

## **Supporting Information**

### **Theoretical studies on carcinogenic activity of diol epoxide derivatives of PAH: proton affinity and aromaticity as decisive descriptors**

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(i) **Table 1.** SCF energy, Zero point energy correction (ZPE) and Enthalpy values of bay-region diol epoxides (bDE). All values in a.u.

| Name of parent PAH                     | E            | ZPE      | H            |
|----------------------------------------|--------------|----------|--------------|
| Dibenzo[a,i]pyrene                     | -1149.894237 | 0.337812 | -1149.536497 |
| Dibenzo[a,h]pyrene                     | -1149.894186 | 0.337873 | -1149.536399 |
| Benzo[a]naphtho[8,1,2-cde]naphthacene. | -1303.525009 | 0.384668 | -1303.117686 |
| Benzo[a]naphtho[2,1,8-hij]naphthacene  | -1303.535373 | 0.384399 | -1303.128352 |
| Tribenzo[a,e,i]pyrene                  | -1303.541588 | 0.384581 | -1303.134136 |
| Dibenzo[a,l]pyrene                     | -1149.864310 | 0.337672 | -1149.506860 |
| Tribenzo[a,c,j]naphthacene             | -1380.945621 | 0.418305 | -1380.502442 |
| Benzo[a]pyrene                         | -996.250371  | 0.291169 | -995.942086  |
| Dibenzo[a,c]naphthacene                | -1227.287402 | 0.371734 | -1226.893740 |
| Dibenzo[a,e]pyrene                     | -1149.897341 | 0.337883 | -1149.539418 |
| Benzo[a]anthracene                     | -920.007432  | 0.278045 | -919.712913  |
| Dibenzo[a,h]anthracene                 | -1073.659128 | 0.324931 | -1073.314980 |
| Dibenzo[a,j]anthracene                 | -1073.658737 | 0.324958 | -1073.314571 |
| Dibenzo[a,c]anthracene                 | -1073.647877 | 0.325270 | -1073.303407 |
| Benzo[g]chrysene                       | -1073.641368 | 0.325548 | -1073.296798 |
| Benzo[c]chrysene                       | -1073.651721 | 0.325413 | -1073.307234 |
| chrysene                               | -920.015000  | 0.278367 | -919.720135  |

(ii) **Table 2.** SCF energy, Zero point energy correction (ZPE) and Enthalpy values of protonated bay-region diol epoxides (bDEH<sup>+</sup>). All values in a.u.

| Name of parent PAH                     | E            | ZPE      | H            |
|----------------------------------------|--------------|----------|--------------|
| Dibenzo[a,i]pyrene                     | -1150.292406 | 0.350114 | -1149.921610 |
| Dibenzo[a,h]pyrene                     | -1150.289676 | 0.350023 | -1149.918950 |
| Benzo[a]naphtho[8,1,2-cde]naphthacene. | -1303.916782 | 0.396372 | -1303.496987 |
| Benzo[a]naphtho[2,1,8-hij]naphthacene  | -1303.932450 | 0.396518 | -1303.512553 |
| Tribenzo[a,e,i]pyrene                  | -1303.939496 | 0.396912 | -1303.518987 |
| Dibenzo[a,l]pyrene                     | -1150.261205 | 0.349735 | -1149.890991 |
| Tribenzo[a,c,j]naphthacene             | -1381.339000 | 0.430224 | -1380.883102 |
| Benzo[a]pyrene                         | -996.639826  | 0.303199 | -996.318701  |
| Dibenzo[a,c]naphthacene                | -1227.677396 | 0.383473 | -1227.271204 |
| Dibenzo[a,e]pyrene                     | -1150.288921 | 0.350112 | -1149.918018 |
| Benzo[a]anthracene                     | -920.390704  | 0.289862 | -920.083554  |
| Dibenzo[a,h]anthracene                 | -1074.044633 | 0.336866 | -1073.687752 |
| Dibenzo[a,j]anthracene                 | -1074.042441 | 0.336670 | -1073.685700 |
| Dibenzo[a,c]anthracene                 | -1074.031954 | 0.336969 | -1073.674958 |
| Benzo[g]chrysene                       | -1074.027635 | 0.337342 | -1073.670409 |
| Benzo[c]chrysene                       | -1074.031336 | 0.336848 | -1073.674501 |
| chrysene                               | -920.389685  | 0.289923 | -920.082361  |

