

Infinite as a Two Fused Helicoidal Trails of Local-Aromatic rings. Evaluation of Magnetic behavior of [12]Infinite and Anionic Species

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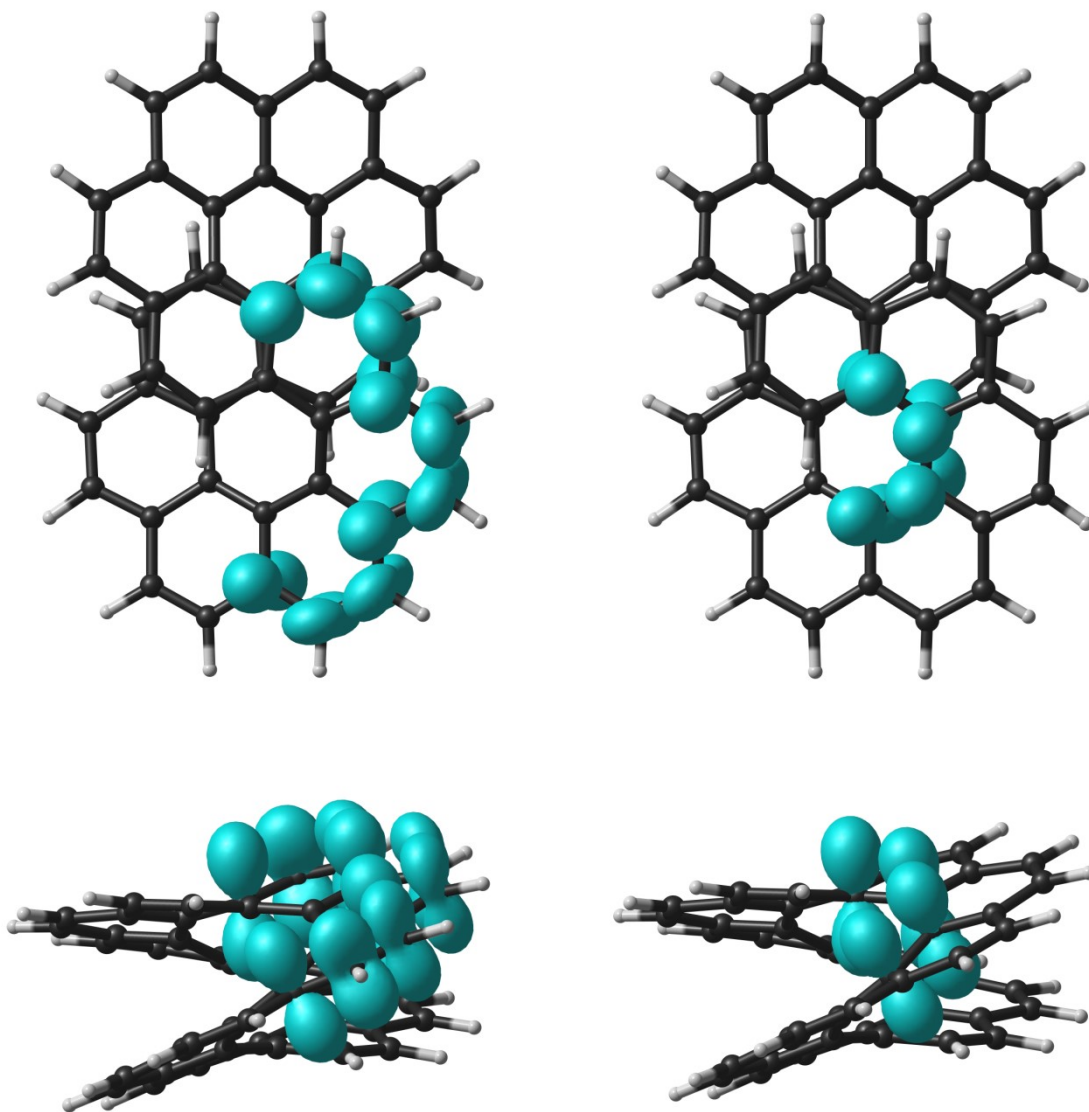


Figure S1. Graphical representation of the shielding tensors for [12]Infiniteene in two views.

Table S1. Calculated isotropic chemical shielding tensor (δ) and different components of the absolute shielding tensor (σ_{ii}) according the principal-axis-system (PAS), and related anisotropy (σ_{aniso}) and asymmetry (η) parameters, at several charges (q). Values in ppm. C-C means, sp²-carbon atoms bonded to carbons. C-H means, sp²-carbon atoms bonded to hydrogen. See color code from right figure.

