Supporting Information

Theoretical insight into the doubly antiaromatic carbon allotrope cyclo[16]carbon

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Figure S1. STM image of constant height mode of the carbon 16 above 0.7 Å of the ring plane with a bias voltage of -3.5 V. A short C-C bond is highlighted by a red arrow. The color scale is given in arbitrary unit.

Figure S2. Color-filled contour line of the STM image of the carbon 16 of constant current mode with LDOS = 0.003 au. A short C-C bond is highlighted by a red arrow. The color scale is given in Å.

Figure S3. Constant current isosurface corresponding to LDOS = 0.003 au of the carbon 16 with a bias voltage of -3.5 V. A short C-C bond is highlighted by a red arrow.
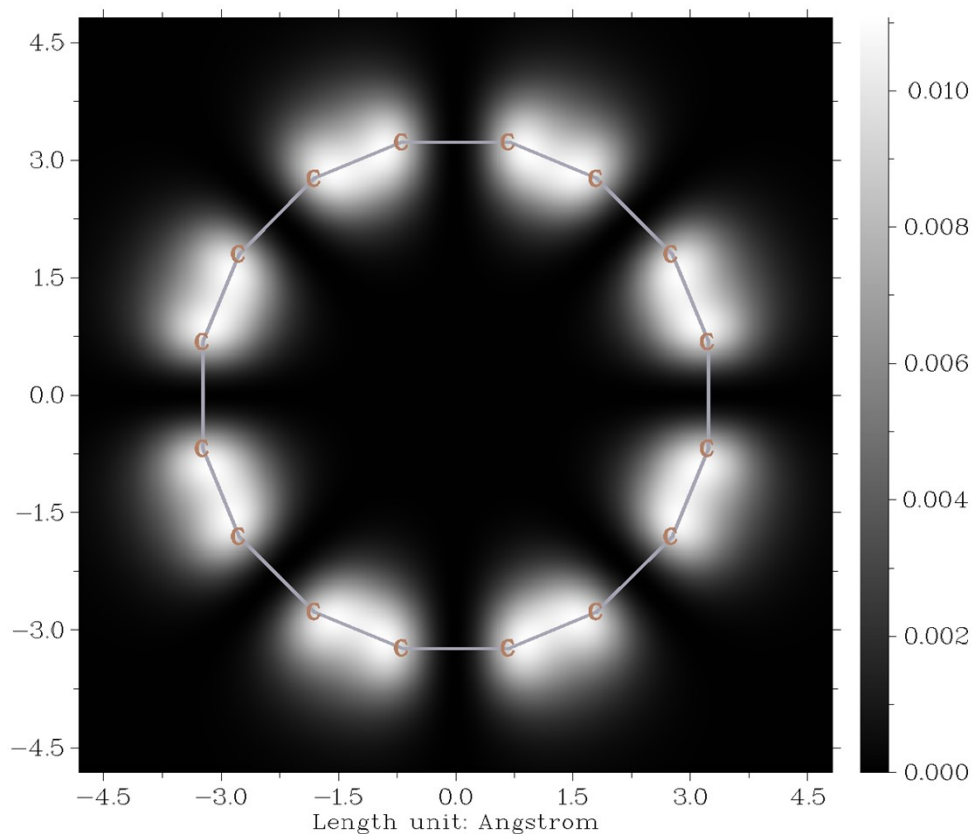
Figure S4. The isosurface of the induced magnetic field for C_{16} and C_{18}, $B_z^{ind} = \pm 8$ ppm, alongside a 1D plot illustrating the shielding values relative to the distance on either side of the C16 ring.

Table S1 Bond orders of two types of C-C bonds in C_{16} obtained using different methods.
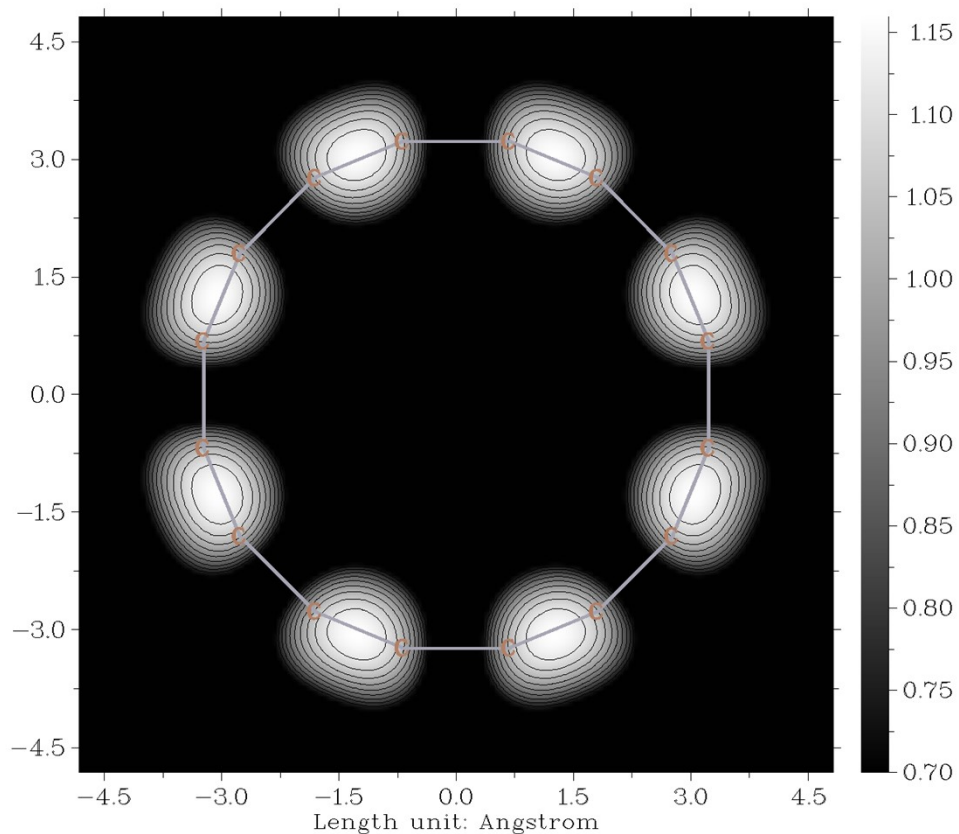
Table S2 Decomposing Mayer bond order of two types of C-C bonds in C_{16}

