Electronic Supplementary Information for PCCP

Supporting Information

Patterns of π-electron delocalization in aromatic and antiaromatic organic compounds in the light of the Hückel's 4n+2 rule

Ferran Feixas,[§] Eduard Matito,[‡] Miquel Solà[*,§] and Jordi Poater[*,§]

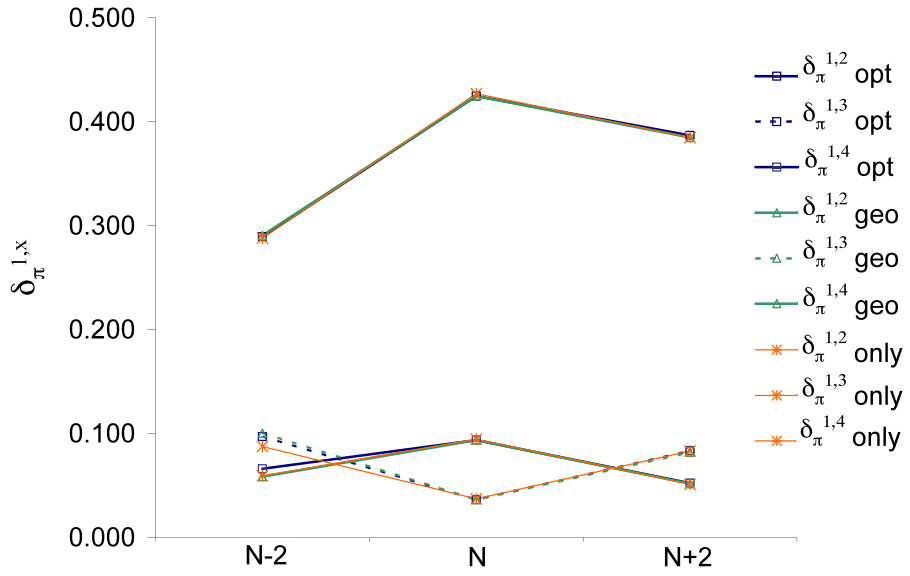
Institut de Química Computacional and Departament de Química, Campus de Montilivi, 17071 Girona, Catalonia, Spain, and Institute of Physics, University of Szczecin, 70-451 Szczecin, Poland

Contents

Section S1. Values of $\delta_\pi^{1,x}$ (in electrons), MCI, and FLU for N, N-2, and N+2 species calculated using three different schemes: (a) full geometry and MO relaxation of all *N*, *N* - 2, and *N* + 2 species (OPT); (b) geometry optimization only for *N* species; *N* - 2 and *N* + 2 keep the geometry of *N*, but the MOs are fully relaxed (GEO); and (c) geometry optimization only for *N* species; *N* - 2 and *N* + 2 keep the geometry and the MOs of the *N* system, and thus, the wave function of *N* species is used throughout the calculations (ONLY). Figures show how the $\delta_\pi^{1,x}$ and MCI are hardly affected by the geometry and electron relaxation.

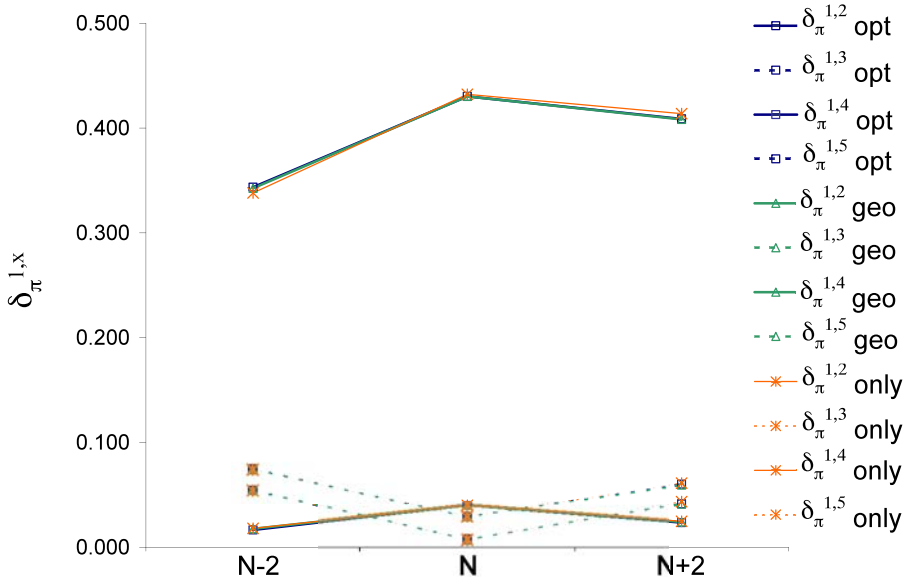
a) C_6H_6

	C_6H_6	N-2	N	N+2
OPT	$\delta_\pi^{1,2}$	0.289	0.425	0.387
GEO	$\delta_\pi^{1,2}$	0.291	0.425	0.385
ONLY	$\delta_\pi^{1,2}$	0.288	0.427	0.385
OPT	$\delta_\pi^{1,3}$	0.097	0.036	0.083
GEO	$\delta_\pi^{1,3}$	0.100	0.036	0.082
ONLY	$\delta_\pi^{1,3}$	0.087	0.037	0.083
OPT	$\delta_\pi^{1,4}$	0.066	0.094	0.052
GEO	$\delta_\pi^{1,4}$	0.058	0.094	0.052
ONLY	$\delta_\pi^{1,4}$	0.059	0.094	0.051
OPT	MCI	-0.020	0.073	0.002
GEO	MCI	-0.020	0.073	0.002
ONLY	MCI	-0.012	0.073	0.003



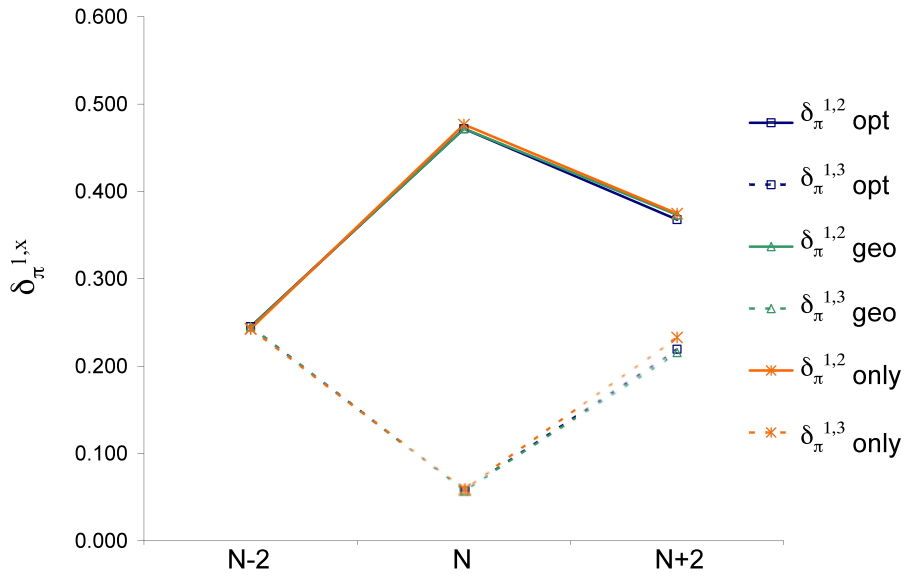
b) C_8H_8

	C_8H_8	N-2	N	N+2
OPT	$\delta_\pi^{1,2}$	0.344	0.430	0.409
GEO	$\delta_\pi^{1,2}$	0.342	0.430	0.408
ONLY	$\delta_\pi^{1,2}$	0.338	0.432	0.414
OPT	$\delta_\pi^{1,3}$	0.074	0.029	0.060
GEO	$\delta_\pi^{1,3}$	0.074	0.029	0.059
ONLY	$\delta_\pi^{1,3}$	0.074	0.029	0.061
OPT	$\delta_\pi^{1,4}$	0.016	0.040	0.023
GEO	$\delta_\pi^{1,4}$	0.018	0.040	0.024
ONLY	$\delta_\pi^{1,4}$	0.018	0.040	0.025
OPT	$\delta_\pi^{1,5}$	0.054	0.007	0.041
GEO	$\delta_\pi^{1,5}$	0.055	0.007	0.041
ONLY	$\delta_\pi^{1,5}$	0.054	0.007	0.044
OPT	MCI	0.040	-0.001	0.014
GEO	MCI	0.040	-0.001	0.014
ONLY	MCI	0.038	-0.001	0.015



