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Coexistence of ferroelectricity and octahedral rotations in ABX_3 perovskites NICOLE BENEDEK, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University — Nearly all cubic perovskite materials are unstable to energy-lowering structural distortions. The most intensively studied distortions are those that induce ferroelectricity and tilts or rotations of the anion octahedra. The phonon dispersion curves of many perovskites contain both types of instability, although competition between the different types of distortions usually leads to ground-state structures in which one type of instability has been eliminated. Hence, whereas there are many perovskites that are *either* ferroelectric or have rotated octahedra, there are very few perovskites that are *both* ferroelectric and have rotated octahedra. We use a combination of Density Functional Theory, group theoretical techniques and crystal chemistry arguments to study the competition between ferroelectric and octahedral rotation distortions in a family of ferroelectric perovskite fluorides and oxides. By considering both "long-range" distortions (phonons) and the local bonding environment of each ion, we are able to build up a picture of which factors favor one type of distortion over the other.

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