Supporting Information

for

Exploitation of Baird aromaticity and Clar's rule for tuning the triplet energies of polycyclic aromatic hydrocarbons

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List of Figures

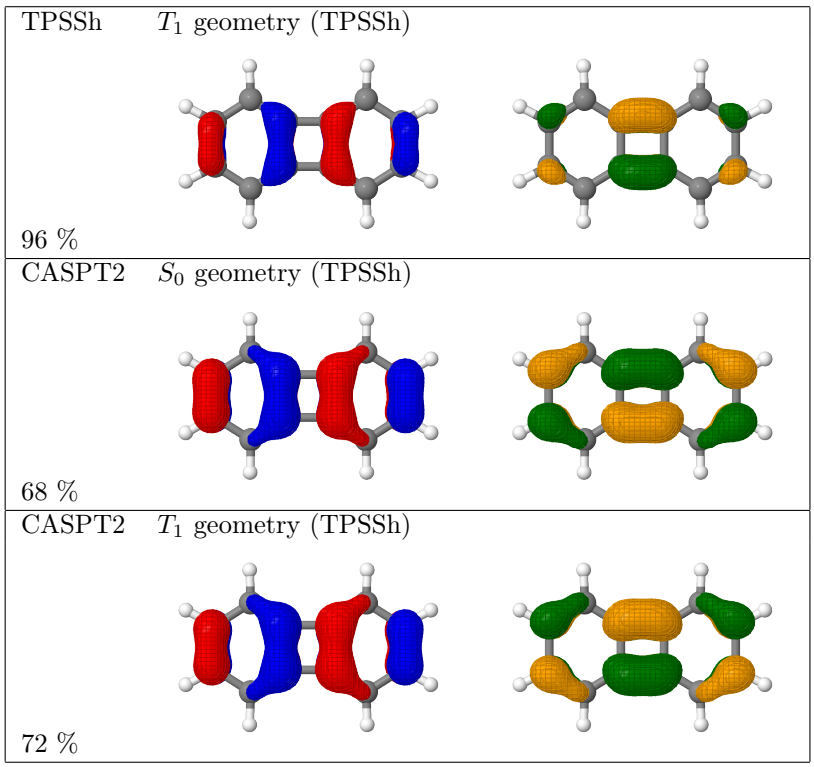

Figure S1: Natural transition orbitals of **2** for different computational methods and geometries.

