Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Magnetically induced ring currents in naphthalene-fused heteroporphyrinoids

Markus Rauhalahti,[a] Dage Sundholm,[a] and Mikael P. Johansson[b,a]

1 Ring-current strengths

Ring currents and pathways computed using three different functionals with varying amount of Hartree–Fock exchange: BP (0%), PBE0 (25%), and BHandHLYP (50%). See main paper for computational details.

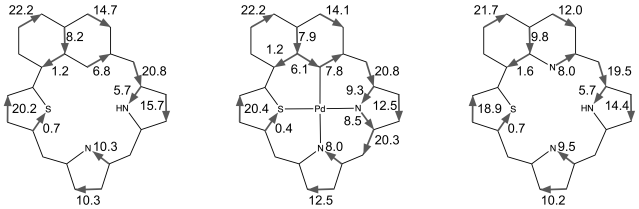

Figure S1 Integrated current strengths (in nA/T) and current pathways of (a) **1**, (b) **2**, and (c) **3**, calculated using the BP functional.

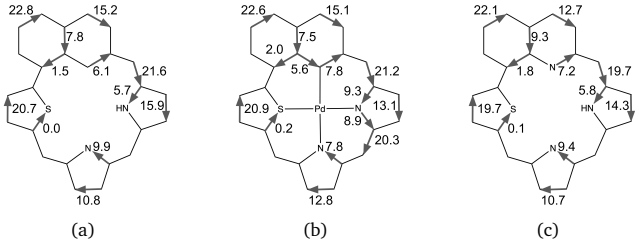

Figure S2 Integrated current strengths (in nA/T) and current pathways of (a) **1**, (b) **2**, and (c) **3**, calculated using the PBE0 functional.

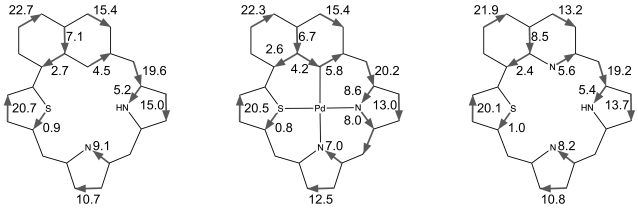

Figure S3 Integrated current strengths (in nA/T) and current pathways of (a) **1**, (b) **2**, and (c) **3**, calculated using the BHandHLYP functional.

[a] *University of Helsinki, Department of Chemistry, Faculty of Science, P.O. Box 55 (A.I. Virtanens plats 1), FI-00014 University of Helsinki, Finland, Markus.Rauhalahti@helsinki.fi, Dage.Sundholm@helsinki.fi*

[b] *CSC – IT Center for Science Ltd., P.O. Box 405, FI-02101 Espoo, Finland, mikael.johansson@csc.fi*

2 Cartesian coordinates of the molecules

Standard XYZ format in Ångström units.

2.1 Molecule 1

```
44
1, optimized at RI-BP86-D3(BJ)/def2-SVP level
S    -1.5606620   -0.3809090    0.0955140
N     0.6224920   -2.1293530    0.0703760
N     2.0026620    0.4653790   -0.0108990
H     1.0517380    0.0783040    0.0682680
C    -3.0814520    0.4903290   -0.0693770
C    -4.1384280   -0.4412660   -0.2194700
H    -5.1853010   -0.1424200   -0.3551010
C    -3.7334800   -1.7801170   -0.1914210
H    -4.4171480   -2.6344400   -0.2919400
C    -2.3380400   -1.9494570   -0.0342670
C    -1.5965810   -3.1491150   -0.0104410
C    -0.1991780   -3.2312610    0.0433910
C     0.5886580   -4.4658530    0.0275920
H     0.1819840   -5.4847810    0.0074080
C     1.9045780   -4.0767610    0.0345740
H     2.8000530   -4.7107970    0.0184850
C     1.8944960   -2.6085380    0.0507720
C     3.0503560   -1.7933560    0.0111590
C     3.0910850   -0.3974480   -0.0311100
C     4.2780000    0.4210130   -0.1002070
H     5.2983500    0.0229020   -0.1346610
C     3.8814640    1.7370650   -0.1114520
H     4.5155230    2.6299290   -0.1580560
C     2.4311530    1.7903510   -0.0502340
C     1.7456440    3.0065630   -0.0107190
C     0.3640360    3.3797350    0.0619090
C    -0.7181140    2.4841610   -0.0808920
H    -0.4753890    1.4594000   -0.3712420
C    -2.0718060    2.8658070    0.0617680
C    -3.1994190    1.9359080    0.0100010
C    -4.5039770    2.4813310    0.0927230
H    -5.3668710    1.8035920    0.0621180
C    -4.7449620    3.8508330    0.2571890
H    -5.7813370    4.2137940    0.3245180
C    -3.6763450    4.7444640    0.3660720
H    -3.8558920    5.8189630    0.5235420
C    -2.3478840    4.2790080    0.2773970
C    -1.2489050    5.1925500    0.3839550
H    -1.4755520    6.2577730    0.5458780
C     0.0549350    4.7673610    0.2935040
H     0.8827630    5.4861540    0.3940560
H    -2.1686690   -4.0881130   -0.0700500
H     4.0259960   -2.3001680   -0.0088740
H     2.4400290    3.8617650    0.0024450
```

