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# Magnetic properties of $Li_2RuO_3$ as studied by NMR and LDA+DMFT calculations[1)]

*I. Yu. Arapova*[+], *A. L. Buzlukov*[+], *A. Yu. Germov*[+], *K. N. Mikhalev*[+], *T.-Y. Tan*[*×], *J.-G. Park*[*×], *S. V. Streltsov*[+○ 2)]

[+] *M.N. Miheev Institute of Metal Physics, 620990 Ekaterinburg, Russia*

[*] *Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 151-747, Korea*

[×] *Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea*

[○] *Ural Federal University, 620002 Ekaterinburg, Russia*

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Low dimensional hexagonal ruthenates attract a lot of attention because of unusual physical properties. $Li_2RuO_3$ has dimerized lattice and shows a spin-gap behavior for $T < 560$ K [1, 2]. At higher temperature $Li_2RuO_3$ was initially supposed to have uniform crystal structure [1]. However, accurate pair distribution function (PDF) analysis of the diffraction data revealed that Ru-Ru dimers still exist for $T > 560$ K, but start to flow over the lattice [3]. This state was called a valence bond liquid (VBL) state. Physical properties of the VBL state has remained largely unexplored.

At the same time, the low temperature phase of $Li_2RuO_3$ is equally interesting. There is a linear contribution to the heat capacity (in spite of insulating temperature behavior of the resistivity) [2] and unusually large (for the system with a spin-gap) magnetic susceptibility [1]. The inelastic neutron scattering show plenty of the low-energy magnetic excitations having a clear momentum modulation [2].

In the present paper the nuclear magnetic resonance (NMR) has been applied for the investigation of the magnetic properties of $Li_2RuO_3$. We found that the NMR shift is proportional to the uniform magnetic susceptibility in a wide temperature range above 100 K, see Fig. 1, which guarantees that a large magnetic response for $100 < T < 560$ K is an intrinsic feature of $Li_2RuO_3$, which cannot be explained by an impurity phase. In its turn spin-lattice relaxation time $T_1$ shows that there is no clear activation-like processes in the low temperature phase expected for the system with a spin gap. In contrast activation behavior is observed for $T > 560$ K.

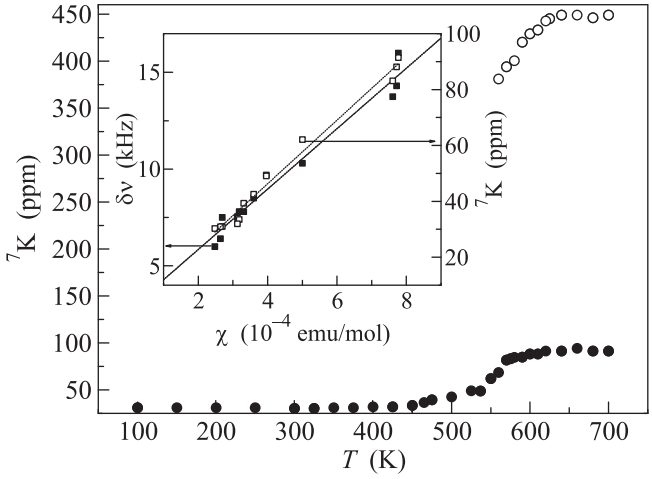


Fig. 1. Temperature dependence of the shifts of the $^7$Li NMR lines. Open and solid circles point positions of Li atoms in Ru layers and out of these layers respectively. In the inset: parametric dependence of the shift (open squares) and the linewidth ($\delta\nu$, solid squares) for the Li atoms out of the Ru layers vs. magnetic susceptibility. Dotted lines are the guide for the eyes

This can be related to the formation of the valence bond liquid state.

Theoretical LDA + DMFT calculations demonstrate that there is indeed a spin gap in the low temperature phase. Magnetic response at higher temperatures is mostly due the $xz/yz$ orbitals of Ru. These are the orbitals, which are not directed to each other and these bonds get broken first with temperature. Bonding between the $xy$ orbitals is much stronger. This is the reason why spin-polarization of these orbitals is minimal even at a very high temperature.

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[2)] e-mail: streltsov.s@gmail.com

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