Electronic Supplementary Information

The pseudo-π model of the Induced Magnetic Field: Fast and Accurate Visualization of Shielding and Deshielding Cones in Planar Conjugated Hydrocarbons and Spherical Fullerenes

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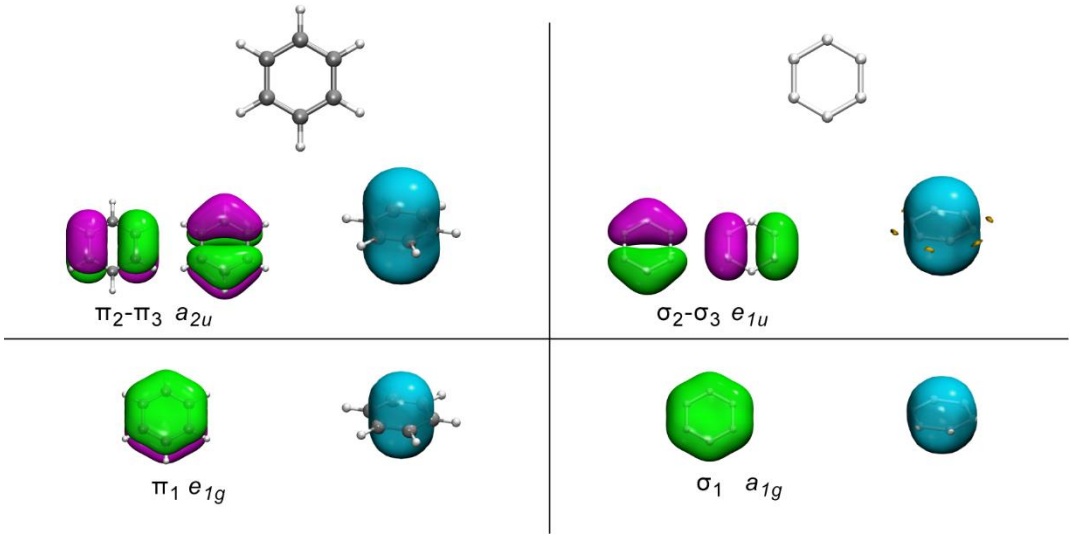

Figure S1. Canonical MOs and their contributions to B_z^{ind} of benzene (PBE/TZ2P) and its hydrogen skeletal model (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.

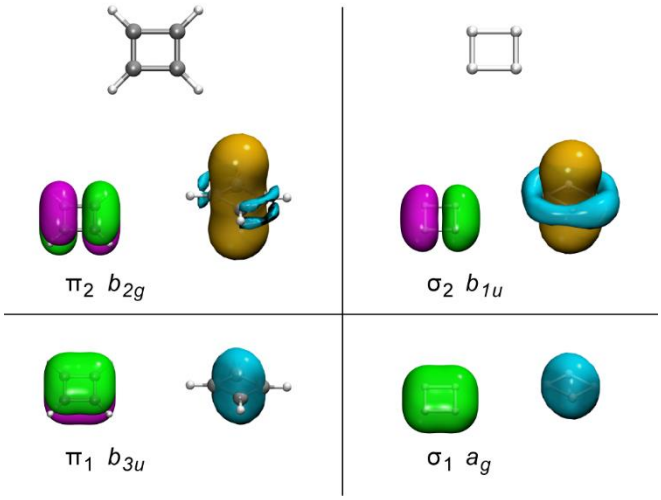

Figure S2. Canonical MOs and their contributions to B_z^{ind} of cyclobutadiene (PBE/TZ2P) and its hydrogen skeletal model (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.