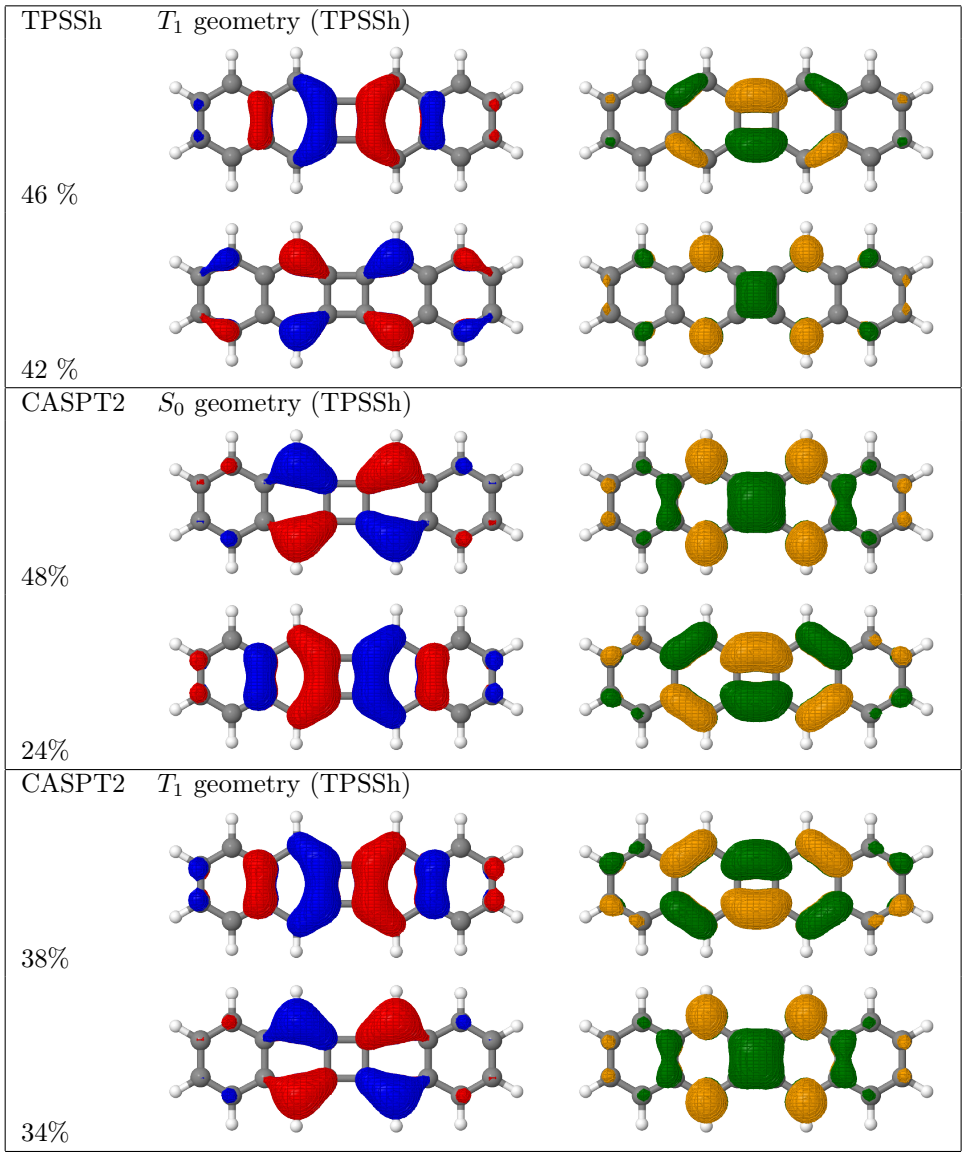

Figure S2: Natural transition orbitals of **3** for different computational methods and geometries.

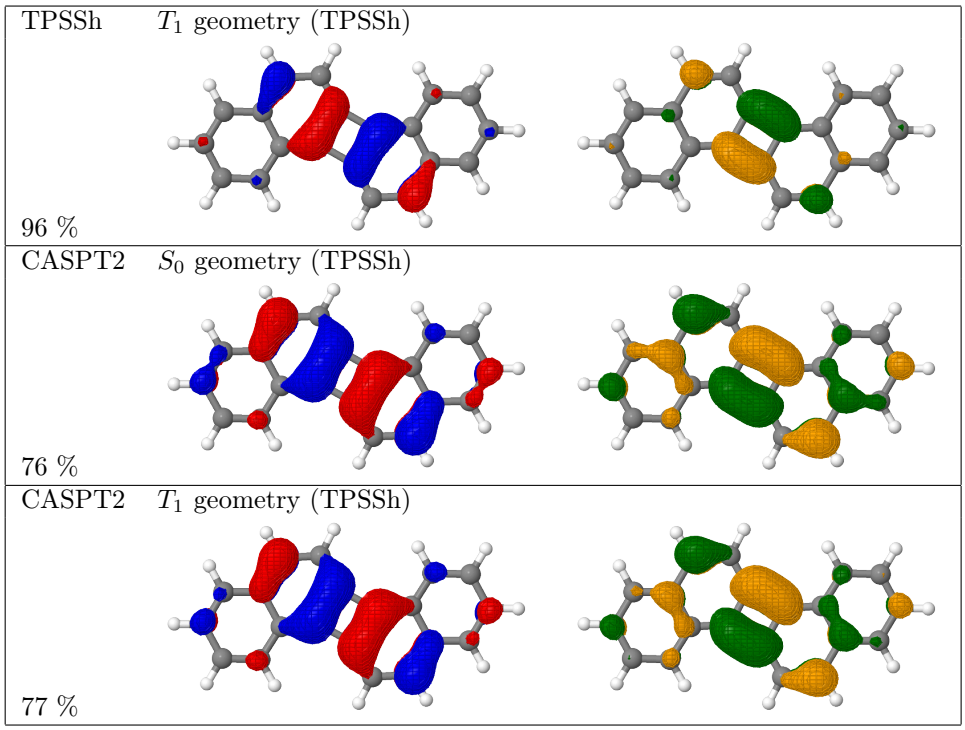

Figure S3: Natural transition orbitals of **4** for different computational methods and geometries.

