

## Supporting Information

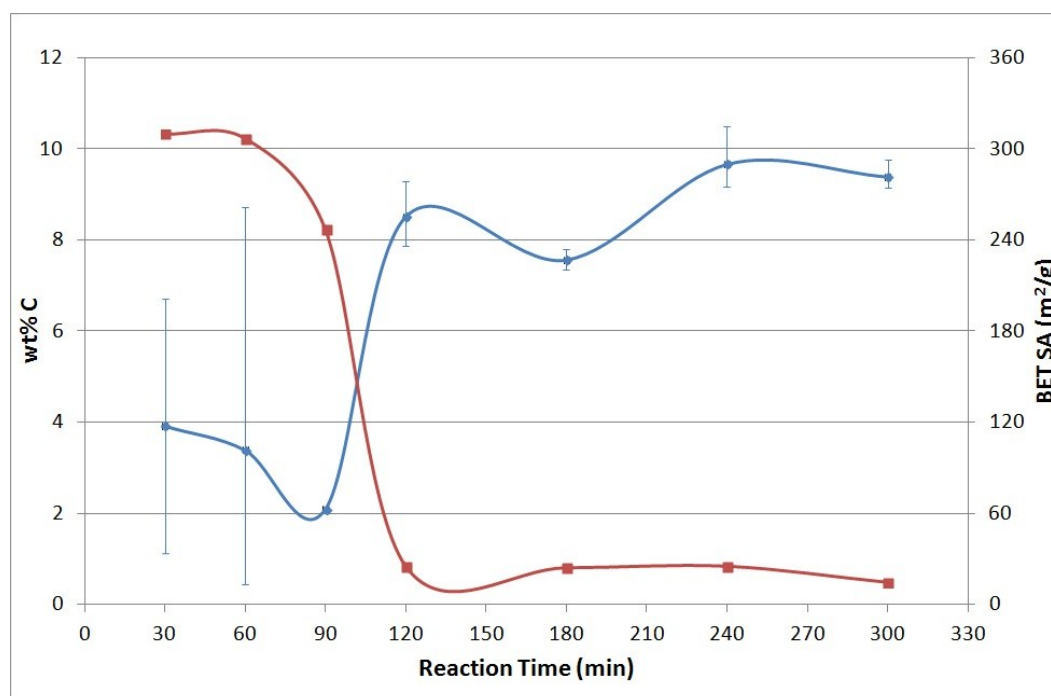
# Radicals in Carbonaceous Residue Deposited on Mordenite from Methanol

*Nicholas A. Spencer<sup>a</sup>, Evert J. Ditzel<sup>b</sup>, Justin S. J. Hargreaves<sup>\*a</sup> and Stephen Sproules<sup>\*a</sup>*

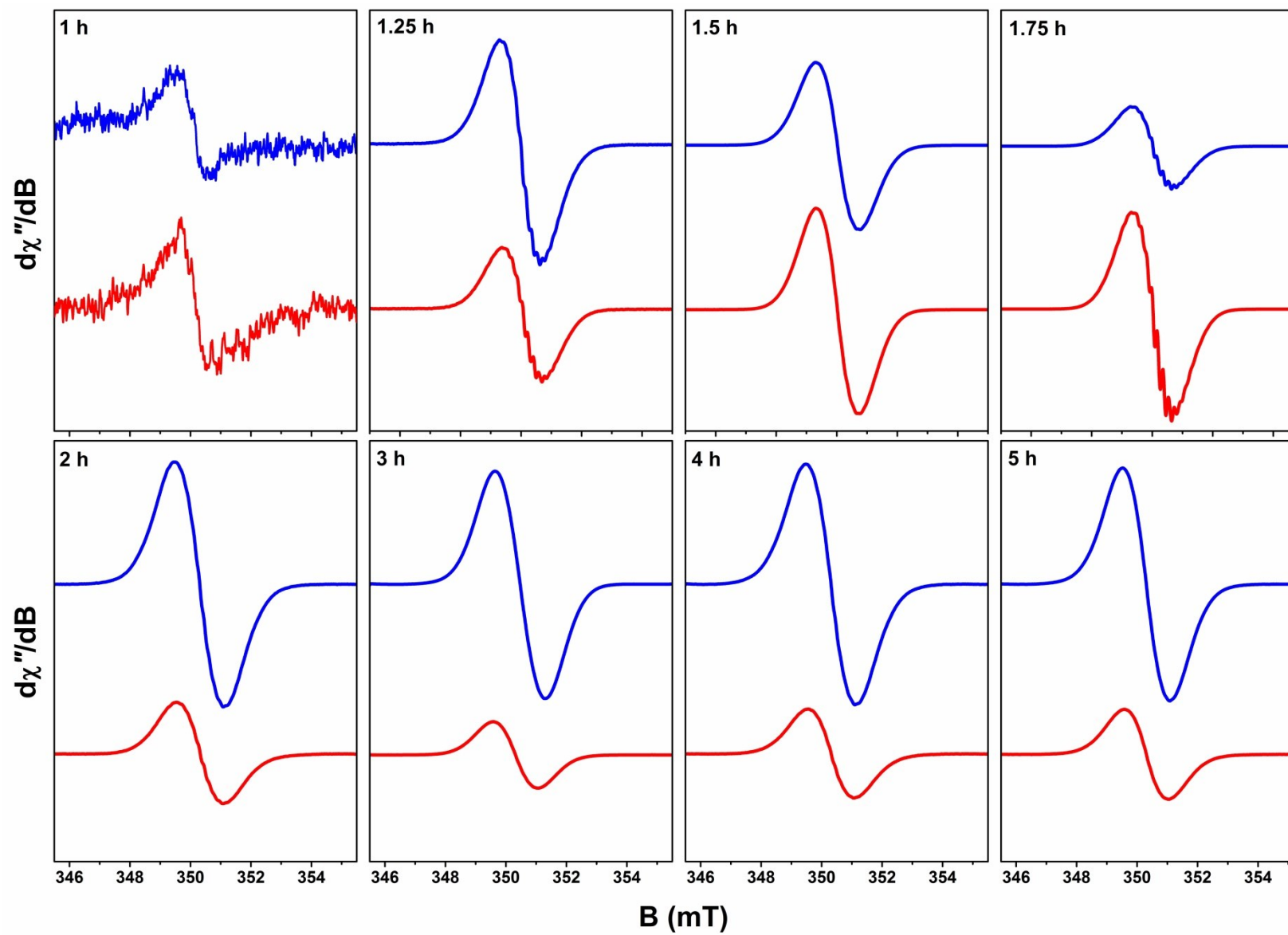
<sup>a</sup>WestCHEM, School of Chemistry, University of Glasgow, Glasgow G12 8QQ, United Kingdom

<sup>b</sup>Hull Research and Technology Centre, BP Chemicals Ltd, Hull HU12 8DS, United Kingdom

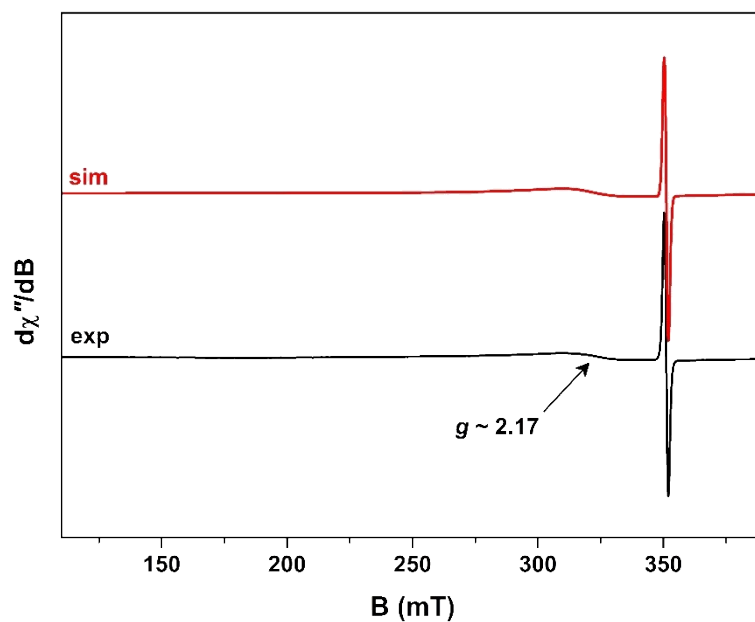
<sup>\*</sup>E-mail: [justin.hargreaves@glasgow.ac.uk](mailto:justin.hargreaves@glasgow.ac.uk); [stephen.sproules@glasgow.ac.uk](mailto:stephen.sproules@glasgow.ac.uk)



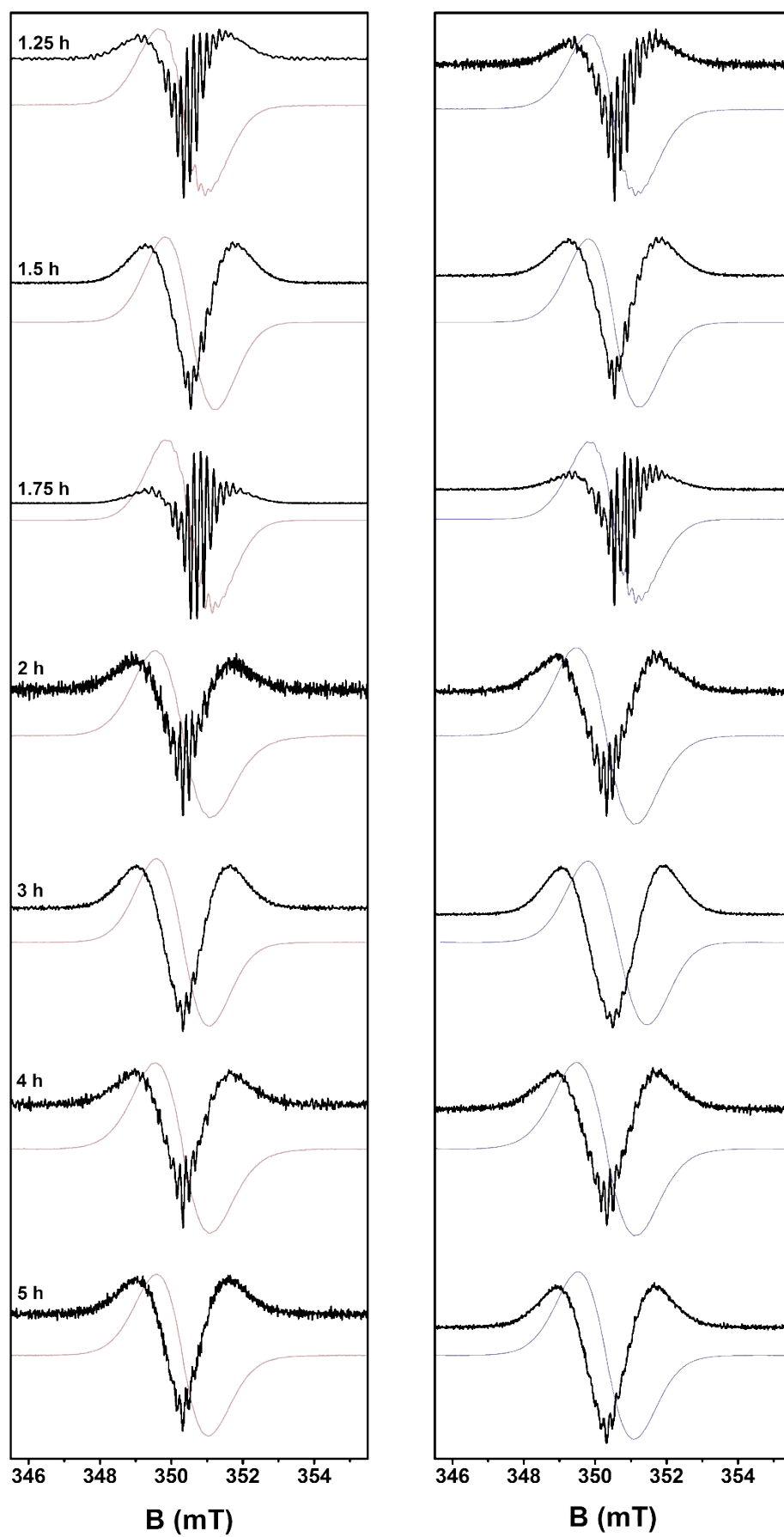
**Fig. S1** Effect of time on stream at 260 °C upon the carbon content (blue) and surface area (red) of H-MOR using a 20% methanol in argon feedstream.



