

*Hierarchical systematics of ordered perovskites: a group-theoretical analysis*

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Perovskites ABX<sub>3</sub> and perovskite-related phases are one of the most fertile families of materials which have numerous important physical properties (such as ferroelectricity, piezoelectricity, superconductivity, colossal magnetoresistance, catalysis, and ionic conductivity). A change in the degree of cation and/or anion order causes changes in the optical, magnetic, and electric (dielectric) properties, as well as electronic and ionic conductivities [1]. One of the most powerful tool of theoretical prediction of new ordered perovskites is a group-theoretic analysis [2].

We presented the general hierarchical picture of possible ordered perovskite phases. In the simplest cases, A-, B - and the X-ordered structures are induced by single-component order parameters. They form aristotypes of cation and anion orders in perovskites. The possibility of the existence of 13 ordered phases in the 1(a) and 1(b) positions (including four binary, two ternary, and five quaternary cationic superstructures) is proved. We limited the analysis of only low-symmetry phases with a number of ordered cations not more than four cations. The possibility of the existence of 261 anion ordered low-symmetry structures, each with a unique space-group symmetry, is established. These results include five binary and 14 ternary anion superstructures [3].

On the basis of these aristotypes, the low-symmetry phases are generated by a combination of different order parameters (parameters describing ordering in different sublattices, the rotation of the oxygen octahedra and ferroelectric properties and others). As an example we considered 1 3 A-site ordered perovskite. We showed different ways of structure genesis of low symmetry phases and emphasized the important role of the full condensate of order parameters in forming the structure and physical properties of perovskites.

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