

# **Planar *versus* twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory**

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Supplementary information

**Table S1.** Optimized ground state structures obtained with the 6-311G(d,p) basis set.

A) GAS-PHASE STRUCTURES

B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.181335  | -0.256131 | -0.041040 |
| 6 | 2.178609  | 0.734058  | 0.071737  |
| 6 | 0.845105  | 0.374746  | 0.042143  |
| 6 | 0.416937  | -0.957481 | -0.102959 |
| 6 | 1.417780  | -1.936404 | -0.218332 |
| 6 | 2.755841  | -1.607947 | -0.188393 |
| 6 | -1.796945 | -0.338392 | -0.026750 |
| 6 | -1.417386 | 1.064477  | 0.117236  |
| 6 | -2.313780 | 2.073000  | 0.221227  |
| 1 | -1.983436 | 3.098501  | 0.326118  |
| 6 | -3.747939 | 1.820733  | 0.197903  |
| 6 | -4.174943 | 0.394839  | 0.055373  |
| 6 | -3.231267 | -0.645375 | -0.052218 |
| 1 | 2.410807  | 1.784442  | 0.164382  |
| 1 | 1.103267  | -2.967793 | -0.324596 |
| 1 | 3.484009  | -2.401902 | -0.261795 |
| 6 | -3.678671 | -1.969304 | -0.183768 |
| 6 | -5.541379 | 0.097672  | 0.029900  |
| 6 | -5.035871 | -2.248517 | -0.206957 |
| 6 | -5.972576 | -1.213611 | -0.100078 |
| 8 | -4.567947 | 2.728540  | 0.291200  |
| 8 | -0.083013 | 1.372413  | 0.149416  |
| 7 | -0.914277 | -1.290985 | -0.131284 |
| 1 | -2.942717 | -2.758595 | -0.265616 |
| 1 | -5.371879 | -3.274471 | -0.308706 |
| 1 | -7.033227 | -1.437664 | -0.119124 |
| 1 | -6.238797 | 0.921963  | 0.114580  |
| 7 | 4.515728  | 0.074456  | -0.007219 |
| 6 | 4.964369  | 1.440022  | 0.266188  |
| 6 | 5.067156  | 2.324440  | -0.981879 |
| 1 | 5.943535  | 1.370364  | 0.747562  |
| 1 | 4.301517  | 1.894878  | 1.005739  |
| 1 | 5.426148  | 3.321513  | -0.711378 |
| 1 | 5.766975  | 1.899087  | -1.705947 |
| 1 | 4.099129  | 2.432281  | -1.475237 |
| 6 | 5.565694  | -0.915956 | -0.248112 |
| 6 | 6.014960  | -1.667718 | 1.010362  |
| 1 | 6.417733  | -0.385482 | -0.681623 |
| 1 | 5.232241  | -1.617219 | -1.016114 |
| 1 | 6.814357  | -2.373056 | 0.765720  |
| 1 | 6.396018  | -0.974895 | 1.765070  |
| 1 | 5.189666  | -2.226775 | 1.456062  |

B3P86

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.171784  | -0.252732 | -0.041212 |
| 6 | 2.172935  | 0.735259  | 0.072476  |
| 6 | 0.842828  | 0.375965  | 0.042290  |
| 6 | 0.417811  | -0.954158 | -0.103749 |
| 6 | 1.416869  | -1.929981 | -0.219881 |
| 6 | 2.751215  | -1.601280 | -0.190051 |
| 6 | -1.786033 | -0.336460 | -0.026953 |
| 6 | -1.407596 | 1.060475  | 0.117300  |
| 6 | -2.303602 | 2.067065  | 0.221871  |
| 1 | -1.972905 | 3.092577  | 0.327457  |
| 6 | -3.732033 | 1.813377  | 0.198577  |
| 6 | -4.154820 | 0.393278  | 0.055751  |
| 6 | -3.213551 | -0.642865 | -0.052341 |
| 1 | 2.406673  | 1.786128  | 0.165985  |
| 1 | 1.101374  | -2.961213 | -0.327019 |
| 1 | 3.482849  | -2.393140 | -0.263990 |
| 6 | -3.656653 | -1.963788 | -0.184537 |
| 6 | -5.517394 | 0.096993  | 0.030519  |
| 6 | -5.010504 | -2.243308 | -0.207638 |
| 6 | -5.946022 | -1.211720 | -0.100051 |
| 8 | -4.553401 | 2.716708  | 0.292148  |
| 8 | -0.080567 | 1.367754  | 0.149575  |
| 7 | -0.906798 | -1.288918 | -0.132284 |
| 1 | -2.916761 | -2.750259 | -0.266870 |
| 1 | -5.345872 | -3.269463 | -0.310159 |
| 1 | -7.006462 | -1.437138 | -0.119141 |
| 1 | -6.212997 | 0.923566  | 0.116175  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 7 | 4.498556 | 0.076782  | -0.006710 |
| 6 | 4.940483 | 1.435558  | 0.261210  |
| 6 | 5.028675 | 2.309666  | -0.984882 |
| 1 | 5.922737 | 1.369785  | 0.737828  |
| 1 | 4.279957 | 1.887664  | 1.005693  |
| 1 | 5.381554 | 3.311148  | -0.725179 |
| 1 | 5.725924 | 1.884017  | -1.710930 |
| 1 | 4.056282 | 2.405621  | -1.472178 |
| 6 | 5.540876 | -0.909320 | -0.241868 |
| 6 | 5.972025 | -1.659412 | 1.013700  |
| 1 | 6.397015 | -0.379149 | -0.668736 |
| 1 | 5.210864 | -1.606815 | -1.015854 |
| 1 | 6.769211 | -2.370039 | 0.779970  |
| 1 | 6.348270 | -0.967777 | 1.771609  |
| 1 | 5.137983 | -2.211931 | 1.451328  |

PBE0

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.170410  | -0.253144 | -0.039943 |
| 6 | 2.171533  | 0.734409  | 0.071936  |
| 6 | 0.841121  | 0.374945  | 0.042734  |
| 6 | 0.416743  | -0.954313 | -0.101570 |
| 6 | 1.415334  | -1.930020 | -0.215450 |
| 6 | 2.749822  | -1.601760 | -0.185516 |
| 6 | -1.784769 | -0.337157 | -0.026510 |
| 6 | -1.404646 | 1.060556  | 0.117739  |
| 6 | -2.300155 | 2.066616  | 0.222870  |
| 1 | -1.968954 | 3.092683  | 0.328673  |
| 6 | -3.729624 | 1.813629  | 0.199683  |
| 6 | -4.153342 | 0.393498  | 0.055667  |
| 6 | -3.213449 | -0.642482 | -0.052769 |
| 1 | 2.404170  | 1.786554  | 0.162804  |
| 1 | 1.099541  | -2.962155 | -0.320687 |
| 1 | 3.481248  | -2.395101 | -0.256697 |
| 6 | -3.656775 | -1.962799 | -0.186121 |
| 6 | -5.516055 | 0.098780  | 0.029644  |
| 6 | -5.010824 | -2.241349 | -0.210166 |
| 6 | -5.945613 | -1.209448 | -0.102244 |
| 8 | -4.549030 | 2.715559  | 0.293854  |
| 8 | -0.080179 | 1.366174  | 0.149070  |
| 7 | -0.908331 | -1.289112 | -0.130712 |
| 1 | -2.916990 | -2.750336 | -0.268718 |
| 1 | -5.346945 | -3.267929 | -0.313680 |
| 1 | -7.006919 | -1.434224 | -0.122027 |
| 1 | -6.211598 | 0.926298  | 0.115779  |
| 7 | 4.496406  | 0.076357  | -0.006936 |
| 6 | 4.938460  | 1.433357  | 0.259019  |
| 6 | 5.028124  | 2.304654  | -0.988112 |
| 1 | 5.921167  | 1.367950  | 0.736606  |
| 1 | 4.278325  | 1.888141  | 1.003287  |
| 1 | 5.381959  | 3.307019  | -0.730460 |
| 1 | 5.725891  | 1.876212  | -1.713165 |
| 1 | 4.055502  | 2.399975  | -1.476713 |
| 6 | 5.537522  | -0.907914 | -0.243002 |
| 6 | 5.972877  | -1.654012 | 1.012616  |
| 1 | 6.392751  | -0.377822 | -0.673854 |
| 1 | 5.206731  | -1.608058 | -1.015314 |
| 1 | 6.770644  | -2.364941 | 0.778804  |
| 1 | 6.350602  | -0.959076 | 1.767851  |
| 1 | 5.139862  | -2.206045 | 1.454614  |