Table S3 The NICS(0) and NICSzz(0) of C_{16} at different level of theory.
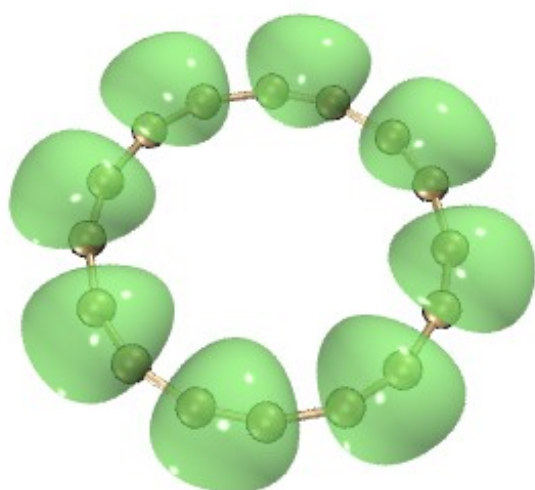
In the STM simulation, the bias voltage was set to -3.5 V. In this case, electrons flow from the carbon 16 to the STM tip, and twp highest occupied MOs (one π^{in} MOs with energy of -8.019 eV one two π^{out} MOs with energy of -8.1434 eV) contribute to the tunneling current.
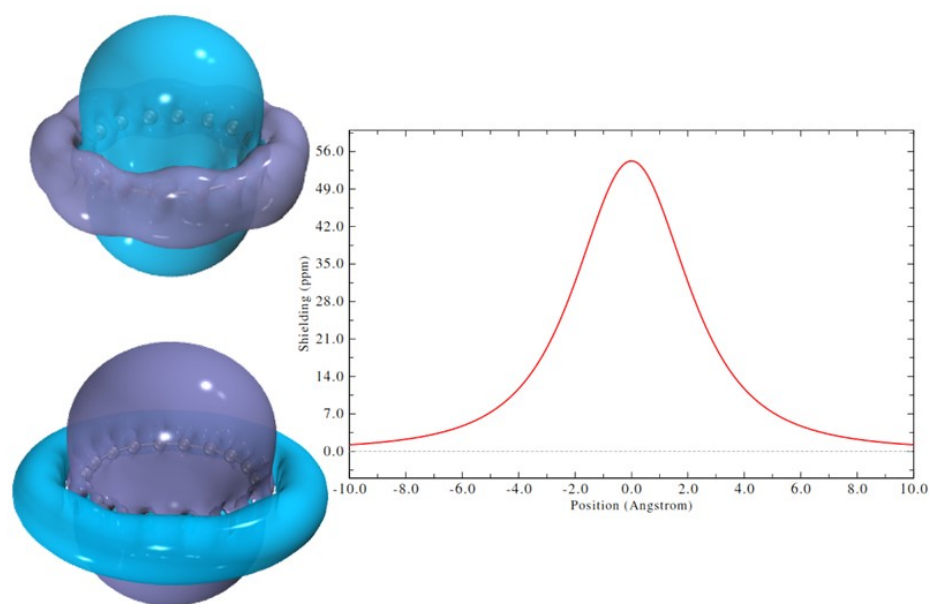

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Figure S4. The isosurface of the induced magnetic field for C_{16} and C_{18}, $B^{ind}_z = \pm 8$ ppm, alongside a 1D plot illustrating the shielding values relative to the distance on either side of the C_{16} ring.

Table S1 Bond orders of two types of C-C bonds in C_{16} obtained using different methods.

bond order	short bond	long bond	diff[a]
Mayer bond order	2.674	1.173	1.501
Fuzzy bond order	2.375	1.359	1.016
Wiberg bond order (Lowdin[b] based)	2.452	1.449	1.003
Wiberg bond order (NAO[c] based)	2.481	1.234	1.247
Laplacian bond order	2.519	1.597	0.922

[a] The bond order difference between two types of C-C bonds.
[b] Lowdin orthogonalization.
[c] Natural atomic orbitals.
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Table S2 Decomposing Mayer bond order of two types of C-C bonds in C_{16}.

MO type[a]	short bond	long bond	diff[b]
π^{in} MOs	1.398	0.113	1.285
π^{out} MOs	1.388	0.154	1.234
δ MOs	1.703	1.284	0.418
sum	4.488	1.552	2.937

[a]The indices of the π^{in} MOs are 33, 35,36, 41, 42, 45, 46, and 48. The indices of the π^{out} are 34, 37, 38, 39, 40, 43, 44, and 47. Other valence of MOs are regarded as δ MOs.
[b] The bond oder difference between two types of C-C bonds.

Table S3 The NICS(0) and NICSzz(0) of C_{16} at different level of theory.

Functional	NICS(0) (ppm)	NICSzz(0) (ppm)
TPSSH	28.4	90.3
B3LYP	25.6	81.8
HSE06	25.8	82.6
PBE0	24.7	79.1
MN15	19.8	64.4
BHandHLYP	16.7	55.3
M06-2X	17.9	58.7
wB97XD	15.8	52.2