Supporting information for “The chemical forces underlying octahedral tilting in halide perovskites”

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Spacegroup P4/mbm compared to Pm3m

In the main paper I state that the comparison of P4/mbm compared to Pm3m is so similar to the comparison of I4/mcm to Pm3m that it did not warrant inclusion in the main article. Nonetheless it is important that this claim be substantiated, therefore I present here the plot of energy differences of P4/mbm and Pm3m. The reader can compare them to Figure 3 of the main text, to test the veracity of my statement.

Figure S1 Energy of Pm3m minus energy of P4/mbm, varying A and B site iconicity (a-c), with dispersion interaction C of 0.0 (a), 40.0 (b) and 100.0 (c); varying A and B site repulsion (d).

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