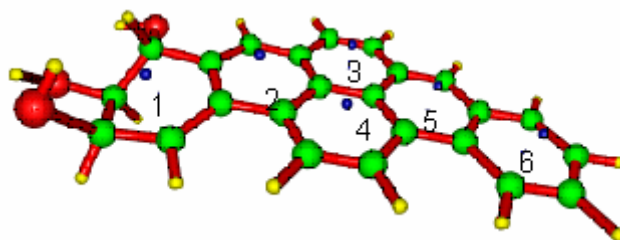
(iii) **Table 3.** SCF energy, Zero point energy correction (ZPE) and Enthalpy values of nonbay-region diol epoxides (nbDE). All values in a.u.

| Name of parent PAH                     | E            | ZPE      | H            |
|----------------------------------------|--------------|----------|--------------|
| Dibenzo[a,i]pyrene                     | -1149.890621 | 0.338020 | -1149.532790 |
| Dibenzo[a,h]pyrene                     | -1149.890478 | 0.338037 | -1149.532651 |
| Benzo[a]naphtho[8,1,2-cde]naphthacene. | -1303.546388 | 0.384512 | -1303.139097 |
| Benzo[a]naphtho[2,1,8-hij]naphthacene  | -1303.532284 | 0.384599 | -1303.125180 |
| Tribenzo[a,e,i]pyrene                  | -1303.537843 | 0.384840 | -1303.130272 |
| Dibenzo[a,l]pyrene                     | -1149.874525 | 0.337775 | -1149.517028 |
| Tribenzo[a,c,j]naphthacene             | -1380.942657 | 0.418596 | -1380.499358 |
| Benzo[a]pyrene                         | -996.246893  | 0.291398 | -995.938517  |
| Dibenzo[a,c]naphthacene                | -1227.310758 | 0.371706 | -1226.916969 |
| Dibenzo[a,e]pyrene                     | -1149.893470 | 0.338142 | -1149.535435 |
| Benzo[a]anthracene                     | -920.020492  | 0.278255 | -919.725794  |
| Dibenzo[a,h]anthracene                 | -1073.656187 | 0.325173 | -1073.311933 |
| Dibenzo[a,j]anthracene                 | -1073.656118 | 0.325154 | -1073.311871 |
| Dibenzo[a,c]anthracene                 | -1073.666371 | 0.324999 | -1073.322002 |
| Benzo[g]chrysene                       | -1073.638735 | 0.325140 | -1073.294577 |
| Benzo[c]chrysene                       | -1073.649360 | 0.325608 | -1073.304834 |
| chrysene                               | -920.011475  | 0.278589 | -919.716526  |

(iv) **Table 4.** SCF energy, Zero point energy correction (ZPE) and Enthalpy values of protonated nonbay-region diol epoxides (nbDEH<sup>+</sup>). All values in a.u.