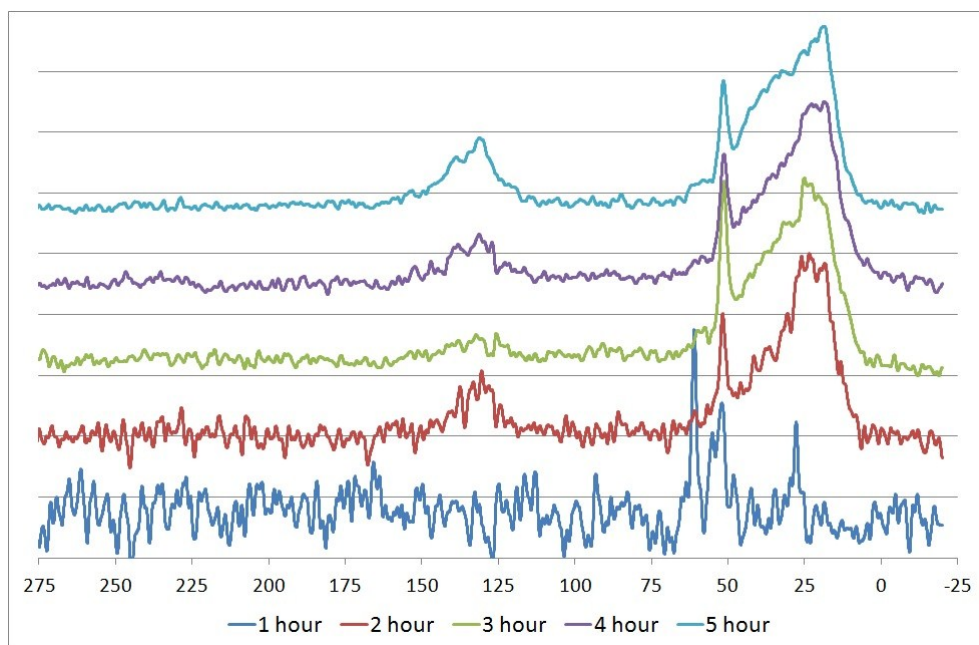
**Fig. S2** Overlay of the EPR spectra showing the relative intensity of fresh (red) and exposed (blue) samples of H-MOR at the time intervals indicated.



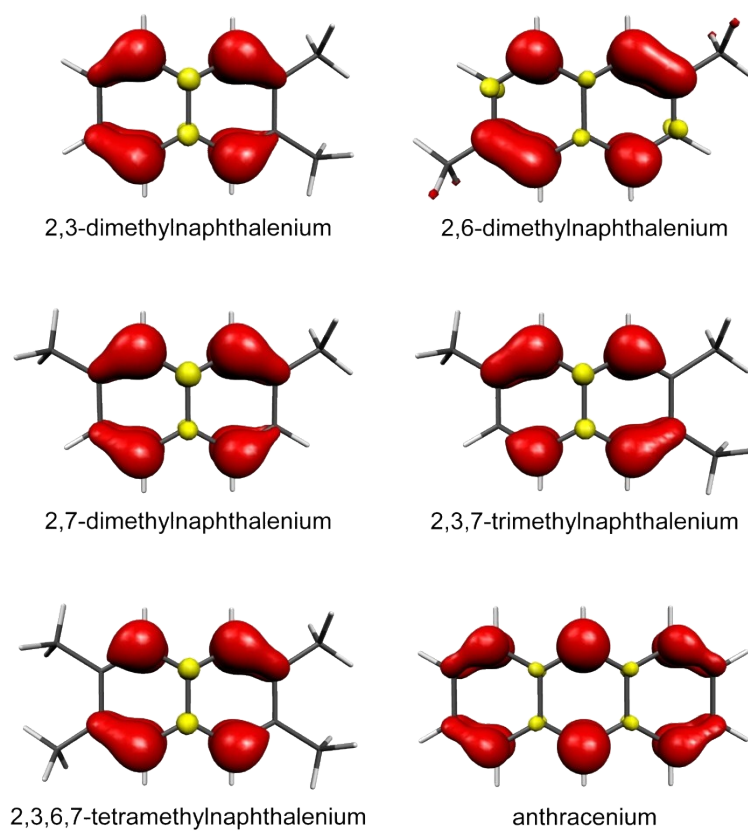
**Fig. S3** X-band EPR spectrum of H-MOR catalyst after 2 h on stream at 293 K (experimental conditions: frequency, 9.8176 GHz; modulation, 0.2 mT; power, 0.63 mW). Experimental spectrum shown in black; simulation is depicted by the red trace. The simulation is composed of two subspectra:  $g = 2.167$ , linewidth = 31.6 mT;  $g = 2.0026$ , linewidth = 1.7 mT.



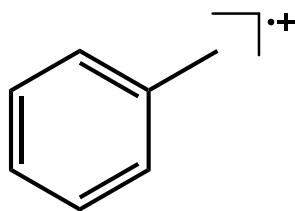
**Fig. S4** Overlay of the first and second derivative EPR spectra of fresh (red) and exposed (blue) samples of H-MOR at the time intervals indicated.



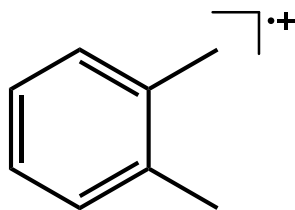
**Fig. S5**  $^{13}\text{C}$  MAS-NMR spectra of post reaction samples obtained using a 20% MeOH/Ar feed at indicated reaction times.



**Fig. S6** Mulliken spin density plots for polymethylaromatic radical cations derived from B3LYP-DFT calculations.

**Table S1**      Geometry Optimised Structures**toluenium**

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.40980 | -0.75699 | 0.00000  |
| C | 0.00000  | -0.87324 | 0.00000  |
| C | 0.82251  | 0.35087  | 0.00000  |
| C | 2.30202  | 0.26492  | 0.00000  |
| C | 0.17942  | 1.59497  | 0.00000  |
| C | -1.20608 | 1.67396  | 0.00000  |
| C | -2.00998 | 0.48244  | 0.00000  |
| C | 0.61168  | -2.22175 | 0.00000  |
| H | -2.01542 | -1.66438 | 0.00000  |
| H | 2.76341  | 1.25808  | 0.00000  |
| H | 2.66492  | -0.29954 | -0.87780 |
| H | 2.66492  | -0.29954 | 0.87780  |
| H | 0.77888  | 2.50578  | 0.00000  |
| H | -1.69992 | 2.64672  | 0.00000  |
| H | -3.09664 | 0.57342  | 0.00000  |
| H | 1.70445  | -2.22412 | 0.00000  |
| H | 0.24835  | -2.79377 | -0.87380 |
| H | 0.24835  | -2.79377 | 0.87380  |

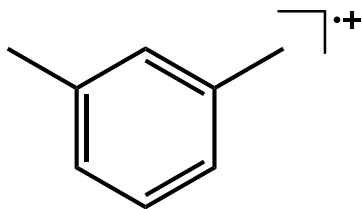
***o*-xylum**

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.40980 | -0.75699 | 0.00000  |
| C | 0.00000  | -0.87324 | 0.00000  |
| C | 0.82251  | 0.35087  | 0.00000  |
| C | 2.30202  | 0.26492  | 0.00000  |
| C | 0.17942  | 1.59497  | 0.00000  |
| C | -1.20608 | 1.67396  | 0.00000  |
| C | -2.00998 | 0.48244  | 0.00000  |
| C | 0.61168  | -2.22175 | 0.00000  |
| H | -2.01542 | -1.66438 | 0.00000  |
| H | 2.76341  | 1.25808  | 0.00000  |
| H | 2.66492  | -0.29954 | -0.87780 |
| H | 2.66492  | -0.29954 | 0.87780  |
| H | 0.77888  | 2.50578  | 0.00000  |
| H | -1.69992 | 2.64672  | 0.00000  |
| H | -3.09664 | 0.57342  | 0.00000  |



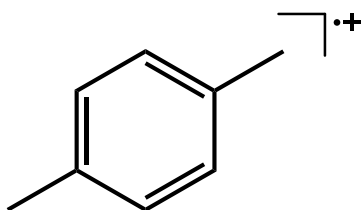
|   |         |          |          |
|---|---------|----------|----------|
| H | 1.70445 | -2.22412 | 0.00000  |
| H | 0.24835 | -2.79377 | -0.87380 |
| H | 0.24835 | -2.79377 | 0.87380  |

*m*-xylum



|   |          |          |          |
|---|----------|----------|----------|
| C | -1.21080 | 0.31263  | 0.00000  |
| C | 0.00000  | 0.99798  | 0.00000  |
| C | 1.21929  | 0.30513  | 0.00000  |
| C | 2.51537  | 1.02679  | 0.00000  |
| C | 1.20215  | -1.14780 | 0.00000  |
| C | 0.00737  | -1.85330 | 0.00000  |
| C | -1.19071 | -1.14315 | 0.00000  |
| C | -2.52375 | 1.00135  | 0.00000  |
| H | 0.00381  | 2.08936  | 0.00000  |
| H | 3.37829  | 0.35247  | 0.00000  |
| H | 2.57677  | 1.69728  | 0.87583  |
| H | 2.57677  | 1.69728  | -0.87583 |
| H | 2.15687  | -1.67620 | 0.00000  |
| H | 0.00488  | -2.94282 | 0.00000  |
| H | -2.14447 | -1.67443 | 0.00000  |
| H | -2.42893 | 2.09237  | 0.00000  |
| H | -3.11876 | 0.68346  | 0.87593  |
| H | -3.11876 | 0.68346  | -0.87593 |

