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^{31}P NMR study of the spin $S = \frac{1}{2}$ quasi-1D Heisenberg antiferromagnet $BaCuP_2O_7$

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There is continued interest in the properties of low-dimensional quantum spin systems due to the novelty of ground states and excitations that such systems exhibit. The emphasis of recent research has been on the magnetic properties of quasi-1D $S = \frac{1}{2}$ and $S = 1$ Heisenberg chains with antiferromagnetic (AF) nearest neighbour interactions. We focus here on the 1D magnetic properties of $S = \frac{1}{2}$ AF chains. Traditionally, there have been very few compounds with relatively negligible inter-chain exchange interactions compared to the intra-chain interactions (J/k_B). Consequently, the temperature T range over which true 1D properties could be observed has been rather limited. An exception to the above is Sr_2CuO_3 which has a very large J/k_B ($\simeq 2000$ K) [1] while long-range magnetic order (LRO) sets in only at about 5 K. A large body of work probing the low-T properties exists for this compound. However, owing to the large J/k_B all investigations were limited to $T \ll J/k_B$.

$BaCuP_2O_7$ contains Cu-O-P-O-Cu chains along the crystallographic c-direction [2]. While there exist pairs of such chains in the structure, the magnetic interaction between the chains might not be significant due to the nearly orthogonal orientation of the inter-chain bond vis-a-vis the intra-chain bond. Consequently, one might expect the magnetic properties to be primarily 1D.

Herein, we report magnetic properties of polycrystalline samples of $BaCuP_2O_7$ as determined from pulsed ^{31}P nuclear magnetic resonance NMR (shift K, spin-lattice relaxation rate $1/T_1$, and line shape) measurements in a large T-range $0.03\,\text{K} \leqslant T \leqslant 300\,\text{K}$, four orders of magnitude in temperature. This range not only covers temperatures well below J/k_B but also up to $T \sim 3J/k_B$. The SQUID-based susceptibility measurements have been made between 1.8 and 400 K. Our work shows that $BaCuP_2O_7$ is a good example of a 1D $S = \frac{1}{2}$ Heisenberg AF above about 1 K whereas clear signs of LRO are seen below 0.85 K. For $T > 1$ K, our results for the static and dynamic magnetic susceptibility are in excellent agreement with the predictions of Sachdev [3] while at lower temperatures there are indications that the magnetic order is exotic.

The structure of $BaCuP_2O_7$ belongs to the triclinic space group $P\bar{1}$. Lattice parameters for our single phase samples were found to be in agreement with previously reported values [2]. The ^{31}P nuclei have spin $I = \frac{1}{2}$ and gyromagnetic ratio $\gamma/(2\pi) = 17.237$ MHz/T. The T dependence of the ^{31}P

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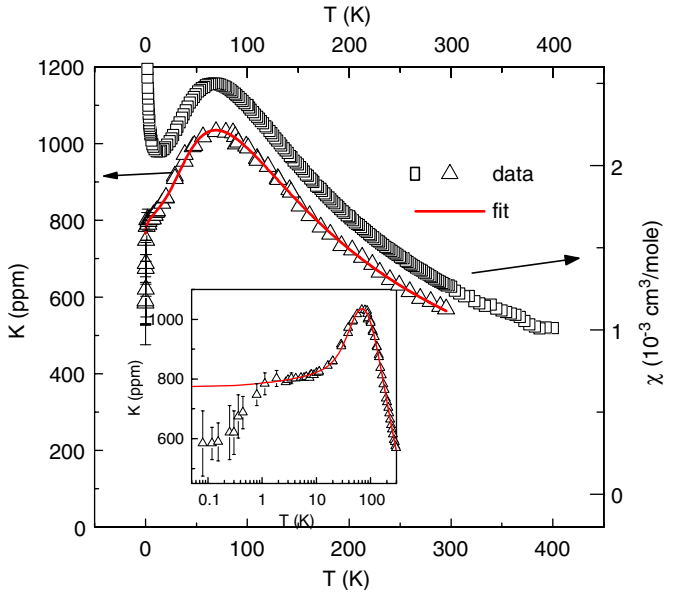

Fig. 1. The T dependence of the ^{31}P NMR shift K is shown along with that of the susceptibility (right and top axes). The inset shows $K(T)$ on a logarithmic T scale. The solid line is a fit to Eq. (1).