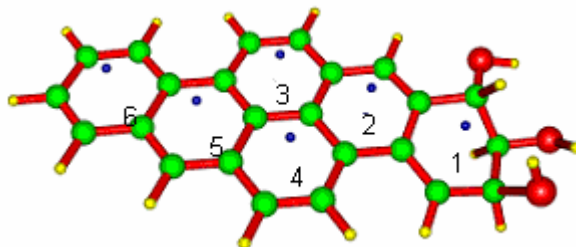
| Name of parent PAH                     | E            | ZPE      | H            |
|----------------------------------------|--------------|----------|--------------|
| Dibenzo[a,i]pyrene                     | -1150.266216 | 0.349689 | -1149.895848 |
| Dibenzo[a,h]pyrene                     | -1150.264899 | 0.349734 | -1149.894489 |
| Benzo[a]naphtha[8,1,2-cde]naphthacene. | -1303.934926 | 0.396560 | -1303.514758 |
| Benzo[a]naphtha[2,1,8-hij]naphthacene  | -1303.921304 | 0.396476 | -1303.501538 |
| Tribenzo[a,e,i]pyrene                  | -1303.915508 | 0.396556 | -1303.495352 |
| Dibenzo[a,l]pyrene                     | -1150.251884 | 0.349447 | -1149.881926 |
| Tribenzo[a,c,j]naphthacene             | -1381.335914 | 0.430643 | -1380.879796 |
| Benzo[a]pyrene                         | -996.616981  | 0.303025 | -996.296095  |
| Dibenzo[a,c]naphthacene                | -1227.690387 | 0.383463 | -1227.283949 |
| Dibenzo[a,e]pyrene                     | -1150.267277 | 0.349740 | -1149.896735 |
| Benzo[a]anthracene                     | -920.393090  | 0.289967 | -920.085794  |
| Dibenzo[a,h]anthracene                 | -1074.038944 | 0.336984 | -1073.682050 |
| Dibenzo[a,j]anthracene                 | -1074.041214 | 0.337068 | -1073.684236 |
| Dibenzo[a,c]anthracene                 | -1074.041140 | 0.336794 | -1073.684111 |
| Benzo[g]chrysene                       | -1074.020369 | 0.336842 | -1073.663707 |
| Benzo[c]chrysene                       | -1074.029380 | 0.337248 | -1073.672356 |
| chrysene                               | -920.383909  | 0.290197 | -920.076439  |

(v) **NICS(1) and NICS(1)<sub>zz</sub> values.** Figure showing the NICS points of bay-region DEH<sup>+</sup> system is shown along with numbering used for the aromatic rings. The same numbering scheme is used for the corresponding nonbay-region DEH<sup>+</sup> systems.



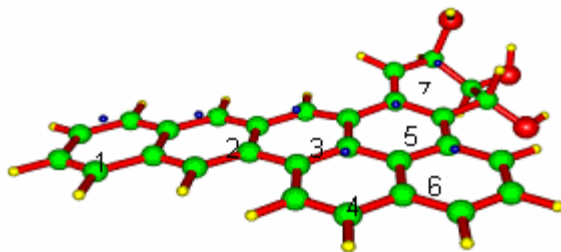
dibenzo[a,i]pyrene (1)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -1.08             | 6.48                  | -0.56              | 9.87                  |
| 2    | -3.47             | -0.03                 | -1.86              | 3.04                  |
| 3    | -7.09             | -5.10                 | -2.54              | 0.46                  |
| 4    | -12.08            | -22.09                | -3.47              | -2.34                 |
| 5    | -8.78             | -11.64                | -5.51              | -8.46                 |
| 6    | -12.90            | -24.32                | -8.43              | -18.79                |
| Sum  | -45.40            | -56.71                | -22.37             | -16.24                |



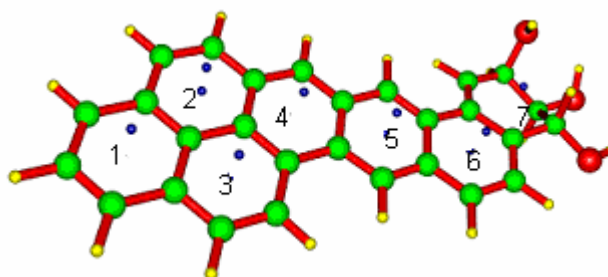
dibenzo[a,h]pyrene (2)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -0.56             | 10.07                 | -0.72              | 8.92                  |
| 2    | -2.50             | 0.94                  | -2.12              | 2.45                  |
| 3    | -8.18             | -16.80                | -3.45              | -2.09                 |
| 4    | -6.85             | -12.75                | -3.48              | -0.45                 |
| 5    | -8.63             | -17.77                | -5.90              | -9.66                 |
| 6    | -10.55            | -25.14                | -8.32              | -18.32                |
| Sum  | -37.27            | -61.46                | -24.00             | -19.15                |