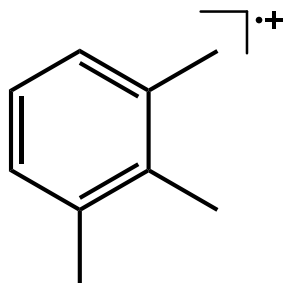
*p*-xylum



|   |          |          |          |
|---|----------|----------|----------|
| C | -1.41506 | -0.01249 | 0.00000  |
| C | -0.73333 | -1.20314 | 0.00000  |
| C | 0.70528  | -1.22793 | 0.00000  |
| C | 1.41506  | -2.52298 | 0.00000  |
| C | 1.41506  | 0.01249  | 0.00000  |
| C | 0.73333  | 1.20314  | 0.00000  |
| C | -0.70528 | 1.22793  | 0.00000  |
| C | -1.41506 | 2.52298  | 0.00000  |
| H | -2.50555 | 0.00224  | 0.00000  |
| H | -1.27341 | -2.15130 | 0.00000  |
| H | 2.50476  | -2.41774 | 0.00000  |
| H | 1.09941  | -3.12536 | -0.87277 |
| H | 1.09941  | -3.12536 | 0.87277  |
| H | 2.50555  | -0.00224 | 0.00000  |

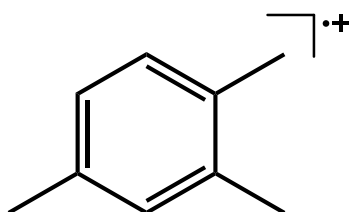
|   |          |         |          |
|---|----------|---------|----------|
| H | 1.27341  | 2.15130 | 0.00000  |
| H | -2.50476 | 2.41773 | 0.00000  |
| H | -1.09942 | 3.12536 | -0.87277 |
| H | -1.09942 | 3.12536 | 0.87277  |

### 1,2,3-trimethylbenzenium



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.007950 | 0.699227  | 0.000000  |
| C | -1.268070 | -0.017273 | 0.000000  |
| C | -2.576500 | 0.717457  | 0.000000  |
| C | -1.240670 | -1.393993 | 0.000000  |
| C | -0.011820 | -2.127983 | 0.000000  |
| C | 1.212650  | -1.418153 | 0.000000  |
| C | 1.250600  | -0.036863 | 0.000000  |
| C | 2.577810  | 0.663297  | 0.000000  |
| C | 0.015580  | 2.180507  | 0.000000  |
| H | -0.033880 | -3.217460 | 0.000000  |
| H | -2.388972 | 1.801354  | 0.000000  |
| H | -3.149829 | 0.444800  | 0.898306  |
| H | -3.149829 | 0.444800  | -0.898306 |
| H | -2.182165 | -1.962840 | -0.000000 |
| H | 2.166246  | -1.966473 | -0.000000 |
| H | 3.386392  | -0.082488 | 0.000000  |
| H | 2.659977  | 1.292817  | 0.898306  |
| H | 2.659977  | 1.292817  | -0.898306 |
| H | 1.058187  | 2.531179  | 0.000000  |
| H | -0.496988 | 2.555101  | 0.898306  |
| H | -0.496988 | 2.555101  | -0.898306 |

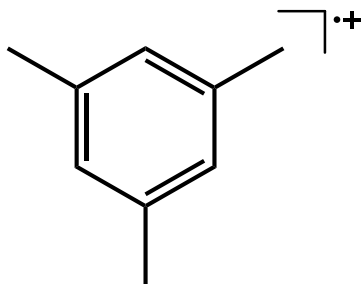
### 1,2,4-trimethylbenzenium



|   |          |          |         |
|---|----------|----------|---------|
| C | -1.20480 | 0.36336  | 0.00000 |
| C | 0.00000  | 1.05830  | 0.00000 |
| C | -0.00825 | 2.55222  | 0.00000 |
| C | 2.56228  | 0.98685  | 0.00000 |
| C | 1.25170  | 0.29726  | 0.00000 |
| C | 1.19830  | -1.11883 | 0.00000 |

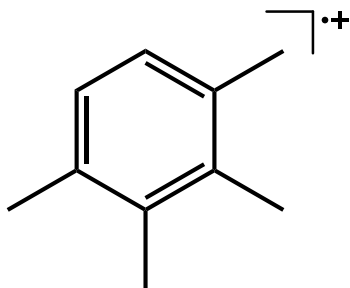
|   |          |          |          |
|---|----------|----------|----------|
| C | -0.00759 | -1.77658 | 0.00000  |
| C | -1.25251 | -1.03887 | 0.00000  |
| C | -2.53271 | -1.78467 | 0.00000  |
| H | -0.04465 | -2.86738 | 0.00000  |
| H | -2.14198 | 0.92367  | 0.00000  |
| H | 0.98939  | 3.00020  | 0.00000  |
| H | -0.55875 | 2.92431  | 0.87980  |
| H | -0.55875 | 2.92431  | -0.87980 |
| H | 3.39739  | 0.27844  | 0.00000  |
| H | 2.65440  | 1.65318  | 0.87668  |
| H | 2.65440  | 1.65318  | -0.87668 |
| H | 2.13273  | -1.68106 | 0.00000  |
| H | -3.40844 | -1.12697 | 0.00000  |
| H | -2.57720 | -2.45806 | 0.87541  |
| H | -2.57720 | -2.45806 | -0.87541 |

### 1,3,5-trimethylbenzenium



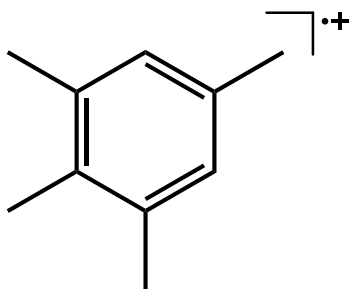
|   |          |          |          |
|---|----------|----------|----------|
| C | 0.02638  | 1.41915  | 0.00000  |
| C | 1.24169  | 0.73413  | 0.00000  |
| C | 1.26108  | -0.66188 | 0.00000  |
| C | 2.53776  | -1.42379 | 0.00000  |
| C | 0.00000  | -1.37884 | 0.00000  |
| C | -1.24330 | -0.73016 | 0.00000  |
| C | -1.21722 | 0.66200  | 0.00000  |
| C | -0.05142 | 2.89841  | 0.00000  |
| C | -2.52858 | -1.51074 | 0.00000  |
| H | 2.17900  | 1.29272  | 0.00000  |
| H | 2.38346  | -2.50843 | 0.00000  |
| H | 3.14779  | -1.14528 | 0.87725  |
| H | 3.14779  | -1.14528 | -0.87725 |
| H | 0.03832  | -2.47065 | 0.00000  |
| H | -2.15462 | 1.22358  | 0.00000  |
| H | 0.93458  | 3.37475  | 0.00000  |
| H | -0.63009 | 3.24780  | 0.87500  |
| H | -0.63009 | 3.24780  | -0.87500 |
| H | -3.40027 | -0.84515 | 0.00000  |
| H | -2.58712 | -2.16078 | 0.88562  |
| H | -2.58712 | -2.16078 | -0.88562 |

### 1,2,3,4-tetramethylbenzenium



|   |          |          |          |
|---|----------|----------|----------|
| C | 0.97864  | 0.02035  | 0.00000  |
| C | 0.00000  | -0.97853 | 0.00000  |
| C | 0.38469  | -2.43126 | 0.00000  |
| C | -2.47480 | -1.62957 | 0.00000  |
| C | -1.40065 | -0.60684 | 0.00000  |
| C | -1.77472 | 0.77278  | 0.00000  |
| C | -0.81789 | 1.74629  | 0.00000  |
| C | 0.57869  | 1.39918  | 0.00000  |
| C | 1.55102  | 2.51826  | 0.00000  |
| C | 2.44478  | -0.31218 | 0.00000  |
| H | -0.48133 | -3.09876 | 0.00000  |
| H | 0.99626  | -2.67363 | 0.88347  |
| H | 0.99626  | -2.67363 | -0.88347 |
| H | -3.47058 | -1.17353 | 0.00000  |
| H | -2.38484 | -2.29605 | 0.87654  |
| H | -2.38484 | -2.29605 | -0.87654 |
| H | -2.83443 | 1.02992  | 0.00000  |
| H | -1.09355 | 2.80222  | 0.00000  |
| H | 2.59915  | 2.21060  | 0.00000  |
| H | 1.36275  | 3.16924  | 0.87380  |
| H | 1.36275  | 3.16924  | -0.87380 |
| H | 2.62703  | -1.38982 | 0.00000  |
| H | 2.94337  | 0.11463  | 0.88449  |
| H | 2.94337  | 0.11463  | -0.88449 |

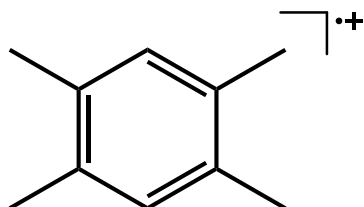
### 1,2,3,5-tetramethylbenzenium



|   |          |          |         |
|---|----------|----------|---------|
| C | 0.00000  | 1.09187  | 0.00000 |
| C | -1.26012 | 0.37537  | 0.00000 |
| C | -2.56855 | 1.11010  | 0.00000 |
| C | -1.23272 | -1.00135 | 0.00000 |
| C | -0.00387 | -1.73534 | 0.00000 |
| C | 1.22060  | -1.02551 | 0.00000 |
| C | 1.25855  | 0.35578  | 0.00000 |
| C | 2.58576  | 1.05594  | 0.00000 |