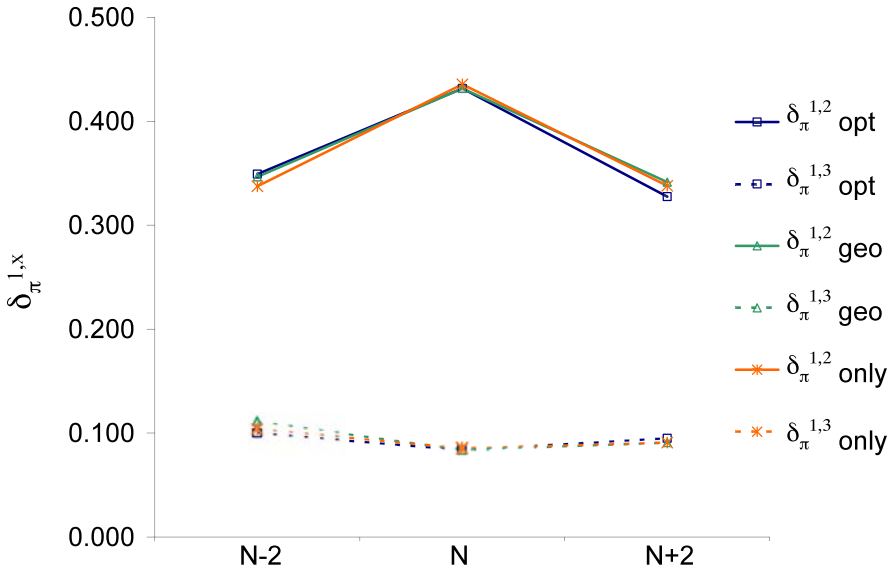
c) C_4H_4

	C_4H_4	N-2	N	N+2
OPT	$\delta_\pi^{1,2}$	0.245	0.472	0.368
GEO	$\delta_\pi^{1,2}$	0.245	0.472	0.373
ONLY	$\delta_\pi^{1,2}$	0.243	0.477	0.375
OPT	$\delta_\pi^{1,3}$	0.245	0.057	0.219
GEO	$\delta_\pi^{1,3}$	0.245	0.057	0.216
ONLY	$\delta_\pi^{1,3}$	0.243	0.059	0.233
OPT	MCI	0.183	0.009	0.064
GEO	MCI	0.183	0.009	0.064
ONLY	MCI	0.181	0.009	0.071



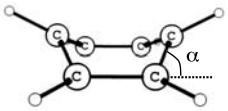
d) $C_5H_5^-$

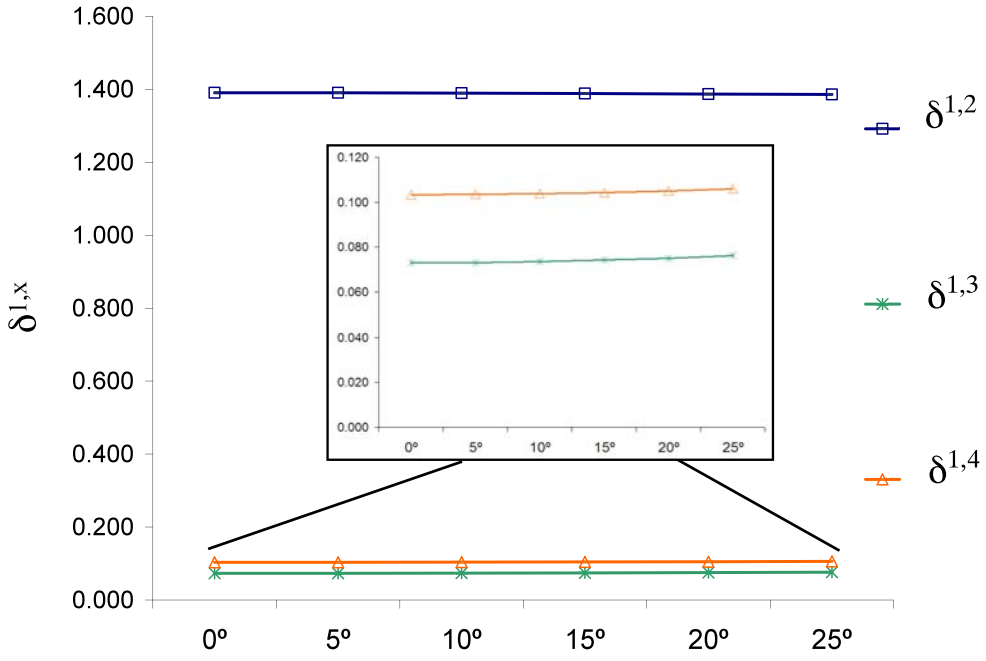
	$C_5H_5^-$	N-2	N	N+2
OPT	$\delta_\pi^{1,2}$	0.349	0.431	0.327
GEO	$\delta_\pi^{1,2}$	0.346	0.431	0.341
ONLY	$\delta_\pi^{1,2}$	0.337	0.436	0.338
OPT	$\delta_\pi^{1,3}$	0.100	0.084	0.095
GEO	$\delta_\pi^{1,3}$	0.111	0.084	0.091
ONLY	$\delta_\pi^{1,3}$	0.104	0.085	0.091
OPT	MCI	-0.021	0.072	0.009
GEO	MCI	-0.028	0.072	0.010
ONLY	MCI	-0.022	0.072	0.005



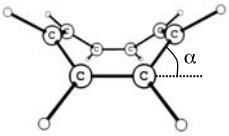
Section S2. Evolution of $\delta_\pi^{1,x}$ (in electrons), MCI, FLU, and HOMA along the out-of-plane boat-like distortion of C_6H_6 and C_8H_8. Figures show how the average crossed terms ($\delta_\pi^{1,x}$), MCI, FLU, and HOMA are hardly affected by the out-of-plane distortion.

a) C_6H_6

C_6H_6	α	0º	5º	10º	15º	20º	25º
	$\delta_\pi^{1,2}$	1.390	1.390	1.389	1.388	1.387	1.386
	$\delta_\pi^{1,3}$	0.073	0.073	0.074	0.074	0.075	0.076
	$\delta_\pi^{1,4}$	0.103	0.103	0.104	0.104	0.105	0.106
	FLU	0.000	0.000	0.000	0.000	0.000	0.000
	MCI	0.0726	0.0725	0.0721	0.0715	0.0706	0.0696
	HOMA	0.99	0.99	0.99	0.99	0.98	0.97



b) C_8H_8

C_8H_8	α	0º	5º	10º	15º	20º	25º	COT
	$\delta_\pi^{1,2}$	1.401	1.401	1.402	1.402	1.403	1.404	1.404
	$\delta_\pi^{1,3}$	0.064	0.064	0.064	0.065	0.065	0.066	0.068
	$\delta_\pi^{1,4}$	0.043	0.043	0.042	0.041	0.040	0.039	0.038
	$\delta_\pi^{1,5}$	0.008	0.008	0.008	0.009	0.009	0.010	0.014
	FLU	0.105	0.105	0.106	0.106	0.107	0.109	0.115
	MCI	-0.0005	-0.0005	-0.0003	0.0000	0.0002	0.0005	0.0009
	HOMA	-0.25	-0.24	-0.23	-0.22	-0.20	-0.20	-0.20

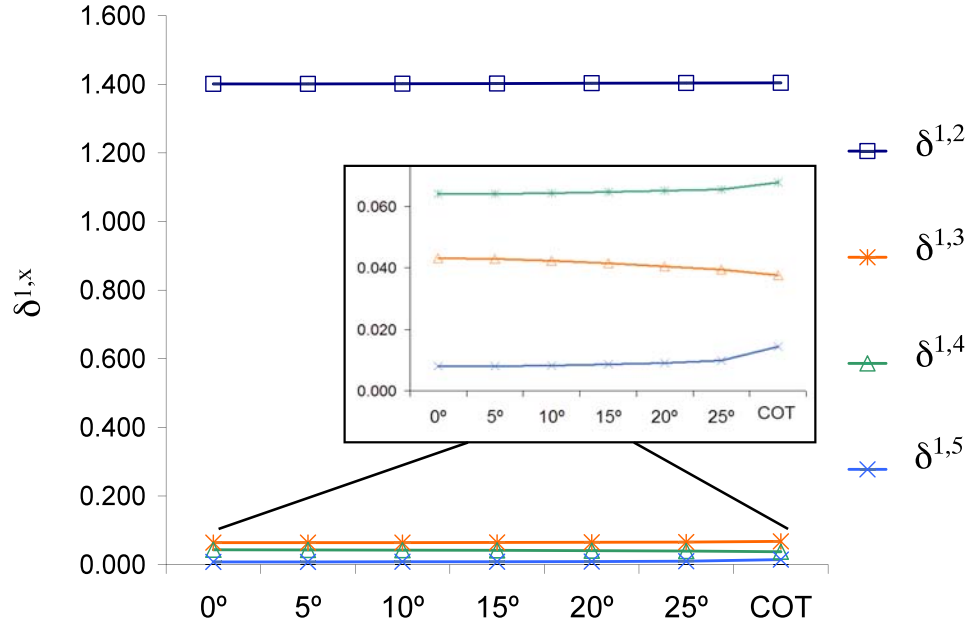
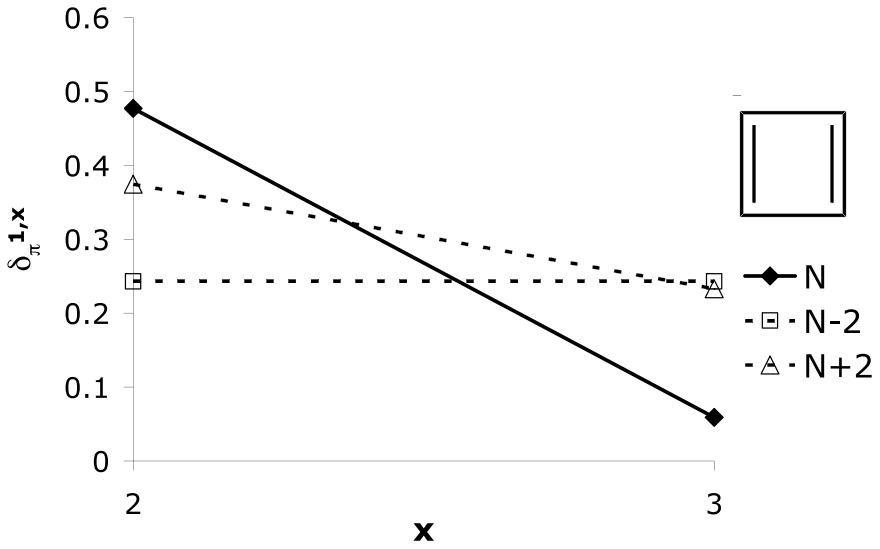
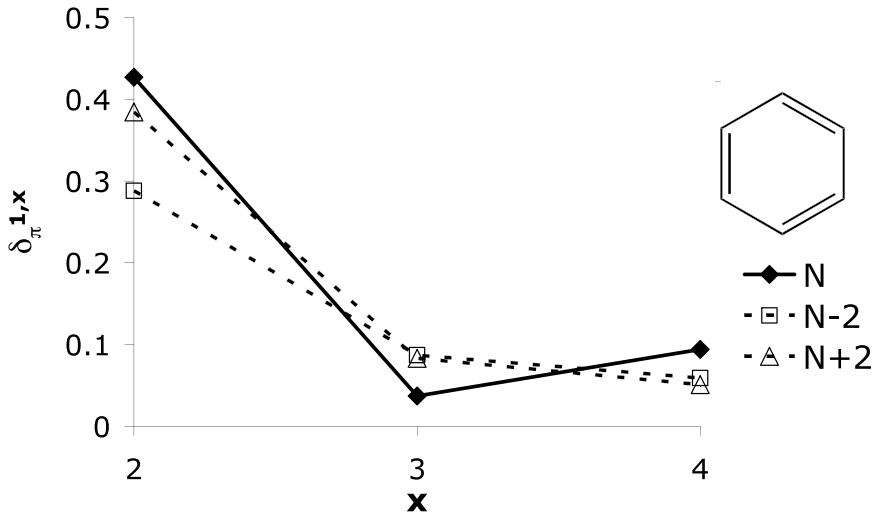


