Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Double aromaticity of B_{40} Fullerene: Induced magnetic field analysis of π and σ delocalization in boron cavernous structure

Nickolas D. Charistos[a] and Alvaro Muñoz-Castro[b]

[a]Aristotle University of Thessaloniki, Department of Chemistry, Laboratory of Quantum and Computational Chemistry, Thessaloniki, Greece, 54 124.

[b]Laboratorio de Química Inorgánica y Materiales Moleculares, Universidad Autonoma de Chile, Llano Subercaceaux 2801, San Miguel, Santiago, Chile.

Contents

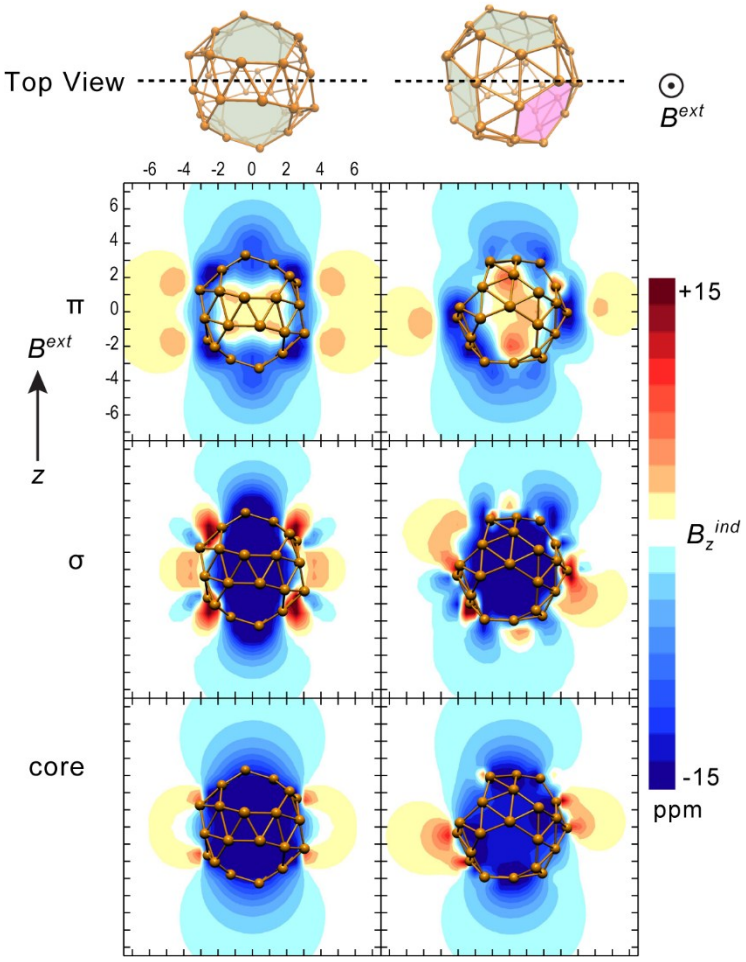

Figure S1. Contour maps of total, π, σ and core contributions to the induced magnetic field of B_{40} fullerene under two different orientations. Left: the magnetic field is applied along the non-principal C_2 rotational axis; Right: the magnetic field is applied perpendicular to a B_6 unit.