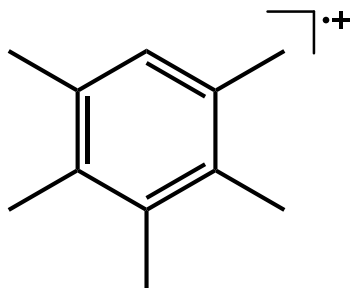
|   |          |          |          |
|---|----------|----------|----------|
| C | 0.02353  | 2.57315  | 0.00000  |
| C | -0.03388 | -3.21746 | 0.00000  |
| H | -2.17070 | -1.56055 | 0.00000  |
| H | -3.40692 | 0.40341  | 0.00000  |
| H | -2.66482 | 1.75853  | -0.88487 |
| H | -2.66482 | 1.75853  | 0.88487  |
| H | 2.15469  | -1.59084 | 0.00000  |
| H | 2.51040  | 2.14668  | 0.00000  |
| H | 3.17068  | 0.75100  | -0.88218 |
| H | 3.17068  | 0.75100  | 0.88218  |
| H | -0.97204 | 3.02294  | 0.00000  |
| H | 0.58401  | 2.94854  | -0.87563 |
| H | 0.58401  | 2.94854  | 0.87563  |
| H | 0.96702  | -3.66216 | 0.00000  |
| H | -0.59898 | -3.58544 | -0.87552 |
| H | -0.59898 | -3.58544 | 0.87552  |

### 1,2,4,5-tetramethylbenzenium



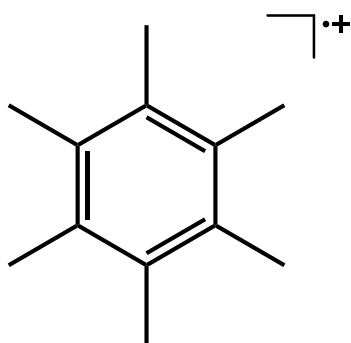
|   |          |          |          |
|---|----------|----------|----------|
| C | -3.38103 | 1.61421  | -0.00000 |
| C | -2.16933 | 0.90484  | -0.00000 |
| C | -0.85885 | 1.63466  | -0.00000 |
| C | -0.89626 | -1.27464 | -0.00000 |
| C | -2.18761 | -0.51146 | -0.00000 |
| C | -3.41724 | -1.18951 | -0.00000 |
| C | -4.61585 | -0.47056 | -0.00000 |
| C | -4.59776 | 0.92636  | -0.00000 |
| C | -5.88995 | 1.68810  | 0.00000  |
| C | -5.92722 | -1.19878 | -0.00000 |
| H | -3.37437 | 2.71419  | -0.00000 |
| H | -0.03355 | 0.90742  | -0.00000 |
| H | -0.79100 | 2.26588  | 0.89831  |
| H | -0.79100 | 2.26588  | -0.89831 |
| H | -1.10771 | -2.35412 | -0.00000 |
| H | -0.31705 | -1.01472 | 0.89831  |
| H | -0.31705 | -1.01472 | -0.89831 |
| H | -3.43887 | -2.28930 | -0.00000 |
| H | -5.67970 | 2.76782  | 0.00000  |
| H | -6.46888 | 1.42754  | 0.89831  |
| H | -6.46888 | 1.42754  | -0.89831 |
| H | -6.75163 | -0.47053 | -0.00000 |
| H | -5.99585 | -1.82992 | 0.89831  |
| H | -5.99585 | -1.82992 | -0.89831 |

### Pentamethylbenzenium



|   |          |          |          |
|---|----------|----------|----------|
| C | 0.00000  | -1.14768 | 0.00000  |
| C | 1.22089  | -0.42564 | 0.00000  |
| C | 2.52554  | -1.14736 | 0.00000  |
| C | 2.48902  | 1.81426  | 0.00000  |
| C | 1.21398  | 1.03966  | 0.00000  |
| C | -0.00004 | 1.70369  | 0.00000  |
| C | -1.21857 | 1.01138  | 0.00000  |
| C | -1.21793 | -0.44847 | 0.00000  |
| C | -2.53052 | -1.15992 | 0.00000  |
| C | -2.48166 | 1.80166  | 0.00000  |
| C | 0.00221  | -2.65826 | 0.00000  |
| H | 3.38803  | -0.47666 | 0.00000  |
| H | 2.60095  | -1.81021 | -0.87891 |
| H | 2.60095  | -1.81021 | 0.87891  |
| H | 2.29415  | 2.89286  | 0.00000  |
| H | 3.10534  | 1.56825  | -0.88129 |
| H | 3.10534  | 1.56825  | 0.88129  |
| H | -0.01474 | 2.79511  | 0.00000  |
| H | -2.42540 | -2.24729 | 0.00000  |
| H | -3.12979 | -0.86986 | -0.88003 |
| H | -3.12979 | -0.86986 | 0.88003  |
| H | -3.39141 | 1.19673  | 0.00000  |
| H | -2.49877 | 2.47130  | -0.87732 |
| H | -2.49877 | 2.47130  | 0.87732  |
| H | 1.01276  | -3.07519 | 0.00000  |
| H | -0.51817 | -3.05228 | -0.88583 |
| H | -0.51817 | -3.05228 | 0.88583  |

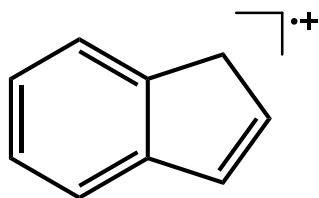
### hexamethylbenzenium



|   |          |         |         |
|---|----------|---------|---------|
| C | 1.24594  | 0.74073 | 0.00000 |
| C | 0.00009  | 1.41224 | 0.00000 |
| C | -0.03817 | 2.90489 | 0.00000 |
| C | -2.54379 | 1.41666 | 0.00000 |

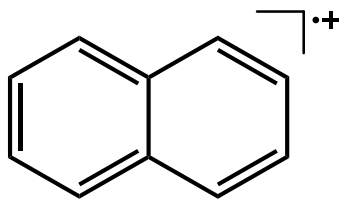
|   |          |          |          |
|---|----------|----------|----------|
| C | -1.25575 | 0.65916  | 0.00000  |
| C | -1.24596 | -0.74068 | 0.00000  |
| C | 0.00000  | -1.41215 | 0.00000  |
| C | 1.25567  | -0.65920 | 0.00000  |
| C | 2.54348  | -1.41715 | 0.00000  |
| C | 0.03871  | -2.90481 | 0.00000  |
| C | 2.54503  | 1.51221  | 0.00000  |
| C | -2.54524 | -1.51187 | 0.00000  |
| H | -1.04887 | 3.31733  | 0.00000  |
| H | 0.49710  | 3.30312  | -0.87883 |
| H | 0.49710  | 3.30312  | 0.87883  |
| H | -3.41698 | 0.76046  | 0.00000  |
| H | -2.60886 | 2.07736  | -0.88091 |
| H | -2.60886 | 2.07736  | 0.88091  |
| H | 3.41695  | -0.76138 | 0.00000  |
| H | 2.60819  | -2.07790 | -0.88090 |
| H | 2.60819  | -2.07790 | 0.88090  |
| H | 1.04963  | -3.31679 | 0.00000  |
| H | -0.49636 | -3.30318 | -0.87888 |
| H | -0.49636 | -3.30318 | 0.87888  |
| H | 2.38939  | 2.59422  | 0.00000  |
| H | 3.14974  | 1.26658  | -0.88597 |
| H | 3.14974  | 1.26658  | 0.88597  |
| H | -2.38999 | -2.59392 | 0.00000  |
| H | -3.14987 | -1.26601 | -0.88595 |
| H | -3.14987 | -1.26601 | 0.88595  |

### Indenium



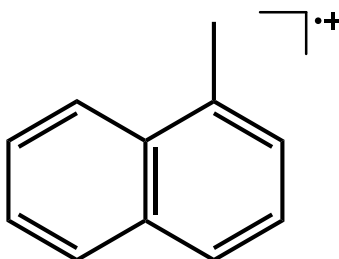
|   |          |          |          |
|---|----------|----------|----------|
| C | -0.94147 | -1.42141 | 0.00019  |
| C | 0.26150  | -0.71799 | 0.00002  |
| C | 0.26143  | 0.71839  | -0.00007 |
| C | -0.94182 | 1.42142  | -0.00020 |
| C | -2.15401 | 0.69877  | -0.00009 |
| C | -2.15396 | -0.69905 | 0.00012  |
| C | 1.64941  | -1.14544 | -0.00030 |
| C | 2.46547  | -0.00007 | 0.00003  |
| C | 1.64926  | 1.14543  | 0.00030  |
| H | -0.95402 | -2.51397 | 0.00027  |
| H | -0.95463 | 2.51400  | -0.00034 |
| H | -3.10220 | 1.23968  | -0.00012 |
| H | -3.10204 | -1.24012 | 0.00022  |
| H | 1.99175  | -2.17967 | -0.00059 |
| H | 3.55396  | 0.00028  | 0.00008  |
| H | 1.99234  | 2.17947  | 0.00053  |

### Naphthalenium



|   |          |          |          |
|---|----------|----------|----------|
| C | -3.64691 | 1.46467  | 0.00000  |
| C | -2.43521 | 0.75529  | 0.00000  |
| C | -1.20962 | 1.43784  | 0.00000  |
| C | -0.00201 | 0.72413  | 0.00000  |
| C | -0.02024 | -0.69215 | 0.00000  |
| C | -1.24585 | -1.37471 | 0.00000  |
| C | -2.45349 | -0.66101 | 0.00000  |
| C | -3.68312 | -1.33905 | 0.00000  |
| C | -4.88173 | -0.62011 | 0.00000  |
| C | -4.86364 | 0.77681  | 0.00000  |
| H | -3.63694 | 2.56462  | -0.00000 |
| H | -1.19262 | 2.53771  | -0.00000 |
| H | 0.95617  | 1.26440  | 0.00000  |
| H | 0.92523  | -1.25437 | 0.00000  |
| H | -1.26286 | -2.47458 | 0.00000  |
| H | -3.70475 | -2.43884 | -0.00000 |
| H | -5.84340 | -1.15414 | 0.00000  |
| H | -5.81125 | 1.33542  | 0.00000  |

### 1-methylnaphthalenium

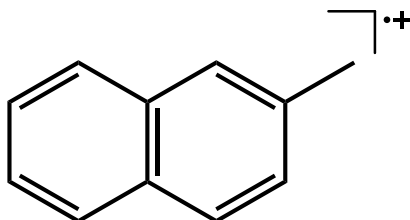


|   |          |          |         |
|---|----------|----------|---------|
| C | -0.95640 | -1.46479 | 0.00000 |
| C | 0.00000  | -0.42607 | 0.00000 |
| C | 1.41350  | -0.68173 | 0.00000 |
| C | 2.30118  | 0.42371  | 0.00000 |
| C | 1.84055  | 1.73460  | 0.00000 |
| C | 0.45955  | 1.99496  | 0.00000 |
| C | -0.47099 | 0.92971  | 0.00000 |
| C | -1.86363 | 1.18549  | 0.00000 |
| C | -2.78814 | 0.13303  | 0.00000 |
| C | -2.33393 | -1.18617 | 0.00000 |
| C | 1.96735  | -2.06771 | 0.00000 |
| H | -0.62954 | -2.50508 | 0.00000 |
| H | 3.37477  | 0.22910  | 0.00000 |
| H | 2.54896  | 2.56338  | 0.00000 |
| H | 0.09365  | 3.02353  | 0.00000 |
| H | -2.21060 | 2.22034  | 0.00000 |
| H | -3.85688 | 0.34791  | 0.00000 |
| H | -3.04645 | -2.01160 | 0.00000 |