Figure S3. Evolution of $\delta_\pi^{1,x}$ (in electrons) in N, N-2, and N+2 species for a) C_4H_4, b) C_6H_6, c) C_8H_8, d) $C_{14}H_{14}$, and e) $C_{16}H_{16}$.

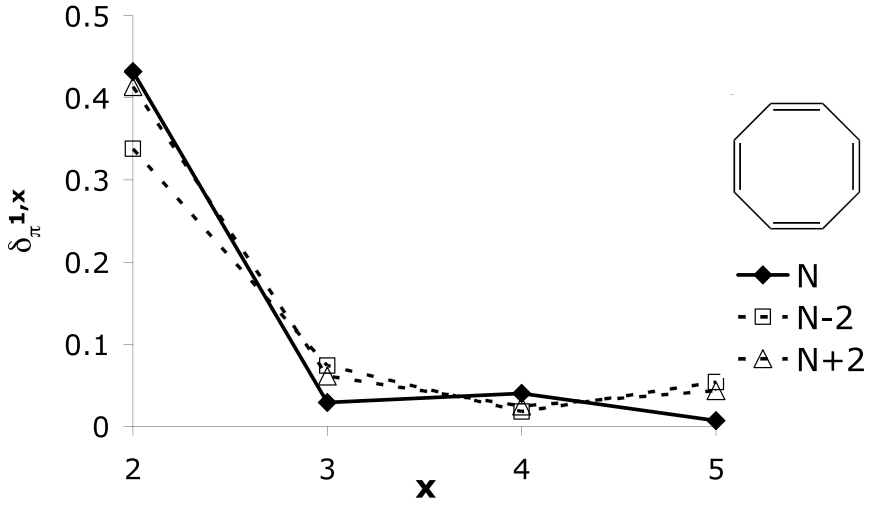
a)



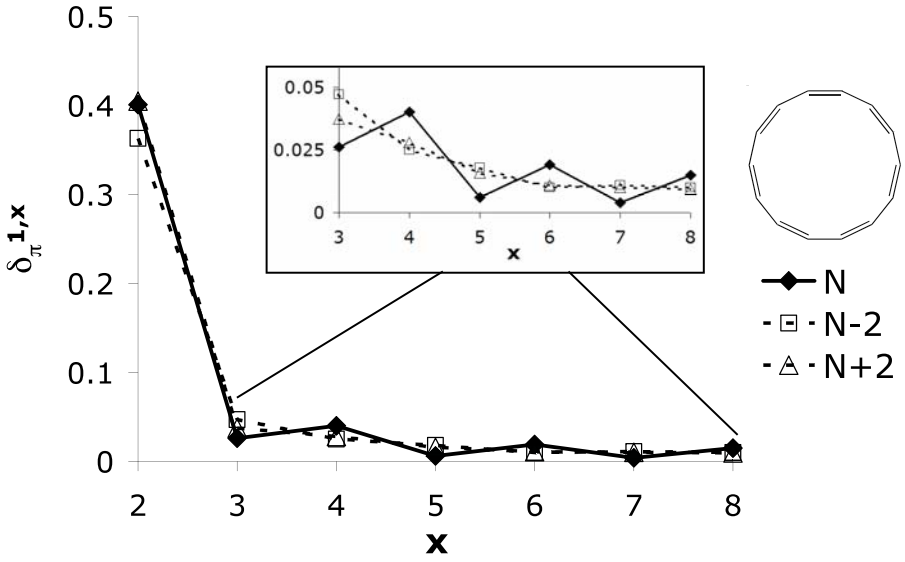
b)



c)


0.5
0.4
0.3
0.2
0.1
0
δ π 1,x
2
3
4
5
x
N
N-2
N+2

d)


0.5
0.4
0.3
0.2
0.1
0
δ π 1,x
2
3
4
5
6
7
8
x
0.05
0.025
0
N
N-2
N+2

e)

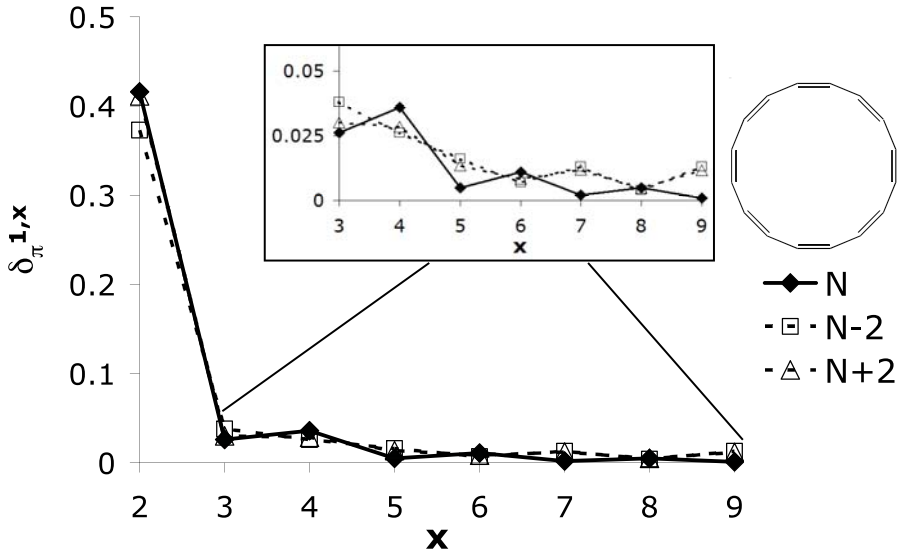
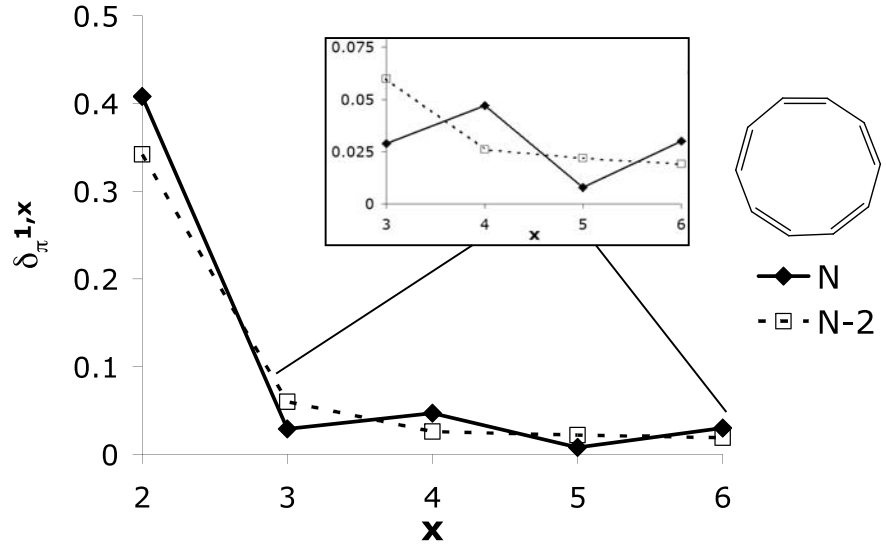
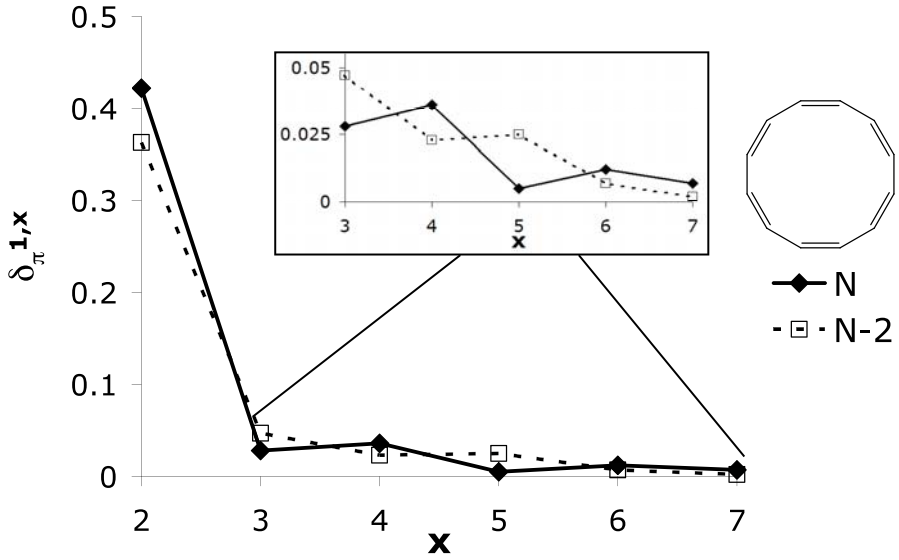