$q=0$		σ_{11}	σ_{22}	σ_{33}	σ_{iso}	δ_{iso}	σ_{aniso}	η asym
1	C-C	-4.2	4.6	185.5	62.0	130.6	185.3	0.07
6	C-C	-5.5	-0.2	191.7	62.0	130.5	194.5	0.04
4	C-C	-5.3	3.4	187.8	62.0	130.5	188.7	0.07
7	C-C	-12.2	5.2	193.7	62.2	130.3	197.2	0.13
5	C-C	-0.7	6.9	186.3	64.2	128.4	183.1	0.06
2	C-C	2.0	12.9	179.2	64.7	127.8	171.7	0.10
9	C-H	-24.7	65.7	155.7	65.5	127.0	135.2	1.00
3	C-C	1.1	13.2	183.4	65.9	126.6	176.2	0.10
8	C-H	-21.5	67.4	154.2	66.7	125.8	131.3	1.02
11	C-H	-24.3	64.9	161.5	67.4	125.2	141.2	0.95
10	C-H	-20.5	67.4	156.1	67.7	124.9	132.6	0.99
13	C-H	-30.4	61.0	179.0	69.9	122.7	163.8	0.84
12	C-H	-16.6	70.4	163.0	72.3	120.3	136.1	0.96
$q=-2$								
4	C-C	-61.3	7.5	131.4	25.9	166.6	158.3	0.65
1	C-C	-76.9	-1.3	160.8	27.5	165.0	200.0	0.57
6	C-C	-62.9	11.2	177.8	42.0	150.5	203.7	0.55
3	C-C	-20.0	10.1	168.0	52.7	139.8	173.0	0.26
13	C-H	-15.3	12.3	181.4	59.5	133.0	183.0	0.23
7	C-C	-32.9	-7.4	222.2	60.7	131.8	242.3	0.16
12	C-H	-44.0	82.3	149.8	62.7	129.8	130.7	1.45
11	C-H	-10.8	83.2	144.5	72.3	120.2	108.3	1.30
10	C-H	-27.5	83.6	182.7	79.6	112.9	154.7	1.08
8	C-H	-23.4	90.7	172.3	79.9	112.6	138.6	1.24
9	C-H	-8.0	82.6	179.5	84.7	107.8	142.2	0.95
5	C-C	8.9	66.8	186.9	87.5	105.0	149.1	0.58
2	C-C	34.8	51.3	190.7	92.3	100.2	147.6	0.17
$q=-4$								
1	C-C	-6.4	-4.8	179.1	56.0	136.5	184.7	0.01
4	C-C	-3.8	19.5	177.5	64.4	128.1	169.7	0.21
13	C-H	-20.2	29.3	200.3	69.8	122.7	195.8	0.38
2	C-C	23.5	29.3	171.2	74.6	117.9	144.9	0.06
7	C-C	-14.8	44.4	199.0	76.2	116.3	184.3	0.48
6	C-C	1.6	39.2	203.1	81.3	111.2	182.7	0.31
5	C-C	8.4	50.1	186.2	81.6	110.9	156.9	0.40
3	C-C	20.2	40.9	183.7	81.6	110.9	153.2	0.20
8	C-H	10.9	97.5	137.1	81.9	110.6	82.8	1.57
11	C-H	-10.6	110.1	147.5	82.4	110.1	97.8	1.85
10	C-H	16.0	94.4	143.3	84.6	107.9	88.1	1.33
9	C-H	12.8	117.2	133.9	88.0	104.5	68.9	2.27
12	C-H	12.7	105.0	160.0	92.5	100.0	101.2	1.37

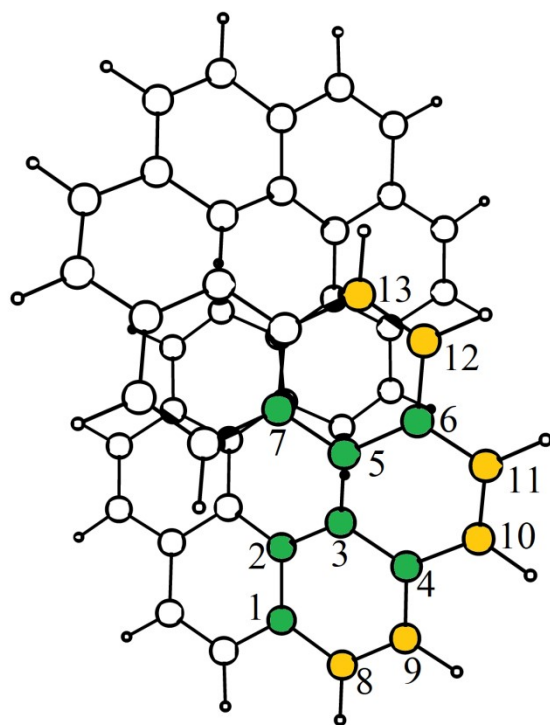
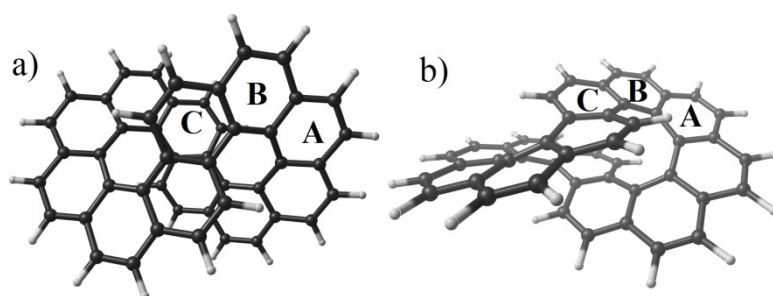