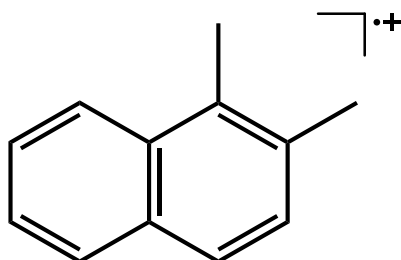
|   |         |          |          |
|---|---------|----------|----------|
| H | 3.06295 | -2.05650 | 0.00000  |
| H | 1.62446 | -2.63061 | -0.88316 |
| H | 1.62446 | -2.63061 | 0.88316  |

### 2-methylnaphthalenium



|   |          |          |          |
|---|----------|----------|----------|
| C | 0.56599  | 1.98824  | 0.00000  |
| C | 0.00000  | 0.68583  | 0.00000  |
| C | -1.39376 | 0.48209  | 0.00000  |
| C | -1.96326 | -0.82115 | 0.00000  |
| C | -3.44899 | -0.98084 | 0.00000  |
| C | -1.09572 | -1.92448 | 0.00000  |
| C | 0.28979  | -1.75140 | 0.00000  |
| C | 0.86916  | -0.45336 | 0.00000  |
| C | 2.26241  | -0.25187 | 0.00000  |
| C | 2.80018  | 1.05043  | 0.00000  |
| C | 1.95643  | 2.16288  | 0.00000  |
| H | -0.09626 | 2.85619  | 0.00000  |
| H | -2.05589 | 1.35148  | 0.00000  |
| H | -3.74864 | -2.03511 | 0.00000  |
| H | -3.88835 | -0.48553 | -0.88156 |
| H | -3.88835 | -0.48553 | 0.88156  |
| H | -1.51036 | -2.93354 | 0.00000  |
| H | 0.94726  | -2.62323 | 0.00000  |
| H | 2.92912  | -1.11632 | 0.00000  |
| H | 3.88228  | 1.18428  | 0.00000  |
| H | 2.37578  | 3.16908  | 0.00000  |

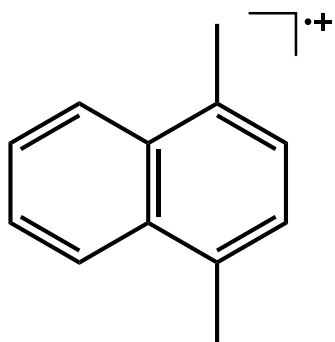
### 1,2-dimethylnaphthalenium



|   |          |          |         |
|---|----------|----------|---------|
| C | -0.03958 | -1.99015 | 0.00000 |
| C | 0.00000  | -0.57487 | 0.00000 |
| C | 1.23652  | 0.15315  | 0.00000 |
| C | 1.20707  | 1.59108  | 0.00000 |
| C | 2.47122  | 2.39469  | 0.00000 |
| C | -0.02812 | 2.25123  | 0.00000 |
| C | -1.23340 | 1.54991  | 0.00000 |
| C | -1.24653 | 0.13208  | 0.00000 |
| C | -2.46107 | -0.58565 | 0.00000 |

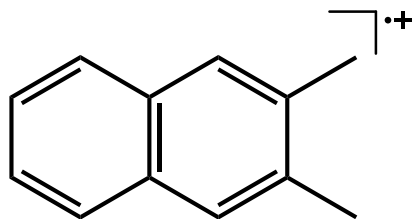
|   |          |          |          |
|---|----------|----------|----------|
| C | -2.46675 | -1.98793 | 0.00000  |
| C | -1.25732 | -2.68469 | 0.00000  |
| C | 2.54040  | -0.57751 | 0.00000  |
| H | 0.88892  | -2.56084 | 0.00000  |
| H | 2.25187  | 3.46871  | 0.00000  |
| H | 3.08937  | 2.16653  | -0.88326 |
| H | 3.08937  | 2.16653  | 0.88326  |
| H | -0.04515 | 3.34197  | 0.00000  |
| H | -2.18075 | 2.09263  | 0.00000  |
| H | -3.40347 | -0.03467 | 0.00000  |
| H | -3.41399 | -2.52779 | 0.00000  |
| H | -1.25258 | -3.77504 | 0.00000  |
| H | 3.39932  | 0.09830  | 0.00000  |
| H | 2.62126  | -1.23219 | -0.88265 |
| H | 2.62126  | -1.23219 | 0.88265  |

### 1,4-dimethylnaphthalenium



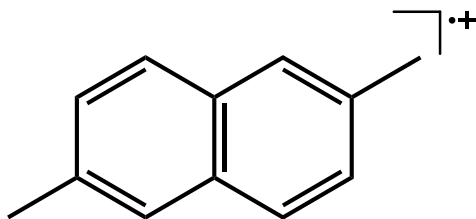
|   |          |          |          |
|---|----------|----------|----------|
| C | -0.93604 | -1.81616 | 0.00000  |
| C | 0.00000  | -0.75875 | 0.00000  |
| C | 1.41198  | -1.01972 | 0.00000  |
| C | 2.29692  | 0.08396  | 0.00000  |
| C | 1.83153  | 1.38599  | 0.00000  |
| C | 0.44444  | 1.68759  | 0.00000  |
| C | -0.48663 | 0.59725  | 0.00000  |
| C | -1.88557 | 0.80937  | 0.00000  |
| C | -2.78819 | -0.25908 | 0.00000  |
| C | -2.31443 | -1.57174 | 0.00000  |
| C | 1.96617  | -2.40617 | 0.00000  |
| C | 0.05166  | 3.12682  | 0.00000  |
| H | -0.58338 | -2.84761 | 0.00000  |
| H | 3.37168  | -0.10410 | 0.00000  |
| H | 2.54423  | 2.21303  | 0.00000  |
| H | -2.27915 | 1.82437  | 0.00000  |
| H | -3.86004 | -0.05935 | 0.00000  |
| H | -3.01185 | -2.40996 | 0.00000  |
| H | 3.06187  | -2.39289 | 0.00000  |
| H | 1.62544  | -2.97038 | -0.88320 |
| H | 1.62544  | -2.97038 | 0.88320  |
| H | -1.02628 | 3.30656  | 0.00000  |
| H | 0.49050  | 3.62728  | -0.87931 |
| H | 0.49050  | 3.62728  | 0.87931  |

### 2,3-dimethylnaphthalenium



|   |          |          |          |
|---|----------|----------|----------|
| C | 0.34507  | 2.40832  | 0.00000  |
| C | 0.00000  | 1.03722  | 0.00000  |
| C | -1.34296 | 0.59599  | 0.00000  |
| C | -1.69689 | -0.77228 | 0.00000  |
| C | -3.15331 | -1.13048 | 0.00000  |
| C | -0.66982 | -1.74621 | 0.00000  |
| C | 0.67268  | -1.31456 | 0.00000  |
| C | 1.03771  | 0.05439  | 0.00000  |
| C | 2.38474  | 0.47492  | 0.00000  |
| C | 2.70629  | 1.84445  | 0.00000  |
| C | 1.69331  | 2.80441  | 0.00000  |
| C | -0.96988 | -3.21738 | 0.00000  |
| H | -0.44612 | 3.16082  | 0.00000  |
| H | -2.13975 | 1.34421  | 0.00000  |
| H | -3.32679 | -2.21069 | 0.00000  |
| H | -3.65111 | -0.69779 | -0.88259 |
| H | -3.65111 | -0.69779 | 0.88259  |
| H | 1.46658  | -2.06579 | 0.00000  |
| H | 3.18032  | -0.27246 | 0.00000  |
| H | 3.75221  | 2.15223  | 0.00000  |
| H | 1.94380  | 3.86545  | 0.00000  |
| H | -0.04622 | -3.80817 | 0.00000  |
| H | -1.56177 | -3.50143 | -0.88420 |
| H | -1.56177 | -3.50143 | 0.88420  |

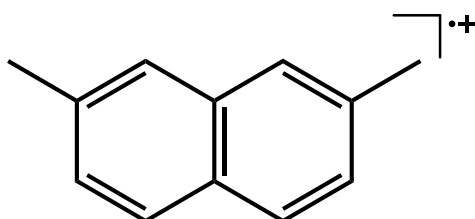
### 2,6-dimethylnaphthalenium



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.569132 | 1.903365  | 0.000000  |
| C | -2.357440 | 1.193987  | 0.000000  |
| C | -1.131849 | 1.876538  | 0.000000  |
| C | 0.075765  | 1.162829  | 0.000000  |
| C | 1.305412  | 1.840917  | 0.000000  |
| C | 0.057533  | -0.253454 | 0.000000  |
| C | -1.168080 | -0.936013 | 0.000000  |
| C | -2.375716 | -0.222313 | 0.000000  |
| C | -3.605346 | -0.900357 | 0.000000  |
| C | -4.803956 | -0.181410 | 0.000000  |
| C | -4.785866 | 1.215508  | 0.000000  |
| C | -6.115327 | -0.909631 | -0.000000 |
| H | -3.559164 | 3.003319  | -0.000000 |

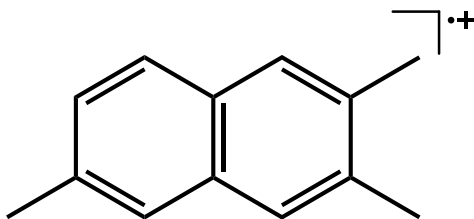
|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.114842 | 2.976406  | -0.000000 |
| H | 2.127665  | 1.110232  | 0.000000  |
| H | 1.375909  | 2.471850  | 0.898306  |
| H | 1.375909  | 2.471850  | -0.898306 |
| H | 1.001542  | -0.818120 | -0.000000 |
| H | -1.185090 | -2.035882 | -0.000000 |
| H | -3.623700 | -2.000204 | -0.000000 |
| H | -5.733471 | 1.774117  | 0.000000  |
| H | -6.939737 | -0.181381 | -0.000000 |
| H | -6.183958 | -1.540770 | 0.898306  |
| H | -6.183958 | -1.540770 | -0.898306 |