0.5
0.4
0.3
0.2
0.1
0
2
3
4
5
6
7
8
9
x
$\delta_{\pi}^{1,x}$
0.05
0.025
0
3
4
5
6
7
8
9
x
N
N-2
N+2

Figure S4. Evolution of $\delta_{\pi}^{1,x}$ (in electrons) in N and N-2 species for a) $C_{10}H_{10}$, b) $C_{12}H_{12}$, c) $C_{11}H_{11}^{+}$, d) $C_{11}H_{11}^{-}$, e) $C_{13}H_{13}^{+}$, f) $C_{13}H_{13}^{-}$, and g) $C_{15}H_{15}^{+}$.

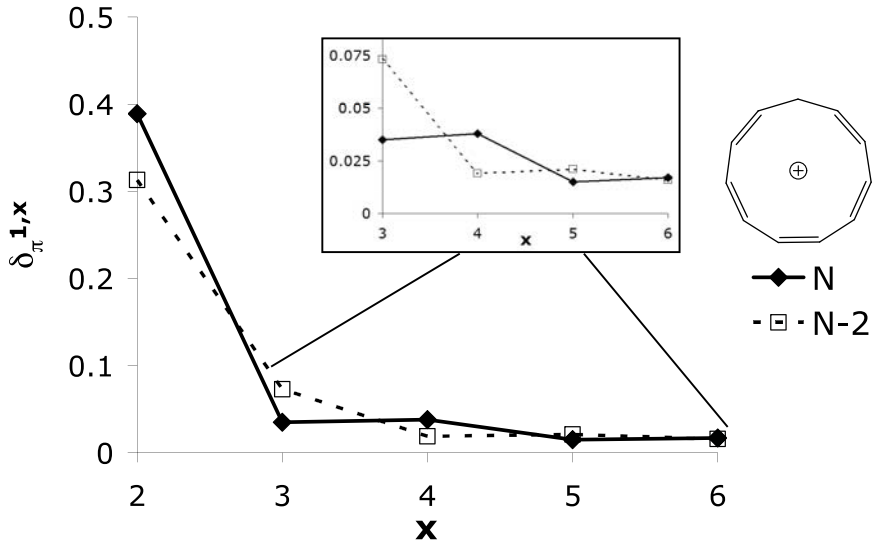
a)



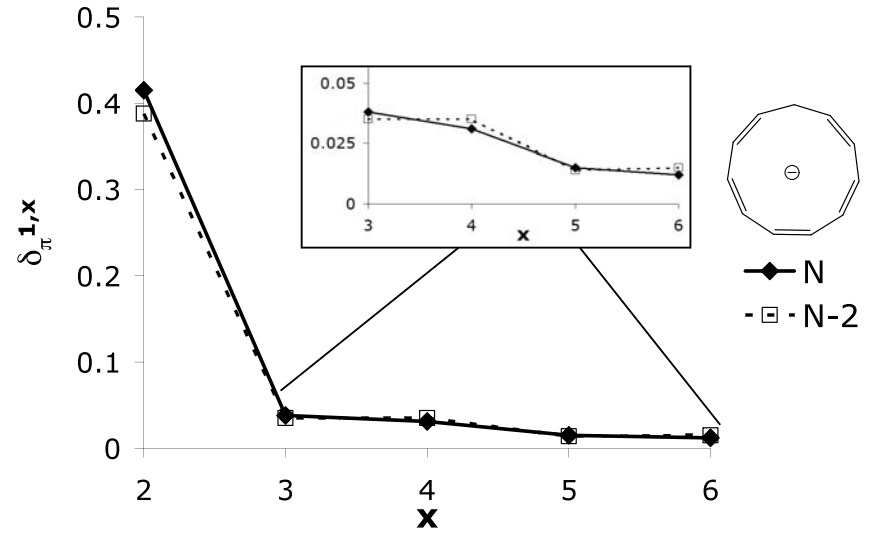
b)



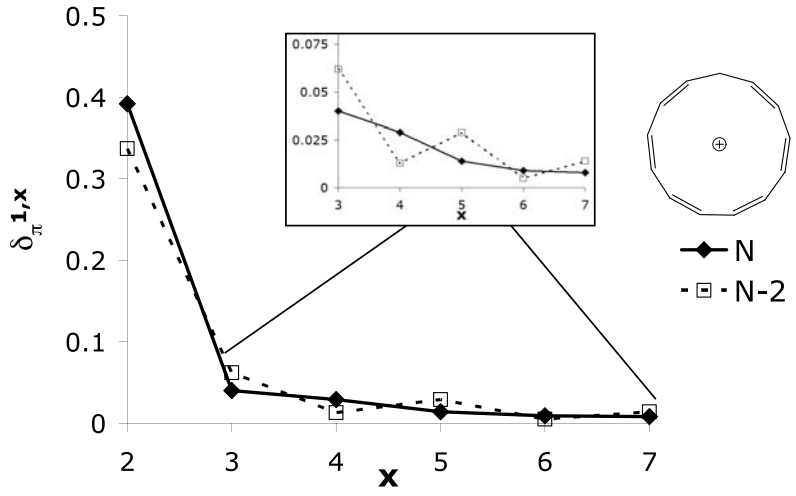
c)


0.5
0.4
0.3
0.2
0.1
0
2
3
4
5
6
x
δπ1,x
0.075
0.05
0.025
0
3
4
5
6
x
⊕
N
N-2

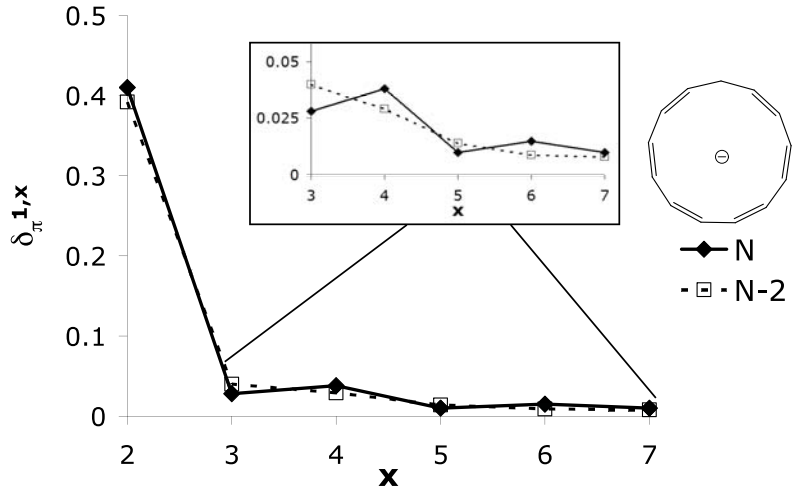
d)


0.5
0.4
0.3
0.2
0.1
0
2
3
4
5
6
x
δπ1,x
0.05
0.025
0
3
4
5
6
x
⊖
N
N-2

e)


0.5
0.4
0.3
0.2
0.1
0
2
3
4
5
6
7
x
δ π 1,x
0.075
0.05
0.025
0
3
4
5
6
7
x
⊕
N
N-2

f)


0.5
0.4
0.3
0.2
0.1
0
2
3
4
5
6
7
x
δ π 1,x
0.05
0.025
0
3
4
5
6
7
x
⊖
N
N-2

g)