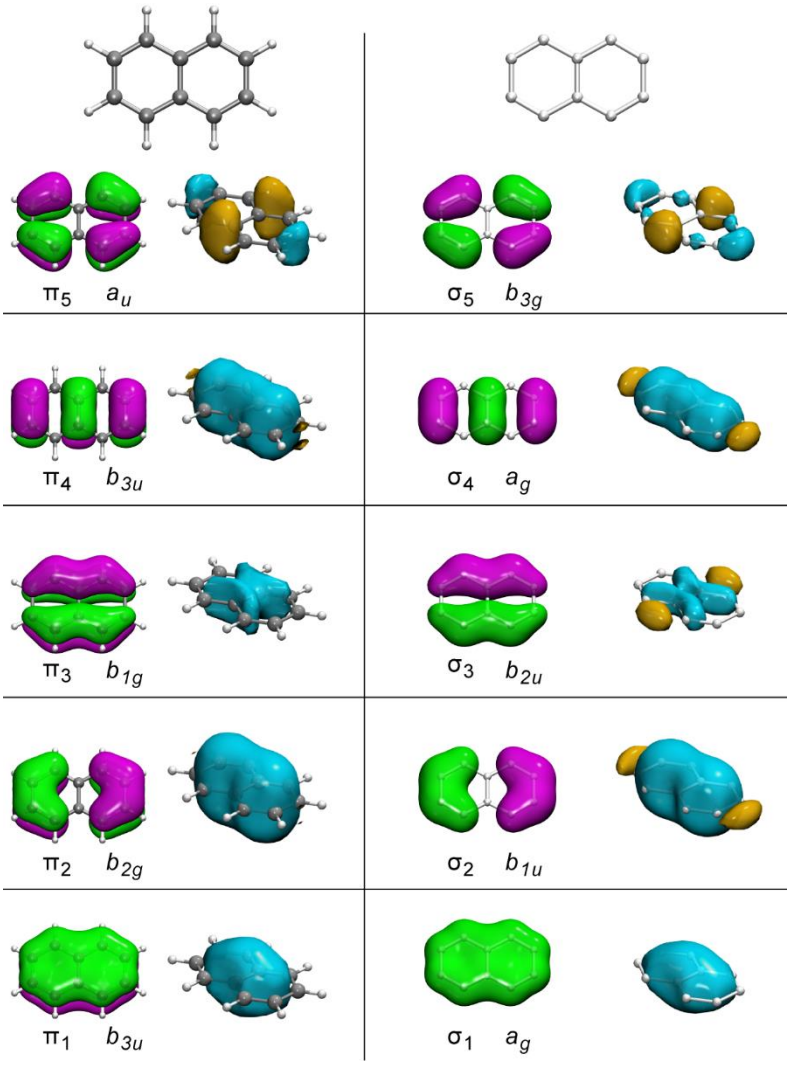

Figure S3. Canonical MOs and their contributions to B_z^{ind} of naphthalene (PBE/TZ2P) and its hydrogen skeletal model (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.

