Electronic Supplementary Material (ESI) for RSC Advances.


# Electronic Supplementary Information to

## On Splitting of the NICS(1) Magnetic Aromaticity Index

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**Table 1SI**. Dihedral angles τ and *T*=RMSD(τ) of the molecules studied

| molecule | $\tau_1$ | $\tau_2$ | $\tau_3$ | $\tau_4$ | $\tau_5$ | $\tau_6$ | $\tau_7$ | $\tau_8$ | *T* |
|---|---|---|---|---|---|---|---|---|---|
| (**1**)A5 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | | | | 0.00 |
| (**1**)A | -9.5073 | 9.4035 | 0.0000 | -9.4035 | 9.5073 | 0.0000 | | | 7.72 |
| (**2**)A5 | -8.5265 | 12.8257 | -12.8277 | 8.5355 | -0.0063 | | | | 8.89 |
| (**2**)A | 0.0049 | -0.0048 | 0.0049 | -0.0048 | 0.0049 | -0.0049 | | | 0.00 |
| (**2**)B | -6.2272 | 6.1593 | -0.0083 | -6.1479 | 6.2283 | -0.0037 | | | 5.05 |
| (**3**)A | -14.9993 | -1.4481 | 10.1681 | -1.4488 | -14.9988 | 22.4614 | | | 13.30 |
| (**3**)B | -0.9718 | -13.8143 | 20.7826 | -13.8140 | -0.9723 | 8.6766 | | | 12.18 |
| (**3**)C | 0.3271 | -2.3873 | 3.3402 | -2.3868 | 0.3267 | 0.7497 | | | 1.97 |
| -4 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | | | 0.00 |
| -5 | -54.6416 | 54.6253 | -54.6262 | 54.6422 | -54.6264 | 54.6267 | | | 54.63 |
| -6 | -103.7096 | 38.2288 | 38.1808 | -103.6805 | 103.7086 | -38.2265 | -38.1822 | 103.6803 | 78.14 |
| (**7**)A5 | 0.2387 | 0.0000 | -0.2387 | 0.3862 | -0.3862 | | | | 0.29 |
| (**7**)A | -9.3834 | 9.3003 | 0.0000 | -9.3003 | 9.3834 | 0.0000 | | | 7.63 |
| (**7**)B | 9.1033 | 0.4678 | -9.4838 | 9.1337 | 0.4291 | -9.6345 | | | 7.63 |
| (**7**)C | 9.4220 | 0.0035 | -9.4633 | 9.5991 | -0.0719 | -9.4943 | | | 7.75 |
| (**8**)A | -10.2122 | -0.6930 | 6.4788 | -0.6930 | -10.2122 | 15.2109 | | | 8.97 |
| (**9**)A | -9.9856 | 15.1438 | -10.3068 | -0.2499 | 6.1963 | -0.7949 | | | 8.89 |
| (**9**)B | -0.4827 | 6.4595 | -0.9227 | -9.9596 | 15.1381 | -10.3519 | | | 8.93 |
| (**10**)A | -15.8886 | 18.4061 | -9.3599 | -3.6389 | 7.0118 | 3.1578 | | | 11.19 |
| (**10**)B | -0.2309 | 7.6904 | -1.5809 | -11.2748 | 17.8445 | -12.5917 | | | 10.53 |
| (**11**)A | -13.9368 | 16.9561 | -9.7252 | -1.0758 | 4.7443 | 3.0193 | | | 10.08 |
| (**11**)B | -0.3052 | 7.3167 | -1.5702 | -10.5243 | 16.7438 | -11.7778 | | | 9.88 |
| (**12**)A | -9.0739 | 14.7888 | -10.4400 | -0.4993 | 7.0226 | -1.9617 | | | 8.79 |
| (**12**)B | -0.2287 | 6.3278 | -1.0377 | -9.7610 | 15.0258 | -10.4700 | | | 8.87 |
| (**13**)A | -11.6353 | 16.3284 | -9.8568 | -2.3193 | 7.8408 | -0.5767 | | | 9.72 |
| (**13**)B | 0.5880 | 6.8917 | -1.9855 | -9.8183 | 16.3360 | -12.1846 | | | 9.69 |
| -14 | 0.0306 | -0.0279 | 0.0034 | 0.0181 | -0.0153 | -0.0090 | | | 0.02 |
| -15 | 0.0901 | -0.1886 | 0.0345 | 0.2174 | -0.3156 | 0.1616 | | | 0.19 |
| -16 | 0.3479 | -0.3525 | -0.0502 | 0.4550 | -0.4593 | 0.0579 | | | 0.33 |
| -17 | -0.0973 | 0.1213 | -0.1276 | 0.1097 | -0.0848 | 0.0786 | | | 0.10 |
| (**18**)5A | -0.3025 | 0.2704 | -0.1341 | -0.0529 | 0.2196 | | | | 0.22 |
| (**18**)A | 9.2161 | -0.1969 | -9.4696 | 10.0892 | -0.8155 | -8.7490 | | | 7.68 |
| (**18**)B | 9.7675 | -0.0191 | -9.4005 | 9.1518 | 0.7560 | -10.2281 | | | 7.88 |
| (**18**)C | 9.3706 | 0.0551 | -9.4550 | 9.5450 | -0.0221 | -9.4854 | | | 7.73 |
| (**18**)D | 9.4164 | 0.0251 | -9.4171 | 9.4895 | 0.0566 | -9.5553 | | | 7.73 |
| (**18**)E | 9.4335 | -0.4769 | -8.6517 | 8.7821 | 0.4194 | -9.4878 | | | 7.43 |