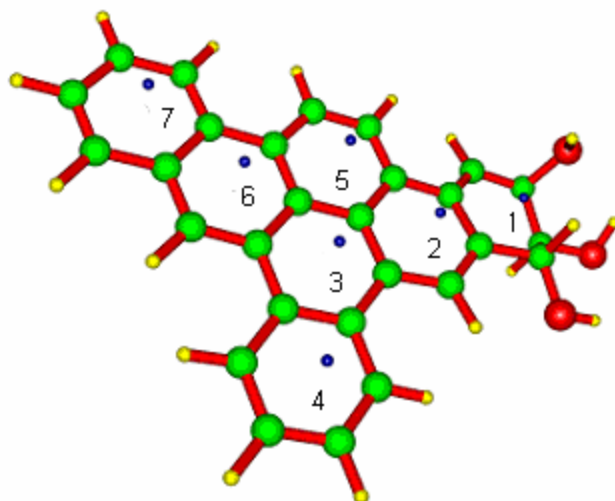
benzo[a]naphtho[8,1,2-cde]naphthacene (**3**)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -10.70            | -25.02                | -1.03              | 8.91                  |
| 2    | -11.60            | -26.55                | -3.66              | -2.65                 |
| 3    | -6.77             | -11.77                | -3.85              | -3.07                 |
| 4    | -8.70             | -18.48                | -8.75              | -18.50                |
| 5    | -0.50             | 7.89                  | -3.90              | -3.16                 |
| 6    | -6.10             | -10.42                | -10.21             | -23.38                |
| 7    | -2.32             | 5.27                  | -9.66              | -22.38                |
| Sum  | -46.70            | -79.08                | -41.07             | -64.25                |

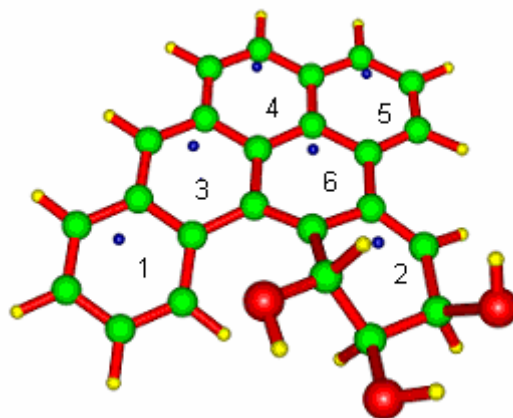


benzo[a]naphtho[2,1,8-hij]naphthacene (**4**)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -11.90            | -28.69                | -10.08             | -23.23                |
| 2    | -6.22             | -11.16                | -4.38              | -5.70                 |
| 3    | -8.90             | -18.94                | -6.14              | -10.60                |
| 4    | -8.40             | -17.01                | -5.35              | -7.96                 |
| 5    | -8.35             | -16.89                | -3.88              | -3.48                 |
| 6    | -2.41             | 1.23                  | -2.56              | 0.43                  |
| 7    | -1.09             | 9.62                  | -0.63              | 10.28                 |
| Sum  | -47.27            | -81.84                | -33.03             | -40.25                |