BMK

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.183449  | -0.254529 | -0.043525 |
| 6 | 2.180700  | 0.739679  | 0.067863  |
| 6 | 0.844084  | 0.377690  | 0.034326  |
| 6 | 0.420641  | -0.956809 | -0.111910 |
| 6 | 1.420539  | -1.938949 | -0.228782 |
| 6 | 2.761193  | -1.610572 | -0.196985 |
| 6 | -1.788186 | -0.343169 | -0.031494 |
| 6 | -1.400213 | 1.070562  | 0.108075  |
| 6 | -2.293825 | 2.081024  | 0.206658  |
| 1 | -1.960312 | 3.107954  | 0.305387  |
| 6 | -3.738558 | 1.828752  | 0.184951  |
| 6 | -4.171345 | 0.394276  | 0.052868  |
| 6 | -3.231785 | -0.648768 | -0.049132 |
| 1 | 2.416502  | 1.790977  | 0.160265  |
| 1 | 1.102944  | -2.971228 | -0.335752 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | 3.494407  | -2.401685 | -0.270846 |
| 6 | -3.679854 | -1.975331 | -0.166116 |
| 6 | -5.541591 | 0.103830  | 0.035404  |
| 6 | -5.041172 | -2.250815 | -0.181097 |
| 6 | -5.977018 | -1.210299 | -0.080830 |
| 8 | -4.549981 | 2.728456  | 0.270829  |
| 8 | -0.078660 | 1.363116  | 0.137508  |
| 7 | -0.912692 | -1.288123 | -0.136866 |
| 1 | -2.945643 | -2.769313 | -0.241676 |
| 1 | -5.380771 | -3.278155 | -0.269877 |
| 1 | -7.039365 | -1.433040 | -0.092985 |
| 1 | -6.235892 | 0.933742  | 0.115769  |
| 7 | 4.511062  | 0.074289  | -0.002410 |
| 6 | 4.955168  | 1.426579  | 0.301915  |
| 6 | 5.044923  | 2.331975  | -0.939980 |
| 1 | 5.940546  | 1.351200  | 0.773425  |
| 1 | 4.292651  | 1.866018  | 1.053399  |
| 1 | 5.392856  | 3.331773  | -0.660909 |
| 1 | 5.747613  | 1.914711  | -1.668219 |
| 1 | 4.070411  | 2.426332  | -1.427493 |
| 6 | 5.555622  | -0.904877 | -0.267123 |
| 6 | 5.995361  | -1.681314 | 0.987148  |
| 1 | 6.411632  | -0.364684 | -0.684597 |
| 1 | 5.220933  | -1.592004 | -1.049419 |
| 1 | 6.794660  | -2.387596 | 0.739760  |
| 1 | 6.370510  | -0.994923 | 1.752868  |
| 1 | 5.158063  | -2.239442 | 1.415736  |

BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.159143  | -0.255681 | -0.039153 |
| 6 | 2.165171  | 0.727500  | 0.069986  |
| 6 | 0.839523  | 0.370515  | 0.041371  |
| 6 | 0.417272  | -0.947696 | -0.099544 |
| 6 | 1.406499  | -1.921176 | -0.210704 |
| 6 | 2.737224  | -1.597229 | -0.180938 |
| 6 | -1.781940 | -0.338554 | -0.026477 |
| 6 | -1.398717 | 1.063214  | 0.116559  |
| 6 | -2.286311 | 2.059686  | 0.219552  |
| 1 | -1.960071 | 3.078288  | 0.323306  |
| 6 | -3.716933 | 1.807037  | 0.196486  |
| 6 | -4.146556 | 0.390412  | 0.054605  |
| 6 | -3.214063 | -0.641273 | -0.052181 |
| 1 | 2.396010  | 1.770409  | 0.159584  |
| 1 | 1.094446  | -2.945621 | -0.313704 |
| 1 | 3.459213  | -2.386568 | -0.250719 |
| 6 | -3.658111 | -1.954745 | -0.183270 |
| 6 | -5.504927 | 0.101679  | 0.029502  |
| 6 | -5.007088 | -2.229011 | -0.206646 |
| 6 | -5.935664 | -1.199844 | -0.100213 |
| 8 | -4.523678 | 2.703036  | 0.288649  |
| 8 | -0.080624 | 1.358312  | 0.146153  |
| 7 | -0.913749 | -1.275485 | -0.127714 |
| 1 | -2.929673 | -2.740269 | -0.264727 |
| 1 | -5.342648 | -3.246843 | -0.308120 |
| 1 | -6.988967 | -1.420344 | -0.119307 |
| 1 | -6.196678 | 0.920289  | 0.113824  |
| 7 | 4.484695  | 0.072718  | -0.007310 |
| 6 | 4.928970  | 1.425966  | 0.267121  |
| 6 | 5.024680  | 2.306110  | -0.971724 |
| 1 | 5.903884  | 1.357703  | 0.739988  |
| 1 | 4.275036  | 1.877069  | 1.005561  |
| 1 | 5.378506  | 3.298041  | -0.705283 |
| 1 | 5.718717  | 1.884103  | -1.692376 |
| 1 | 4.061163  | 2.408260  | -1.459170 |
| 6 | 5.524242  | -0.908876 | -0.252766 |
| 6 | 5.971090  | -1.657969 | 0.995328  |
| 1 | 6.370974  | -0.382422 | -0.682433 |
| 1 | 5.193202  | -1.603824 | -1.016644 |
| 1 | 6.761971  | -2.362031 | 0.752214  |
| 1 | 6.352500  | -0.969411 | 1.743268  |
| 1 | 5.149195  | -2.208630 | 1.440117  |

