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Analysis of the Magnetically Induced Current Density for Molecules Consisting of Annelated Aromatic and Antiaromatic Hydrocarbon Rings

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1 Molecular structures

1.1 Napthalene N

C	−2.4239877771	−0.7092123350	0.0000000000
C	−2.4258236994	0.7028714430	0.0000000000
C	−1.2429156010	1.3958224984	0.0000000000
C	−0.0009446203	0.7141908768	0.0000000000
C	0.0009320449	−0.7142533492	0.0000000000
C	−1.2392792414	−1.3990863487	0.0000000000
C	1.2392743998	1.3990745106	0.0000000000
C	2.4239741948	0.7092492718	0.0000000000
C	2.4258452365	−0.7028539155	0.0000000000
C	1.2429845239	−1.3958427517	0.0000000000
H	−1.2430349924	2.4799169802	0.0000000000
H	−3.3681484659	1.2368190787	0.0000000000
H	−3.3649245625	−1.2456027285	0.0000000000
H	−1.2365780682	−2.4831819152	0.0000000000
H	1.2430596378	−2.4799402260	0.0000000000
H	3.3681892964	−1.2367731361	0.0000000000
H	3.3649166408	1.2456325167	0.0000000000
H	1.2364610534	2.4831695300	0.0000000000

1.2 Pentalene P

C	−1.9664671876	−0.9095562828	0.0000000000
C	−1.6343947468	0.5468291829	0.0000000000
C	−0.2892817529	0.6676054729	0.0000000000
C	0.2893102243	−0.6676895171	0.0000000000
C	−0.8241065699	−1.6296616746	0.0000000000
C	0.8240148296	1.6296928234	0.0000000000
C	1.9664551800	0.9096218748	0.0000000000
C	1.6344453706	−0.5469281795	0.0000000000
H	0.7410694226	2.7059732267	0.0000000000
H	2.9728926300	1.3016263161	0.0000000000
H	2.3730829325	−1.3373943850	0.0000000000
H	−0.7411898652	−2.7058942472	0.0000000000
H	−2.9728565576	−1.3014835890	0.0000000000
H	−2.3729739096	1.3372589784	0.0000000000

1.3 Molecule 1

C	−1.1919985	0.0000000	0.2143763
C	−1.1916189	0.0000000	−1.2070427
C	0.0000000	0.0000000	0.9310596
C	1.1919985	0.0000000	0.2143763
C	1.1916189	0.0000000	−1.2070427
C	0.0000000	0.0000000	−1.9251478
C	2.5992031	0.0000000	0.6206891
C	2.5887457	0.0000000	−1.6755440
C	3.4071823	0.0000000	−0.5952759
C	4.8095815	0.0000000	−0.1911462
C	4.8253972	0.0000000	1.1656841
C	3.4387694	0.0000000	1.6844968
C	−2.5992031	0.0000000	0.6206891
C	−2.5887457	0.0000000	−1.6755440
C	−3.4071823	0.0000000	−0.5952759
C	−3.4387694	0.0000000	1.6844968
C	−4.8095815	0.0000000	−0.1911462
C	−4.8253972	0.0000000	1.1656841
H	3.1827912	0.0000000	2.7349182
H	5.7055999	0.0000000	1.7921594
H	5.6672152	0.0000000	−0.8462555
H	2.8765648	0.0000000	−2.7190699
H	0.0000000	0.0000000	−3.0095842

H	−2.8765648	0.0000000	−2.7190699
H	−5.6672152	0.0000000	−0.8462555
H	−5.7055999	0.0000000	1.7921594
H	−3.1827912	0.0000000	2.7349182
H	0.0000000	0.0000000	2.0144132

1.4 Molecule 2

H	2.6714823	−5.0132990	0.0000000
C	2.1417717	−1.8699621	0.0000000
H	3.2100287	−1.6959719	0.0000000
H	1.6213625	4.2446684	0.0000000
H	0.2900636	−6.1460158	0.0000000
C	0.4931062	−5.0846957	0.0000000
C	1.7185043	−4.5071190	0.0000000
C	1.5003967	−3.0616581	0.0000000
C	1.1310058	−0.7933877	0.0000000
C	1.2996171	0.5895335	0.0000000
H	2.2901971	1.0295639	0.0000000
C	0.1596995	1.3835861	0.0000000
C	−0.0553300	2.8336120	0.0000000
C	0.5601368	4.0382236	0.0000000
H	−2.6714823	5.0132990	0.0000000
H	−1.6213625	−4.2446684	0.0000000
C	−0.5601368	−4.0382236	0.0000000
C	0.0553300	−2.8336120	0.0000000
C	−0.1596995	−1.3835861	0.0000000
C	−1.2996171	−0.5895335	0.0000000
H	−2.2901971	−1.0295639	0.0000000
C	−1.1310058	0.7933877	0.0000000
C	−2.1417717	1.8699621	0.0000000
H	−3.2100287	1.6959719	0.0000000
C	−1.5003967	3.0616581	0.0000000
C	−1.7185043	4.5071190	0.0000000
C	−0.4931062	5.0846957	0.0000000
H	−0.2900636	6.1460158	0.0000000