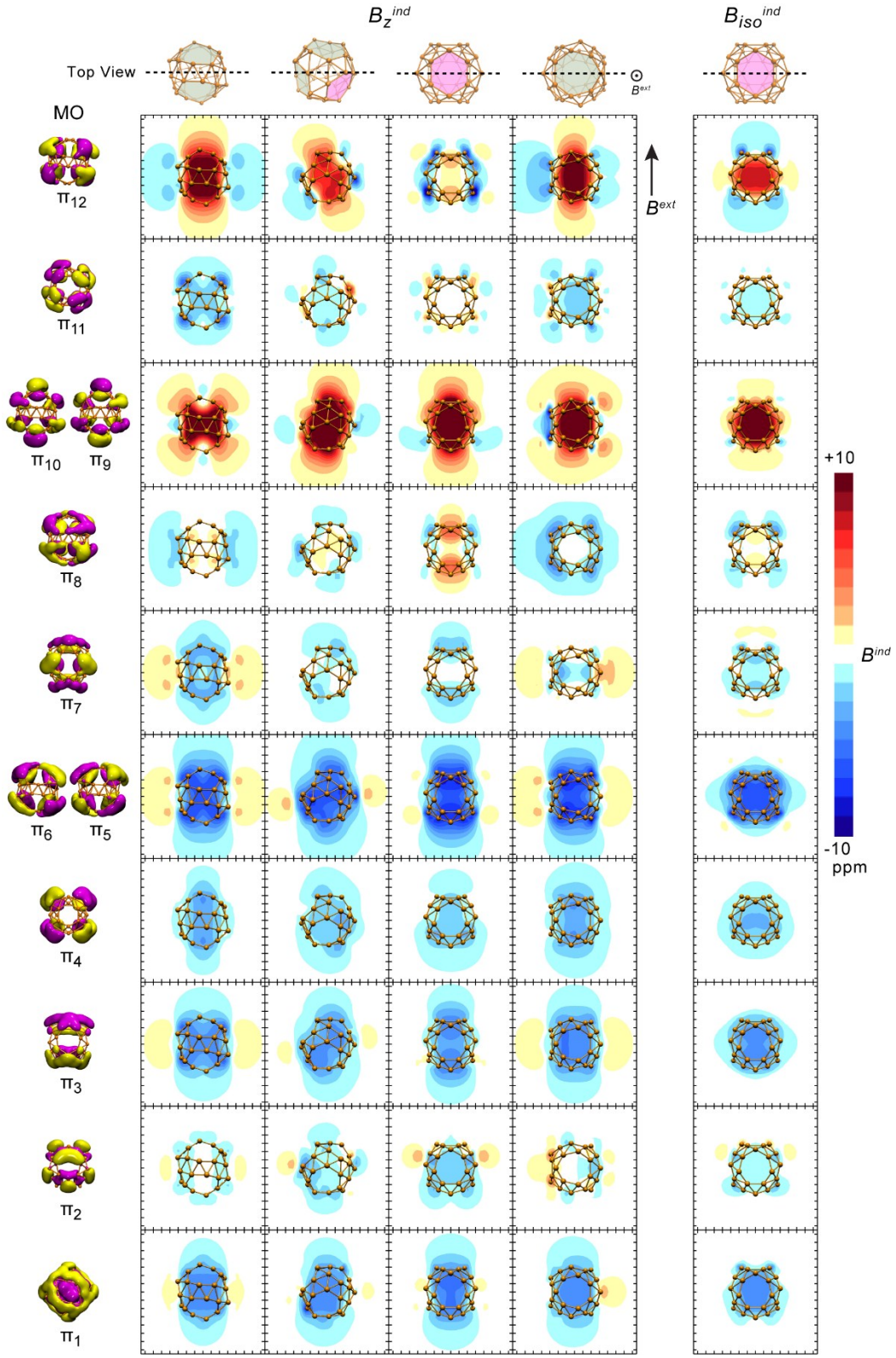

Figure S2. π-type orbitals of B_{40} fullerene and their corresponding maps of CMO contributions to the induced magnetic field under four different orientations (left) and their orientational averaged response (right).