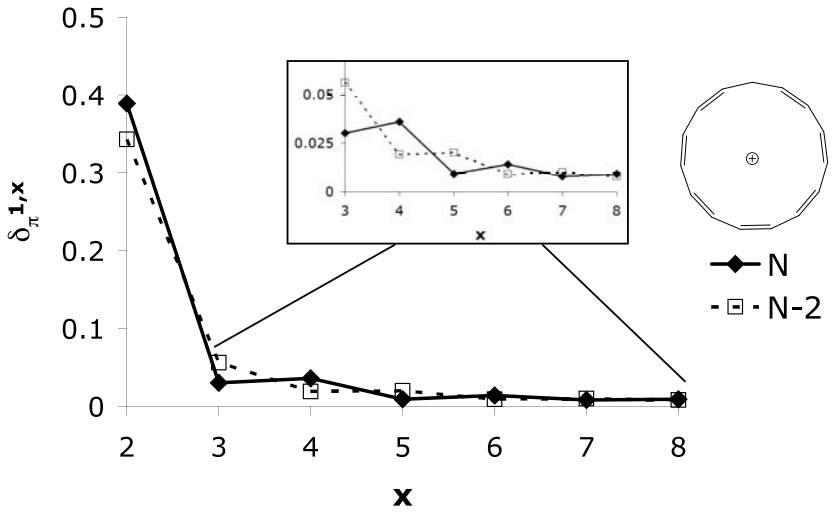
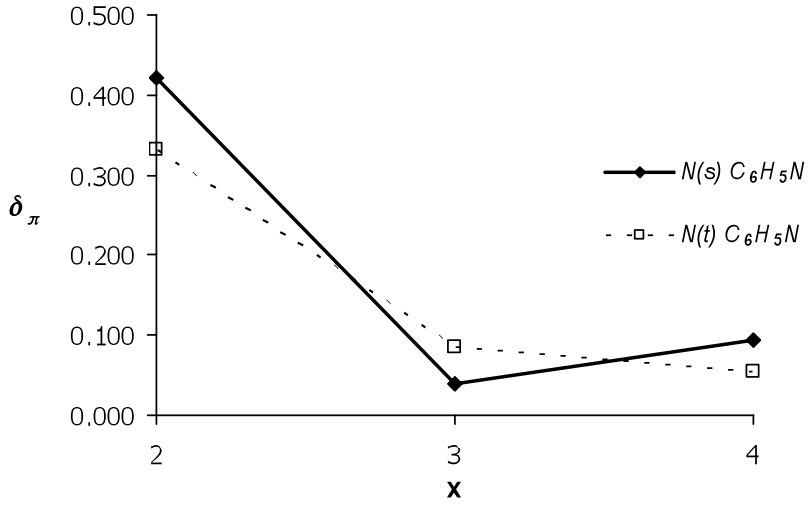

0.5
0.4
0.3
0.2
0.1
0
2
3
4
5
6
7
8
x
δ π 1,x
0.05
0.025
0
3
4
5
6
7
8
x
⊕
N
N-2

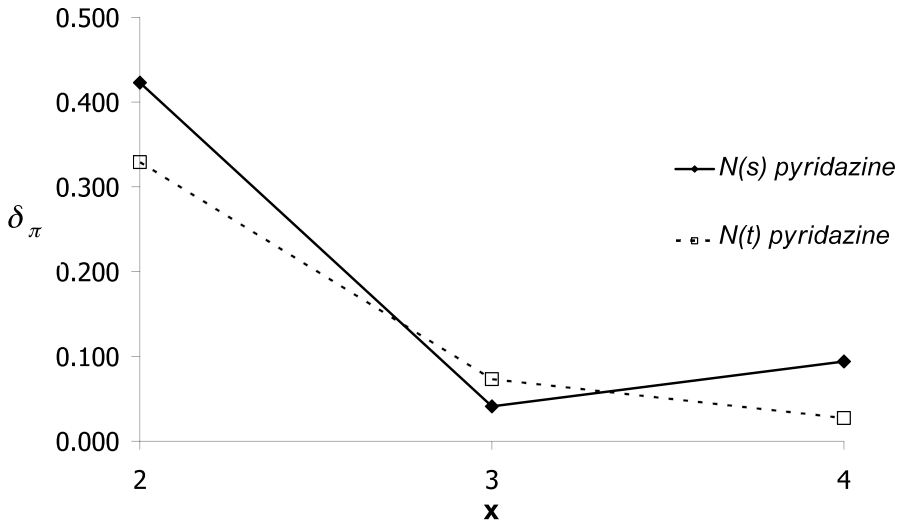
Table S5. $\delta_\pi^{1,x}$ (in electrons), MCI, FLU, HOMA, NICS(0), NICS(1), $NICS(0)_{zz}$, and $NICS(1)_{zz}$ results for the rings studied at the lowest-lying singlet and triplet states for a) C_6H_5N, b) pyridazine, c) pyimidine, d) triazine, and e) $C_7H_7^+$. Figures show the evolution of $\delta_\pi^{1,x}$ (in electrons) in N(s) and N(t) species.

		$\delta_\pi^{1,2}$	$\delta_\pi^{1,3}$	$\delta_\pi^{1,4}$	MCI	FLU	HOMA	NICS(0)	NICS(1)	$NICS(0)_{zz}$	$NICS(1)_{zz}$
C_6H_5N	***N(s)***	0.422	0.040	0.093	0.069	0.001	1.00	-7.46	-10.91	-13.21	-28.72
	N(t)	0.332	0.086	0.054	-0.009	0.006	0.76	13.38	12.20	74.82	45.84
pyridazine	***N(s)***	0.423	0.041	0.094	0.070	0.003	0.98	-5.65	-11.09	-11.52	-28.33
	N(t)	0.329	0.073	0.027	-0.002	0.035	-0.53	19.16	15.77	85.24	52.67
pyrimidine	***N(s)***	0.415	0.041	0.091	0.066	0.001	1.00	-6.03	-10.55	-11.05	-27.59
	N(t)	0.328	0.084	0.047	-0.008	0.011	0.79	22.35	18.96	100.79	62.14
triazine	***N(s)***	0.410	0.039	0.087	0.064	0.003	1.00	-4.48	-10.10	-7.87	-25.92
	N(t)	0.329	0.075	0.029	0.003	0.032	0.24	49.23	33.94	179.78	107.18
$C_7H_7^+$	***N(s)***	0.389	0.050	0.050	0.058	0.000	0.98	-6.39	-9.88	-16.29	-26.55
	N(t)	0.329	0.073	0.034	-0.009	0.025	0.26	79.69	62.06	245.04	190.04

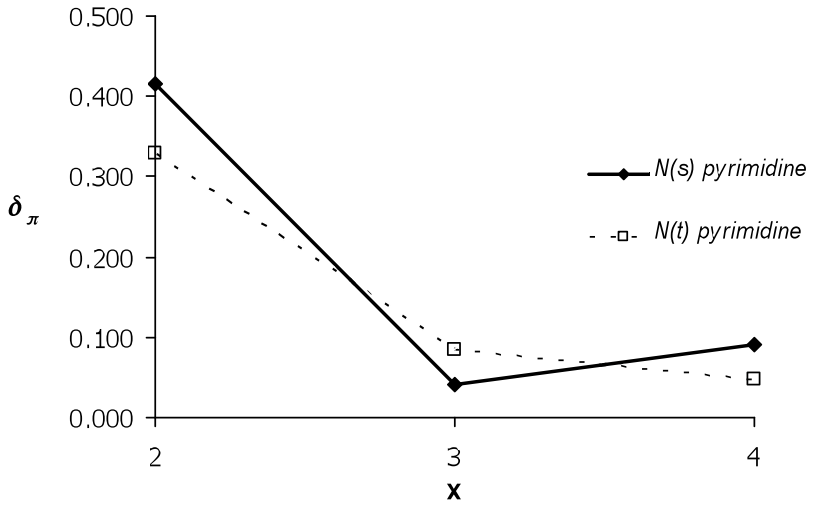
a)



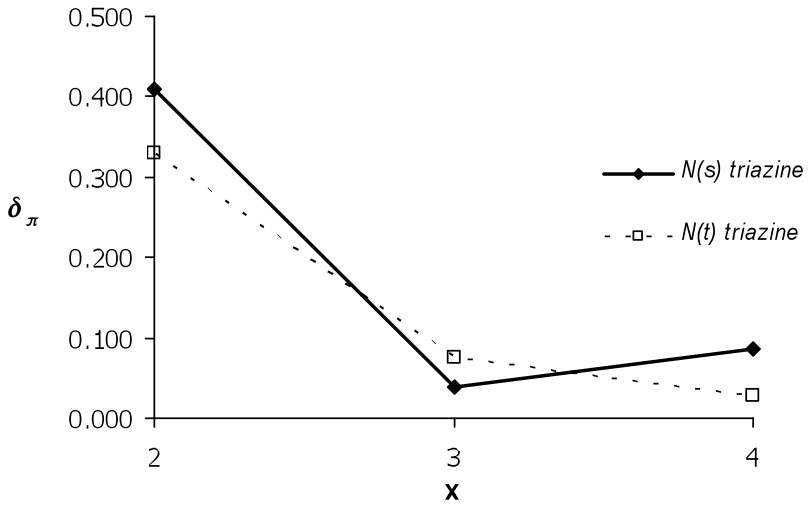
b)


0.500
0.400
0.300
0.200
0.100
0.000
δ π
2
3
4
x
N(s) pyridazine
N(t) pyridazine

c)


0.500
0.400
0.300
0.200
0.100
0.000
δ π
2
3
4
x
N(s) pyrimidine
N(t) pyrimidine

d)


0.500
0.400
0.300
0.200
0.100
0.000
δπ
2
3
4
X
N(s) triazine
N(t) triazine

e)