CAM-B3LYP

|   |          |           |           |
|---|----------|-----------|-----------|
| 6 | 3.170360 | -0.255341 | -0.039342 |
| 6 | 2.174201 | 0.730424  | 0.070860  |
| 6 | 0.844328 | 0.371449  | 0.041997  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 0.421144  | -0.950334 | -0.100379 |
| 6 | 1.413590  | -1.926473 | -0.212551 |
| 6 | 2.747776  | -1.601201 | -0.182300 |
| 6 | -1.786323 | -0.339736 | -0.026684 |
| 6 | -1.404769 | 1.066964  | 0.118194  |
| 6 | -2.296214 | 2.066263  | 0.222658  |
| 1 | -1.968631 | 3.091626  | 0.328177  |
| 6 | -3.730036 | 1.811945  | 0.199320  |
| 6 | -4.158969 | 0.389595  | 0.055159  |
| 6 | -3.223203 | -0.643977 | -0.052965 |
| 1 | 2.405037  | 1.780647  | 0.161024  |
| 1 | 1.096994  | -2.956777 | -0.316860 |
| 1 | 3.475432  | -2.395067 | -0.252417 |
| 6 | -3.666722 | -1.960895 | -0.185985 |
| 6 | -5.520211 | 0.099142  | 0.029433  |
| 6 | -5.019504 | -2.237460 | -0.210054 |
| 6 | -5.951193 | -1.206404 | -0.102294 |
| 8 | -4.544833 | 2.711959  | 0.293075  |
| 8 | -0.079330 | 1.368116  | 0.148531  |
| 7 | -0.915823 | -1.282514 | -0.129306 |
| 1 | -2.930232 | -2.748813 | -0.268566 |
| 1 | -5.356354 | -3.262092 | -0.313454 |
| 1 | -7.011239 | -1.429066 | -0.121968 |
| 1 | -6.214653 | 0.924996  | 0.115434  |
| 7 | 4.500661  | 0.074022  | -0.007261 |
| 6 | 4.944762  | 1.433399  | 0.262925  |
| 6 | 5.032236  | 2.310608  | -0.983049 |
| 1 | 5.927212  | 1.367756  | 0.735997  |
| 1 | 4.287892  | 1.886630  | 1.007573  |
| 1 | 5.386164  | 3.310859  | -0.723171 |
| 1 | 5.727595  | 1.884576  | -1.709419 |
| 1 | 4.060308  | 2.407506  | -1.468842 |
| 6 | 5.543518  | -0.912300 | -0.248967 |
| 6 | 5.983531  | -1.661690 | 1.005776  |
| 1 | 6.397117  | -0.383801 | -0.679537 |
| 1 | 5.211492  | -1.611099 | -1.018610 |
| 1 | 6.779794  | -2.371239 | 0.769132  |
| 1 | 6.362471  | -0.968064 | 1.759309  |
| 1 | 5.153251  | -2.213585 | 1.448803  |

LC-wPBE

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.165163  | -0.254417 | -0.038929 |
| 6 | 2.172950  | 0.728969  | 0.068923  |
| 6 | 0.843351  | 0.370313  | 0.040423  |
| 6 | 0.423090  | -0.945570 | -0.099905 |
| 6 | 1.411915  | -1.920292 | -0.209471 |
| 6 | 2.744387  | -1.597392 | -0.178841 |
| 6 | -1.779415 | -0.339830 | -0.027537 |
| 6 | -1.396474 | 1.070188  | 0.118619  |
| 6 | -2.286397 | 2.064060  | 0.225208  |
| 1 | -1.959698 | 3.090370  | 0.331829  |
| 6 | -3.722371 | 1.808061  | 0.202931  |
| 6 | -4.151711 | 0.386340  | 0.055970  |
| 6 | -3.219499 | -0.642038 | -0.054261 |
| 1 | 2.403294  | 1.781072  | 0.157490  |
| 1 | 1.094075  | -2.951539 | -0.312519 |
| 1 | 3.472387  | -2.393553 | -0.246573 |
| 6 | -3.658614 | -1.955845 | -0.189978 |
| 6 | -5.510158 | 0.098147  | 0.030204  |
| 6 | -5.009074 | -2.232942 | -0.214618 |
| 6 | -5.939549 | -1.205108 | -0.104416 |
| 8 | -4.535162 | 2.704808  | 0.299324  |
| 8 | -0.075730 | 1.369611  | 0.146733  |
| 7 | -0.918660 | -1.280256 | -0.129678 |
| 1 | -2.919083 | -2.742750 | -0.274404 |
| 1 | -5.345443 | -3.258548 | -0.320585 |
| 1 | -7.000488 | -1.428448 | -0.124406 |
| 1 | -6.205559 | 0.924808  | 0.118603  |
| 7 | 4.493029  | 0.073456  | -0.007526 |
| 6 | 4.935124  | 1.429055  | 0.256590  |
| 6 | 5.016853  | 2.295266  | -0.992058 |
| 1 | 5.919156  | 1.365814  | 0.728296  |
| 1 | 4.280814  | 1.884483  | 1.003458  |
| 1 | 5.363089  | 3.300438  | -0.742702 |
| 1 | 5.714821  | 1.866532  | -1.714255 |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 4.043877 | 2.378891  | -1.478702 |
| 6 | 5.531253 | -0.911459 | -0.243808 |
| 6 | 5.961852 | -1.653506 | 1.013147  |
| 1 | 6.387249 | -0.385074 | -0.673921 |
| 1 | 5.201552 | -1.611108 | -1.014929 |
| 1 | 6.752923 | -2.371399 | 0.786296  |
| 1 | 6.342778 | -0.955828 | 1.761855  |
| 1 | 5.124755 | -2.193933 | 1.457979  |

## N-HEPTANE STRUCTURES

### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.181787  | -0.254936 | -0.040761 |
| 6 | 2.177220  | 0.735747  | 0.071663  |
| 6 | 0.845523  | 0.374773  | 0.040926  |
| 6 | 0.416717  | -0.958768 | -0.104634 |
| 6 | 1.419483  | -1.938363 | -0.219967 |
| 6 | 2.755749  | -1.608894 | -0.189463 |
| 6 | -1.797194 | -0.338178 | -0.028169 |
| 6 | -1.417870 | 1.062224  | 0.116065  |
| 6 | -2.315143 | 2.072437  | 0.221077  |
| 1 | -1.981819 | 3.097121  | 0.325926  |
| 6 | -3.746182 | 1.820541  | 0.198594  |
| 6 | -4.174506 | 0.396135  | 0.056433  |
| 6 | -3.230673 | -0.644986 | -0.053271 |
| 1 | 2.410265  | 1.785844  | 0.164573  |
| 1 | 1.107299  | -2.970438 | -0.326680 |
| 1 | 3.484804  | -2.401839 | -0.262956 |
| 6 | -3.679938 | -1.968646 | -0.185899 |
| 6 | -5.541515 | 0.097902  | 0.032826  |
| 6 | -5.037166 | -2.247979 | -0.207540 |
| 6 | -5.973847 | -1.212890 | -0.097839 |
| 8 | -4.568458 | 2.730753  | 0.292537  |
| 8 | -0.085605 | 1.370938  | 0.147783  |
| 7 | -0.911892 | -1.290944 | -0.133110 |
| 1 | -2.945838 | -2.759350 | -0.270016 |
| 1 | -5.373328 | -3.273691 | -0.310163 |
| 1 | -7.034499 | -1.436482 | -0.115283 |
| 1 | -6.241220 | 0.919935  | 0.119523  |
| 7 | 4.512149  | 0.074150  | -0.005409 |
| 6 | 4.963119  | 1.441419  | 0.265264  |
| 6 | 5.074089  | 2.317930  | -0.987045 |
| 1 | 5.939564  | 1.369654  | 0.750759  |
| 1 | 4.298149  | 1.900625  | 0.999680  |
| 1 | 5.436339  | 3.314135  | -0.718565 |
| 1 | 5.775617  | 1.885721  | -1.705240 |
| 1 | 4.108508  | 2.428499  | -1.484746 |
| 6 | 5.564899  | -0.916632 | -0.244504 |
| 6 | 6.015041  | -1.661859 | 1.016879  |
| 1 | 6.414443  | -0.384249 | -0.679343 |
| 1 | 5.232470  | -1.620352 | -1.010150 |
| 1 | 6.818190  | -2.363098 | 0.773739  |
| 1 | 6.391758  | -0.964795 | 1.769689  |
| 1 | 5.192433  | -2.225070 | 1.462522  |

