Electric Field Gradient Comparisons in Perovskites\textsuperscript{1} \ DANDAN MAO, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — Piezoelectric and dielectric properties of Pb-based complex ferroelectric alloys with the A(B′B”B”’)O\textsubscript{3} perovskite structure depend on composition and the local ordering of the B-site cations. A prototypical example is Pb(Sc\textsubscript{1/2}Ta\textsubscript{1/2})O\textsubscript{3} (PST), which is a normal ferroelectric when the B atoms are ordered and becomes a relaxor when they are disordered. Electric field gradients (EFG) are sensitive to variations in local structure, and they can be probed using high-field nuclear magnetic resonance experiments. Calculations of EFGs are presented using the LAPW method within the local density approximation. We examine trends in B-site EFGs as a function of composition and order in PST, Pb(Zr\textsubscript{1−x}Ti\textsubscript{x})O\textsubscript{3} (PZT), Pb(Sc\textsubscript{2/3}W\textsubscript{1/3})O\textsubscript{3} (PSW), and Pb(Mg\textsubscript{1/3}Nb\textsubscript{2/3})O\textsubscript{3} (PMN). We discuss these results in terms of B- and Pb-atom off-centerings, and B-atom ordering.

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