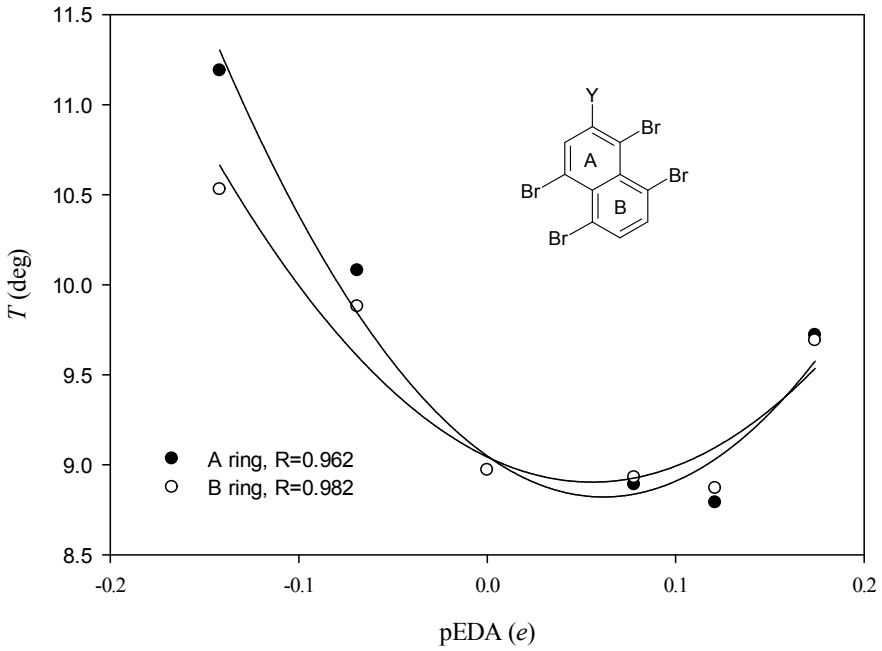



**Figure 1SI**. Quadratic correlations between the ring deformation in substituted 1,4,5,8-tetrabromonaphthalene (**8**) and the pEDA substituent effect descriptor

