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Structural distortions in AlF_3 derived using density functional methods L. L. BOYER, M. J. MEHL, DAN FINKENSTADT, Center for Computational Materials Science, Naval Research Laboratory — The crystal structure of AlF_3 at high temperatures has a simple cubic lattice. Below $\sim$ 730K the structure transforms to a rhombohedral (α-phase) structure with R$\overline{3}$c symmetry, due to an unstable R_5^- phonon. Density-functional based methods, from the least accurate rigid-ion model to highly-accurate all-electron Kohn-Sham models, yield the triply degenerate R_5^- phonon that becomes unstable with decreasing volume at some critical volume V_c. Significant variations for V_c and the equilibrium volume V_0 among the models lead to large uncertainties for the energy differences between the cubic and rhombohedral structures, indicating that present density functional models are not reliable for accurate quantitative results in this case.

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