_1^{-1}(T)$ measured in a constant magnetic field of 5.2 T is very different in two different T-regions. At temperatures above a crossover temperature of approximately 5 K, T_1^{-1} is, on the average, temperature independent and at temperatures below 5 K it decreases very rapidly with decreasing temperature. These results for the spin-lattice relaxation rate are very similar to the cases of $Ca_{0.995}La_{0.005}B_6$ and SrB_6 [6].

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