Analysis of local and global aromaticity in Si_3C_5 and Si_4C_8 Clusters. Aromatic species containing planar tetracoordinate carbon

Juan Torres-Vega,[1] Diego R. Alcoba,[2,3] Ofelia B. Oña,[4] Alejandro Vásquez-Espinal,[5] Rodrigo Báez-Grez,[5] Luis Lain,[6] Alicia Torre,[6] Victor Garcia*[7] and William Tiznado*[5]

[1] Centro de Investigaciones Tecnológicas, Biomédicas y Medioambientales, Calle José Santos Chocano 199, Urb. San Joaquín, Callao, Perú.
[2] Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, 1428 Buenos Aires, Argentina.
[3] Instituto de Física de Buenos Aires, Consejo Nacional de Investigaciones Científicas y Técnicas, Ciudad Universitaria, 1428 Buenos Aires, Argentina.
[4] Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, Universidad Nacional de La Plata, CCT La Plata, Consejo Nacional de Investigaciones Científicas y Técnicas. Diag. 113 y 64 (S/N), Sucursal 4, CC 16, 1900 La Plata, Argentina.
[5] Computational and Theoretical Chemistry Group, Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, República 498, Santiago, Chile.
[6] Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco. Apdo. 644, E-48080 Bilbao, Spain.
[7] Departamento Académico de Fisicoquímica - Facultad de Química e Ingeniería Química, Universidad Nacional Mayor de San Marcos, Lima, Perú.

SUPPORTING INFORMATION

Table S1. Cartesian coordinates of the studied systems.

Si_3C_5				Si_4C_8			
				Si	-2.992387000	1.783878000	0.000329000
				C	-0.000002000	0.710356000	0.000006000
Si	1.734453000	1.828109000	-0.000355000	C	1.345736000	1.182177000	-0.000152000
Si	-2.939689000	-0.000020000	-0.001748000	Si	2.992386000	1.783866000	-0.000379000
Si	1.734467000	-1.828091000	-0.001028000	C	-1.345745000	1.182169000	0.000168000
C	1.001829000	0.000001000	0.000998000	C	0.000002000	-0.710352000	0.000139000
C	0.114198000	-1.169992000	0.000838000	C	-1.345733000	-1.182180000	0.000298000
C	0.114192000	1.169996000	0.001036000	Si	-2.992372000	-1.783881000	0.000282000
C	-1.243078000	-0.699136000	0.002667000	C	2.217927000	0.000009000	-0.000225000
C	-1.243084000	0.699137000	0.002657000	C	1.345741000	-1.182172000	0.000036000
				Si	2.992381000	-1.783876000	-0.000097000
				C	-2.217932000	-0.000001000	0.000331000
$Si_2C_5H_2$				$C_5H_5^-$			
C	1.159242000	0.511515000	0.001002000	C	-1.141441000	0.370987000	0.000000000
C	0.691174000	1.852859000	0.000706000	C	0.000000000	1.200061000	0.000000000
Si	1.786054000	-1.127046000	0.001912000	C	1.141370000	0.370802000	0.000000000
H	1.327680000	2.730150000	0.001179000	C	0.705386000	-0.970930000	0.000000000
C	0.000066000	-0.394592000	0.000315000	C	-0.705393000	-0.970929000	0.000000000
C	-1.159826000	0.510530000	-0.000862000	H	-2.174702000	0.707423000	0.000000000
C	-0.692922000	1.852281000	-0.001424000	H	0.000116000	2.286754000	0.000000000
Si	-1.785309000	-1.128546000	-0.000811000	H	2.174960000	0.706057000	0.000000000

H	-1.330169000	2.729036000	-0.002410000	H	1.344113000	-1.850112000	0.000000000
				H	-1.344020000	-1.850070000	0.000000000

$C_8H_6^{2-}$

C	0.000000000	0.724045000	0.000000000
C	1.366619000	1.166982000	0.000000000
C	-1.366619000	1.166982000	0.000000000
C	0.000000000	-0.724045000	0.000000000
C	-1.366619000	-1.166982000	0.000000000
C	2.185326000	0.000000000	0.000000000
C	1.366619000	-1.166982000	0.000000000
C	-2.185326000	0.000000000	0.000000000
H	1.731600000	2.195531000	0.000000000
H	3.278591000	0.000000000	0.000000000
H	1.731600000	-2.195531000	0.000000000
H	-1.731600000	2.195531000	0.000000000
H	-3.278591000	0.000000000	0.000000000
H	-1.731600000	-2.195531000	0.000000000