### B3P86

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.171784  | -0.251753 | -0.041724 |
| 6 | 2.171307  | 0.736938  | 0.071273  |
| 6 | 0.842946  | 0.376119  | 0.039680  |
| 6 | 0.417244  | -0.955367 | -0.106750 |
| 6 | 1.418078  | -1.932007 | -0.223046 |
| 6 | 2.750649  | -1.602330 | -0.192505 |
| 6 | -1.786644 | -0.336101 | -0.028926 |
| 6 | -1.408367 | 1.058460  | 0.114629  |
| 6 | -2.305169 | 2.066907  | 0.219523  |
| 1 | -1.971328 | 3.091653  | 0.324193  |
| 6 | -3.730565 | 1.813591  | 0.197455  |
| 6 | -4.154754 | 0.394786  | 0.056600  |
| 6 | -3.213341 | -0.642417 | -0.052823 |
| 1 | 2.406076  | 1.787509  | 0.164987  |
| 1 | 1.104953  | -2.963947 | -0.330680 |
| 1 | 3.483141  | -2.393247 | -0.266522 |
| 6 | -3.658347 | -1.963268 | -0.184131 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -5.517899 | 0.097313  | 0.034169  |
| 6 | -5.012262 | -2.242999 | -0.204683 |
| 6 | -5.947735 | -1.211103 | -0.095244 |
| 8 | -4.554222 | 2.719354  | 0.290941  |
| 8 | -0.083376 | 1.366409  | 0.146164  |
| 7 | -0.904817 | -1.288748 | -0.134847 |
| 1 | -2.920478 | -2.751429 | -0.267963 |
| 1 | -5.347760 | -3.269103 | -0.306509 |
| 1 | -7.008213 | -1.436042 | -0.111969 |
| 1 | -6.215975 | 0.921548  | 0.121122  |
| 7 | 4.494687  | 0.076040  | -0.004740 |
| 6 | 4.939217  | 1.435444  | 0.264583  |
| 6 | 5.039744  | 2.304371  | -0.983576 |
| 1 | 5.917401  | 1.365821  | 0.748019  |
| 1 | 4.274868  | 1.890878  | 1.003065  |
| 1 | 5.397428  | 3.303663  | -0.722895 |
| 1 | 5.739374  | 1.872264  | -1.703407 |
| 1 | 4.070910  | 2.406266  | -1.476920 |
| 6 | 5.539836  | -0.909770 | -0.239859 |
| 6 | 5.973397  | -1.654359 | 1.017517  |
| 1 | 6.392928  | -0.376996 | -0.668499 |
| 1 | 5.210504  | -1.609243 | -1.011783 |
| 1 | 6.774944  | -2.359770 | 0.783906  |
| 1 | 6.345261  | -0.959110 | 1.774147  |
| 1 | 5.142954  | -2.212571 | 1.454989  |

PBE0

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.170652  | -0.252163 | -0.040511 |
| 6 | 2.170161  | 0.736015  | 0.071035  |
| 6 | 0.841421  | 0.374993  | 0.040474  |
| 6 | 0.416407  | -0.955575 | -0.104375 |
| 6 | 1.416729  | -1.932099 | -0.218509 |
| 6 | 2.749487  | -1.602819 | -0.187965 |
| 6 | -1.785166 | -0.336913 | -0.028226 |
| 6 | -1.405173 | 1.058520  | 0.115447  |
| 6 | -2.301447 | 2.066451  | 0.220761  |
| 1 | -1.967137 | 3.091760  | 0.325675  |
| 6 | -3.727930 | 1.813817  | 0.198679  |
| 6 | -4.153033 | 0.394891  | 0.056463  |
| 6 | -3.213039 | -0.642143 | -0.053167 |
| 1 | 2.403776  | 1.787864  | 0.162305  |
| 1 | 1.103319  | -2.964950 | -0.324247 |
| 1 | 3.481723  | -2.395257 | -0.259210 |
| 6 | -3.658252 | -1.962404 | -0.185711 |
| 6 | -5.516332 | 0.099071  | 0.033006  |
| 6 | -5.012386 | -2.241120 | -0.207413 |
| 6 | -5.947125 | -1.208864 | -0.097799 |
| 8 | -4.549601 | 2.718091  | 0.292362  |
| 8 | -0.082756 | 1.364656  | 0.146283  |
| 7 | -0.906196 | -1.288968 | -0.133071 |
| 1 | -2.920471 | -2.751627 | -0.269706 |
| 1 | -5.348663 | -3.267637 | -0.310276 |
| 1 | -7.008474 | -1.433137 | -0.115388 |
| 1 | -6.214301 | 0.924306  | 0.120329  |
| 7 | 4.492851  | 0.075814  | -0.005205 |
| 6 | 4.937053  | 1.433541  | 0.262097  |
| 6 | 5.036397  | 2.300518  | -0.986720 |
| 1 | 5.916519  | 1.364766  | 0.744914  |
| 1 | 4.273998  | 1.890871  | 1.001711  |
| 1 | 5.394628  | 3.300839  | -0.728066 |
| 1 | 5.735718  | 1.866657  | -1.706960 |
| 1 | 4.066488  | 2.401328  | -1.479815 |
| 6 | 5.536815  | -0.908047 | -0.241216 |
| 6 | 5.973521  | -1.649896 | 1.015841  |
| 1 | 6.389471  | -0.375208 | -0.672742 |
| 1 | 5.207299  | -1.609500 | -1.012351 |
| 1 | 6.775460  | -2.355799 | 0.782048  |
| 1 | 6.346737  | -0.952176 | 1.770639  |
| 1 | 5.143614  | -2.207641 | 1.456769  |

BMK

|   |          |           |           |
|---|----------|-----------|-----------|
| 6 | 3.184207 | -0.253341 | -0.044164 |
| 6 | 2.179535 | 0.741330  | 0.066355  |
| 6 | 0.844674 | 0.377471  | 0.031459  |
| 6 | 0.420503 | -0.958182 | -0.115383 |
| 6 | 1.422475 | -1.941032 | -0.232112 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 2.761335  | -1.611584 | -0.199315 |
| 6 | -1.788326 | -0.343069 | -0.033977 |
| 6 | -1.400443 | 1.068189  | 0.106189  |
| 6 | -2.294599 | 2.080531  | 0.206894  |
| 1 | -1.958050 | 3.106595  | 0.305794  |
| 6 | -3.736094 | 1.828770  | 0.186654  |
| 6 | -4.170772 | 0.395755  | 0.054807  |
| 6 | -3.231213 | -0.648363 | -0.050619 |
| 1 | 2.415519  | 1.792557  | 0.159270  |
| 1 | 1.107397  | -2.974121 | -0.339613 |
| 1 | 3.495370  | -2.401953 | -0.272929 |
| 6 | -3.681492 | -1.974566 | -0.169122 |
| 6 | -5.541672 | 0.104297  | 0.040227  |
| 6 | -5.042899 | -2.250008 | -0.181672 |
| 6 | -5.978450 | -1.209284 | -0.077123 |
| 8 | -4.549223 | 2.731013  | 0.273641  |
| 8 | -0.080958 | 1.361352  | 0.134315  |
| 7 | -0.910245 | -1.287886 | -0.140360 |
| 1 | -2.950212 | -2.770781 | -0.248170 |
| 1 | -5.382748 | -3.277137 | -0.271756 |
| 1 | -7.040929 | -1.431302 | -0.086959 |
| 1 | -6.239201 | 0.930960  | 0.123720  |
| 7 | 4.507960  | 0.073975  | -0.000661 |
| 6 | 4.953968  | 1.427951  | 0.300713  |
| 6 | 5.051094  | 2.325852  | -0.945460 |
| 1 | 5.936976  | 1.350829  | 0.775992  |
| 1 | 4.289697  | 1.871934  | 1.047584  |
| 1 | 5.402746  | 3.324774  | -0.668527 |
| 1 | 5.754806  | 1.901702  | -1.668658 |
| 1 | 4.078470  | 2.423504  | -1.436281 |
| 6 | 5.555322  | -0.905876 | -0.261021 |
| 6 | 5.992671  | -1.676013 | 0.997360  |
| 1 | 6.410327  | -0.364309 | -0.677747 |
| 1 | 5.223591  | -1.595686 | -1.041807 |
| 1 | 6.796777  | -2.377879 | 0.753752  |
| 1 | 6.360958  | -0.985352 | 1.762492  |
| 1 | 5.157010  | -2.238841 | 1.423211  |

BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.159878  | -0.254611 | -0.039445 |
| 6 | 2.164199  | 0.728927  | 0.069744  |
| 6 | 0.840040  | 0.370242  | 0.039783  |
| 6 | 0.417270  | -0.948818 | -0.102157 |
| 6 | 1.408171  | -1.922895 | -0.213754 |
| 6 | 2.737367  | -1.598022 | -0.183218 |
| 6 | -1.782034 | -0.338494 | -0.028154 |
| 6 | -1.398846 | 1.061201  | 0.115375  |
| 6 | -2.287127 | 2.059283  | 0.219372  |
| 1 | -1.958345 | 3.077185  | 0.323166  |
| 6 | -3.714695 | 1.806723  | 0.196927  |
| 6 | -4.145871 | 0.391516  | 0.055688  |
| 6 | -3.213431 | -0.641073 | -0.053059 |
| 1 | 2.395680  | 1.771572  | 0.160235  |
| 1 | 1.098390  | -2.947979 | -0.317648 |
| 1 | 3.460046  | -2.386545 | -0.253435 |
| 6 | -3.659236 | -1.954263 | -0.184641 |
| 6 | -5.504779 | 0.102045  | 0.032675  |
| 6 | -5.008351 | -2.228499 | -0.206188 |
| 6 | -5.936759 | -1.199064 | -0.097257 |
| 8 | -4.523481 | 2.705065  | 0.289493  |
| 8 | -0.082866 | 1.356630  | 0.144600  |
| 7 | -0.911611 | -1.275178 | -0.130289 |
| 1 | -2.932792 | -2.741353 | -0.268097 |
| 1 | -5.344147 | -3.246112 | -0.308041 |
| 1 | -6.990091 | -1.418997 | -0.114590 |
| 1 | -6.198761 | 0.918433  | 0.118803  |
| 7 | 4.481790  | 0.072504  | -0.005836 |
| 6 | 4.927689  | 1.427204  | 0.266736  |
| 6 | 5.028911  | 2.301747  | -0.975166 |
| 1 | 5.900698  | 1.357366  | 0.742304  |
| 1 | 4.272301  | 1.881426  | 1.001606  |
| 1 | 5.386286  | 3.292604  | -0.710173 |
| 1 | 5.723124  | 1.874185  | -1.692271 |
| 1 | 4.066671  | 2.407102  | -1.464674 |
| 6 | 5.523788  | -0.909526 | -0.248862 |
| 6 | 5.969874  | -1.653806 | 1.001890  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 6.369074 | -0.381595 | -0.678451 |
| 1 | 5.194437 | -1.606387 | -1.011315 |
| 1 | 6.764562 | -2.353970 | 0.760747  |
| 1 | 6.346245 | -0.961962 | 1.749239  |
| 1 | 5.149798 | -2.208720 | 1.444998  |

CAM-B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.166002  | -0.253466 | -0.038845 |
| 6 | 2.172146  | 0.730101  | 0.069305  |
| 6 | 0.843808  | 0.369575  | 0.039530  |
| 6 | 0.423054  | -0.946762 | -0.101862 |
| 6 | 1.413415  | -1.921974 | -0.212014 |
| 6 | 2.744619  | -1.598086 | -0.180721 |
| 6 | -1.779726 | -0.340032 | -0.028684 |
| 6 | -1.396622 | 1.068396  | 0.117719  |
| 6 | -2.286951 | 2.063888  | 0.224477  |
| 1 | -1.957758 | 3.089561  | 0.330882  |
| 6 | -3.720126 | 1.807897  | 0.202303  |
| 6 | -4.151311 | 0.387373  | 0.056520  |
| 6 | -3.219401 | -0.642008 | -0.054689 |
| 1 | 2.403137  | 1.781979  | 0.158791  |
| 1 | 1.098192  | -2.954014 | -0.315990 |
| 1 | 3.473276  | -2.393524 | -0.248941 |
| 6 | -3.660298 | -1.955559 | -0.190149 |
| 6 | -5.510300 | 0.098854  | 0.032479  |
| 6 | -5.010998 | -2.232412 | -0.213240 |
| 6 | -5.941091 | -1.204088 | -0.101651 |
| 8 | -4.534607 | 2.706634  | 0.298228  |
| 8 | -0.077927 | 1.367755  | 0.146054  |
| 7 | -0.917206 | -1.279991 | -0.131497 |
| 1 | -2.923003 | -2.744372 | -0.275803 |
| 1 | -5.347796 | -3.257839 | -0.318968 |
| 1 | -7.002132 | -1.426700 | -0.120148 |
| 1 | -6.207924 | 0.923405  | 0.121821  |
| 7 | 4.490611  | 0.073312  | -0.005843 |
| 6 | 4.934126  | 1.430023  | 0.257424  |
| 6 | 5.020408  | 2.292227  | -0.993221 |
| 1 | 5.916692  | 1.365063  | 0.731150  |
| 1 | 4.278878  | 1.887776  | 1.001772  |
| 1 | 5.370298  | 3.296107  | -0.744339 |
| 1 | 5.718315  | 1.859014  | -1.712765 |
| 1 | 4.048400  | 2.379736  | -1.481343 |
| 6 | 5.531068  | -0.911442 | -0.241935 |
| 6 | 5.962429  | -1.650568 | 1.015981  |
| 1 | 6.385303  | -0.382925 | -0.672057 |
| 1 | 5.202675  | -1.612072 | -1.012408 |
| 1 | 6.756848  | -2.364489 | 0.788947  |
| 1 | 6.339764  | -0.950801 | 1.764508  |
| 1 | 5.127759  | -2.195877 | 1.459659  |