1.5 Molecule 3

C	2.5170999	0.2032691	0.0000000
C	1.4705771	1.1355879	0.0000000
C	0.1274769	0.7145928	0.0000000
C	−0.1274769	−0.7145928	0.0000000
C	2.2639926	−1.1744425	0.0000000
C	0.9612153	−1.6204081	0.0000000
C	−0.9612153	1.6204081	0.0000000
C	−2.2639926	1.1744425	0.0000000
C	−1.4705771	−1.1355879	0.0000000
C	−2.5170999	−0.2032691	0.0000000
C	−3.8086083	−0.9238234	0.0000000
C	−2.1048129	−2.4639903	0.0000000
C	−3.5531927	−2.2508408	0.0000000
C	−1.8848296	−3.7998307	0.0000000
C	−3.2030966	−4.4830778	0.0000000
C	−4.1963007	−3.5633122	0.0000000
C	2.1048129	2.4639903	0.0000000
C	3.8086083	0.9238234	0.0000000
C	3.5531927	2.2508408	0.0000000
C	1.8848296	3.7998307	0.0000000
C	4.1963007	3.5633122	0.0000000
C	3.2030966	4.4830778	0.0000000
H	5.2577530	3.7578700	0.0000000
H	3.3271308	5.5562921	0.0000000
H	0.9394289	4.3231225	0.0000000

H	4.7748949	0.4364254	0.0000000
H	3.0840914	−1.8828310	0.0000000
H	0.7560655	−2.6818248	0.0000000
H	−0.7560655	2.6818248	0.0000000
H	−3.0840914	1.8828310	0.0000000
H	−4.7748949	−0.4364254	0.0000000
H	−5.2577530	−3.7578700	0.0000000
H	−3.3271308	−5.5562921	0.0000000
H	−0.9394289	−4.3231225	0.0000000

2 Calculated NMR shieldings

At the B3LYP/def2-TZVP level, the ^{1}H NMR shielding for tetramethylsilan (TMS) and H_2O are 31.91 ppm and 31.79 ppm, respectively.

2.1 Naphtalene N

No.	Type	Mult.	Isotropic
1	c	1	53.01685609
2	c	1	53.01952952
3	c	1	50.02630032
4	c	1	42.57079116
5	c	1	42.57328756
6	c	1	50.03291654
7	c	1	50.02778895
8	c	1	53.02403742
9	c	1	53.01986925
10	c	1	50.03301855
11	h	1	23.74556837
12	h	1	24.13143064
13	h	1	24.13161554
14	h	1	23.74656598
15	h	1	23.74678161
16	h	1	24.13229672
17	h	1	24.13202515
18	h	1	23.74574591

2.2 Pentalene P

No.	Type	Mult.	Isotropic
1	c	1	41.49946492
2	c	1	37.14675934
3	c	1	22.45085635
4	c	1	22.45150620
5	c	1	46.16084942
6	c	1	46.15583682
7	c	1	41.47994186
8	c	1	37.13140765
9	h	1	26.96556211
10	h	1	27.08140640
11	h	1	26.92265037
12	h	1	26.96707232
13	h	1	27.08297326
14	h	1	26.92459399

2.3 Molecule 1

No.	Type	Mult.	Isotropic
1	c	2	32.58257530
2	c	2	28.64113832
3	c	1	63.89072304
6	c	1	58.02974379
7	c	2	28.89106309
8	c	2	37.73416717
9	c	2	23.10489412
10	c	2	52.28031428

11	c	2	40.30587916
12	c	2	46.15761879
19	h	2	26.28262303
20	h	2	26.24752071
21	h	2	26.40406223
22	h	2	26.28808397
23	h	1	26.38626378
28	h	1	26.20188799

2.4 Molecule 2

No.	Type	Mult.	Isotropic
1	h	2	26.47919378
2	c	2	39.00653360
3	h	2	26.29375921
4	h	2	26.44060862
5	h	2	26.30048536
6	c	2	38.66223512
7	c	2	53.61460671
8	c	2	20.49532800
9	c	2	24.06033770
10	c	2	61.27065615
11	h	2	26.29120791
12	c	2	37.59372503
13	c	2	28.21658244
14	c	2	48.67289106

2.5 Molecule 3

No.	Type	Mult.	Isotropic
1	c	2	27.94610710
2	c	2	38.44682643
3	c	2	45.34415878
5	c	2	56.29664215
6	c	2	55.66062778
11	c	2	37.08845813
12	c	2	25.88216847
13	c	2	19.25610605
14	c	2	42.68235102
15	c	2	38.15818184
16	c	2	51.52530803
23	h	2	26.73675520
24	h	2	26.58254771
25	h	2	26.43147339
26	h	2	26.40822108
27	h	2	25.68347899
28	h	2	25.45164278

3 Current strengths

Current strengths calculated for the molecular structure of molecule **1** with phenyl substituents. The molecular structure repored in Ref. 1 of the paper was used. The current density was calculated at the B3LYP/def2-TZVP level.

Plane	Diatropic	Paratropic	Net Current
b:	9.92	-7.46	2.46
c:	5.14	-14.49	-9.35
d:	8.32	-8.58	-0.27
e:	5.53	-15.16	-9.63
g:	8.30	-9.23	-0.93

Current strengths calculated for the molecular structure of molecule **3** with phenyl substituents. The molecular structure repored in Ref. 1 of the paper was used. The current density was calculated at the B3LYP/def2-TZVP level.

Plane	Diatropic	Paratropic	Net Current
a:	8.06	-7.80	0.26
b:	11.38	-7.63	3.75

c:	13.40	−1.94	11.46
d:	4.13	−21.31	−17.18
e:	4.87	−19.23	−14.36
f:	9.10	−12.93	−3.84
g:	4.90	−19.13	−14.23