

Electronic Supplementary Information for:

**Theoretical characterization of a series of N₅-based aromatic
hyperhalogen anions**

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Fig. S1 The HOMO orbital energies of N_5^- and $M(N_5)_{k+1}^-$ ($M = \text{Li, Be, and B}$) anions.

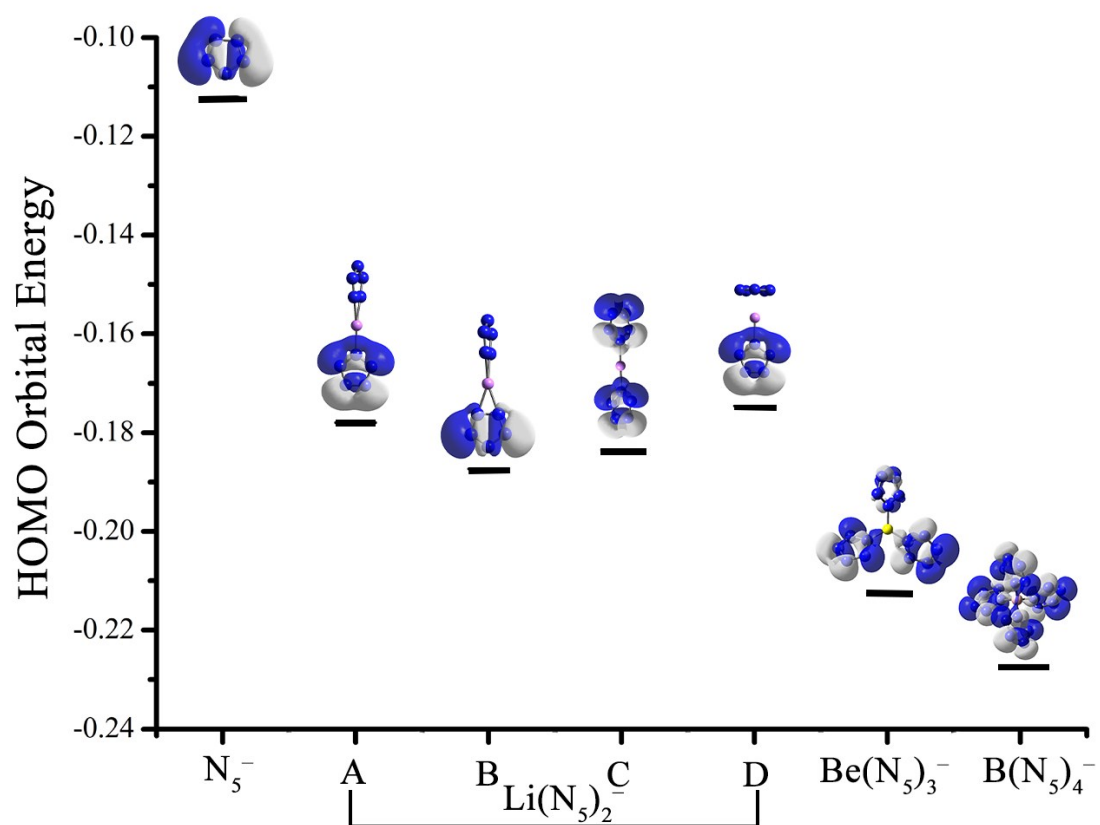


Fig. S2. Equilibrium structures of the $M(N_5)_k$ ($M = \text{Li}, \text{Be}, \text{and B}$) and $M_2(N_5)_{2k}$ ($M = \text{Li and Be}$) clusters at the B3LYP/6-311+G(3df) level.