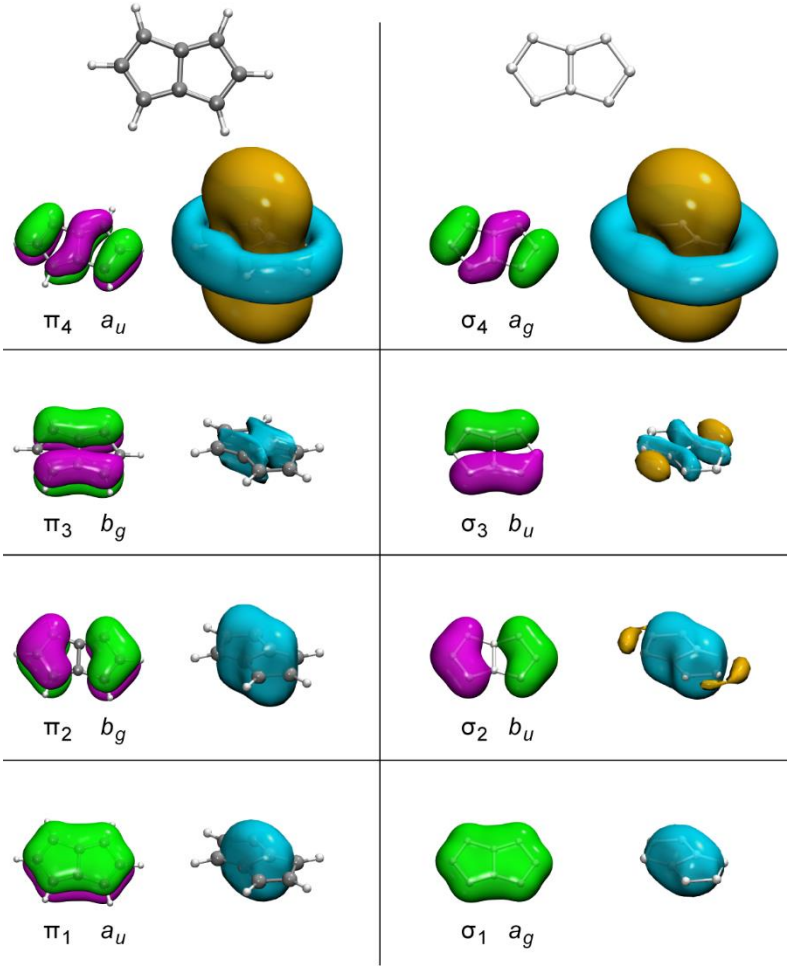

Figure S4. Canonical MOs and their contributions to B_z^{ind} of pentalene (PBE/TZ2P) and its hydrogen skeletal model (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.

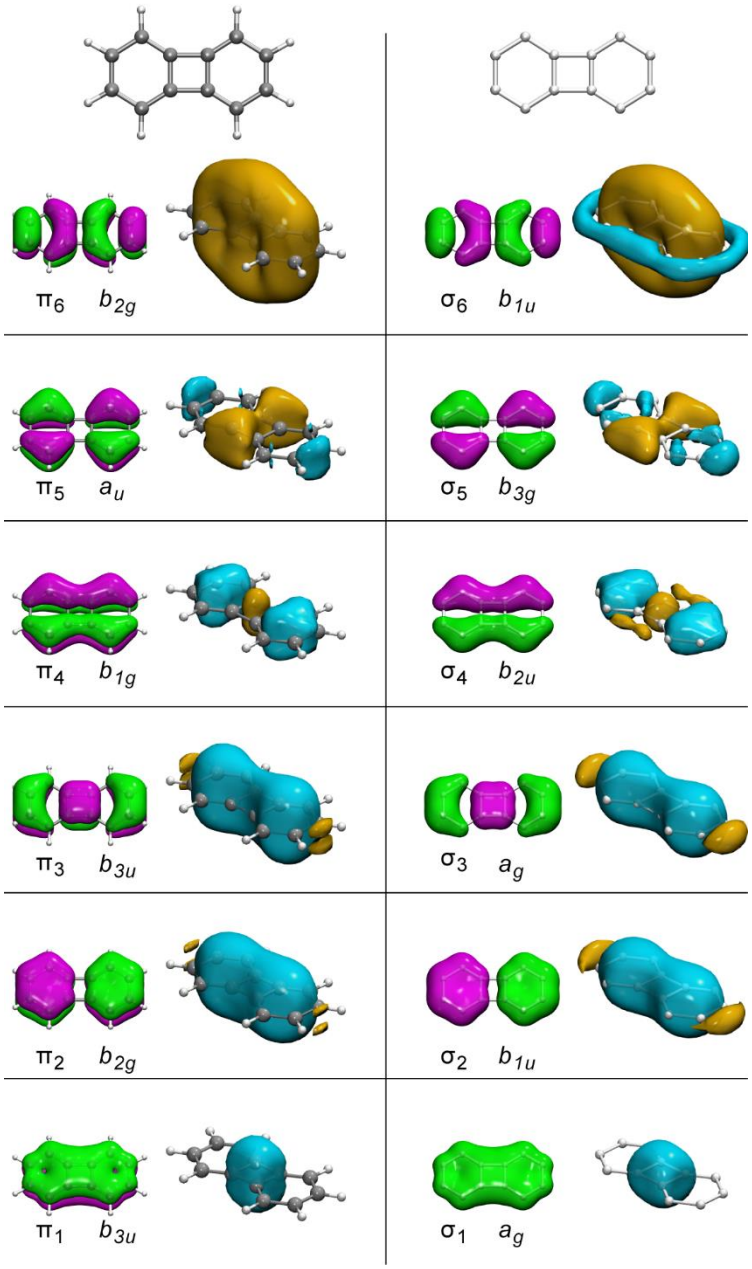

Figure S5. Canonical MOs and their contributions to B_z^{ind} of biphenylene (PBE/TZ2P) and its hydrogen skeletal model (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.

