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Orbital Dimer Model for Spin-Glass State in $Y_2Mo_2O_7$ JOSEPH PADDISON, Churchill College, University of Cambridge, CB3 0DS, UK, PETER THYGESEN, ANDREW GOODWIN, RONGHUAN ZHANG, MICHAEL HAYWARD, Department of Chemistry, University of Oxford, OX1 3QR, UK, KARENA CHAPMAN, KEVIN BEYER, Advanced Photon Source, Argonne National Lab., IL 60439, USA, HELEN PLAYFORD, DAVID KEEN, STFC-ISIS, Rutherford Appleton Lab., Didcot OX11 0QX, UK, MATTHEW TUCKER, Spallation Neutron Source, Oak Ridge National Lab., TN 37831, USA — The formation of a spin glass generally requires that magnetic interactions are both frustrated and disordered. Consequently, the origin of spin-glass behavior in $Y_2Mo_2O_7$ – in which magnetic Mo^{4+} ions occupy a frustrated pyrochlore lattice with minimal compositional disorder – is a longstanding question. We use neutron and X-ray pair-distribution function (PDF) analysis to develop a disorder model that resolves apparent incompatibilities between previous PDF, EXAFS and NMR studies, and provides a new and physical explanation of the exchange disorder responsible for spin-glass formation. We show that Mo^{4+} ions displace according to a local "2-in/2-out" rule on Mo_4 tetrahedra, driven by orbital dimerization of Jahn-Teller active Mo^{4+} ions. Long-range orbital order is prevented by the macroscopic degeneracy of dimer coverings permitted by the pyrochlore lattice. Cooperative O^{2-} displacements yield a distribution of Mo–O–Mo angles, introducing disorder into magnetic interactions. Our presentation shows how frustration of atomic displacements can assume the role of compositional disorder in driving a spin-glass transition, and reveals a link between ice-like and spin-glass physics.

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