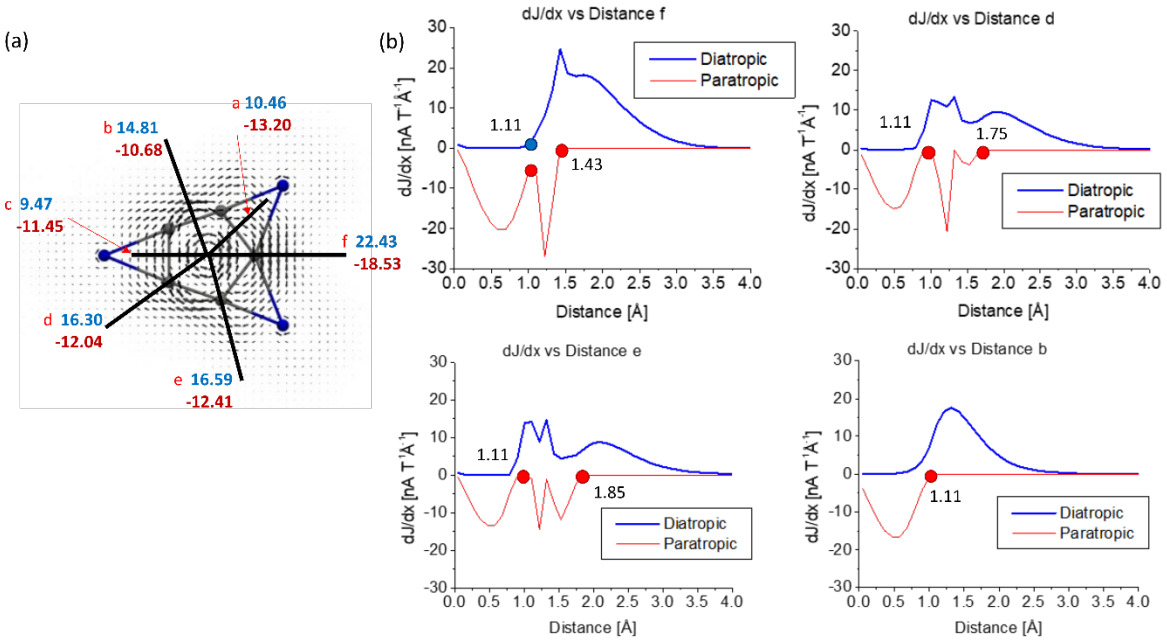

Figure S1. (a) Vector plot visualization of the current density of Si_3C_5 in a plane placed 0.5 Å above the molecular plane and top view of integration planes. (b) Integration profiles along the integration planes of Si_3C_5.

