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Study of B1 (NaCl-type) to B2 (CsCl-type) pressure-induced structural phase transition in BaS, BaSe and BaTe using first-principles computations[1] SANJAY KHARE, Dept. of Physics, University of Toledo, XIUQUAN ZHOU, Dept. of Chemistry, University of Toledo, JASON L. ROEHL, Dept. of Physics, University of Toledo, CORA LIND, Dept. of Chemistry, University of Toledo — We have studied the pressure-induced phase transitions from NaCl-type (B1) to CsCl-type (B2) structure in BaS, BaSe and BaTe by using *ab initio* density functional theory computations in the local density approximation. The Buerger and WTM[2] mechanisms were explored by mapping the enthalpy contours in two and four dimensional configuration space for the two mechanisms, respectively. Transition pressures for BaS, BaSe and BaTe were determined to be 5.5 GPa, 4.9 GPa and 3.4 GPa, respectively. From these configuration space landscapes, a low enthalpy barrier path was constructed for the transitions to proceed at three different pressures. We obtained barriers of 0.18, 0.16 and 0.15 eV/pair (17.4, 15.4 and 14.5 kJ/mol) for the Buerger mechanism and 0.13, 0.13 and 0.12 eV/pair (12.5, 12.5 and 11.6 kJ/mol) for the WTM mechanism at the transition pressures for BaS, BaSe and BaTe, respectively, indicating that the WTM mechanism is slightly more favorable in these compounds. We describe the difference of the two mechanisms by differences in their symmetry and atomic coordination.

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[2]M. Watanabe *et. al*, Acta Crystallogr., Sect. A **33**, 294 (1977).

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