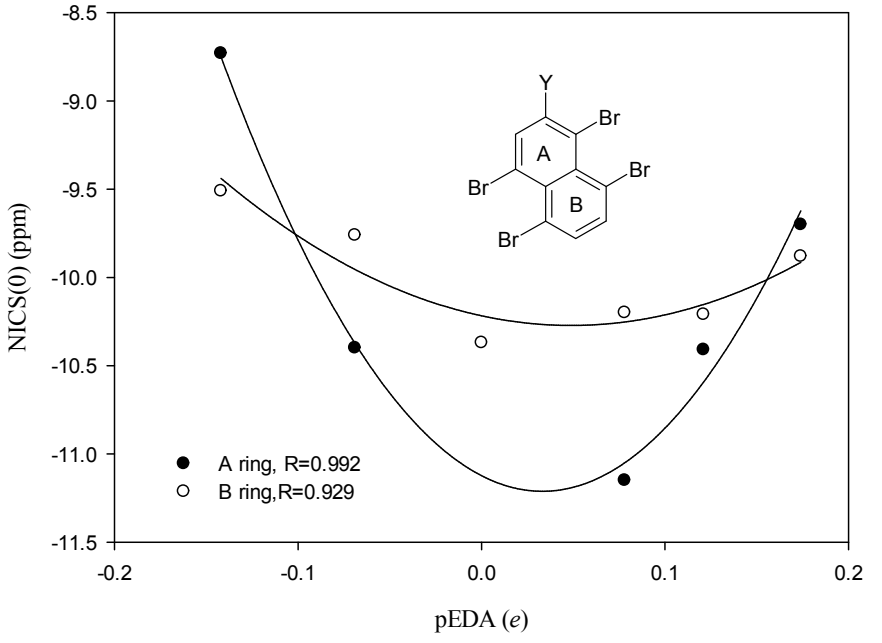



**Figure 2SI**. Quadratic correlations between NICS(0) index in substituted 1,4,5,8-tetrabromonaphthalene (**8**) and the pEDA substituent effect descriptor

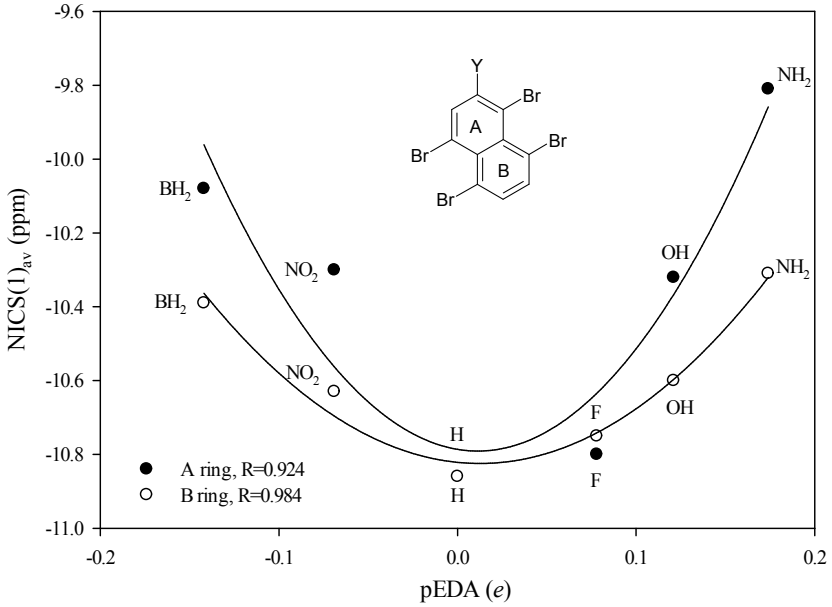



**Figure 3SI**. Quadratic correlations between NICS(1)$_{av}$ index in substituted 1,4,5,8-tetrabromonaphthalene (**8**) and the pEDA substituent effect descriptor

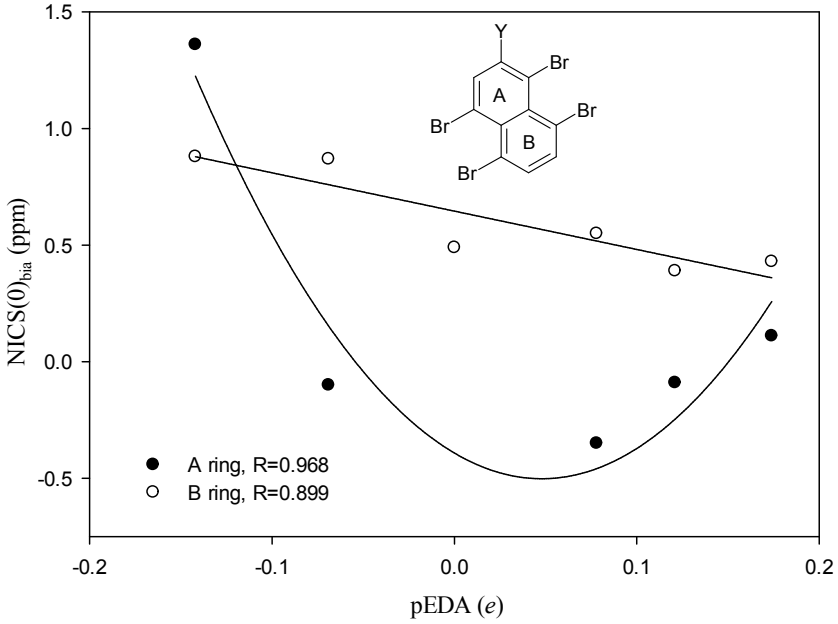



**Figure 4SI**. Quadratic correlations between NICS(0)$_{bia}$ index in substituted 1,4,5,8-tetrabromonaphthalene (**8**) and the pEDA substituent effect descriptor