2.2 Molecule 2

```
43
2, optimized at RI-BP86-D3(BJ)/def2-SVP level
Pd    0.0987150    0.1235990    0.1478320
S    -2.0316310   -0.1340380    0.6683090
N     0.2122200   -2.0456780    0.1207090
N     2.1242260    0.2034500   -0.0526630
C    -3.1138590    0.9821640   -0.1112400
C    -4.1889100    0.2651880   -0.6584050
H    -5.0311070    0.7553510   -1.1641150
C    -4.0432230   -1.1388410   -0.5902510
H    -4.7613830   -1.8514750   -1.0187630
C    -2.8258790   -1.5545170   -0.0231470
C    -2.1858510   -2.8022750    0.0329770
C    -0.8052790   -3.0024120    0.1480620
C    -0.2236810   -4.3352010    0.1754320
H    -0.8063490   -5.2638600    0.2006840
C     1.1361680   -4.1801460    0.1457950
H     1.9128010   -4.9543360    0.1402490
C     1.3959430   -2.7500220    0.0935520
C     2.6785340   -2.2091770   -0.0354490
C     3.0023700   -0.8512190   -0.1288680
C     4.3564580   -0.3379880   -0.2727210
H     5.2509430   -0.9656440   -0.3641000
C     4.2705420    1.0317400   -0.2609970
H     5.0793680    1.7680330   -0.3371300
C     2.8627330    1.3578840   -0.1087280
C     2.3372420    2.6274820    0.0336800
C     0.9825800    3.0472340    0.1807890
C    -0.2036200    2.2242320    0.1360690
C    -1.4796540    2.9432240    0.1445790
C    -2.8299260    2.3839690   -0.0312080
C    -3.9752910    3.2114570   -0.1363910
H    -4.9529500    2.7242810   -0.2525840
C    -3.9151670    4.5988560   -0.0307530
H    -4.8285260    5.2079020   -0.0958090
C    -2.6708580    5.1819170    0.1905880
H    -2.5759100    6.2735590    0.2950420
C    -1.4904690    4.4088100    0.2688500
C    -0.2759260    5.1355070    0.4330680
H    -0.3218130    6.2263400    0.5679670
C     0.9119860    4.4776440    0.3647350
H     1.8589420    5.0326950    0.4427580
H     3.5143950   -2.9213810   -0.0778930
H     3.0858490    3.4339440    0.0278330
H    -2.8012930   -3.7007150   -0.1294180
```

2.3 Molecule 3

```
3, optimized at RI-BP86-D3(BJ)/def2-SVP level
S     0.1124823    1.3607543    0.0000000
N     2.9259659    0.7973230    0.0000000
N     1.7316024   -1.7581160    0.0000000
H     1.4801492   -0.7561674    0.0000000
C    -1.4837123    2.0936717    0.0000000
C    -1.3841951    3.5073934    0.0000000
H    -2.2584687    4.1694338    0.0000000
C    -0.0738243    3.9813307    0.0000000
H     0.2023014    5.0451057    0.0000000
C     0.8946664    2.9499118    0.0000000
C     2.2905725    3.1419441    0.0000000
C     3.2545437    2.1279385    0.0000000
C     4.7078752    2.3055621    0.0000000
H     5.2373014    3.2666190    0.0000000
C     5.2438559    1.0406716    0.0000000
H     6.3025934    0.7523810    0.0000000
C     4.1027118    0.1193548    0.0000000
C     4.1697521   -1.2938379    0.0000000
C     3.0651456   -2.1461143    0.0000000
C     3.0901513   -3.5902175    0.0000000
H     4.0067086   -4.1908711    0.0000000
C     1.7885431   -4.0283475    0.0000000
H     1.4257387   -5.0626785    0.0000000
C     0.9085278   -2.8680660    0.0000000
C    -0.4781046   -3.0206805    0.0000000
C    -1.6338860   -2.1724779    0.0000000
C    -2.7541461   -0.1169550    0.0000000
C    -2.7158256    1.3396895    0.0000000
C    -3.9477315    2.0399076    0.0000000
H    -3.9363921    3.1373052    0.0000000
C    -5.1876797    1.3918879    0.0000000
H    -6.1121076    1.9881458    0.0000000
C    -5.2472706   -0.0049150    0.0000000
H    -6.2149427   -0.5300190    0.0000000
C    -4.0592196   -0.7616097    0.0000000
C    -4.0786246   -2.1897397    0.0000000
H    -5.0473243   -2.7132882    0.0000000
C    -2.8965698   -2.8815277    0.0000000
H    -2.8879592   -3.9812520    0.0000000
H     2.6424139    4.1861499    0.0000000
H     5.1602486   -1.7705434    0.0000000
H    -0.7493009   -4.0873553    0.0000000
N    -1.5965660   -0.8177018    0.0000000
```