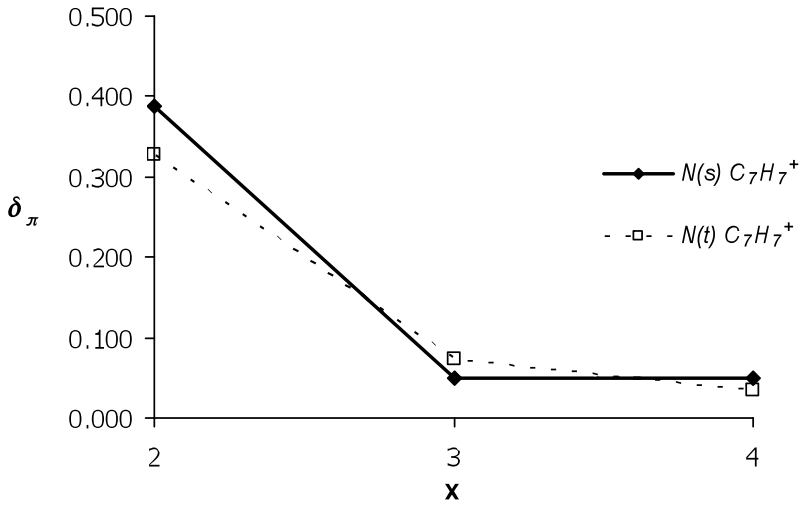
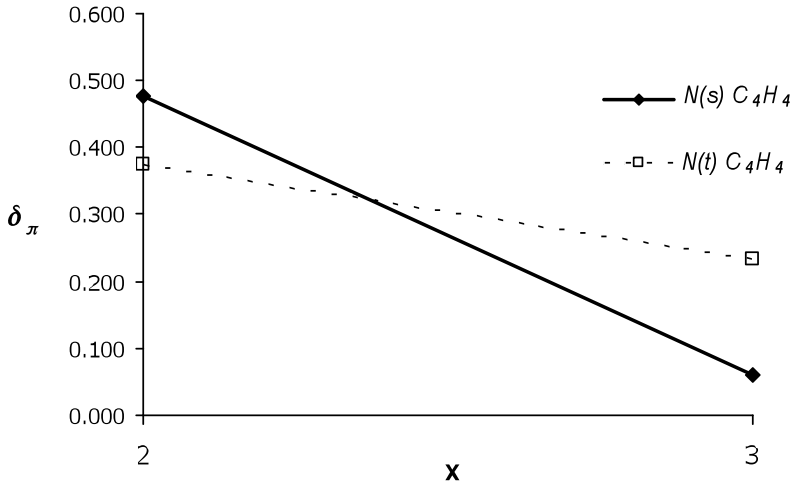

0.500
0.400
0.300
0.200
0.100
0.000
δπ
2
3
4
X
N(s) C7H7+
N(t) C7H7+

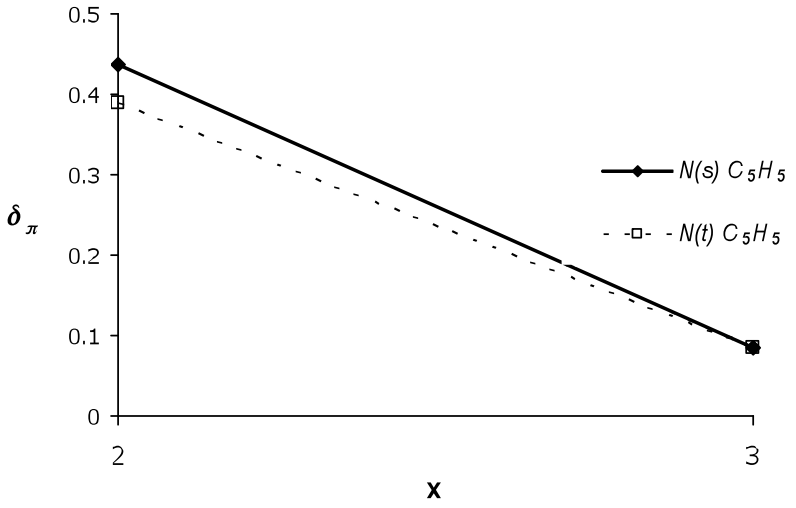
Table S6. $\delta_\pi^{1,x}$ (in electrons), MCI, FLU, HOMA, NICS(0), NICS(1), $NICS(0)_{zz}$, and $NICS(1)_{zz}$ results for the rings studied at the lowest-lying singlet and triplet states for a) C_4H_4, b) $C_5H_5^-$, c) C_5H_4NH, d) C_5H_4O, e) $C_5H_4S^+$, f) $C_5H_4P^-$, g) C_5H_4BH, h) $C_5H_4SiH^+$, and i) $C_5H_4F_2$. Figures show the evolution of $\delta_\pi^{1,x}$ (in electrons) in N(s) and N(t) species.

		$\delta^\pi_{(1-2)}$	$\delta^\pi_{(1-3)}$	MCI	FLU	HOMA	NICS(0)	NICS(1)	$NICS(0)_{zz}$	$NICS(1)_{zz}$
C_4H_4	***N(s)***	0.477	0.059	0.009	0.211	-4.10	25.35	16.45	109.39	55.50
	N(t)	0.375	0.233	0.063	0.012	0.32	-3.10	-7.95	22.16	-17.03
$C_5H_5^-$	***N(s)***	0.436	0.085	0.072	0.000	0.84	-15.61	-12.29	-15.93	-33.42
	N(t)	0.389	0.084	0.014	0.019	0.36	14.90	9.84	64.94	37.64
C_5H_4NH	***N(s)***	0.417	0.086	0.050	0.008	0.86	-14.74	-11.10	-12.31	-30.96
	N(t)	0.314	0.068	0.001	0.039	-0.18	13.00	11.26	68.88	36.30
C_5H_4O	***N(s)***	0.407	0.081	0.029	0.017	0.21	-12.68	-10.26	-8.80	-27.23
	N(t)	0.300	0.070	0.002	0.035	-0.97	6.62	5.37	48.74	19.66
C_5H_4S	***N(s)***	0.417	0.082	0.041	0.017	0.82	-13.86	-11.27	-9.22	-28.06
	N(t)	0.304	0.072	0.000	0.058	-1.08	7.16	6.65	50.63	25.14
$C_5H_4P^-$	***N(s)***	0.440	0.088	0.068	*	*	-14.54	-11.80	-14.98	-31.56
	N(t)	0.345	0.080	-0.002	*	*	40.15	36.87	140.23	111.26
C_5H_4BH	***N(s)***	0.361	0.053	-0.003	*	*	19.89	11.45	64.77	38.23
	N(t)	0.256	0.104	0.015	*	*	-0.15	-7.88	0.42	-20.36
$C_5H_4SiH^+$	***N(s)***	0.359	0.065	-0.006	*	*	15.74	10.59	57.75	37.40
	N(t)	0.281	0.108	0.025	*	*	-3.59	-8.54	-3.12	-20.27
$C_5H_4F_2$	***N(s)***	0.358	0.043	-0.005	*	*	3.09	0.10	29.61	7.22
	N(t)	0.244	0.078	0.010	*	*	-2.08	-5.14	13.26	-8.47

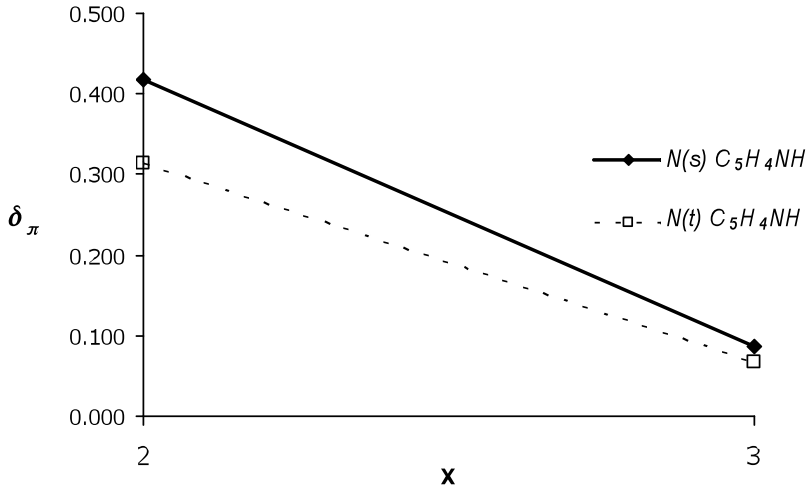
a)


0.600
0.500
0.400
0.300
0.200
0.100
0.000
δπ
2
3
x
N(s) C4H4
N(t) C4H4

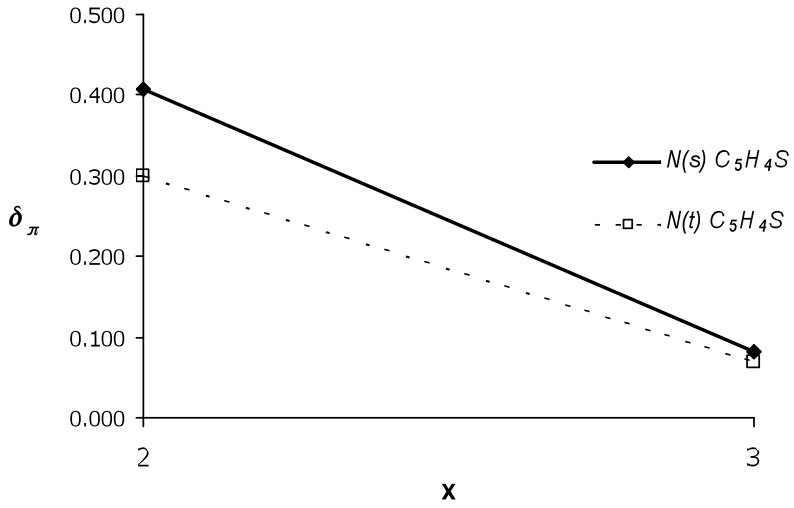
b)