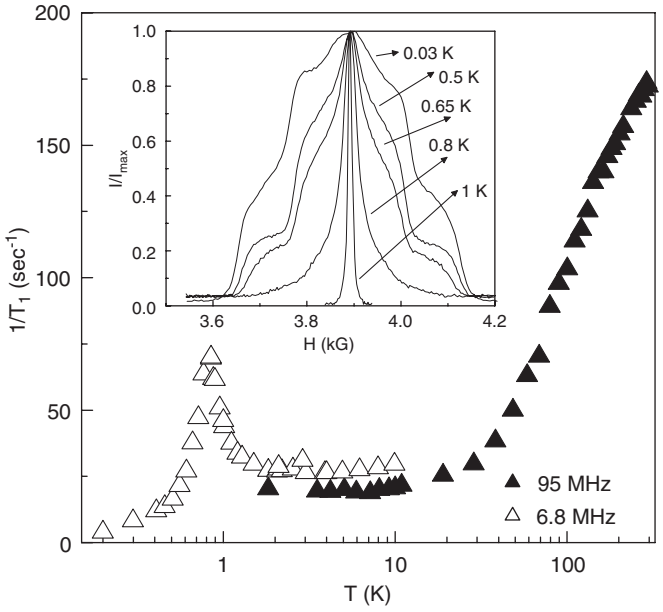

Fig. 2. ^{31}P NMR $1/T_1$ is plotted as a function of temperature T. The inset shows field swept spectra at various temperatures below 1 K, using a radio frequency of 6.8 MHz.

NMR shift $K(T)$ is shown in Fig. 1. The qualitative shape of the curve is seen to be similar to that of the bulk susceptibility χ.

Indeed a plot of K versus χ (not shown) with T as an implicit parameter yields a straight line. This implies that the ^{31}P nucleus senses the copper spin susceptibility via a super-transferred hyperfine coupling. Therefore, measurements of the temperature dependence of ^{31}P NMR parameters such as K, the line shape, and $1/T_1$ are expected to yield information about the static and dynamic magnetic properties of $BaCuP_2O_7$. The broad maximum seen in $K(T)$ is indicative of low-dimensional magnetic behaviour. Since the T dependence of the spin susceptibility of a $S=\frac{1}{2}$ Heisenberg AF chain $\chi_{\rm spin}(T,J)$ is known [4], we fit the variation of K with T to the following equation:

$$K = K_0 + \left(\frac{A}{N_{\rm A}\mu_{\rm B}}\right)\chi_{\rm spin}(T,J), \qquad (1)$$

where K_0 is the chemical shift, A is the hyperfine coupling of the ^{31}P nucleus to the Cu magnetic moments, $N_{\rm A}$ is the Avogadro number, and $\mu_{\rm B}$ is the Bohr magneton. The parameters obtained from the fit are $K_0 = 73 \pm 20$ ppm, $A = 2182 \pm 20\,{\rm Oe}/\mu_{\rm B}$, and $J/k_{\rm B} = 108 \pm 2$ K. It is clear from Fig. 1 that the data are well fit by Eq. (1) for $T > 1$ K whereas a sharp decrease is seen below 1 K. This suggests a magnetic transition and further evidence is detailed below.

The T dependence of ^{31}P $1/T_1$ is shown in Fig. 2. The T independent behaviour seen between 2 K and 10 K is in accord with predictions of Sachdev that, for $T \ll J/k_{\rm B}$, the relaxation is dominated by the fluctuations of the staggered susceptibility at the AF wave vector $\mathbf{q} = \pi/a$. The nearly linear T dependence at higher T arises due to the dominance of the uniform susceptibility. The sharp peak seen at 0.85 K suggests a transition to LRO. The ^{31}P NMR line shape is also observed to broaden drastically below about 0.85 K with the appearance of two symmetrically located shoulders on either side of the central line (see inset of Fig. 2). Whereas an unambiguous interpretation of the line shape appears difficult at this stage, we suggest [5] the possibility of a transition to an incommensurate magnetic order with a two-dimensional modulation of the phase of the magnetization [6].

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