**2,7-dimethylnaphthalenium**



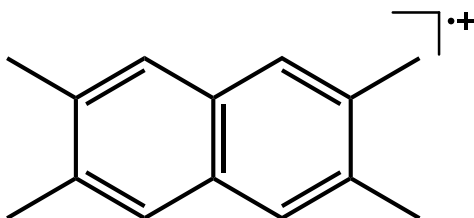
|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.569132 | 1.903365  | 0.000000  |
| C | -2.357440 | 1.193987  | 0.000000  |
| C | -1.131849 | 1.876538  | 0.000000  |
| C | 0.075765  | 1.162829  | 0.000000  |
| C | 1.269369  | -0.962767 | 0.000000  |
| C | 0.057533  | -0.253454 | 0.000000  |
| C | -1.168080 | -0.936013 | 0.000000  |
| C | -2.375716 | -0.222313 | 0.000000  |
| C | -3.605346 | -0.900357 | 0.000000  |
| C | -4.803956 | -0.181410 | 0.000000  |
| C | -4.785866 | 1.215508  | 0.000000  |
| C | -6.115327 | -0.909631 | -0.000000 |
| H | -3.559164 | 3.003319  | -0.000000 |
| H | -1.114842 | 2.976406  | -0.000000 |
| H | 1.033944  | 1.703100  | -0.000000 |
| H | 1.062470  | -2.043134 | 0.000000  |
| H | 1.847486  | -0.700417 | 0.898306  |
| H | 1.847486  | -0.700417 | -0.898306 |
| H | -1.185090 | -2.035882 | -0.000000 |
| H | -3.623700 | -2.000204 | -0.000000 |
| H | -5.733471 | 1.774117  | 0.000000  |
| H | -6.939737 | -0.181381 | -0.000000 |
| H | -6.183958 | -1.540770 | 0.898306  |
| H | -6.183958 | -1.540770 | -0.898306 |

### 2,3,6-trimethylnaphthalenium



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.296046 | 1.649457  | -0.000055 |
| C | -2.083310 | 0.944093  | -0.000047 |
| C | -0.832264 | 1.596395  | -0.000089 |
| C | 0.384826  | 0.898226  | -0.000021 |
| C | 1.659669  | 1.690515  | 0.000107  |
| C | 0.362103  | -0.506884 | -0.000058 |
| C | -0.882977 | -1.166538 | -0.000037 |
| C | -2.103703 | -0.477042 | -0.000013 |
| C | -3.350879 | -1.136792 | 0.000022  |
| C | -4.539270 | -0.414963 | 0.000093  |
| C | -4.539083 | 0.982534  | 0.000005  |
| C | 1.621102  | -1.323127 | -0.000040 |
| C | -5.825134 | 1.750352  | -0.000026 |
| H | -3.275856 | 2.733498  | -0.000078 |
| H | -0.812865 | 2.680810  | -0.000228 |
| H | 2.546280  | 1.063068  | -0.000290 |
| H | 1.701042  | 2.340466  | 0.878259  |
| H | 1.700753  | 2.341265  | -0.877461 |
| H | -0.898113 | -2.250654 | -0.000007 |
| H | -3.378656 | -2.219973 | -0.000069 |
| H | -5.481811 | -0.947734 | 0.000060  |
| H | 1.396012  | -2.388428 | -0.000578 |
| H | 2.232249  | -1.102972 | 0.878738  |
| H | 2.232855  | -1.102228 | -0.878198 |
| H | -5.654021 | 2.825943  | -0.001107 |
| H | -6.423166 | 1.493823  | 0.878470  |
| H | -6.424157 | 1.492185  | -0.877352 |

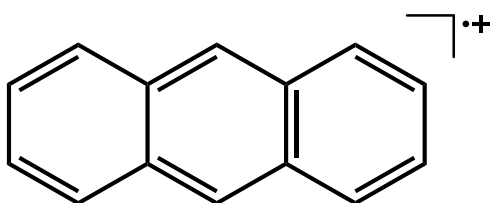
### 2,3,6,7-tetramethylnaphthalenium



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.306043 | 1.650618  | -0.000196 |
| C | -2.081885 | 0.951752  | -0.000150 |
| C | -0.840178 | 1.598943  | -0.000068 |
| C | 0.379386  | 0.893224  | 0.000032  |
| C | 1.650970  | 1.686563  | 0.000219  |
| C | 0.359159  | -0.512738 | -0.000056 |
| C | -0.880762 | -1.166507 | -0.000057 |
| C | -2.104973 | -0.467610 | -0.000129 |
| C | -3.346653 | -1.114774 | -0.000125 |
| C | -4.566200 | -0.409096 | -0.000072 |

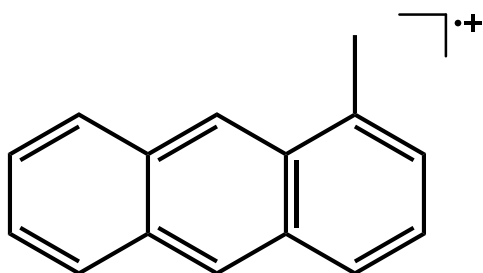
|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.545959 | 0.996868  | -0.000180 |
| C | 1.622232  | -1.326950 | -0.000123 |
| C | -5.809011 | 1.811011  | -0.000132 |
| C | -5.837892 | -1.202246 | 0.000203  |
| H | -3.284117 | 2.734671  | -0.000131 |
| H | -0.814819 | 2.683250  | -0.000078 |
| H | 2.539750  | 1.062445  | 0.000041  |
| H | 1.688544  | 2.338535  | 0.877586  |
| H | 1.688498  | 2.339048  | -0.876761 |
| H | -0.902816 | -2.250579 | -0.000153 |
| H | -3.372062 | -2.199053 | 0.000150  |
| H | 1.397003  | -2.392438 | -0.000715 |
| H | 2.232885  | -1.108766 | 0.879127  |
| H | 2.233417  | -1.107933 | -0.878786 |
| H | -5.583789 | 2.876504  | -0.000646 |
| H | -6.419608 | 1.592660  | 0.879109  |
| H | -6.420204 | 1.591967  | -0.878776 |
| H | -6.726558 | -0.577982 | 0.000193  |
| H | -5.875466 | -1.854247 | 0.877544  |
| H | -5.875637 | -1.854588 | -0.876872 |

anthracenium



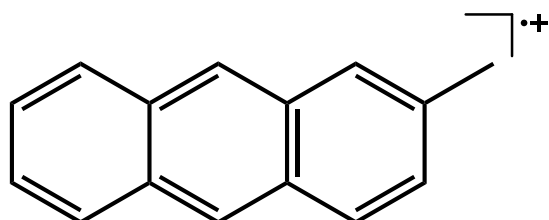
|   |          |          |         |
|---|----------|----------|---------|
| C | -2.47008 | 1.40934  | 0.00000 |
| C | -1.23198 | 0.72154  | 0.00000 |
| C | 0.00000  | 1.40910  | 0.00000 |
| C | 1.23198  | 0.72154  | 0.00000 |
| C | 2.47008  | 1.40934  | 0.00000 |
| C | 3.67114  | 0.70355  | 0.00000 |
| C | 3.67114  | -0.70355 | 0.00000 |
| C | 2.47008  | -1.40934 | 0.00000 |
| C | 1.23198  | -0.72154 | 0.00000 |
| C | -0.00000 | -1.40910 | 0.00000 |
| C | -1.23198 | -0.72154 | 0.00000 |
| C | -2.47008 | -1.40934 | 0.00000 |
| C | -3.67114 | -0.70355 | 0.00000 |
| C | -3.67114 | 0.70355  | 0.00000 |
| H | -2.47336 | 2.50084  | 0.00000 |
| H | 0.00000  | 2.50186  | 0.00000 |
| H | 2.47336  | 2.50084  | 0.00000 |
| H | 4.61753  | 1.24544  | 0.00000 |
| H | 4.61753  | -1.24544 | 0.00000 |
| H | 2.47336  | -2.50084 | 0.00000 |
| H | -0.00000 | -2.50186 | 0.00000 |
| H | -2.47336 | -2.50084 | 0.00000 |
| H | -4.61753 | -1.24544 | 0.00000 |
| H | -4.61753 | 1.24544  | 0.00000 |

### 1-methylantracenium



|   |          |          |          |
|---|----------|----------|----------|
| C | 2.19023  | -1.91958 | 0.00000  |
| C | 1.03939  | -1.09427 | 0.00000  |
| C | 1.13655  | 0.31503  | 0.00000  |
| C | 0.00000  | 1.14576  | 0.00000  |
| C | 0.10121  | 2.57522  | 0.00000  |
| C | -1.08434 | 3.32494  | 0.00000  |
| C | -2.34950 | 2.71911  | 0.00000  |
| C | -2.46583 | 1.33166  | 0.00000  |
| C | -1.30509 | 0.52280  | 0.00000  |
| C | -1.40474 | -0.88383 | 0.00000  |
| C | -0.26312 | -1.71075 | 0.00000  |
| C | -0.35812 | -3.12473 | 0.00000  |
| C | 0.79201  | -3.90829 | 0.00000  |
| C | 2.06511  | -3.30604 | 0.00000  |
| C | 1.42807  | 3.27499  | 0.00000  |
| H | 3.17834  | -1.45605 | 0.00000  |
| H | 2.13261  | 0.76129  | 0.00000  |
| H | -1.01571 | 4.41452  | 0.00000  |
| H | -3.24554 | 3.34085  | 0.00000  |
| H | -3.44829 | 0.85680  | 0.00000  |
| H | -2.39608 | -1.34357 | 0.00000  |
| H | -1.34461 | -3.59225 | 0.00000  |
| H | 0.70762  | -4.99560 | 0.00000  |
| H | 2.95936  | -3.93038 | 0.00000  |
| H | 1.29166  | 4.36264  | 0.00000  |
| H | 2.02478  | 3.00481  | -0.88533 |
| H | 2.02478  | 3.00481  | 0.88533  |

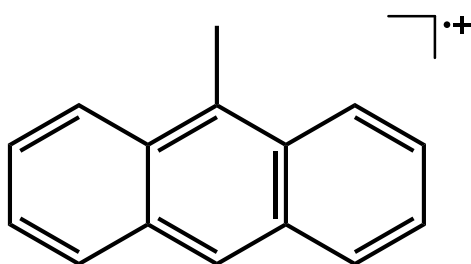
### 2-methylantracenium



|   |          |          |         |
|---|----------|----------|---------|
| C | 2.72061  | -1.58862 | 0.00000 |
| C | 1.43873  | -0.98325 | 0.00000 |
| C | 1.27904  | 0.41782  | 0.00000 |
| C | 0.00000  | 1.01749  | 0.00000 |
| C | -0.16244 | 2.42011  | 0.00000 |
| C | -1.43423 | 3.01563  | 0.00000 |
| C | -2.57008 | 2.17325  | 0.00000 |
| C | -2.44785 | 0.78938  | 0.00000 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.17054 | 0.17396  | 0.00000  |
| C | -1.01273 | -1.22312 | 0.00000  |
| C | 0.26626  | -1.82472 | 0.00000  |
| C | 0.42973  | -3.23032 | 0.00000  |
| C | 1.70338  | -3.79461 | 0.00000  |
| C | 2.84768  | -2.97432 | 0.00000  |
| C | -1.57315 | 4.50962  | 0.00000  |
| H | 3.60848  | -0.95363 | 0.00000  |
| H | 2.16673  | 1.05527  | 0.00000  |
| H | 0.72844  | 3.05273  | 0.00000  |
| H | -3.56445 | 2.62321  | 0.00000  |
| H | -3.34061 | 0.16105  | 0.00000  |
| H | -1.90028 | -1.86081 | 0.00000  |
| H | -0.45530 | -3.86923 | 0.00000  |
| H | 1.81483  | -4.87951 | 0.00000  |
| H | 3.83952  | -3.42775 | 0.00000  |
| H | -2.62491 | 4.82024  | 0.00000  |
| H | -1.07946 | 4.94429  | -0.88339 |
| H | -1.07946 | 4.94429  | 0.88339  |

