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Magnetic dipolar fields in quasi-one-dimensional paramagnetic metal $Li_{0.9}Mo_6O_{17}$ GUOQING WU, College of Physics Science and Technology, Yangzhou University, W. GILBERT CLARK, STUART BROWN, Dept. of Physics and Astron., UCLA — A general calculation for the magnetic dipolar fields in paramagnetic systems with non-Cartesian lattice coordinates is described and the field in the Q1D metal $Li_{0.9}Mo_6O_{17}$ is calculated with observations at the ^{7}Li site. We find that the "easy axis" is along the lattice *c*-axis, as it shows that, with sample rotations around the *b*-axis, the so called "magic angle" (θ_{max}) corresponding to the magnetic dipolar field minimum is right at the angle 54.7° from the *c*-axis, while the principle axis (p_z) of the electric field gradient (EFG) is along *a* as determined from our ^{7}Li-NMR experiments. Thus the lattice *c* and *a* axes are not only the symmetry axes of the lattice structure, but also the symmetry axes for the orientation of the magnetic dipole moments and for the distribution of the surrounding electric charges, respectively. This later character is very unusual as compared with other Q1D and 2D materials. Our calculation also shows that the dipolar field contributes to the local fields significantly at the Li site as one of its major local field sources, with a shift in maximum from ∼2ppm above 100 K to ∼7ppm at 5 K, agreeing with our ^{7}Li-NMR experimental observations and helping the property understanding.

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