LC-wPBE

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.166002  | -0.253466 | -0.038845 |
| 6 | 2.172146  | 0.730101  | 0.069305  |
| 6 | 0.843808  | 0.369575  | 0.039530  |
| 6 | 0.423054  | -0.946762 | -0.101862 |
| 6 | 1.413415  | -1.921974 | -0.212014 |
| 6 | 2.744619  | -1.598086 | -0.180721 |
| 6 | -1.779726 | -0.340032 | -0.028684 |
| 6 | -1.396622 | 1.068396  | 0.117719  |
| 6 | -2.286951 | 2.063888  | 0.224477  |
| 1 | -1.957758 | 3.089561  | 0.330882  |
| 6 | -3.720126 | 1.807897  | 0.202303  |
| 6 | -4.151311 | 0.387373  | 0.056520  |
| 6 | -3.219401 | -0.642008 | -0.054689 |
| 1 | 2.403137  | 1.781979  | 0.158791  |
| 1 | 1.098192  | -2.954014 | -0.315990 |
| 1 | 3.473276  | -2.393524 | -0.248941 |
| 6 | -3.660298 | -1.955559 | -0.190149 |
| 6 | -5.510300 | 0.098854  | 0.032479  |
| 6 | -5.010998 | -2.232412 | -0.213240 |
| 6 | -5.941091 | -1.204088 | -0.101651 |
| 8 | -4.534607 | 2.706634  | 0.298228  |
| 8 | -0.077927 | 1.367755  | 0.146054  |
| 7 | -0.917206 | -1.279991 | -0.131497 |
| 1 | -2.923003 | -2.744372 | -0.275803 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -5.347796 | -3.257839 | -0.318968 |
| 1 | -7.002132 | -1.426700 | -0.120148 |
| 1 | -6.207924 | 0.923405  | 0.121821  |
| 7 | 4.490611  | 0.073312  | -0.005843 |
| 6 | 4.934126  | 1.430023  | 0.257424  |
| 6 | 5.020408  | 2.292227  | -0.993221 |
| 1 | 5.916692  | 1.365063  | 0.731150  |
| 1 | 4.278878  | 1.887776  | 1.001772  |
| 1 | 5.370298  | 3.296107  | -0.744339 |
| 1 | 5.718315  | 1.859014  | -1.712765 |
| 1 | 4.048400  | 2.379736  | -1.481343 |
| 6 | 5.531068  | -0.911442 | -0.241935 |
| 6 | 5.962429  | -1.650568 | 1.015981  |
| 1 | 6.385303  | -0.382925 | -0.672057 |
| 1 | 5.202675  | -1.612072 | -1.012408 |
| 1 | 6.756848  | -2.364489 | 0.788947  |
| 1 | 6.339764  | -0.950801 | 1.764508  |
| 1 | 5.127759  | -2.195877 | 1.459659  |

**Table S2.** Optimized TD-DFT structures for the lowest singlet state (S1) obtained with the 6-311G(d,p) basis set.

A) GAS-PHASE STRUCTURES  
B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.177091  | -0.252636 | -0.043319 |
| 6 | 2.168033  | 0.726187  | 0.064180  |
| 6 | 0.834290  | 0.361861  | 0.033268  |
| 6 | 0.402068  | -0.989474 | -0.108783 |
| 6 | 1.427917  | -1.955935 | -0.217318 |
| 6 | 2.762068  | -1.613186 | -0.187152 |
| 6 | -1.803967 | -0.348032 | -0.031612 |
| 6 | -1.420193 | 1.025673  | 0.104502  |
| 6 | -2.312067 | 2.060389  | 0.213605  |
| 1 | -1.959060 | 3.079182  | 0.313340  |
| 6 | -3.751341 | 1.829953  | 0.197210  |
| 6 | -4.174716 | 0.414693  | 0.059228  |
| 6 | -3.220181 | -0.631696 | -0.050928 |
| 1 | 2.391333  | 1.779088  | 0.155074  |
| 1 | 1.123998  | -2.990562 | -0.319924 |
| 1 | 3.497992  | -2.400878 | -0.257143 |
| 6 | -3.677076 | -1.961592 | -0.180098 |
| 6 | -5.538399 | 0.108055  | 0.037581  |
| 6 | -5.034012 | -2.241081 | -0.198669 |
| 6 | -5.972527 | -1.206250 | -0.089893 |
| 8 | -4.554816 | 2.761339  | 0.291722  |
| 8 | -0.086944 | 1.362824  | 0.134246  |
| 7 | -0.909650 | -1.358530 | -0.140863 |
| 1 | -2.939261 | -2.749120 | -0.263015 |
| 1 | -5.369453 | -3.267711 | -0.298433 |
| 1 | -7.033427 | -1.429104 | -0.105452 |
| 1 | -6.239023 | 0.930227  | 0.123323  |
| 7 | 4.514871  | 0.083611  | -0.004473 |
| 6 | 4.953118  | 1.449158  | 0.278453  |
| 6 | 5.052530  | 2.339370  | -0.968190 |
| 1 | 5.932588  | 1.383240  | 0.759637  |
| 1 | 4.281537  | 1.894750  | 1.015467  |
| 1 | 5.401249  | 3.337258  | -0.688013 |
| 1 | 5.759984  | 1.924331  | -1.690442 |
| 1 | 4.084986  | 2.440532  | -1.463200 |
| 6 | 5.572116  | -0.896892 | -0.249443 |
| 6 | 6.030404  | -1.642801 | 1.011133  |
| 1 | 6.418415  | -0.357433 | -0.683154 |
| 1 | 5.241532  | -1.601877 | -1.014584 |
| 1 | 6.836752  | -2.338543 | 0.762577  |
| 1 | 6.405537  | -0.946199 | 1.764943  |
| 1 | 5.210914  | -2.210637 | 1.456072  |

B3P86

|   |          |           |           |
|---|----------|-----------|-----------|
| 6 | 3.167397 | -0.249616 | -0.043886 |
| 6 | 2.162293 | 0.726997  | 0.064285  |
| 6 | 0.831688 | 0.362732  | 0.032520  |
| 6 | 0.402848 | -0.985506 | -0.110478 |
| 6 | 1.426337 | -1.948731 | -0.219542 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 2.757264  | -1.606158 | -0.189221 |
| 6 | -1.792161 | -0.347134 | -0.032570 |
| 6 | -1.409567 | 1.022072  | 0.103939  |
| 6 | -2.301393 | 2.054037  | 0.214552  |
| 1 | -1.947920 | 3.072941  | 0.314714  |
| 6 | -3.735413 | 1.822834  | 0.198385  |
| 6 | -4.154856 | 0.413035  | 0.060132  |
| 6 | -3.203204 | -0.628846 | -0.051146 |
| 1 | 2.386836  | 1.780472  | 0.156021  |
| 1 | 1.121337  | -2.983208 | -0.323053 |
| 1 | 3.496248  | -2.392174 | -0.259580 |
| 6 | -3.655445 | -1.955479 | -0.180876 |
| 6 | -5.514751 | 0.107169  | 0.039363  |
| 6 | -5.009098 | -2.235798 | -0.198786 |
| 6 | -5.946429 | -1.204507 | -0.088689 |
| 8 | -4.539499 | 2.750129  | 0.292873  |
| 8 | -0.084387 | 1.359092  | 0.133347  |
| 7 | -0.903658 | -1.356587 | -0.142872 |
| 1 | -2.913211 | -2.739825 | -0.264618 |
| 1 | -5.343621 | -3.262704 | -0.299325 |
| 1 | -7.007122 | -1.428686 | -0.103838 |
| 1 | -6.213644 | 0.931498  | 0.126541  |
| 7 | 4.497864  | 0.085607  | -0.004108 |
| 6 | 4.929327  | 1.443936  | 0.274026  |
| 6 | 5.015533  | 2.323913  | -0.970531 |
| 1 | 5.911483  | 1.381948  | 0.751375  |
| 1 | 4.259195  | 1.886941  | 1.015147  |
| 1 | 5.358212  | 3.326109  | -0.700576 |
| 1 | 5.720974  | 1.908597  | -1.694295 |
| 1 | 4.044097  | 2.413450  | -1.460298 |
| 6 | 5.547333  | -0.890474 | -0.242887 |
| 6 | 5.987557  | -1.634304 | 1.015176  |
| 1 | 6.397883  | -0.351495 | -0.670071 |
| 1 | 5.220270  | -1.592264 | -1.013586 |
| 1 | 6.792439  | -2.334820 | 0.777920  |
| 1 | 6.357174  | -0.938528 | 1.772209  |
| 1 | 5.159455  | -2.196186 | 1.451823  |

