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High sensitivity of ^{17}O NMR to p-d hybridization in transition metal perovskites: first principles calculations of large anisotropic chemical shielding[1] DANIEL L. PECHKIS, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — First principles calculations are used to show that O chemical shielding tensors, $\hat{\sigma}$, are a sensitive indicator of local structure in transition metal ABO_3 perovskites, due to their strong dependence on covalent O(2p)-B(nd) interactions.[2] This indicates that ^{17}O NMR spectroscopy, coupled with first principles calculations, can be an especially useful tool to study the local structure in complex perovskite alloys. Our principal findings are 1) a large anisotropy between deshielded $\sigma_x \simeq \sigma_y$ and shielded σ_z components; 2) a nearly linear variation of isotropic $\sigma_{\rm iso}$ and uniaxial $\sigma_{\rm ax}$ components, as a function of the B-O-B bond asymmetry, across all the systems studied; 3) the demonstration that the anisotropy and linear variation arise from large paramagnetic contributions to σ_x and σ_y, due to virtual transitions between O(2p) and unoccupied B(nd) states. 4) Very good agreement with recent $BaTiO_3$ and $SrTiO_3$ single crystal ^{17}O NMR measurements of isotropic $\delta_{\rm iso}$ and uniaxial $\delta_{\rm ax}$ chemical shifts, and good agreement with $PbTiO_3$ and $PbZrO_3$ powder spectrum $\delta_{\rm iso}$ measurements.[2]

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[2]Pechkis et al., JCP **131**, 184511 (2009); references therein.

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