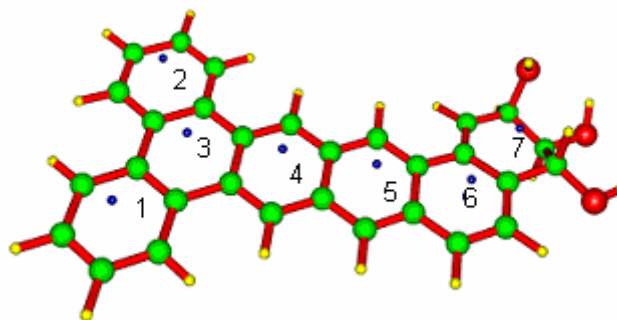


| tribenzo[a,e,i]pyrene (5) |                   |                       |                    |                       |
|---------------------------|-------------------|-----------------------|--------------------|-----------------------|
| Ring                      | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|                           | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1                         | -1.02             | 10.33                 | -0.83              | 8.91                  |
| 2                         | -2.19             | 2.62                  | -2.31              | 2.05                  |
| 3                         | -4.39             | -4.34                 | -1.39              | 4.69                  |
| 4                         | -9.49             | -21.64                | -9.61              | -22.09                |
| 5                         | -9.62             | -20.89                | -3.78              | -2.92                 |
| 6                         | -7.68             | -14.70                | -5.03              | -6.78                 |
| 7                         | -10.80            | -25.92                | -8.09              | -17.72                |
| Sum                       | -45.22            | -74.54                | -31.05             | -33.85                |



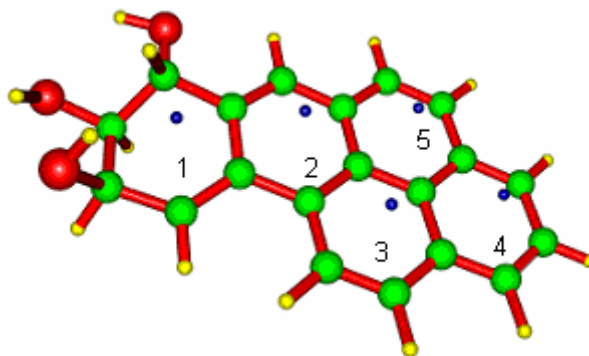
| dibenzo[a,l]pyrene (6) |                   |                       |                    |                       |
|------------------------|-------------------|-----------------------|--------------------|-----------------------|
| Ring                   | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|                        | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1                      | -9.84             | -18.13                | -9.69              | -17.32                |
| 2                      | -3.57             | 7.19                  | -3.16              | 6.99                  |
| 3                      | -5.15             | -6.99                 | -1.80              | 3.67                  |
| 4                      | -7.55             | -14.96                | -8.13              | -14.66                |
| 5                      | -11.04            | -24.75                | -3.76              | -0.95                 |

|     |        |        |        |        |
|-----|--------|--------|--------|--------|
| 6   | -1.59  | 6.00   | -2.88  | 2.12   |
| Sum | -38.74 | -51.64 | -29.42 | -20.14 |



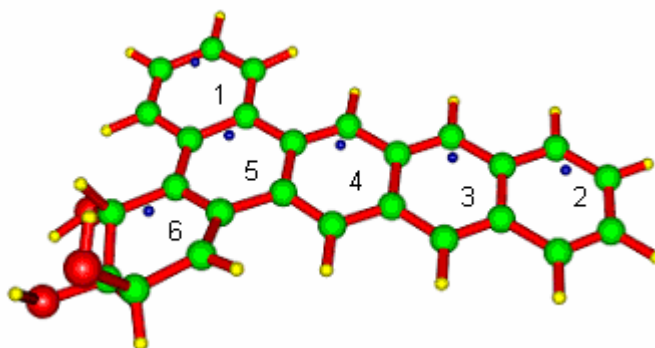
tribenzo[a,c,j]naphthacene (7)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -10.41            | -24.59                | -9.12              | -20.64                |
| 2    | -9.63             | -22.32                | -10.24             | -24.21                |
| 3    | -4.13             | -3.84                 | -3.61              | -2.29                 |
| 4    | -9.14             | -19.26                | -6.76              | -12.07                |
| 5    | -7.96             | -15.80                | -5.11              | -7.11                 |
| 6    | -2.47             | 1.12                  | -3.02              | -0.86                 |
| 7    | -1.21             | 9.53                  | -1.01              | 9.14                  |
| Sum  | -44.95            | -75.15                | -38.87             | -58.03                |