0.5
0.4
0.3
0.2
0.1
0
δπ
2
3
x
N(s) C5H5
N(t) C5H5

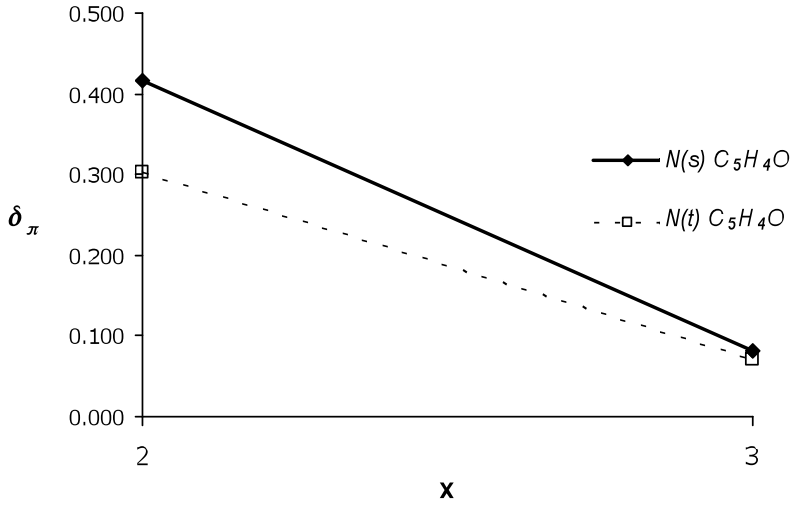
c)


0.500
0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4NH
N(t) C5H4NH

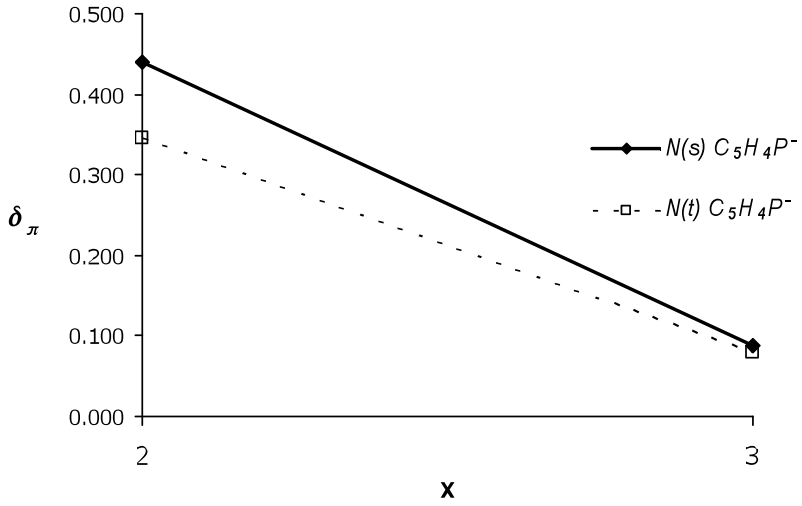
d)


0.500
0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4S
N(t) C5H4S

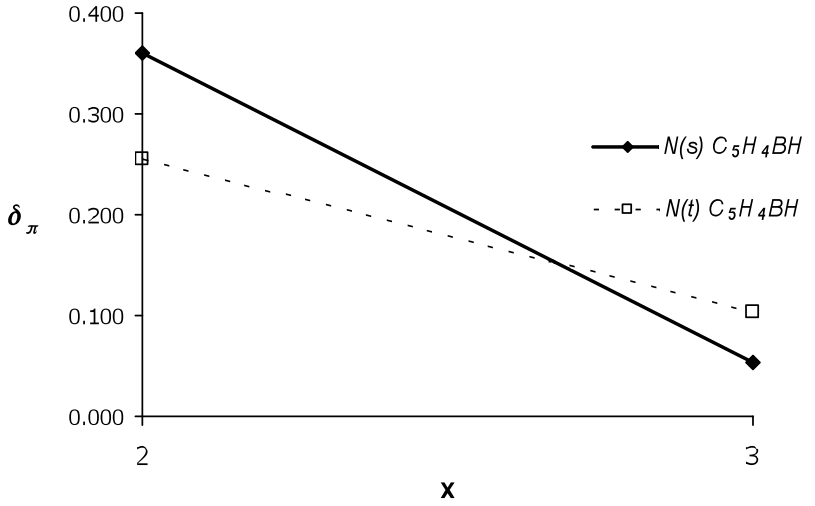
e)


0.500
0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4O
N(t) C5H4O

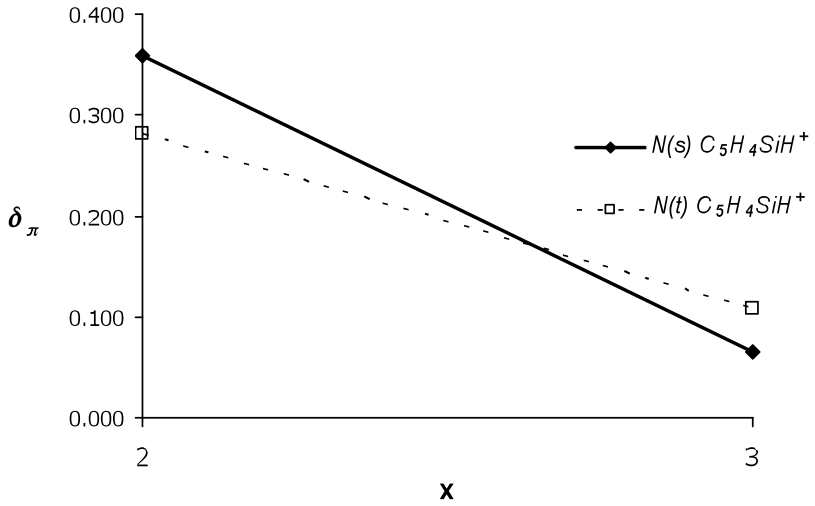
f)


0.500
0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4P-
N(t) C5H4P-

g)


0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4BH
N(t) C5H4BH

h)


0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4SiH+
N(t) C5H4SiH+

i)

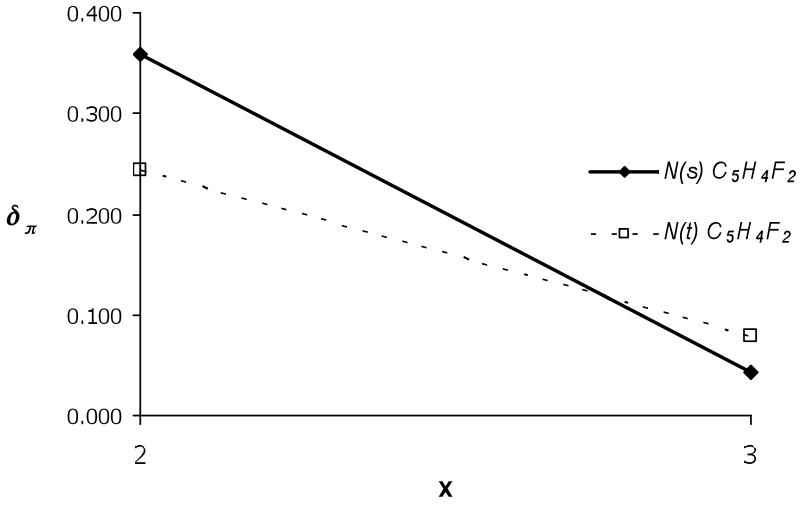

0.400
0.300
0.200
0.100
0.000
δ π
2
3
x
N(s) C5H4F2
N(t) C5H4F2

Table S7. MCI, FLU, HOMA, NICS(0), NICS(1), $NICS(0)_{zz}$, and $NICS(1)_{zz}$ results for the rings studied. *A* and *B* refer to the different rings in the PAH (see Schemes 2 and 3).

