Electronic Supplementary Material (ESI) for RSC Advances.

Theoretical Studies of 3D-to-planar Structural Transition in $Si_nAl_{5-n}^{+1, 0, -1}$ (n=0-5) Clusters

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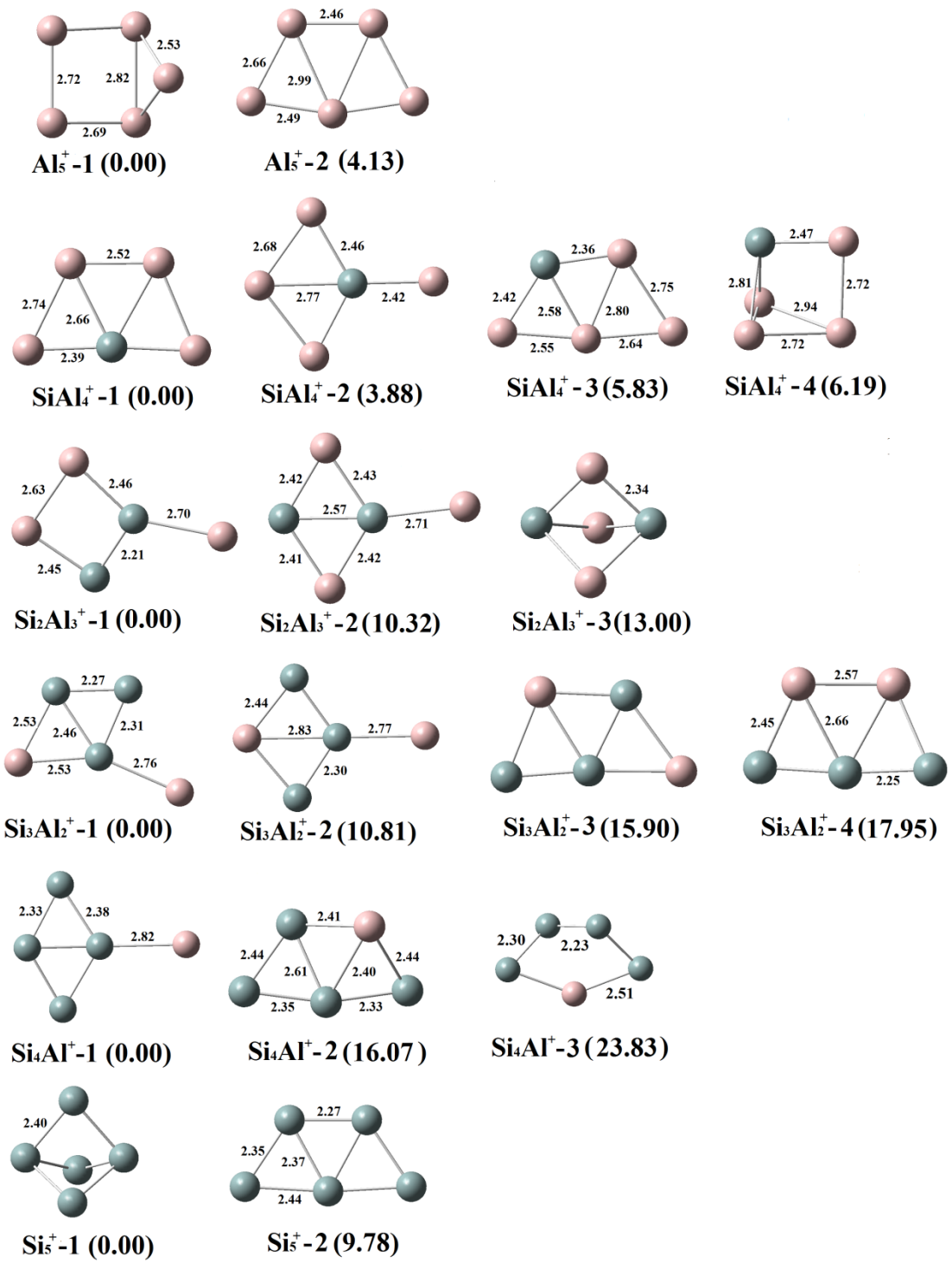

Figure S1 B3LYP-Optimized geometries of $Si_nAl_{5-n}^+$ (n=0-5) clusters. The relative energies calculated at CCSD(T)/6-311+G(2d) level are shown in bracket. Bond length and relative energy are presented in the units of Å and kcal/mol.

