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Microscopic Insight into the Isosymmetric Jahn-Teller Bond Axis Reorientation in Na_3MnF_6 NENIAN CHARLES, JAMES RONDINELLI, Drexel University — Using first-principles density functional theory calculations, we investigate the hydrostatic pressure-induced spontaneous reorientation of the Jahn-Teller bond axis in the fluoride cryolite Na_3MnF_6. We find a first-order isosymmetric transition occurs between crystallographically equivalent monoclinic structures at approximately 2.15 GPa, consistent with earlier experimental studies. Analogous calculations for Na_3ScF_6 show no evidence of a transition up to 6.82 GPa. Mode crystallography analysis of the pressure-dependent structures in the vicinity of the transition reveals a clear evolution of the Jahn-Teller bond distortions in cooperation with an asymmetrical stretching of the equatorial fluorine atoms in the MnF_6 octahedral units. We identify a change in orbital occupancy of the e_g manifold in the d^4 Jahn-Teller active Mn(III) to be responsible for the transition, which stabilizes one monoclinic $P2_1/n$ variant over the other. From our results, we conjecture that the same transition may be accessible in epitaxially grown thin films of Na_3MnF_6 with a modest biaxial tensile strain.

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