

Supporting Info

# Alternation of Aromatic-Nonaromatic Rings in Belt-like Structures. Behavior of [6.8]<sub>3</sub>cyclacene in Magnetic Fields.

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1) Figure S1. Comparison of the induced magnetic field for [6,8]<sub>3</sub>cyclacene (**1**), Cyclooctadiene (COT) and Benzene (Bz).

2) Optimized geometry for [6,8]<sub>3</sub>cyclacene in Å.

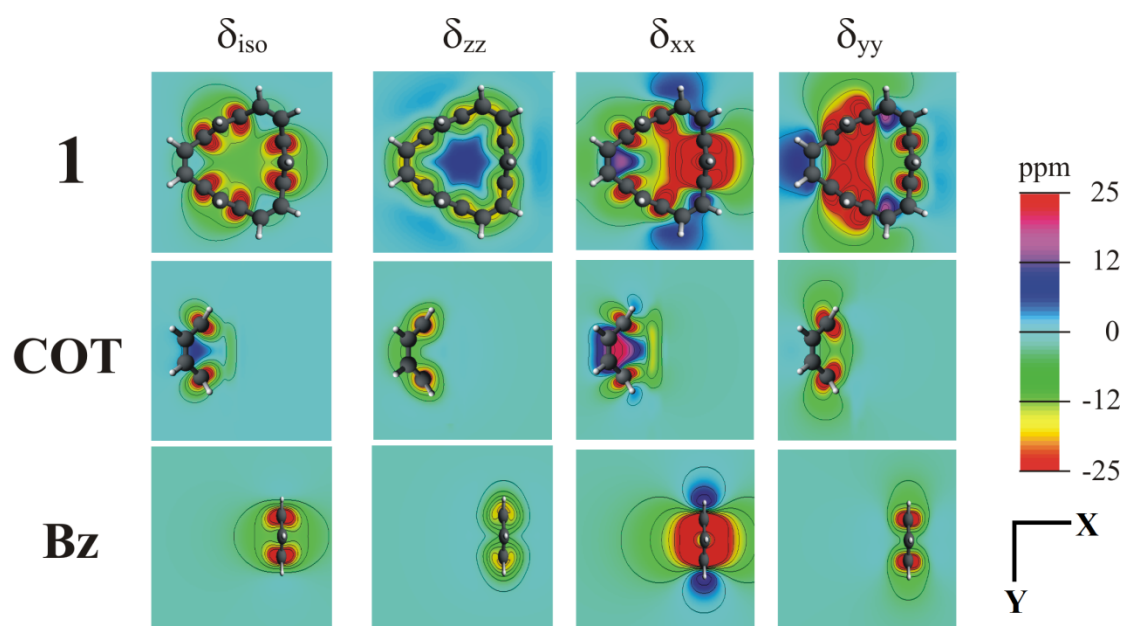


Figure S1. Comparison of the induced magnetic field for [6,8]<sub>3</sub>cyclacene (**1**), Cyclooctadiene (COT) and Benzene (Bz).

Optimized geometry for [6,8]<sub>3</sub>cyclacene in Å.

0 imaginary Freqs. Smaller vibrational mode at 86.5 cm<sup>-1</sup>.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.262315 | 1.468365  | -0.704919 |
| C | -1.237775 | 2.143889  | -1.379202 |
| H | -1.232349 | 2.134492  | -2.470409 |
| C | -0.140483 | 2.693405  | -0.704919 |
| C | -0.140483 | 2.693405  | 0.704919  |
| C | -1.237775 | 2.143889  | 1.379202  |
| H | -1.232349 | 2.134492  | 2.470409  |
| C | -2.262315 | 1.468365  | 0.704919  |
| C | 1.035862  | 3.136098  | -1.498422 |
| H | 0.907982  | 3.990491  | -2.167593 |
| C | 2.198009  | 2.465132  | -1.498422 |
| H | 3.001876  | 2.781581  | -2.167593 |
| C | 1.035862  | 3.136098  | 1.498422  |
| H | 0.907982  | 3.990491  | 2.167593  |
| C | 2.198009  | 2.465132  | 1.498422  |
| H | 3.001876  | 2.781581  | 2.167593  |
| C | 2.402799  | 1.225040  | -0.704919 |
| C | 2.475550  | 0.000000  | -1.379202 |
| H | 2.464699  | 0.000000  | -2.470409 |
| C | 2.402799  | -1.225040 | -0.704919 |
| C | 2.402799  | -1.225040 | 0.704919  |
| C | 2.475550  | 0.000000  | 1.379202  |
| H | 2.464699  | 0.000000  | 2.470409  |
| C | 2.402799  | 1.225040  | 0.704919  |
| C | 2.198009  | -2.465132 | -1.498422 |
| H | 3.001876  | -2.781581 | -2.167593 |
| C | 1.035862  | -3.136098 | -1.498422 |
| H | 0.907982  | -3.990491 | -2.167593 |
| C | 2.198009  | -2.465132 | 1.498422  |
| H | 3.001876  | -2.781581 | 2.167593  |
| C | 1.035862  | -3.136098 | 1.498422  |
| H | 0.907982  | -3.990491 | 2.167593  |
| C | -0.140483 | -2.693405 | -0.704919 |
| C | -1.237775 | -2.143889 | -1.379202 |
| H | -1.232349 | -2.134492 | -2.470409 |
| C | -2.262315 | -1.468365 | -0.704919 |
| C | -2.262315 | -1.468365 | 0.704919  |
| C | -1.237775 | -2.143889 | 1.379202  |
| H | -1.232349 | -2.134492 | 2.470409  |
| C | -0.140483 | -2.693405 | 0.704919  |
| C | -3.233871 | -0.670966 | -1.498422 |
| H | -3.909858 | -1.208910 | -2.167593 |
| C | -3.233871 | 0.670966  | -1.498422 |
| H | -3.909858 | 1.208910  | -2.167593 |
| C | -3.233871 | -0.670966 | 1.498422  |
| H | -3.909858 | -1.208910 | 2.167593  |
| C | -3.233871 | 0.670966  | 1.498422  |
| H | -3.909858 | 1.208910  | 2.167593  |