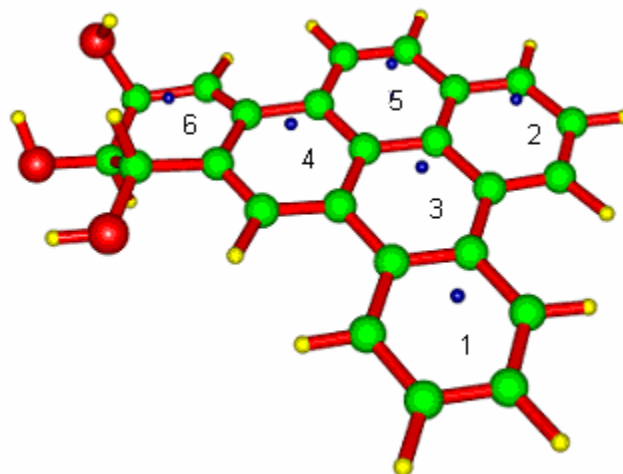
benzo[a]pyrene (8)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -0.77             | 10.11                 | -0.61              | 9.39                  |
| 2    | -2.92             | -0.33                 | -2.56              | 0.93                  |
| 3    | -8.79             | -18.83                | -3.54              | -2.60                 |
| 4    | -9.58             | -21.61                | -7.63              | -15.85                |
| 5    | -6.01             | -10.29                | -3.82              | -3.57                 |
| Sum  | -28.06            | -40.94                | -18.15             | -11.70                |



dibenzo[a,c]naphthacene (**9**)

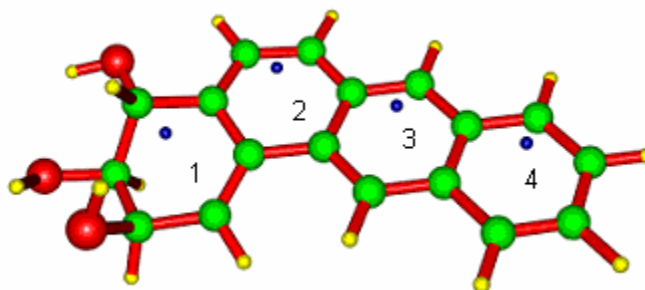
| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -5.85             | -9.55                 | -8.26              | -18.18                |
| 2    | -10.06            | -23.39                | -1.06              | 8.66                  |
| 3    | -11.26            | -26.04                | -3.61              | -2.68                 |
| 4    | -8.28             | -16.96                | -5.28              | -7.67                 |
| 5    | -1.51             | 4.67                  | -2.98              | -0.53                 |
| 6    | -2.78             | 4.49                  | -10.02             | -23.52                |
| Sum  | -39.72            | -66.77                | -31.21             | -43.92                |



dibenzo[a,e]pyrene (**10**)

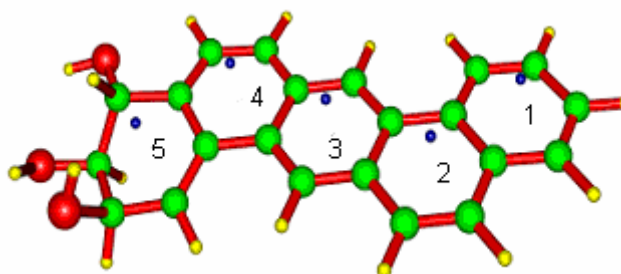
| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -9.49             | -21.76                | -9.63              | -22.19                |
| 2    | -9.80             | -22.18                | -7.17              | -14.39                |
| 3    | -4.39             | -4.57                 | -2.12              | 2.35                  |
| 4    | -2.47             | 1.53                  | -3.03              | -0.18                 |
| 5    | -8.83             | -18.71                | -4.18              | -4.39                 |

|     |        |        |        |        |
|-----|--------|--------|--------|--------|
| 6   | -0.90  | 10.49  | -0.88  | 8.50   |
| Sum | -17.78 | -55.20 | -27.01 | -30.30 |