PBE0

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.166241  | -0.248569 | -0.042733 |
| 6 | 2.160173  | 0.727298  | 0.065112  |
| 6 | 0.830256  | 0.363251  | 0.035296  |
| 6 | 0.400238  | -0.986913 | -0.106905 |
| 6 | 1.426375  | -1.950310 | -0.214772 |
| 6 | 2.755170  | -1.606702 | -0.185132 |
| 6 | -1.790974 | -0.346979 | -0.030309 |
| 6 | -1.407132 | 1.020131  | 0.106618  |
| 6 | -2.298164 | 2.052983  | 0.216412  |
| 1 | -1.943391 | 3.072116  | 0.317694  |
| 6 | -3.733450 | 1.822625  | 0.199793  |
| 6 | -4.152856 | 0.413310  | 0.059698  |
| 6 | -3.201510 | -0.628225 | -0.050916 |
| 1 | 2.383652  | 1.781980  | 0.154738  |
| 1 | 1.121593  | -2.985768 | -0.316447 |
| 1 | 3.494864  | -2.393340 | -0.253508 |
| 6 | -3.654106 | -1.954483 | -0.182357 |
| 6 | -5.512897 | 0.108545  | 0.036611  |
| 6 | -5.007663 | -2.233771 | -0.202617 |
| 6 | -5.945066 | -1.202386 | -0.093199 |
| 8 | -4.534658 | 2.749307  | 0.296078  |
| 8 | -0.084528 | 1.356814  | 0.136578  |
| 7 | -0.901196 | -1.357129 | -0.139726 |
| 1 | -2.912139 | -2.740102 | -0.265837 |
| 1 | -5.342623 | -3.261205 | -0.304472 |
| 1 | -7.006504 | -1.426399 | -0.110064 |
| 1 | -6.211938 | 0.933727  | 0.123550  |
| 7 | 4.494163  | 0.085487  | -0.005275 |
| 6 | 4.926513  | 1.443092  | 0.267440  |
| 6 | 5.012108  | 2.317371  | -0.979925 |
| 1 | 5.909748  | 1.381984  | 0.744439  |
| 1 | 4.258148  | 1.890092  | 1.008830  |
| 1 | 5.356186  | 3.321121  | -0.714980 |
| 1 | 5.716845  | 1.897785  | -1.703096 |
| 1 | 4.039668  | 2.405355  | -1.469665 |
| 6 | 5.543112  | -0.889242 | -0.243315 |
| 6 | 5.986934  | -1.627136 | 1.015687  |

|   |          |           |           |
|---|----------|-----------|-----------|
| 1 | 6.392503 | -0.350314 | -0.674824 |
| 1 | 5.216292 | -1.594406 | -1.012061 |
| 1 | 6.793045 | -2.327776 | 0.780005  |
| 1 | 6.356923 | -0.926987 | 1.769616  |
| 1 | 5.160018 | -2.188673 | 1.456924  |

BMK

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.178582  | -0.246805 | -0.045328 |
| 6 | 2.166895  | 0.736972  | 0.060670  |
| 6 | 0.832410  | 0.374312  | 0.026277  |
| 6 | 0.399503  | -0.990286 | -0.117877 |
| 6 | 1.435348  | -1.962653 | -0.228530 |
| 6 | 2.764618  | -1.616950 | -0.195675 |
| 6 | -1.795680 | -0.344470 | -0.037430 |
| 6 | -1.406561 | 1.028875  | 0.092765  |
| 6 | -2.296092 | 2.067928  | 0.199924  |
| 1 | -1.939128 | 3.087927  | 0.295322  |
| 6 | -3.746448 | 1.836628  | 0.188819  |
| 6 | -4.170523 | 0.414001  | 0.059490  |
| 6 | -3.213725 | -0.631460 | -0.049543 |
| 1 | 2.396945  | 1.790300  | 0.150350  |
| 1 | 1.128519  | -2.998209 | -0.331722 |
| 1 | 3.508801  | -2.399230 | -0.265062 |
| 6 | -3.666620 | -1.966521 | -0.169354 |
| 6 | -5.536822 | 0.106806  | 0.047407  |
| 6 | -5.025176 | -2.247548 | -0.178342 |
| 6 | -5.968536 | -1.211172 | -0.070017 |
| 8 | -4.540069 | 2.760764  | 0.280929  |
| 8 | -0.084113 | 1.357195  | 0.119237  |
| 7 | -0.896193 | -1.354548 | -0.148202 |
| 1 | -2.924874 | -2.753172 | -0.251643 |
| 1 | -5.360319 | -3.276512 | -0.268993 |
| 1 | -7.029888 | -1.438315 | -0.077449 |
| 1 | -6.239356 | 0.929876  | 0.133331  |
| 7 | 4.503700  | 0.083859  | 0.001955  |
| 6 | 4.940115  | 1.438524  | 0.306129  |
| 6 | 5.027022  | 2.339738  | -0.940601 |
| 1 | 5.925686  | 1.367934  | 0.777700  |
| 1 | 4.270946  | 1.874677  | 1.053227  |
| 1 | 5.367518  | 3.341504  | -0.659842 |
| 1 | 5.735622  | 1.926106  | -1.664910 |
| 1 | 4.052891  | 2.426546  | -1.429734 |
| 6 | 5.557566  | -0.886866 | -0.260216 |
| 6 | 6.001463  | -1.652716 | 1.000086  |
| 1 | 6.408452  | -0.337946 | -0.676546 |
| 1 | 5.229978  | -1.579637 | -1.039796 |
| 1 | 6.811891  | -2.347089 | 0.755799  |
| 1 | 6.363398  | -0.959518 | 1.765759  |
| 1 | 5.169782  | -2.222105 | 1.424700  |

BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.154055  | -0.247819 | -0.041456 |
| 6 | 2.149158  | 0.725192  | 0.066856  |
| 6 | 0.826790  | 0.369717  | 0.037262  |
| 6 | 0.394081  | -0.980758 | -0.105912 |
| 6 | 1.422570  | -1.945797 | -0.214616 |
| 6 | 2.739131  | -1.605069 | -0.184701 |
| 6 | -1.788129 | -0.336489 | -0.028814 |
| 6 | -1.407780 | 1.023463  | 0.108440  |
| 6 | -2.290012 | 2.048667  | 0.217283  |
| 1 | -1.939449 | 3.059673  | 0.319315  |
| 6 | -3.722479 | 1.816020  | 0.199965  |
| 6 | -4.141573 | 0.408850  | 0.059071  |
| 6 | -3.191721 | -0.625607 | -0.050994 |
| 1 | 2.373429  | 1.769841  | 0.157420  |
| 1 | 1.120099  | -2.972779 | -0.316076 |
| 1 | 3.472162  | -2.384879 | -0.254094 |
| 6 | -3.639981 | -1.948416 | -0.183269 |
| 6 | -5.494982 | 0.103896  | 0.035062  |
| 6 | -4.986560 | -2.227684 | -0.204380 |
| 6 | -5.921815 | -1.202346 | -0.095320 |
| 8 | -4.518702 | 2.731543  | 0.296458  |
| 8 | -0.084388 | 1.354178  | 0.138307  |
| 7 | -0.891011 | -1.340180 | -0.138219 |
| 1 | -2.906504 | -2.729086 | -0.266675 |
| 1 | -5.317718 | -3.247260 | -0.306312 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -6.974320 | -1.426925 | -0.112791 |
| 1 | -6.193809 | 0.916995  | 0.121030  |
| 7 | 4.473258  | 0.082136  | -0.005506 |
| 6 | 4.911398  | 1.439782  | 0.264920  |
| 6 | 5.001485  | 2.311438  | -0.981137 |
| 1 | 5.886950  | 1.375722  | 0.736349  |
| 1 | 4.252286  | 1.888789  | 0.999302  |
| 1 | 5.349838  | 3.305788  | -0.717444 |
| 1 | 5.698430  | 1.890104  | -1.699067 |
| 1 | 4.036748  | 2.405855  | -1.467134 |
| 6 | 5.524055  | -0.892232 | -0.243217 |
| 6 | 5.971735  | -1.625861 | 1.014138  |
| 1 | 6.365501  | -0.357231 | -0.671932 |
| 1 | 5.201765  | -1.594643 | -1.003019 |
| 1 | 6.774505  | -2.318536 | 0.778475  |
| 1 | 6.337898  | -0.927893 | 1.760604  |
| 1 | 5.154628  | -2.186676 | 1.454917  |

