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Local structure of the lone-pair pyrochlore $Bi_2Ti_2O_7$ and the search for polar ordering DANIEL SHOEMAKER, RAM SESHADRI, Materials Dept, University of California Santa Barbara, ANDREW HECTOR, School of Chemistry, University of Southampton, ANNA LLOBET, THOMAS PROFFEN, Lujan Neutron Scattering Center, Los Alamos National Laboratory — Pyrochlore oxides of the formula $A_2B_2O_7$ contain geometrically frustrated A and B sublattices, leading to a multitude of complex phenomena including high dielectric constants, glassy spin interactions, and low-temperature peaks in heat capacity. In $Bi_2Ti_2O_7$, large atomic displacements (~ 0.4 Å) on the diamond-type OBi_4 sublattice cannot cooperatively order to accommodate the Bi lone pair. Instead, polar distortions form a charge ice with no long-range order, and powder diffraction finds $Bi_2Ti_2O_7$ to remain centrosymmetric at 2 K. We move beyond Rietveld analysis to describe the real-space, local structure of this highly disordered oxide. By conducting large-box reverse Monte Carlo (RMC) simulations on neutron total scattering data, we produce a model that contains details invisible to traditional crystallographic techniques. In addition to describing the local structure of $Bi_2Ti_2O_7$, we present capabilities of the RMC technique and its application to complex disorder in other crystalline materials.

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