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Intrinsic disorder in the candidate quantum spin ice $\text{Pr}_2\text{Zr}_2\text{O}_7$

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Quantum spin liquids with long-range entanglement are of great interest for applications in quantum technology. The quantum spin ice $\text{Pr}_2\text{Zr}_2\text{O}_7$ is a promising example, where it is believed that structural disorder plays a key role in enhancing quantum mechanical effects by introducing strains that split the ground state doublet akin to the effect of a local disordered transverse field. However, the precise defect structure responsible for this behaviour is unknown. Here I will demonstrate how we have determined the intrinsic defect structure of $\text{Pr}_2\text{Zr}_2\text{O}_7$ using neutron and x-ray scattering techniques supported by density functional theory. Our results explain the single-ion magnetism by considering the non-magnetic singlets that arise as a result of the defect structure. These singlets account for additional features in the neutron-measured crystal electric field excitations. This makes a significant contribution towards the observed broadening of pinch points in the magnetic diffuse scattering, which was previously attributed purely to quantum effects.

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