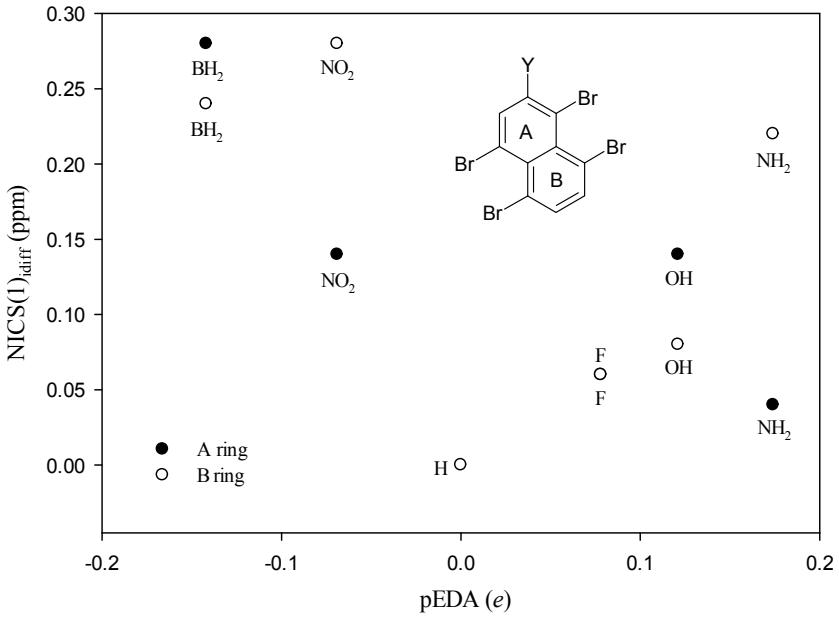
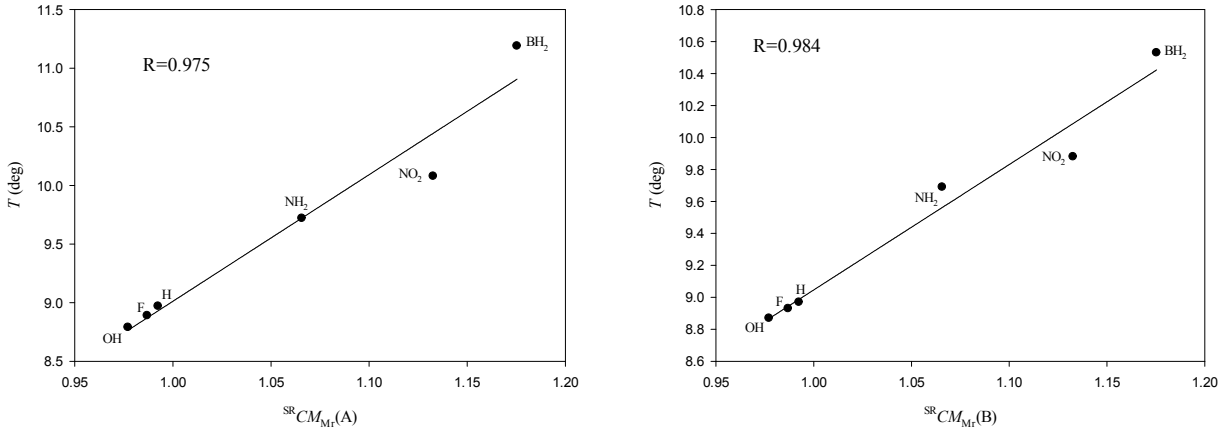



**Figure 5SI**. Plot of NICS(1)$_{diff}$ index in substituted 1,4,5,8-tetrabromonaphthalene (**8**) and the pEDA substituent effect descriptor




(A) (B)

**Figure 6SI**. Linear correlation between $^{SR}CM_{Mr}$ chirality measure and deformation *T* of the ring A (a) and B (b) in the series of the monosubstituted tetrabromonaphthalenes