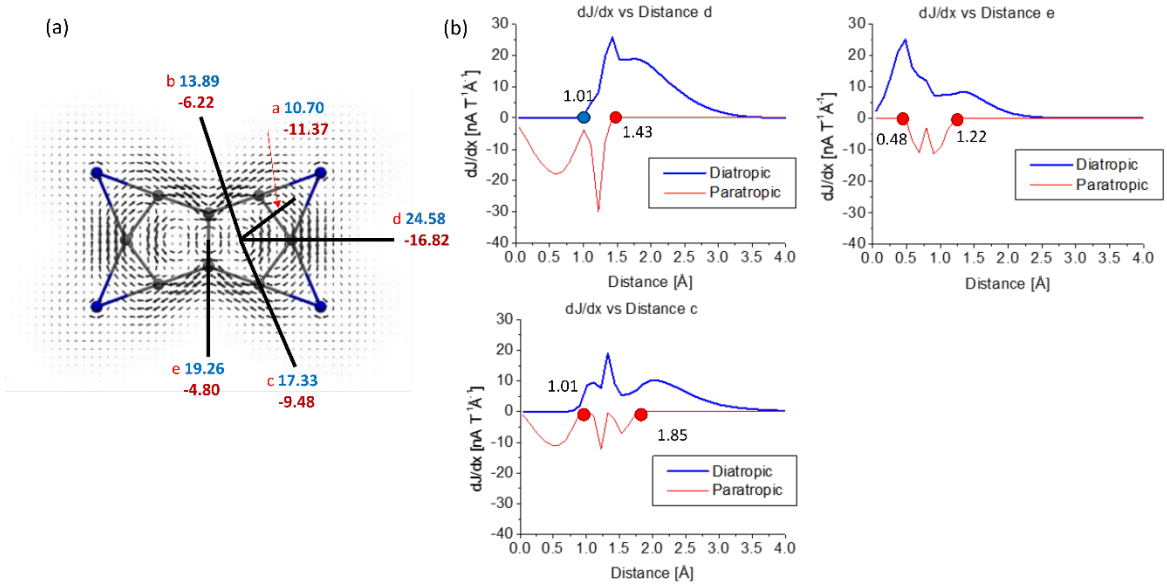

Figure S2. (a) Vector plot visualization of the current density of Si_4C_8 in a plane placed 0.5 Å above the molecular plane and top view of integration planes. (b) Integration profiles along the integration planes of Si_4C_8.

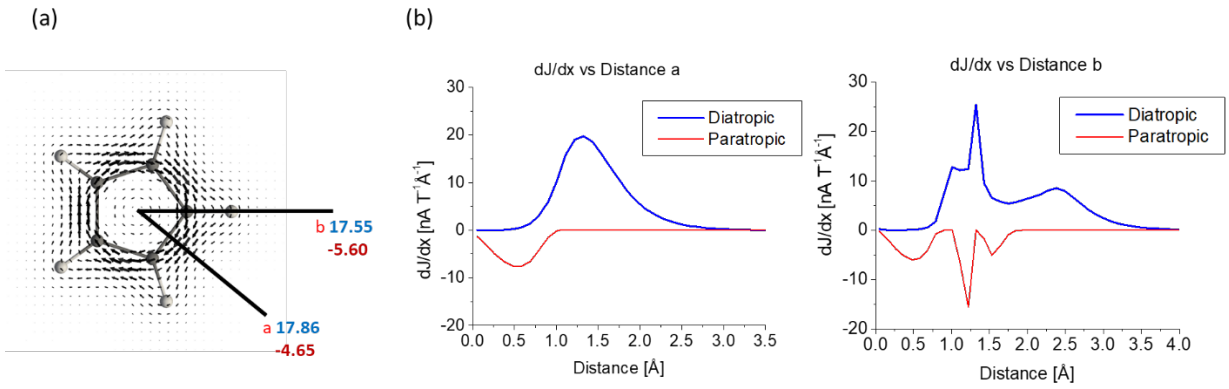

Figure S3. (a) Vector plot visualization of the current density of $C_5H_5^-$ in a plane placed 0.5 Å above the molecular plane and top view of integration planes (RCS are also reported in nA T^{-1}). (c) Integration profiles along the integration planes of $C_5H_5^-$.