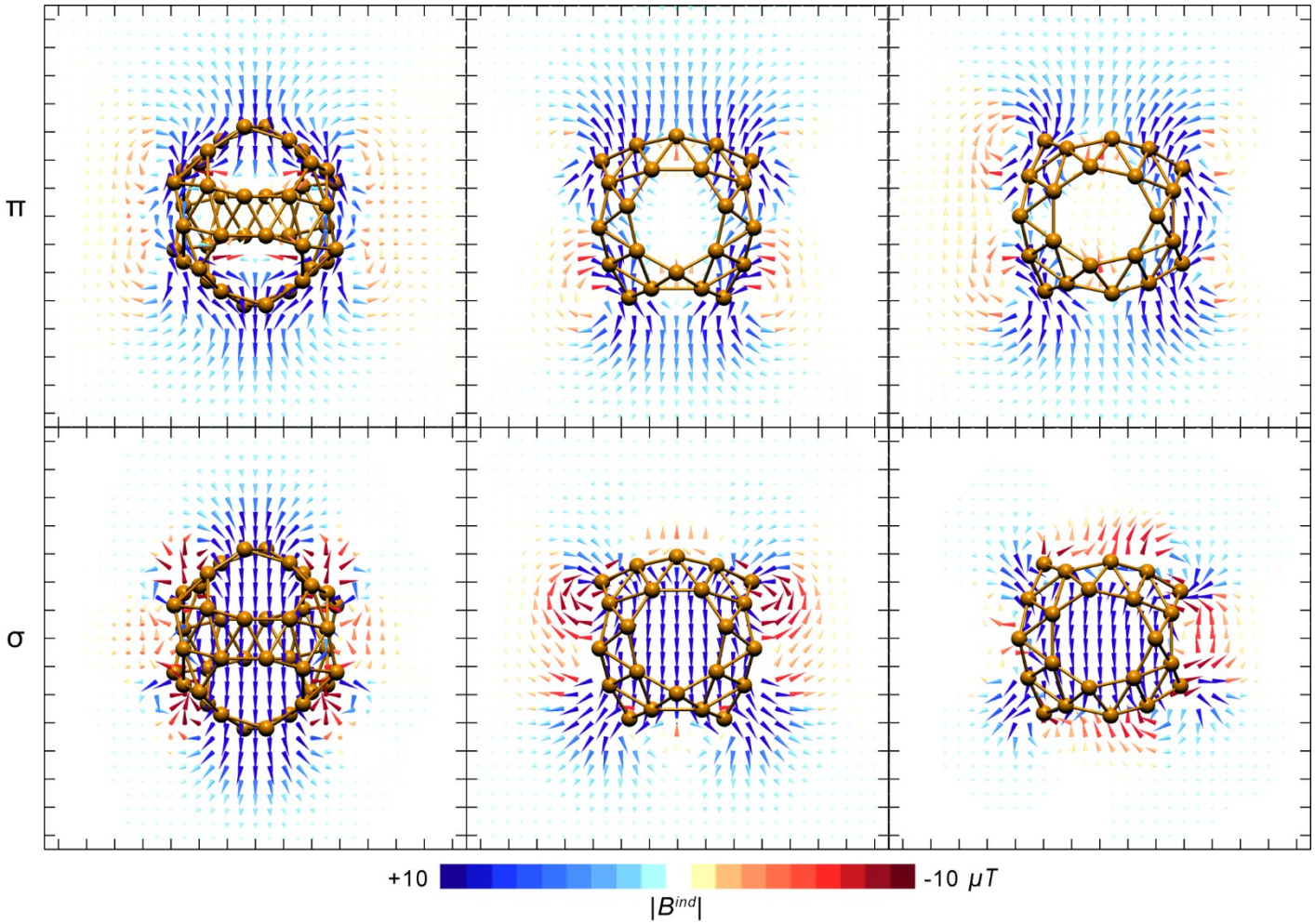

Figure S3. Field lines of the magnetic field induced by the π and σ sets of orbitals of B_{40} fullerene. The external field is applied upwards. Blue vectors denote shielding (downwards) response and red vectors denote deshielding (upwards) response. Color scale represents the magnitude of induced field $|B_{\pi}^{ind}|$ in μTesla.

Table S1. Total and dissected $NICS_{zz}$ values (ppm) of unique B_3 triangles 1 Å above the cage surface

B_3*	Total	π	σ	Core
a	-32.5	-11.2	-11.6	-9.7
b	-30.1	-11.1	-9.2	-9.8
c	-14.4	-5.7	2.8	-11.4
d	-21.6	-6.7	-4.6	-10.3
e	-34.6	-9.6	-15.8	-9.3
f	-28.7	-8.3	-10.6	-9.8
g	-34.1	-9.0	-15.5	-9.5

*B_3 labelling as in Figure 1.

Table S2. Total and dissected $NICS_{zz}$ values (ppm) of unique B_3 triangles 1 Å below the cage surface

B_3*	Total	π	σ	Core
a	-52.1	-8.4	-24.7	-18.9
b	-45.9	-2.9	-23.8	-19.1
c	-39.2	5.9	-25.4	-19.8
d	-41.6	1.9	-24.0	-19.5
e	-51.6	-5.8	-26.9	-18.8
f	-46.4	-0.7	-26.7	-19.1
g	-53.4	-6.5	-27.9	-19.1

*B_3 labelling as in Figure 1.