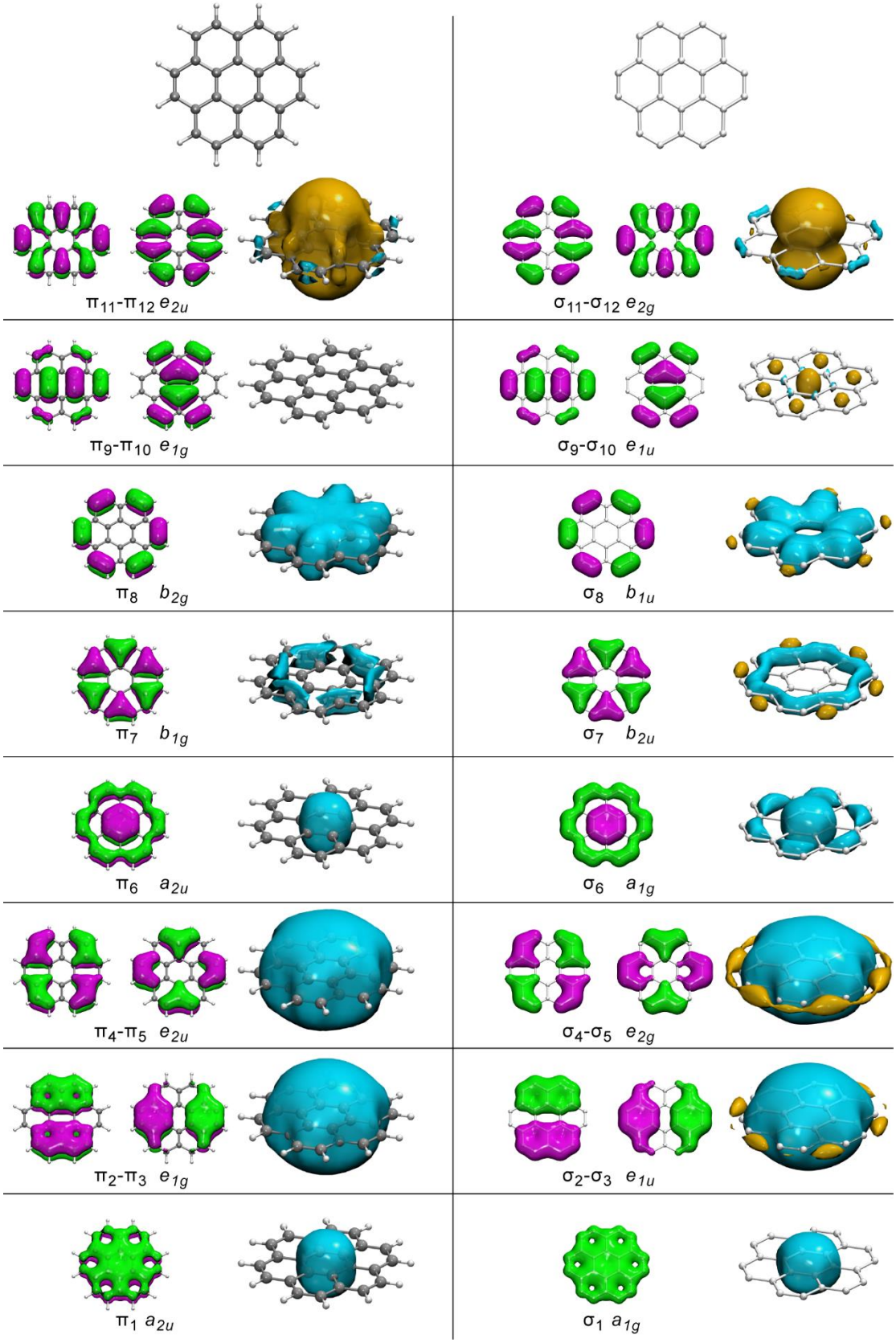

Figure S6. Canonical MOs and their contributions to B_z^{ind} of coronene (PBE/TZ2P) and its hydrogen skeletal model (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.