**9-methylanthracenium**

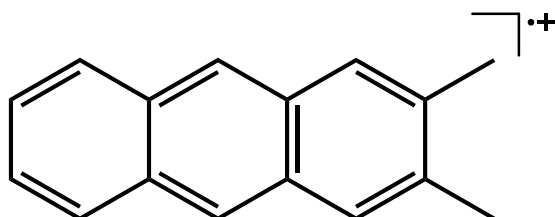


|   |          |          |          |
|---|----------|----------|----------|
| C | 2.49192  | 1.14006  | 0.00000  |
| C | 1.23296  | 0.49117  | 0.00000  |
| C | 0.00000  | 1.22449  | 0.00000  |
| C | -1.23991 | 0.50775  | 0.00000  |
| C | -2.50271 | 1.15311  | 0.00000  |
| C | -3.69084 | 0.42560  | 0.00000  |
| C | -3.67368 | -0.97930 | 0.00000  |
| C | -2.45746 | -1.65161 | 0.00000  |
| C | -1.23324 | -0.93779 | 0.00000  |
| C | -0.00915 | -1.63173 | 0.00000  |
| C | 1.22158  | -0.95013 | 0.00000  |
| C | 2.44483  | -1.66669 | 0.00000  |
| C | 3.66046  | -0.99404 | 0.00000  |
| C | 3.67964  | 0.41178  | 0.00000  |
| C | 0.04716  | 2.72149  | 0.00000  |
| H | 2.54420  | 2.22812  | 0.00000  |
| H | -2.56444 | 2.23963  | 0.00000  |
| H | -4.64306 | 0.95730  | 0.00000  |
| H | -4.60955 | -1.53885 | 0.00000  |
| H | -2.43010 | -2.74286 | 0.00000  |
| H | -0.01557 | -2.72413 | 0.00000  |
| H | 2.41679  | -2.75794 | 0.00000  |
| H | 4.59629  | -1.55370 | 0.00000  |
| H | 4.63316  | 0.94133  | 0.00000  |
| H | -0.94002 | 3.18838  | 0.00000  |
| H | 0.59146  | 3.08892  | -0.88389 |



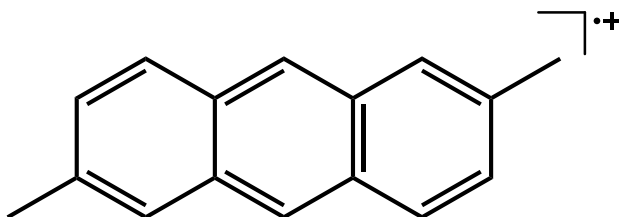
H 0.59146 3.08892 0.88389

### 2,3-dimethylantracenium



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.287272 | 1.919239  | 0.000188  |
| C | -3.066399 | 1.214148  | -0.000013 |
| C | -1.826948 | 1.879336  | -0.000090 |
| C | -0.615093 | 1.172688  | -0.000188 |
| C | 0.629642  | 1.824804  | -0.000239 |
| C | 1.835306  | 1.128342  | -0.000131 |
| C | 1.817010  | -0.291454 | -0.000017 |
| C | 0.591705  | -0.950829 | -0.000023 |
| C | -0.635910 | -0.259902 | -0.000122 |
| C | -1.868278 | -0.926009 | -0.000120 |
| C | -3.087815 | -0.220837 | -0.000121 |
| C | -4.329491 | -0.886180 | -0.000152 |
| C | -5.512278 | -0.165455 | 0.000010  |
| C | -5.491287 | 1.236159  | 0.000180  |
| C | 3.114906  | 1.915119  | -0.000084 |
| C | 3.089019  | -1.090909 | 0.000187  |
| H | -4.273742 | 3.002467  | 0.000311  |
| H | -1.808332 | 2.963509  | 0.000035  |
| H | 0.647345  | 2.909052  | -0.000385 |
| H | 0.574821  | -2.034776 | 0.000164  |
| H | -1.886354 | -2.010203 | -0.000044 |
| H | -4.351070 | -1.969225 | -0.000258 |
| H | -6.459641 | -0.688295 | -0.000042 |
| H | -6.422039 | 1.788021  | 0.000355  |
| H | 3.999781  | 1.285449  | -0.000138 |
| H | 3.158572  | 2.564991  | 0.877830  |
| H | 3.158557  | 2.565175  | -0.877858 |
| H | 2.876581  | -2.159051 | -0.000064 |
| H | 3.697304  | -0.864163 | 0.879078  |
| H | 3.697841  | -0.863876 | -0.878252 |

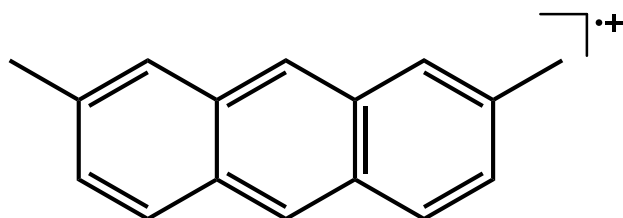
### 2,6-dimethylantracenium



|   |           |          |          |
|---|-----------|----------|----------|
| C | -3.589641 | 1.910972 | 0.000133 |
| C | -2.362053 | 1.212136 | 0.000152 |
| C | -1.129394 | 1.873446 | 0.000176 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.089186  | 1.164164  | 0.000088  |
| C | 1.326699  | 1.825424  | -0.000017 |
| C | 2.531668  | 1.121186  | -0.000120 |
| C | 2.488926  | -0.286106 | -0.000051 |
| C | 1.289560  | -0.970022 | 0.000134  |
| C | 0.061967  | -0.271216 | 0.000154  |
| C | -1.170701 | -0.932519 | 0.000176  |
| C | -2.389277 | -0.223235 | 0.000083  |
| C | -3.626814 | -0.884501 | -0.000027 |
| C | -4.831759 | -0.180259 | -0.000130 |
| C | -4.789001 | 1.227063  | -0.000067 |
| C | 3.838217  | 1.854959  | -0.000204 |
| C | -6.138327 | -0.913988 | -0.000199 |
| H | -3.581837 | 2.994334  | 0.000281  |
| H | -1.108256 | 2.957576  | 0.000307  |
| H | 1.340653  | 2.909556  | -0.000053 |
| H | 3.418005  | -0.842179 | -0.000094 |
| H | 1.281793  | -2.053385 | 0.000281  |
| H | -1.191831 | -2.016651 | 0.000309  |
| H | -3.640664 | -1.968634 | -0.000062 |
| H | -5.718137 | 1.783044  | -0.000109 |
| H | 4.681609  | 1.166003  | -0.000893 |
| H | 3.917390  | 2.500566  | 0.878337  |
| H | 3.916755  | 2.501607  | -0.878029 |
| H | -6.981700 | -0.225007 | -0.000866 |
| H | -6.217502 | -1.559606 | 0.878334  |
| H | -6.216902 | -1.560629 | -0.878026 |

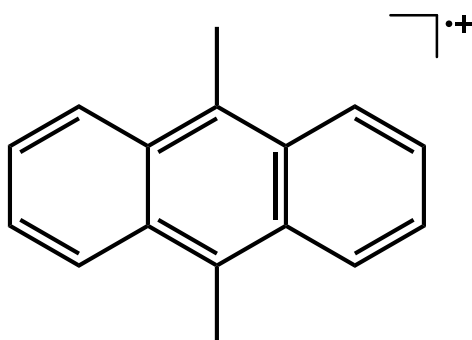
**2,7-dimethylantracenium**



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.587780 | 1.902272  | 0.000036  |
| C | -2.364989 | 1.199950  | 0.000019  |
| C | -1.126901 | 1.866514  | 0.000044  |
| C | 0.091699  | 1.160666  | 0.000004  |
| C | 1.331161  | 1.823619  | -0.000063 |
| C | 2.536712  | 1.119896  | -0.000061 |
| C | 2.493497  | -0.285975 | 0.000038  |
| C | 1.292290  | -0.970888 | 0.000163  |
| C | 0.067213  | -0.273873 | 0.000076  |
| C | -1.167912 | -0.937821 | 0.000048  |
| C | -2.381982 | -0.234092 | -0.000062 |
| C | -3.628256 | -0.894093 | -0.000156 |
| C | -4.805713 | -0.174244 | -0.000125 |
| C | -4.809701 | 1.236415  | -0.000036 |
| C | 3.844983  | 1.851865  | -0.000074 |
| C | -6.111257 | 1.982301  | -0.000005 |
| H | -3.567270 | 2.986212  | 0.000211  |
| H | -1.108643 | 2.950748  | 0.000138  |
| H | 1.344862  | 2.907767  | -0.000127 |

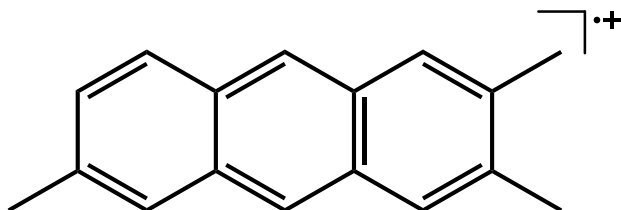
|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 3.422132  | -0.842886 | 0.000072  |
| H | 1.285598  | -2.054262 | 0.000319  |
| H | -1.185703 | -2.022011 | 0.000172  |
| H | -3.653754 | -1.977147 | -0.000297 |
| H | -5.750588 | -0.703654 | -0.000262 |
| H | 4.686497  | 1.160408  | -0.000664 |
| H | 3.926591  | 2.496780  | 0.878630  |
| H | 3.926103  | 2.497734  | -0.878117 |
| H | -5.958439 | 3.060894  | -0.000595 |
| H | -6.705112 | 1.716251  | 0.878421  |
| H | -6.705705 | 1.715350  | -0.877748 |