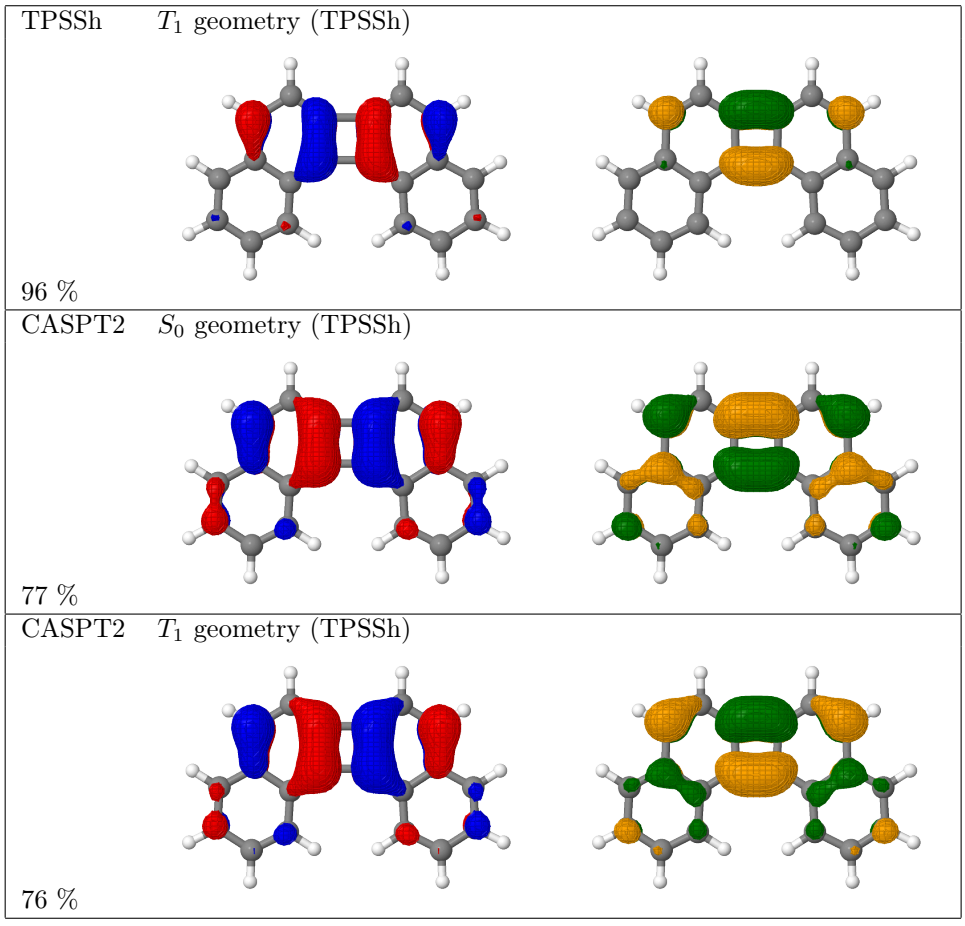

Figure S4: Natural transition orbitals of **5** for different computational methods and geometries.

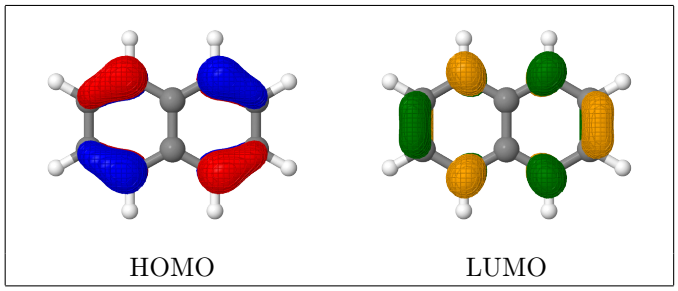

Figure S5: Frontier orbitals of naphthalene computed at the Hartree-Fock level of theory.