3 NMR shielding constants at BP level

3.1 Molecule 1

# NO.	TYPE	ISOTROPIC
1	S	206.01933632
2	N	-22.54259583
3	N	105.03597948
4	H	33.31148450
5	C	26.34591268
6	C	53.86443679
7	H	20.24745623
8	C	50.02286186
9	H	21.35782371
10	C	35.29507336
11	C	62.62873363
12	C	24.37144648
13	C	43.27216180
14	H	22.20542247
15	C	44.99489398
16	H	22.30900351
17	C	20.97414280
18	C	77.66116372
19	C	35.73394807
20	C	51.53323556
21	H	22.14507773
22	C	45.29524774
23	H	21.98654213
24	C	40.52471050
25	C	67.84278054
26	C	45.05181247
27	C	56.52080529
28	H	34.22523274
29	C	52.93824481
30	C	51.37205034
31	C	53.97201078
32	H	19.78789382
33	C	57.21862061
34	H	21.92008073
35	C	53.73591369
36	H	21.65777280
37	C	45.57426735
38	C	46.85724682
39	H	21.70431521
40	C	46.14980061
41	H	21.60156400
42	H	20.91192726
43	H	21.73519299
44	H	21.24175600

3.2 Molecule 2

1	Pd	131.65165551
2	S	266.21610935
3	N	58.39843414
4	N	46.94575209
5	C	34.55225062
6	C	57.72285032
7	H	21.55095540
8	C	53.63973287
9	H	21.99460550
10	C	31.19771755
11	C	68.98129750
12	C	28.22972397
13	C	45.44968789
14	H	22.35493871
15	C	44.74530161
16	H	22.26213055
17	C	31.68105859
18	C	76.14148441
19	C	33.41246936
20	C	46.51942289
21	H	22.23134082
22	C	46.02056056
23	H	22.14160669
24	C	38.64689144
25	C	50.56212939
26	C	43.84298460
27	C	8.84841226
28	C	43.29963935
29	C	49.86065078
30	C	53.87756659
31	H	20.06151785
32	C	56.77739129
33	H	22.03029692
34	C	49.47430323
35	H	21.59680239
36	C	42.11150383
37	C	48.67609319
38	H	21.88225277
39	C	39.96081956
40	H	21.42726048
41	H	21.75409668
42	H	20.92168928
43	H	21.05296347

3.3 Molecule 3

1	S	180.88590940
2	N	-29.73809193
3	N	97.89244949
4	H	31.70192869
5	C	26.01109257
6	C	53.56125030
7	H	20.36251439
8	C	45.75126256
9	H	21.36598590
10	C	28.76132368
11	C	57.50477121
12	C	24.85425659
13	C	43.50685648
14	H	22.33003140
15	C	46.02260606
16	H	22.48723223
17	C	20.64115302
18	C	75.59991624
19	C	34.94966642
20	C	50.02885543
21	H	22.27945396
22	C	44.77851240
23	H	22.21534960
24	C	39.50722786
25	C	69.85204758
26	C	29.20136398
27	C	35.21817985
28	C	50.57215577
29	C	54.71908629
30	H	19.95069159
31	C	57.91955382
32	H	22.17190925
33	C	55.93534341
34	H	22.05679401
35	C	50.86135583
36	C	42.48842911
37	H	21.91740334
38	C	46.06325304
39	H	21.84949691
40	H	20.88419747
41	H	21.97407084
42	H	21.49484078
43	N	-61.90348368