### 9,10-dimethylantracenium



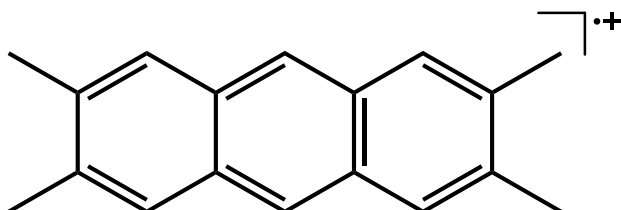
|   |          |          |          |
|---|----------|----------|----------|
| C | -0.03683 | -2.83938 | 0.00000  |
| C | 0.00000  | -1.42234 | 0.00000  |
| C | 1.25246  | -0.72958 | 0.00000  |
| C | 1.25099  | 0.69912  | 0.00000  |
| C | 2.45648  | 1.44943  | 0.00000  |
| C | 2.45384  | 2.83871  | 0.00000  |
| C | 1.23780  | 3.53859  | 0.00000  |
| C | 0.03685  | 2.83944  | 0.00000  |
| C | 0.00009  | 1.42239  | 0.00000  |
| C | -1.25236 | 0.72954  | 0.00000  |
| C | -1.25083 | -0.69906 | 0.00000  |
| C | -2.45641 | -1.44918 | 0.00000  |
| C | -2.45387 | -2.83846 | 0.00000  |
| C | -1.23785 | -3.53843 | 0.00000  |
| C | 2.52384  | -1.52384 | 0.00000  |
| C | -2.52404 | 1.52328  | 0.00000  |
| H | 0.89536  | -3.40181 | 0.00000  |
| H | 3.41618  | 0.93752  | 0.00000  |
| H | 3.39992  | 3.38111  | 0.00000  |
| H | 1.23112  | 4.62918  | 0.00000  |
| H | -0.89535 | 3.40185  | 0.00000  |
| H | -3.41602 | -0.93706 | 0.00000  |
| H | -3.39999 | -3.38079 | 0.00000  |
| H | -1.23124 | -4.62902 | 0.00000  |
| H | 3.42401  | -0.90656 | 0.00000  |
| H | 2.56958  | -2.17881 | -0.88407 |
| H | 2.56958  | -2.17881 | 0.88407  |
| H | -3.42389 | 0.90546  | 0.00000  |
| H | -2.57011 | 2.17819  | -0.88409 |
| H | -2.57011 | 2.17819  | 0.88409  |

### 2,3,6-trimethylantracenium



|   |          |          |          |
|---|----------|----------|----------|
| C | 2.71555  | 1.69564  | -0.00003 |
| C | 1.51974  | 0.93515  | 0.00000  |
| C | 0.24706  | 1.53782  | -0.00002 |
| C | -0.93393 | 0.76594  | -0.00003 |
| C | -2.21723 | 1.35348  | -0.00017 |
| C | -3.39226 | 0.59182  | -0.00032 |
| C | -3.29823 | -0.83325 | -0.00020 |
| C | -2.03334 | -1.42836 | -0.00014 |
| C | -0.83735 | -0.67102 | -0.00005 |
| C | 0.43286  | -1.27544 | 0.00001  |
| C | 1.61907  | -0.50386 | 0.00003  |
| C | 2.89608  | -1.10530 | 0.00007  |
| C | 4.07189  | -0.33969 | 0.00005  |
| C | 3.95565  | 1.06998  | -0.00002 |
| C | -4.71459 | 1.30846  | 0.00019  |
| C | 5.41627  | -1.00822 | 0.00008  |
| C | -4.52615 | -1.70038 | 0.00008  |
| H | 2.65227  | 2.78574  | -0.00007 |
| H | 0.17215  | 2.62821  | -0.00004 |
| H | -2.29287 | 2.44391  | -0.00030 |
| H | -1.95880 | -2.51864 | -0.00012 |
| H | 0.50758  | -2.36581 | 0.00002  |
| H | 2.96320  | -2.19608 | 0.00011  |
| H | 4.86282  | 1.67712  | -0.00005 |
| H | -5.57148 | 0.62753  | -0.01140 |
| H | -4.79025 | 1.97136  | -0.87604 |
| H | -4.79976 | 1.95198  | 0.89005  |
| H | 6.23363  | -0.27675 | 0.00010  |
| H | 5.52838  | -1.65619 | -0.88335 |
| H | 5.52833  | -1.65620 | 0.88349  |
| H | -4.25643 | -2.76355 | 0.00068  |
| H | -5.15247 | -1.50515 | -0.88434 |
| H | -5.15277 | -1.50415 | 0.88405  |

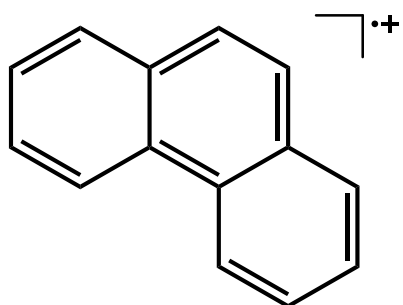
### 2,3,6,7-tetramethylantracenium



|   |           |          |           |
|---|-----------|----------|-----------|
| C | -3.590890 | 1.900422 | -0.000109 |
| C | -2.364346 | 1.207987 | -0.000216 |
| C | -1.129073 | 1.872848 | -0.000212 |
| C | 0.085469  | 1.164081 | -0.000228 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.330512  | 1.814100  | -0.000172 |
| C | 2.534905  | 1.116672  | -0.000053 |
| C | 2.515441  | -0.303444 | -0.000060 |
| C | 1.290225  | -0.960657 | -0.000131 |
| C | 0.063662  | -0.268218 | -0.000209 |
| C | -1.171616 | -0.933076 | -0.000232 |
| C | -2.386161 | -0.224308 | -0.000242 |
| C | -3.631228 | -0.874303 | -0.000191 |
| C | -4.835596 | -0.176862 | -0.000054 |
| C | -4.816095 | 1.243238  | -0.000060 |
| C | 3.816686  | 1.901526  | 0.000168  |
| C | -6.088040 | 2.044421  | 0.000074  |
| C | -6.117387 | -0.961719 | 0.000187  |
| C | 3.787436  | -1.104591 | 0.000093  |
| H | -3.572292 | 2.984452  | 0.000002  |
| H | -1.108927 | 2.957112  | -0.000106 |
| H | 1.349726  | 2.898420  | -0.000227 |
| H | 1.271655  | -2.044688 | -0.000022 |
| H | -1.191758 | -2.017343 | -0.000129 |
| H | -3.650382 | -1.958618 | -0.000252 |
| H | 4.700173  | 1.269647  | -0.000051 |
| H | 3.862991  | 2.550811  | 0.878337  |
| H | 3.862953  | 2.551436  | -0.877534 |
| H | -5.873983 | 3.112371  | -0.000371 |
| H | -6.696973 | 1.819634  | 0.879021  |
| H | -6.697591 | 1.819055  | -0.878289 |
| H | 3.573424  | -2.172556 | -0.000354 |
| H | 4.396340  | -0.879832 | 0.879069  |
| H | 4.396993  | -0.879248 | -0.878274 |
| H | -7.000911 | -0.329882 | 0.000001  |
| H | -6.163686 | -1.611005 | 0.878352  |
| H | -6.163698 | -1.611610 | -0.877523 |

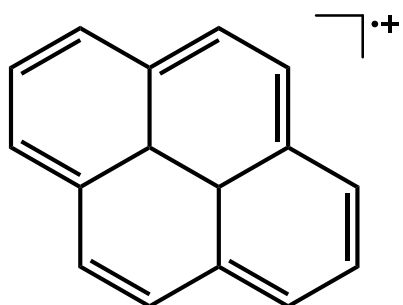
Phenanthrenium



|   |          |          |         |
|---|----------|----------|---------|
| C | 0.66171  | 2.06522  | 0.00000 |
| C | 0.00000  | 0.83181  | 0.00000 |
| C | 0.69633  | -0.45509 | 0.00000 |
| C | -0.07777 | -1.66838 | 0.00000 |
| C | -1.48453 | -1.60007 | 0.00000 |
| C | -2.15145 | -0.36797 | 0.00000 |
| C | -1.43935 | 0.84722  | 0.00000 |
| C | -2.14422 | 2.09056  | 0.00000 |
| C | -1.45765 | 3.29138  | 0.00000 |
| C | -0.05291 | 3.27420  | 0.00000 |
| C | 2.09077  | -0.57532 | 0.00000 |
| C | 2.71250  | -1.83466 | 0.00000 |

|   |          |          |         |
|---|----------|----------|---------|
| C | 1.95865  | -3.02013 | 0.00000 |
| C | 0.57769  | -2.93850 | 0.00000 |
| H | 1.75044  | 2.11087  | 0.00000 |
| H | -2.06381 | -2.52522 | 0.00000 |
| H | -3.24289 | -0.34771 | 0.00000 |
| H | -3.23551 | 2.07165  | 0.00000 |
| H | -1.99626 | 4.23886  | 0.00000 |
| H | 0.50065  | 4.21437  | 0.00000 |
| H | 2.72396  | 0.31139  | 0.00000 |
| H | 3.80246  | -1.88484 | 0.00000 |
| H | 2.45749  | -3.98916 | 0.00000 |
| H | -0.03510 | -3.84187 | 0.00000 |

**Pyrenium**



|   |          |          |          |
|---|----------|----------|----------|
| C | 3.54238  | -0.00001 | 0.00000  |
| C | 2.84662  | 1.20882  | 0.00006  |
| C | 1.42287  | 1.23576  | 0.00004  |
| C | 0.69377  | 2.45422  | -0.00002 |
| C | -0.69376 | 2.45426  | -0.00002 |
| C | -1.42286 | 1.23580  | 0.00002  |
| C | -2.84655 | 1.20881  | -0.00005 |
| C | -3.54242 | -0.00002 | -0.00003 |
| C | -2.84665 | -1.20880 | 0.00006  |
| C | -1.42288 | -1.23571 | 0.00005  |
| C | -0.69383 | -2.45419 | 0.00003  |
| C | 0.69374  | -2.45423 | -0.00006 |
| C | 1.42289  | -1.23585 | -0.00002 |
| C | 2.84661  | -1.20885 | -0.00004 |
| C | 0.70898  | -0.00000 | 0.00002  |
| C | -0.70893 | -0.00000 | -0.00002 |
| H | 4.63244  | -0.00003 | -0.00002 |
| H | 3.39210  | 2.15453  | 0.00019  |
| H | 1.23892  | 3.39981  | -0.00014 |
| H | -1.23886 | 3.39987  | 0.00001  |
| H | -3.39209 | 2.15450  | -0.00010 |
| H | -4.63248 | 0.00014  | -0.00007 |
| H | -3.39198 | -2.15462 | 0.00015  |
| H | -1.23892 | -3.39980 | 0.00014  |
| H | 1.23877  | -3.39988 | -0.00020 |
| H | 3.39215  | -2.15452 | -0.00008 |