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Exploting magnetic interactions in Kitaev anti-ferromagnet Na_2PrO_3

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Our goal is to analyze the magnetic properties of the Kitaev material Na_2PrO_3 by comparing Neutron Scattering (NS) and Muon Spin Spectroscopy (μSR) experiments, with the addition of ab initio calculations.

Alkali-metal lanthanide oxides are an exciting field of study due to their frustrated geometry and possibly anisotropic magnetic interactions, as shown in Fig.1.

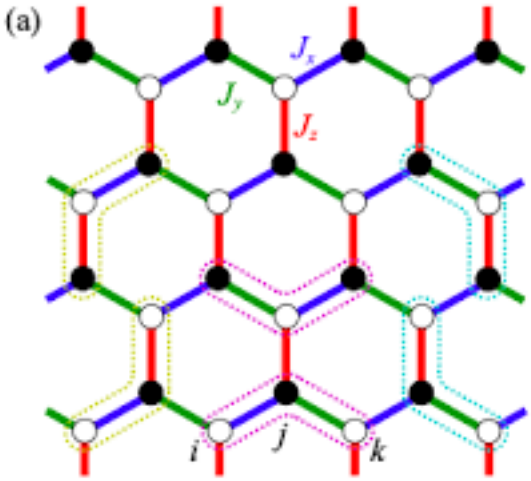

Figure 1: Schematic diagram of Kitaev honeycomb lattice, with anisotropic bond interactions J_x, J_y, J_z.

In this class of materials, also known as Kitaev materials, the SOC energy is comparable to that induced by crystal-field excitations (CEF), and the small spatial extent of f-electron orbitals promotes anisotropic Kitaev terms.

Na_2PrO_3 crystallizes with a monoclinic unit cell, where edge-sharing PrO_6 octahedra forms a honeycomb lattice. The effective paramagnetic moment is 0.99 μB, less than the free Pr^{4+} ion moment (2.54 μB), and the origin of its small value is still under debate. In addition, it displays a magnetic ordering transition at T_N = 4.6 K. Previous powder diffraction measurements could not detect any signs of magnetic ordering, despite evidence in specific heat and magnetometry measurements. Moreover, preliminary magnetic neutron diffraction results do not reveal any clear magnetic Bragg peaks, probably due to the low value of Na_2PrO_3 effective paramagnetic moment.

The principal question that motivated our work was to try to explain the small effective paramagnetic moment, considering the presence of the magnetic ordering. Thanks to the muon's extreme sensitivity to small-moment

magnetism, here μSR is highly relevant. From this, Na_2PrO_3 shows coherent oscillations of the muon asymmetry below T_N, reflecting the presence of an anti-ferromagnetic (AFM) ordering.

In comparison with experimental data, combined ab initio calculations and dipolar simulations were performed in order to elucidate the nature of AFM ordering inside this material and to try to explain the small value of the effective paramagnetic moment.

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