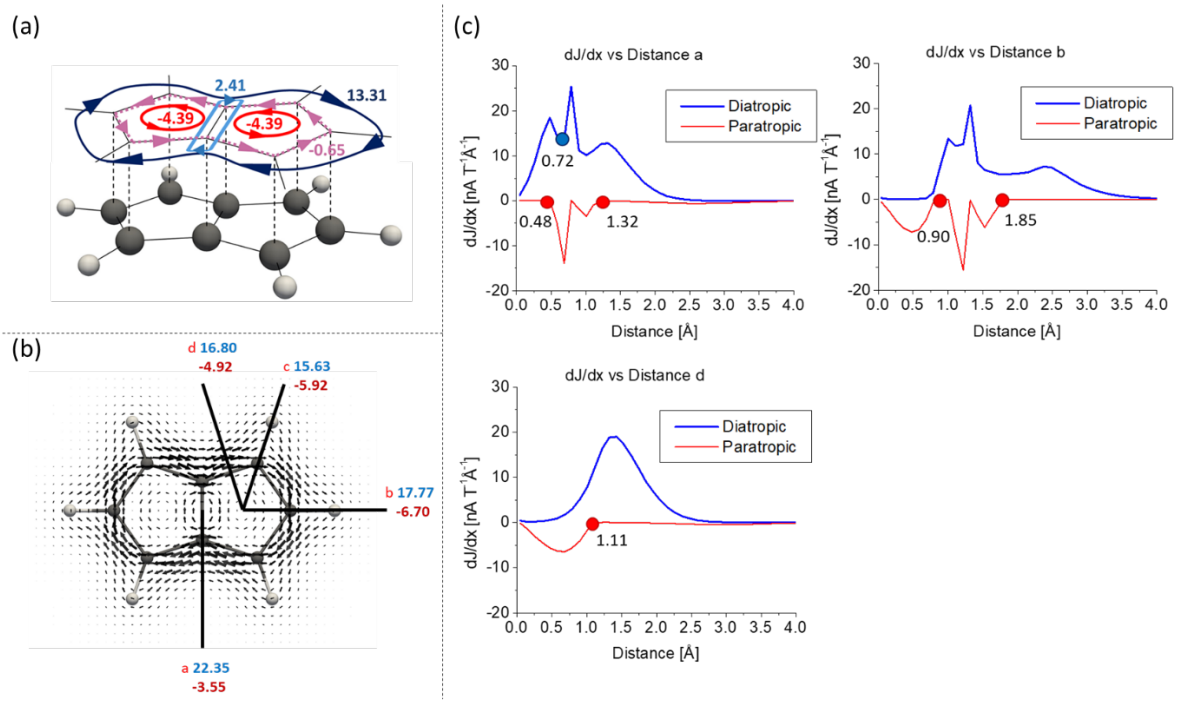

Figure S4. (a) Schematic representation of local and global currents. (b) Vector plot visualization of the current density of $C_8H_6^{2-}$ in a plane placed 0.5 Å above the molecular plane and top view of integration planes. (c) Integration profiles along the integration planes of $C_8H_6^{2-}$.

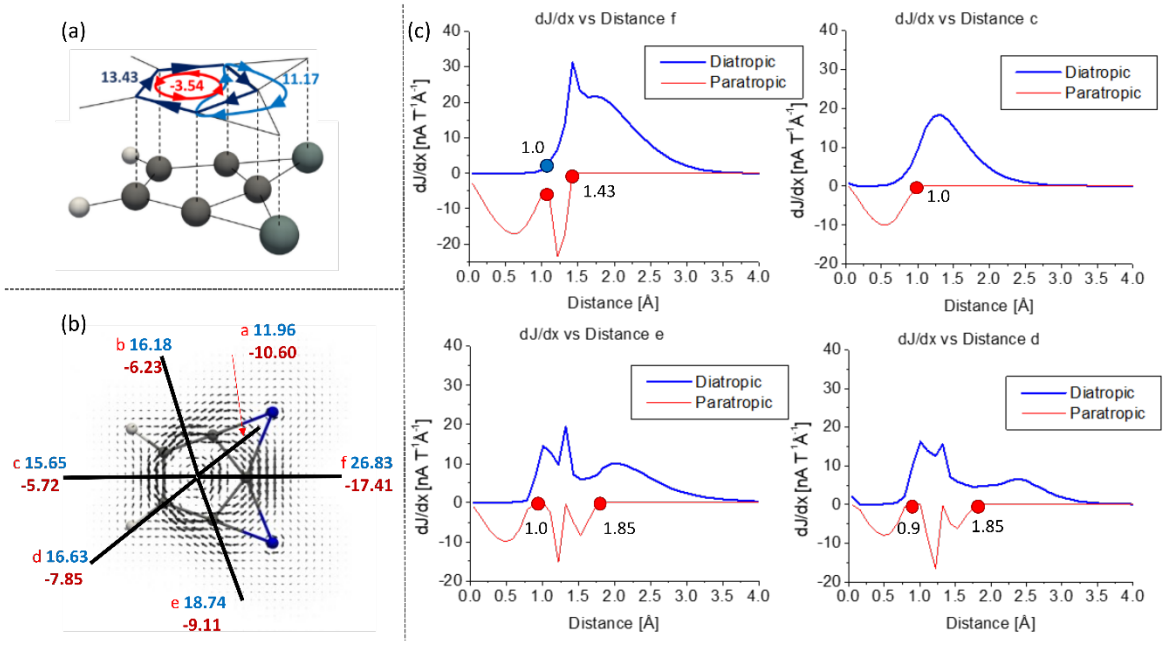

Figure S5. (a) Schematic representation of local and global currents. (b) Vector plot visualization of the current density of $Si_2C_5H_2$ in a plane placed 0.5 Å above the molecular plane and top view of integration planes. (c) Integration profiles along the integration planes of $Si_2C_5H_2$.