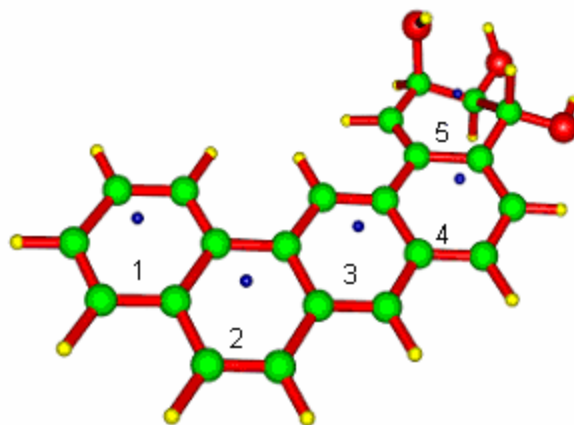
benzo[a]anthracene (**11**)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -0.91             | 9.57                  | -0.91              | 8.89                  |
| 2    | -3.08             | -1.05                 | -4.50              | -5.48                 |
| 3    | -9.46             | -20.71                | -4.78              | -6.88                 |
| 4    | -10.21            | -24.17                | -10.29             | -24.46                |
| Sum  | -23.66            | -36.36                | -20.48             | -27.92                |



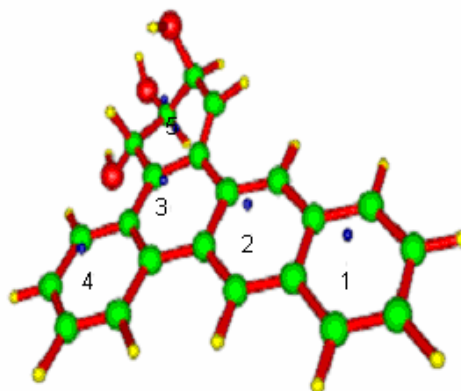
dibenzo[a,h]anthracene (**12**)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -11.31            | -27.53                | -9.48              | -21.89                |
| 2    | -7.31             | -14.48                | -5.71              | -9.71                 |
| 3    | -8.99             | -19.02                | -5.60              | -8.67                 |
| 4    | -2.86             | -0.35                 | -3.25              | -1.64                 |
| 5    | -0.93             | 9.69                  | -0.80              | 9.38                  |
| Sum  | -31.39            | -51.69                | -24.84             | -32.52                |



dibenzo[a,j]anthracene (**13**)

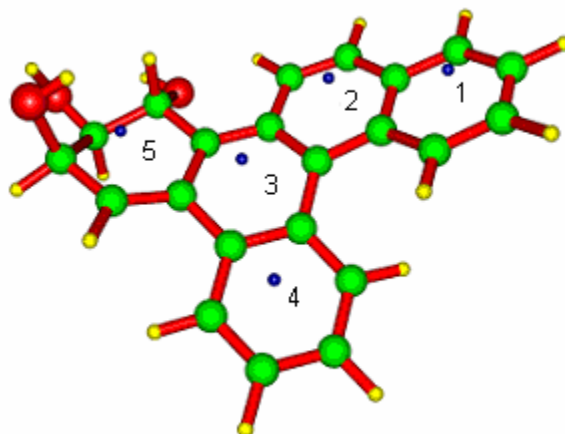
| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -10.68            | -25.67                | -10.58             | -25.37                |
| 2    | -7.53             | -14.98                | -5.52              | -8.91                 |
| 3    | -8.87             | -18.72                | -5.89              | -9.53                 |
| 4    | -2.88             | -0.40                 | -3.35              | -1.98                 |
| 5    | -0.90             | 9.81                  | -0.85              | 9.39                  |
| Sum  | -30.86            | -49.95                | -26.20             | -36.39                |



dibenzo[a,c]anthracene (**14**)