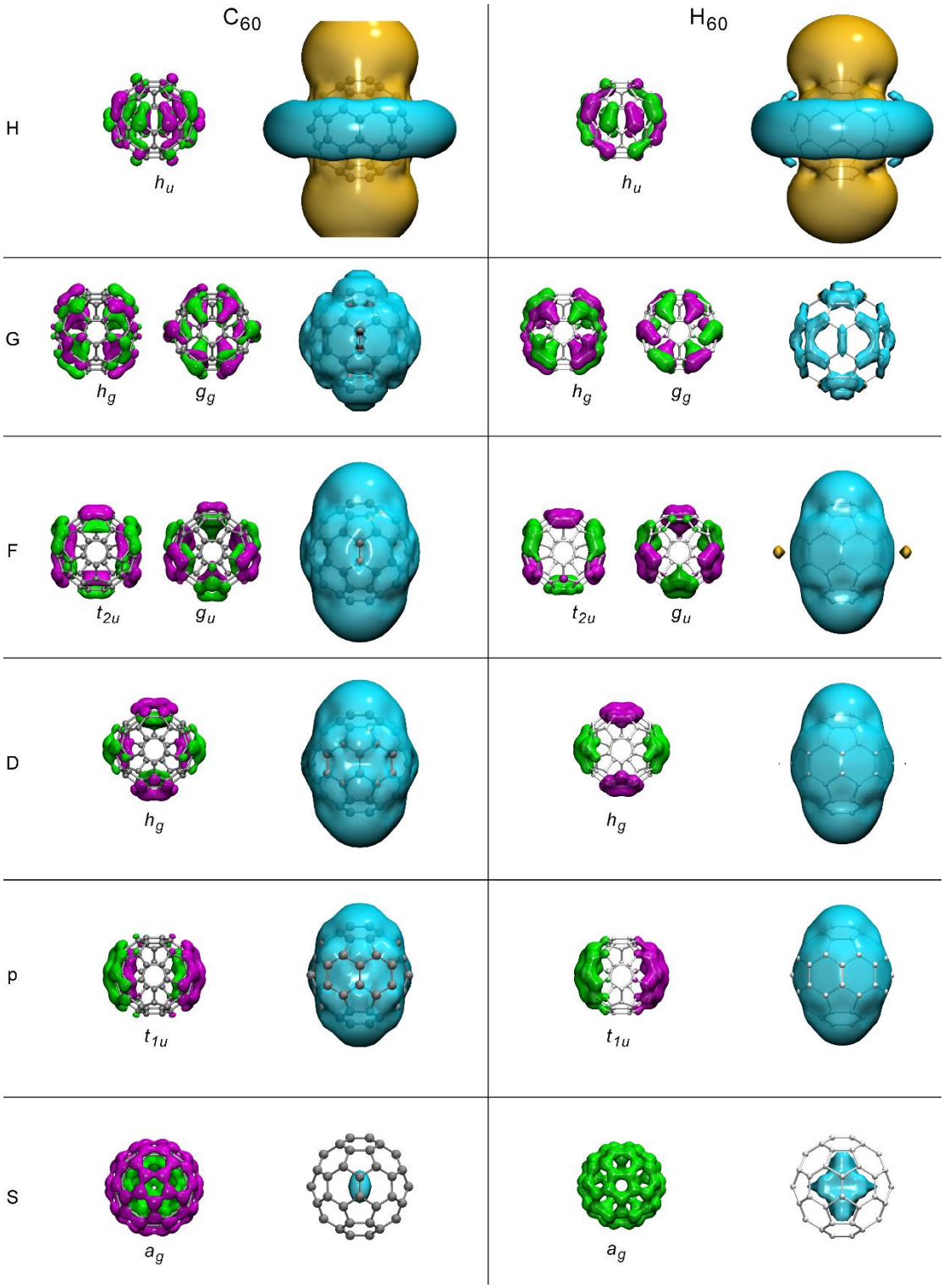

Figure S7. Representative MOs of spherical shells and contributions of each spherical shell to B_z^{ind} of C_{60} (PBE/DZP) and its hydrogen skeletal model H_{60} (PBE/SZ). Cyan/orange isosurface at -/+ 5 ppm.