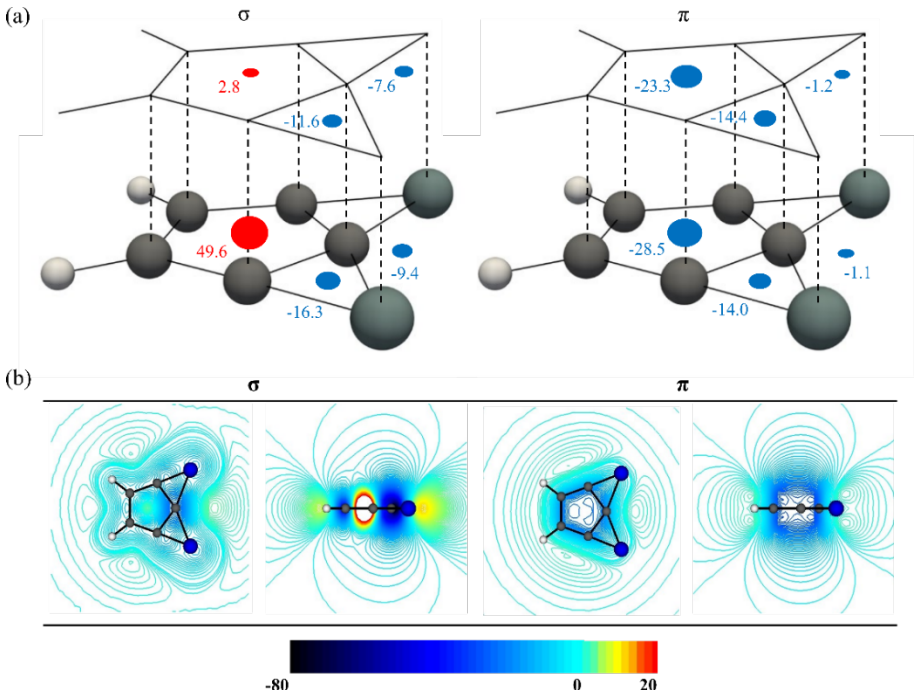

Figure S6. (a) Computed values (in ppm) of σ- and π-components (left and right sides) of $NICS_{zz}$ at and above the ring centers (local and global) of $Si_2C_5H_2$ (at the GIAO-B3LYP/6-311+G*// B3LYP/6-311+G* level). The blue/red dots denote diatropic/paratropic character, and the dot size is in line with the $NICS_{zz}$ magnitude. (b) Isolines of of the σ- and π-componentes of NICSzz for $Si_2C_5H_2$ (at the GIAO-B3LYP/6-311+G*// B3LYP/6-311+G* level). The isolines are plotted in both the molecular plane (left) and a plane perpendicular to the molecular plane (right). The color scale at the bottom is in ppm.

