

Structural Transitions in Perovskites: Successes of a Group Theoretical Approach

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The author has made extensive use of group theory, as implemented in computer program ISOTROPY (<http://physics1.byu.edu/~stokes/isisotropy.html>), to underpin the study of structural variation and structural phase transitions in perovskites. A review of the work appears in the literature [1].

The approach will be illustrated for the double perovskites, $A_2BB'X_6$, where alternation of B -site cations is coupled with the ubiquitous BX_6 octahedral tilting. The symmetries of the cation ordering, in-phase and out-of-phase tilting are identified, respectively, with irreducible representation R_1^+ , M_3^+ , R_4^+ of the parent space group $Pm\bar{3}m$. Program ISOTROPY is used to enumerate the structures and possible phase transitions [1]. The results have guided recent structure determinations of Sr_2YNbO_6 and Sr_2YTaO_6 [2], as well as detailed studies of temperature-induced transitions in $BaBiO_3$ and Ba_2BiSbO_6 .

In another development [3], we used ISOTROPY to assist in constructing the free energy expansion for a combination of Jahn-Teller distortion (Γ_3^+) and octahedral tilting (R_4^+) in $PrAlO_3$. We proposed a mechanism for the coupling of J-T distortion to the octahedral tilting via a common tetragonal strain - such a mechanism can account for the three phase transitions observed.

[1] Howard C.J., Stokes H.T., *Acta Cryst.*, 2005, **A61**, 93. [2] Howard C.J., Barnes P.W., Kennedy B.J., Woodward P.M., *Acta Cryst.* B, submitted. [3] Carpenter M.A., Howard C.J., Kennedy B.J., Knight K.S., *Phys. Rev. B*, submitted.

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