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Simple point-ion electrostatic model explains the cation ordering in A2BO4 spinel oxides[1] VLADAN STEVANOVIC, MAYEUL D'AVEZAC, ALEX ZUNGER, NREL, Golden CO — The A2BO4 spinel oxides are distinguished by having either a normal or an inverse distribution of the A, B cations over the octahedrally and tetrahedrally coordinated sites. While normal spinel represents a single structure (A-octahedral, B-tetrahedral) the inverse spinel is similar to a 50-50 alloy with octahedral sublattice occupied randomly by A and B. We show that a simple point-ion electrostatic (PIE) model parameterized by the oxygen displacement parameter u and by the relative formal cation valencies ZA vs ZB provides a simple rule: if ZA>ZB the structure is normal for u>0.2592 and inverse for u<0.2578, while if ZA<ZB the structure is normal for u<0.2550 and inverse for u>0.2578. This rule is illustrated for the known spinel oxides, proving to be 98 % successful (PRL 105, 075501). Moreover, in inverse spinels the PIE model also explains the origin of the experimentally observed ordered phase that emerges from the random alloy at low T.

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