Table S2. NICS(0) values in ppm for the rings: A, B, and C, and at the middle of the central C-C...C-C cross-section, at the center of the stacked six-membered rings, and at the center of a representative helical axis, for the different charge states (q) at different levels of theory. In addition, HOMO-LUMO gap (HL) values are given in eV.

q=0	A	B	C	Cross-section	Inter-ring	Helical axis	HL
BP86	-5.3	-6.6	-6.8	-10.9	-9.3	6.0	2.05
PBE	-5.2	-6.6	-6.7	-10.9	-9.3	6.0	2.05
OPBE	-5.6	-6.9	-7.1	-11.0	-9.5	6.1	2.09
PBE0	-4.9	-6.3	-6.2	-10.4	-8.9	7.1	3.43
q=-2							
BP86	11.6	14.4	11.5	15.5	4.6	-37.2	0.20
PBE	11.9	14.6	11.6	15.5	4.6	-37.3	0.20
OPBE	12.4	14.7	11.0	15.0	4.1	-37.7	0.20
PBE0	11.7	16.3	15.0	21.6	8.1	-42.6	1.09
q=-4							
BP86	-1.1	-10.7	-13.0	-21.2	-16.7	2.0	0.22
PBE	0.3	-8.5	-11.2	-19.3	-15.2	-1.7	0.07
OPBE	-0.5	-10.8	-12.9	-21.3	-16.4	2.3	0.12
PBE0	2.3	-9.9	-14.1	-27.6	-20.4	-1.8	0.91



Up (a) and side (b) views of the calculated structure for [12]Helicene. Three different types of six membered rings are denoted as A, B, and C,

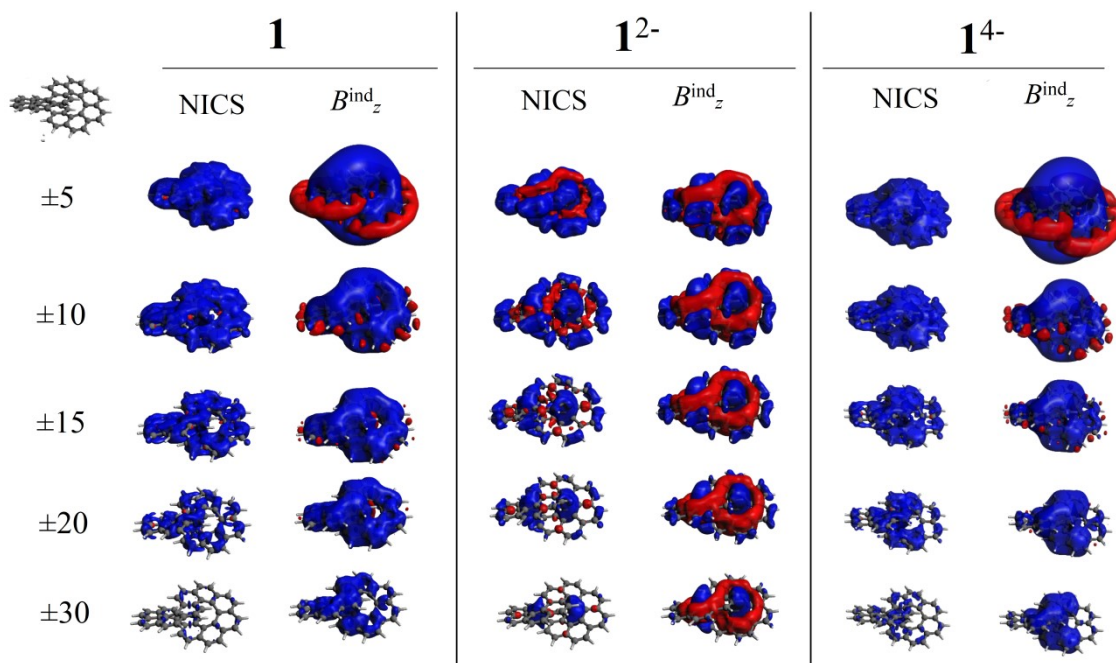


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