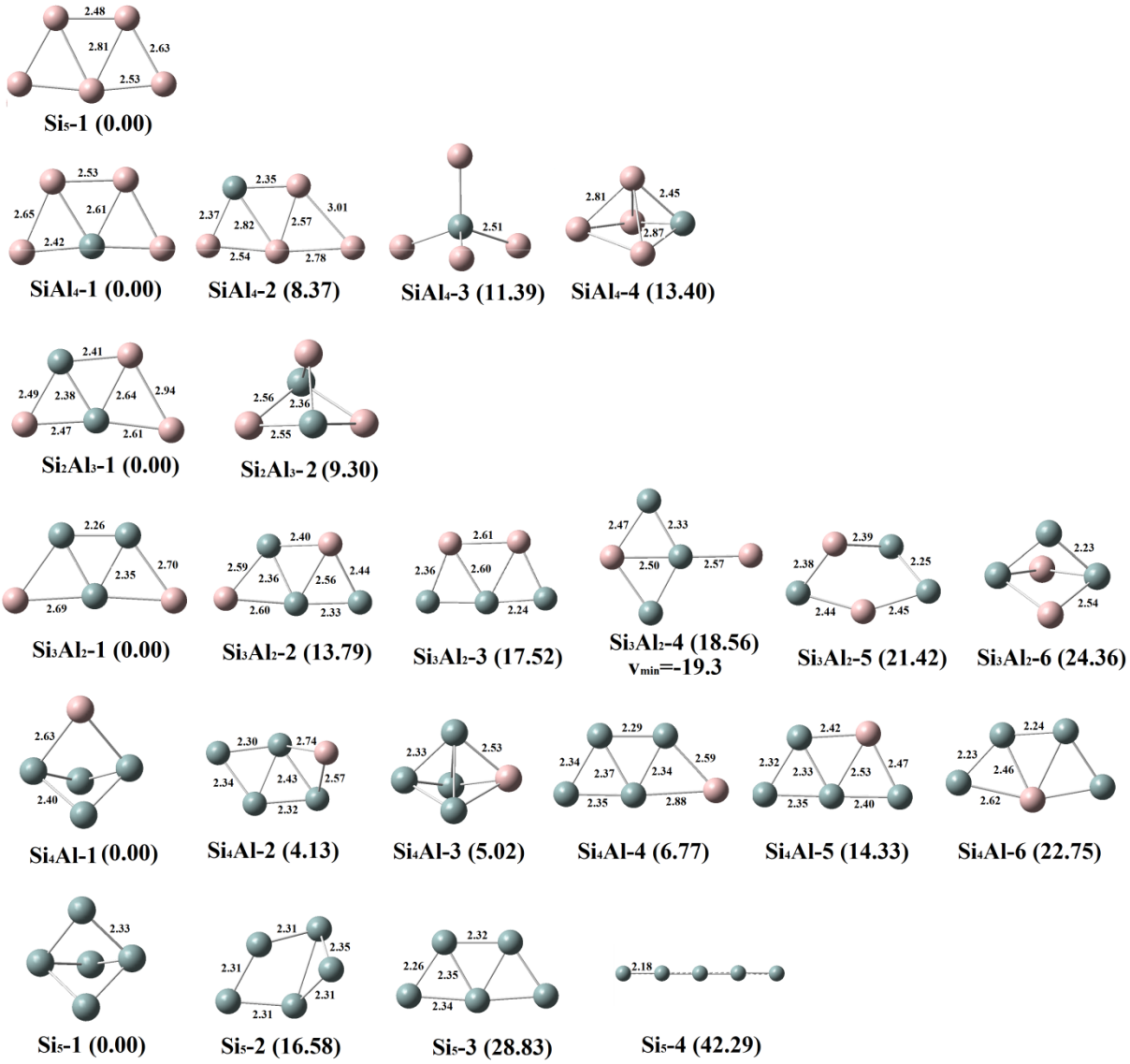

Figure S2 B3LYP-Optimized geometries of Si_nAl_{5-n} (n=0-5) clusters. The relative energies calculated at CCSD(T)/6-311+G(2d) level are shown in bracket. Bond length and relative energy are presented in the units of Å and kcal/mol.