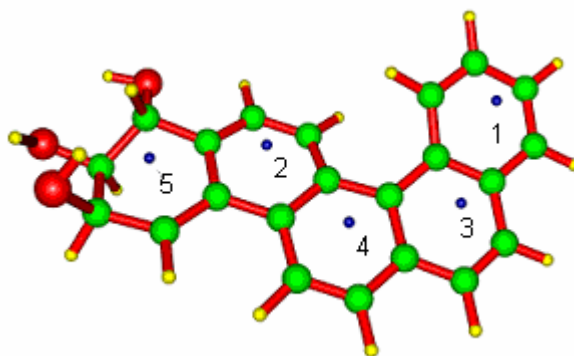
| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -10.39            | -24.33                | -1.10              | 9.17                  |
| 2    | -9.58             | -21.06                | -3.98              | -3.33                 |
| 3    | -1.86             | 3.65                  | -2.72              | 0.14                  |
| 4    | -6.00             | -10.24                | -10.10             | -23.80                |
| 5    | -2.48             | 4.93                  | -7.50              | -15.75                |

|     |        |        |        |        |
|-----|--------|--------|--------|--------|
| Sum | -30.31 | -47.04 | -25.40 | -33.57 |
|-----|--------|--------|--------|--------|



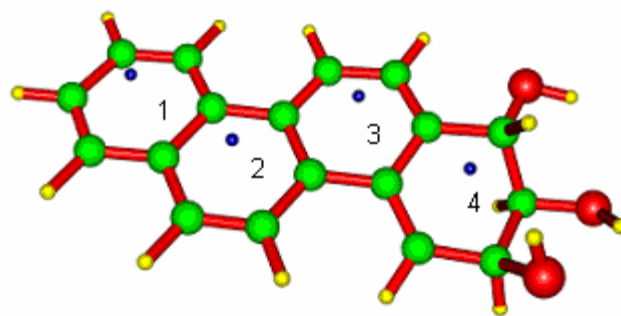
benzo[g]chrysene (**15**)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -11.45            | -20.85                | -9.39              | -17.45                |
| 2    | -5.12             | -3.77                 | -3.01              | 0.71                  |
| 3    | -2.81             | 1.44                  | -9.82              | -18.94                |
| 4    | -9.54             | -19.74                | -4.89              | -2.11                 |
| 5    | -2.41             | 3.43                  | -4.33              | 4.10                  |
| Sum  | -31.33            | -39.49                | -31.44             | -33.69                |



benzo[c]chrysene (**16**)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -13.84            | -30.41                | -10.65             | -20.42                |
| 2    | -2.25             | 1.60                  | -4.85              | -4.83                 |
| 3    | -9.03             | -17.49                | -6.34              | -11.17                |
| 4    | -8.05             | -17.17                | -5.62              | -8.60                 |
| 5    | -1.17             | 6.64                  | -1.85              | 7.77                  |
| Sum  | -34.34            | -56.83                | -29.30             | -37.25                |



chrysene (17)

| Ring | bDEH <sup>+</sup> |                       | nbDEH <sup>+</sup> |                       |
|------|-------------------|-----------------------|--------------------|-----------------------|
|      | NICS(1)           | NICS(1) <sub>zz</sub> | NICS(1)            | NICS(1) <sub>zz</sub> |
| 1    | -11.14            | -26.95                | -8.48              | -18.43                |
| 2    | -8.28             | -17.36                | -5.39              | -8.30                 |
| 3    | -3.61             | -2.77                 | -4.03              | -3.82                 |
| 4    | -0.79             | 9.99                  | -0.88              | 8.80                  |
| Sum  | -23.82            | -37.10                | -18.78             | -21.75                |