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**$^{17}$O Nuclear Magnetic Resonance Chemical Shielding Calculations of PZT Solid Solutions**[1] DANIEL L. PECHKIS[2], ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — First principles B3LYP calculations of $^{17}$O NMR in $PbTiO_3$, $Pb(Zr_{\frac{1}{2}}Ti_{\frac{1}{2}})O_3$ (PZT), and $PbZrO_3$ will be presented. These systems were modeled with finite size quantum clusters embedded in point charge arrays. The embedding reproduces the Ewald Coulomb potential to better simulate the crystal environment.[3] For polar systems, the calculations were performed in the presence of an external electric field to cancel surface depolarization effects.[4] PZT was modeled using three chemically ordered structures: P4mm, P2mm, and R3m. Two groupings of $^{17}$O isotropic chemical shifts $\delta_{iso}$ are seen in all of our PZT calculations with [001] ordering. One is at $\delta_{iso} \approx 400$ppm and the other is at $\delta_{iso} \approx 650$ppm. We relate these to variations in the Ti-O and Zr-O bond lengths and use this to interpret recent experimental measurements.[5]

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[3]M. K. Klintenberg, S. E. Derenzo, and M. J. Weber. Comput. Phys. Commun.**131**, 120, (2000).
[4]S. Li and K. Rabe. APS March Meeting abstract (2007).
[5]A. Baldwin, P.A. Thomas and R. Dupree, J. Phys: Cond. Matt. **17**, 7159 (2005).

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