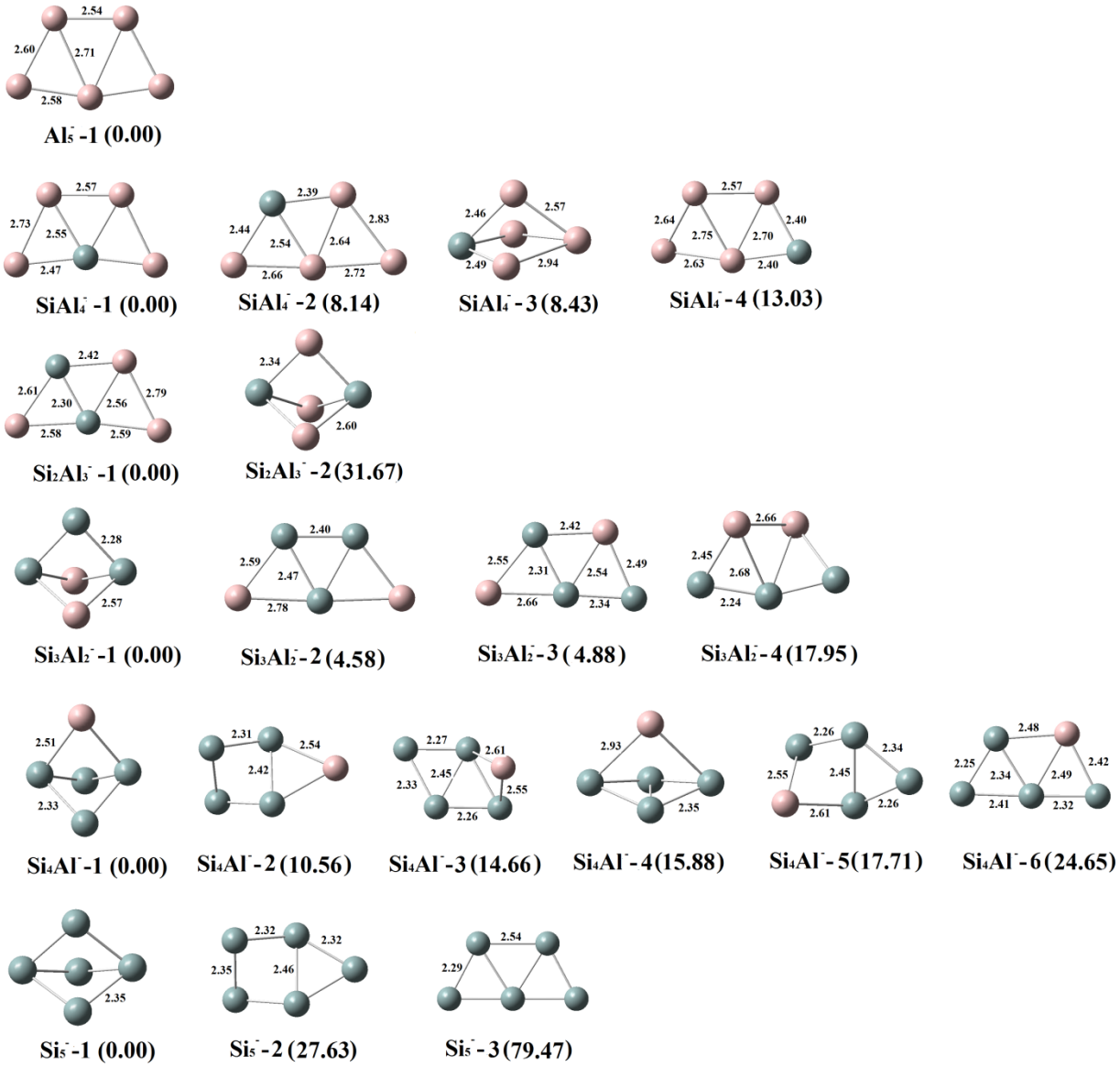

Figure S3 B3LYP-Optimized geometries of $Si_nAl_{5-n}^-$ (n=0-5) clusters. The relative energies calculated at CCSD(T)/6-311+G(2d) level are shown in bracket. Bond length and relative energy are presented in the units of Å and kcal/mol.