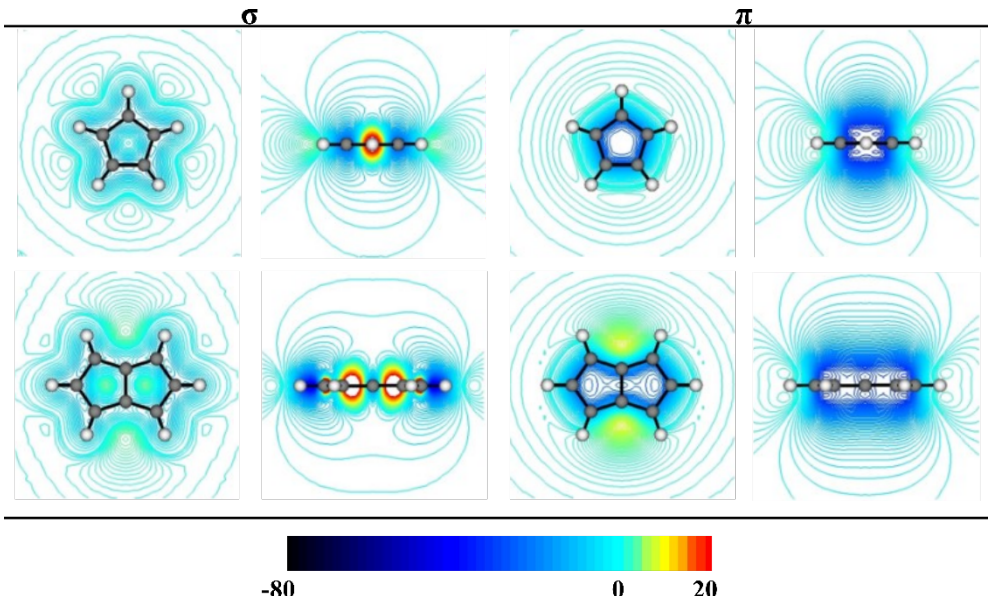

Figure S7. Isolines of of the σ- and π-components of NICSzz for both the cyclopentadienyl anion ($C_5H_5^-$) and the pentalene dianion ($C_8H_6^{2-}$) (at the GIAO-B3LYP/6-311+G*// B3LYP/6-311+G* level). The isolines are plotted in both the molecular plane (left) and a plane perpendicular to the molecular plane (right). The color scale at the bottom is in ppm.

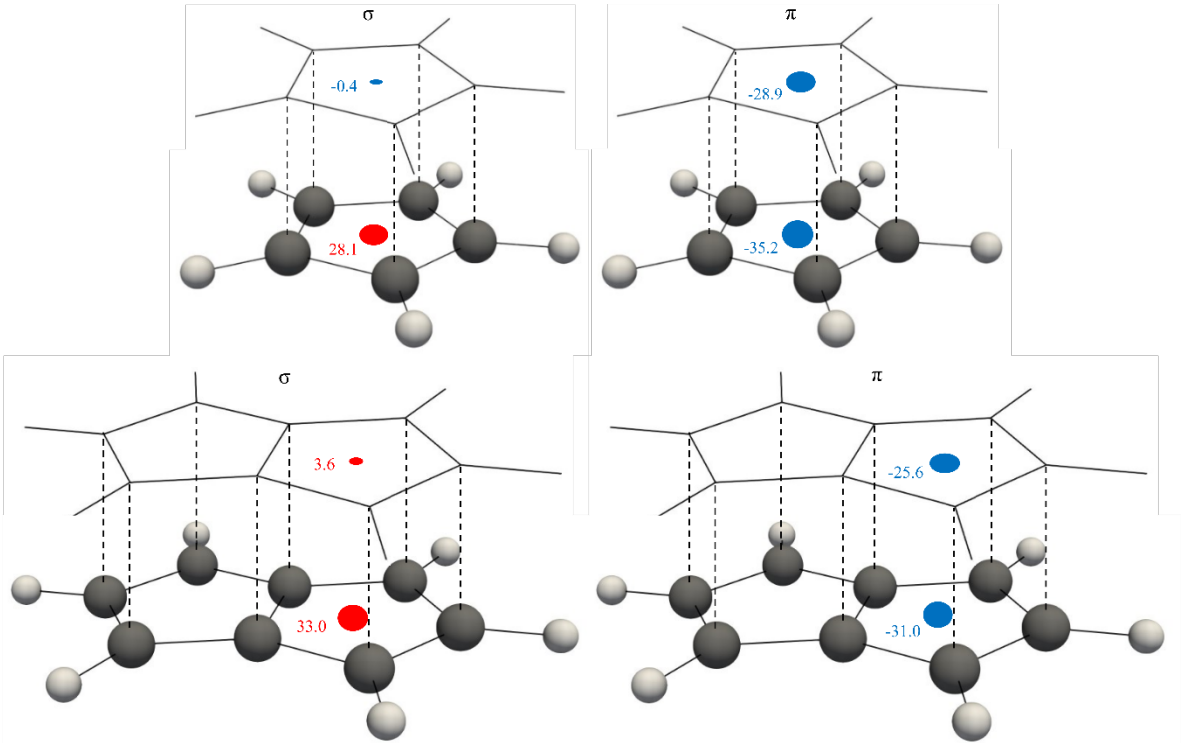

Figure S8. Computed values (in ppm) of σ- and π-components (left and right sides) of $NICS_{zz}$ at and above the ring centers (local and global) of both the cyclopentadienyl anion ($C_5H_5^-$) and the pentalene dianion ($C_8H_6^{2-}$) (at the GIAO-B3LYP/6-311+G*// B3LYP/6-311+G* level). The blue/red dots denote diatropic/paratropic character, and the dot size is in line with the $NICS_{zz}$ magnitude.