Supplementary Information for:

## Structures and Properties of CoB<sub>19</sub><sup>+/0/-</sup> Clusters

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**Figure S1.** Low-lying isomers and relative energies of  $CoB_{19}^+$  clusters. For the first ten isomers, the first line is the relative energies at the level of CCSD(T)/Co/Stuttgart/B/cc-pVTZ level.

**Figure S2.** Low-lying isomers and relative energies of  $CoB_{19}$  clusters. For the first ten isomers, the first line is the relative energies at the level of CCSD(T)/Co/Stuttgart/B/cc-pVTZ level.

**Figure S3.** Low-lying isomers and relative energies of  $CoB_{19}^-$  clusters. For the first ten isomers, the first line is the relative energies at the level of CCSD(T)/Co/Stuttgart/B/cc-pVTZ level.