A) MCI, FLU, and HOMA

	MCI			FLU			HOMA		
	N-2	*N*	*N+2*	*N-2*	*N*	*N+2*	*N-2*	*N*	*N+2*
C_6H_6	-0.020	0.073	0.002	0.044	0.000	0.038	-0.953	0.991	-1.079
C_5H_5N	-0.010	0.069	0.004	0.056	0.001	0.044	-1.340	0.996	-0.073
pyridazine	0.000	0.070	0.002	0.109	0.003	0.024	-0.294	0.979	-1.179
pyrimidine	0.001	0.066	0.002	0.106	0.001	0.039	-0.641	0.999	0.114
pyrazine	0.006	0.066	0.003	0.077	0.003	0.044	-1.934	0.996	0.383
triazine	-0.016	0.064	0.002	0.031	0.003	0.052	0.934	1.000	0.086
$C_7H_7^+$	-0.005	0.058	-0.017	0.052	0.000	0.038	-1.058	0.984	0.015
C_4H_4	0.183	0.009	0.064	0.033	0.211	0.017	0.138	-4.101	-0.718
C_8H_8	0.040	-0.001	0.014	0.009	0.105	0.006	0.896	-0.241	0.810
$C_5H_5^-$	-0.028	0.072	0.010	0.054	0.000	0.036	-1.173	0.837	-6.476
C_4H_4NH	-0.014	0.050	0.011	0.074	0.008	0.017	-0.207	0.860	-1.036
C_4H_4O	-0.010	0.029	0.013	0.081	0.017	0.021	-0.221	0.206	-0.011
C_4H_4S	-0.021	0.041	0.014	0.034	0.017	0.040	0.131	0.819	-1.774
$C_4H_4P^-$	-0.019	0.068	0.014	[a]	[a]	[a]	[a]	[a]	[a]
C_4H_4BH	0.022	-0.003	0.040	[a]	[a]	[a]	[a]	[a]	[a]
$C_4H_4SiH^+$	0.037	-0.006	0.057	[a]	[a]	[a]	[a]	[a]	[a]
$C_4H_4F_2$	0.017	-0.005	0.023	[a]	[a]	[a]	[a]	[a]	[a]
naphthalene	0.020	0.039	0.018	0.028	0.018	0.025	0.667	0.785	0.302
quinoline^A	0.021	0.037	0.016	0.036	0.023	0.031	0.749	0.823	0.377
quinoline^B	0.008	0.038	0.020	0.054	0.022	0.027	0.318	0.796	0.334
anthracene^A	0.028	0.029	0.025	0.016	0.031	0.016	0.813	0.630	0.618
anthracene^B	0.013	0.027	0.012	0.031	0.018	0.030	0.673	0.723	0.351
phenanthrene^A	0.019	0.047	0.020	0.030	0.010	0.029	0.603	0.870	0.335
phenanthrene^B	0.010	0.018	0.008	0.050	0.038	0.053	0.197	0.461	-0.464
biphenylene^A	0.008	0.056	0.010	0.035	0.011	0.032	0.412	0.845	0.033
biphenylene^B	0.054	0.021	0.016	0.087	0.089	0.089	-0.448	-1.035	-1.590
acenaphthene^A	0.005	0.011	0.034	0.084	0.094	0.020	-0.408	0.152	0.529
acenaphthene^B	0.014	0.038	0.019	0.036	0.021	0.024	0.582	0.848	0.568
pyracylene^A	0.015	0.032	0.019	0.042	0.021	0.027	0.463	0.761	0.633
pyracylene^B	0.017	0.012	0.030	0.052	0.081	0.022	0.528	-0.168	0.582
C_6H_6 (t)	0.079	-0.002	0.036	0.012	0.025	0.006	0.392	-0.537	0.476
C_8H_8 (t)	-0.002	0.028	0.007	0.029	0.002	0.012	-0.046	0.890	0.612

[a] There are no reference parameters for the P-C, B–C, Si-C and F-C bonds.

B) NICS(0) and NICS(1)

	NICS(0)			NICS(1)		
	N-2	*N*	*N+2*	*N-2*	*N*	*N+2*
C_6H_6	80.46	-8.89	113.25	60.07	-11.13	93.76
C_5H_5N	34.53	-7.46	111.48	17.82	-10.91	91.61
pyridazine	[b]	-5.65	37.55	[b]	-11.09	30.24
pyrimidine	[b]	-6.03	57.94	[b]	-10.55	45.74
pyrazine	22.51	-5.87	72.14	7.07	-10.93	57.36
triazine	29.13	-4.48	75.32	13.18	-10.10	57.63
$C_7H_7^+$	317.72	-6.39	159.84	265.21	-9.88	130.72
C_4H_4	15.58	25.35	-22.46	-8.58	16.45	-8.95
C_8H_8	-6.70	40.20	-16.58	-9.15	31.74	-13.87
$C_5H_5^-$	111.03	-15.61	[b]	85.97	-12.29	[b]
C_4H_4NH	58.25	-14.74	[b]	39.06	-11.10	[b]
C_4H_4O	29.75	-12.68	85.38	15.07	-10.26	49.67
C_4H_4S	26.52	-13.86	[b]	15.62	-11.27	[b]
$C_4H_4P^-$	62.26	-14.54	[b]	45.79	-11.80	[b]
C_4H_4BH	14.10	19.89	-13.96	-5.98	11.45	-9.39
$C_4H_4SiH^+$	10.22	15.74	-15.00	-5.23	10.59	-10.05
$C_4H_4F_2$	10.46	3.09	-11.96	-3.99	0.10	-6.22
naphthalene	25.98	-8.91	43.42	16.06	-11.26	34.74
quinoline[A]	31.87	-7.94	40.74	20.82	-11.17	31.11
quinoline[B]	48.08	-9.28	32.25	32.43	-11.51	25.43
anthracene[A]	10.94	-8.09	16.12	4.13	-10.53	11.38
anthracene[B]	16.41	-11.91	19.35	9.20	-13.77	13.05
phenanthrene[A]	26.75	-9.21	52.88	17.62	-11.48	41.48
phenanthrene[B]	23.64	-6.16	39.56	15.61	-9.08	29.79
biphenylene[A]	-3.81	-3.09	-11.04	-8.69	-5.48	-10.05
biphenylene[B]	-1.74	18.73	-19.07	-12.66	8.76	-18.63
acenaphthene[A]	44.07	3.82	-17.18	2.38	-0.63	-15.49
acenaphthene[B]	29.65	-7.23	6.58	-3.20	-9.62	3.24
pyracylene[A]	-10.77	0.47	-4.88	-13.94	-2.79	-7.03
pyracylene[B]	-7.71	16.85	-19.03	-14.21	10.31	-17.55
C_6H_6 (t)	-0.2322	28.7187	[b]	-8.4744	20.6024	[b]
C_8H_8 (t)	38.4236	-11.6512	29.0993	29.2637	-11.5248	24.2375

[b] NICS values could not be calculated at the correct state with N-2 or N+2 π electrons.

C) $NICS(0)_{zz}$ and $NICS(1)_{zz}$

	NICS(0)zz			NICS(1)zz		
	N-2	*N*	*N+2*	*N-2*	*N*	*N+2*
C_6H_6	240.14	-14.50	354.40	186.03	-29.33	281.33
C_5H_5N	92.51	-13.21	357.03	58.41	-28.72	276.60
pyridazine	[b]	-11.52	133.96	[b]	-28.33	93.48
pyrimidine	[b]	-11.05	191.60	[b]	-27.59	138.29
pyrazine	57.66	-12.65	235.77	27.43	-28.51	174.10
triazine	130.77	-7.87	243.99	49.09	-25.92	173.55
$C_7H_7^+$	956.32	-16.29	491.14	801.96	-26.55	394.63
C_4H_4	33.96	109.39	5.51	-11.34	55.50	-23.41
C_8H_8	-20.04	126.99	-39.56	-25.38	97.63	-39.63
$C_5H_5^-$	334.40	-15.93	[b]	264.04	-33.42	[b]
C_4H_4NH	181.48	-12.31	[b]	124.55	-30.96	[b]
C_4H_4O	95.58	-8.80	60.94	54.11	-27.23	33.12
C_4H_4S	84.80	-9.22	[b]	54.83	-28.06	[b]
$C_4H_4P^-$	183.84	-14.98	[b]	145.96	-31.56	[b]
C_4H_4BH	10.13	64.77	-16.19	-12.76	38.23	-30.67
$C_4H_4SiH^+$	6.53	57.75	-15.45	-11.56	37.40	-29.42
$C_4H_4F_2$	19.45	29.61	0.76	-3.28	7.22	-15.78
naphthalene	84.86	-12.38	151.86	54.16	-28.67	109.06
quinoline[A]	110.12	-11.64	141.02	73.59	-28.27	97.02
quinoline[B]	137.15	-14.52	117.54	99.85	-29.56	81.21
anthracene[A]	42.32	-9.72	68.50	61.25	-26.13	39.49
anthracene[B]	61.25	-19.06	79.73	34.51	-34.96	46.71
phenanthrene[A]	89.54	-12.83	178.44	58.92	-29.06	129.49
phenanthrene[B]	82.42	-2.07	139.76	53.70	-20.66	94.95
biphenylene[A]	-4.62	4.97	-14.02	-20.30	-11.66	-26.21
biphenylene[B]	15.43	87.12	-12.11	-25.43	37.60	-48.48
acenaphthene[A]	142.67	33.65	-20.26	97.67	5.73	-41.04
acenaphthene[B]	17.90	-6.15	39.76	-3.16	-23.11	15.02
pyracylene[A]	-18.10	18.44	5.02	-34.63	-1.98	-15.03
pyracylene[B]	-10.26	71.73	-26.46	-33.79	38.72	-46.57
C_6H_6 (t)	-1.5070	99.2615	[b]	-19.6135	65.7673	[b]
C_8H_8 (t)	119.1554	-29.3314	98.9257	91.2020	-32.4397	76.6442

[b] NICS values cannot be calculated at the correct state with N-2 or N+2 π electrons.