#### CAM-B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.165105  | -0.246827 | -0.041878 |
| 6 | 2.159082  | 0.728341  | 0.067393  |
| 6 | 0.832269  | 0.369437  | 0.037772  |
| 6 | 0.398132  | -0.985119 | -0.106613 |
| 6 | 1.430515  | -1.952074 | -0.216147 |
| 6 | 2.750200  | -1.608734 | -0.185899 |
| 6 | -1.793505 | -0.339453 | -0.028902 |
| 6 | -1.413278 | 1.022446  | 0.109364  |
| 6 | -2.297995 | 2.053097  | 0.219417  |
| 1 | -1.944798 | 3.070538  | 0.322761  |
| 6 | -3.734866 | 1.819863  | 0.201799  |
| 6 | -4.154144 | 0.408686  | 0.059481  |
| 6 | -3.202649 | -0.628522 | -0.051441 |
| 1 | 2.382681  | 1.780421  | 0.158247  |
| 1 | 1.124270  | -2.985205 | -0.318642 |
| 1 | 3.489490  | -2.392535 | -0.255595 |
| 6 | -3.653242 | -1.953677 | -0.184949 |
| 6 | -5.512435 | 0.104142  | 0.035081  |
| 6 | -5.003738 | -2.232799 | -0.206502 |
| 6 | -5.941464 | -1.204070 | -0.096530 |
| 8 | -4.536193 | 2.742206  | 0.299532  |
| 8 | -0.083388 | 1.359503  | 0.140174  |
| 7 | -0.892513 | -1.348767 | -0.139476 |
| 1 | -2.913482 | -2.738466 | -0.269208 |
| 1 | -5.337615 | -3.258806 | -0.309861 |
| 1 | -7.000932 | -1.429681 | -0.114442 |
| 1 | -6.212107 | 0.926105  | 0.122430  |
| 7 | 4.489915  | 0.083738  | -0.005630 |
| 6 | 4.927819  | 1.446982  | 0.262671  |
| 6 | 5.010613  | 2.317297  | -0.989110 |
| 1 | 5.910569  | 1.384997  | 0.734942  |
| 1 | 4.265174  | 1.897192  | 1.003373  |
| 1 | 5.358131  | 3.319859  | -0.730348 |
| 1 | 5.710066  | 1.893503  | -1.712586 |
| 1 | 4.038081  | 2.406681  | -1.474595 |
| 6 | 5.544091  | -0.894945 | -0.241235 |
| 6 | 5.986886  | -1.629046 | 1.021762  |
| 1 | 6.391649  | -0.357361 | -0.671779 |
| 1 | 5.220426  | -1.601086 | -1.006728 |
| 1 | 6.794751  | -2.327104 | 0.791346  |
| 1 | 6.351828  | -0.926268 | 1.773403  |
| 1 | 5.162275  | -2.191396 | 1.462145  |

#### B)N-HEPTANE STRUCTURES

##### B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.177701  | -0.255971 | -0.043071 |
| 6 | 2.166114  | 0.726356  | 0.063887  |
| 6 | 0.834089  | 0.363687  | 0.031056  |
| 6 | 0.404501  | -0.985588 | -0.110926 |
| 6 | 1.428821  | -1.954777 | -0.219244 |
| 6 | 2.763517  | -1.615952 | -0.188591 |
| 6 | -1.802871 | -0.345741 | -0.033521 |
| 6 | -1.423102 | 1.028883  | 0.102675  |
| 6 | -2.317165 | 2.061049  | 0.211541  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 1 | -1.963005 | 3.079644  | 0.311060  |
| 6 | -3.750755 | 1.830547  | 0.197371  |
| 6 | -4.174438 | 0.415234  | 0.060194  |
| 6 | -3.219643 | -0.631687 | -0.051569 |
| 1 | 2.392394  | 1.778437  | 0.155075  |
| 1 | 1.124528  | -2.989260 | -0.322342 |
| 1 | 3.498329  | -2.404311 | -0.258356 |
| 6 | -3.676185 | -1.961975 | -0.180500 |
| 6 | -5.537581 | 0.105763  | 0.041076  |
| 6 | -5.032387 | -2.244131 | -0.197087 |
| 6 | -5.970800 | -1.209137 | -0.086105 |
| 8 | -4.563327 | 2.759856  | 0.293845  |
| 8 | -0.086724 | 1.367339  | 0.131543  |
| 7 | -0.910544 | -1.354864 | -0.143301 |
| 1 | -2.939042 | -2.749753 | -0.265103 |
| 1 | -5.367211 | -3.270781 | -0.296735 |
| 1 | -7.031669 | -1.432361 | -0.099535 |
| 1 | -6.241583 | 0.924744  | 0.128685  |
| 7 | 4.510144  | 0.082474  | -0.003181 |
| 6 | 4.950770  | 1.449595  | 0.278833  |
| 6 | 5.065651  | 2.329720  | -0.973305 |
| 1 | 5.925376  | 1.379746  | 0.768090  |
| 1 | 4.274436  | 1.901001  | 1.006874  |
| 1 | 5.420976  | 3.325184  | -0.694061 |
| 1 | 5.775263  | 1.904219  | -1.687000 |
| 1 | 4.102189  | 2.437091  | -1.474946 |
| 6 | 5.571124  | -0.897147 | -0.246788 |
| 6 | 6.029816  | -1.636175 | 1.017481  |
| 1 | 6.414416  | -0.354236 | -0.680588 |
| 1 | 5.241162  | -1.604489 | -1.009294 |
| 1 | 6.839541  | -2.327499 | 0.769078  |
| 1 | 6.401136  | -0.935496 | 1.769058  |
| 1 | 5.212922  | -2.208041 | 1.461862  |

#### B3P86

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.167683  | -0.252962 | -0.044923 |
| 6 | 2.160347  | 0.727190  | 0.062820  |
| 6 | 0.831296  | 0.364784  | 0.028621  |
| 6 | 0.405155  | -0.981407 | -0.114673 |
| 6 | 1.427019  | -1.947284 | -0.224637 |
| 6 | 2.758591  | -1.608756 | -0.193637 |
| 6 | -1.791132 | -0.344548 | -0.035311 |
| 6 | -1.412488 | 1.025797  | 0.100346  |
| 6 | -2.306454 | 2.055286  | 0.209491  |
| 1 | -1.951702 | 3.074014  | 0.308698  |
| 6 | -3.734974 | 1.823928  | 0.196176  |
| 6 | -4.154654 | 0.413718  | 0.060979  |
| 6 | -3.202726 | -0.628754 | -0.051104 |
| 1 | 2.388092  | 1.779779  | 0.155435  |
| 1 | 1.121686  | -2.981562 | -0.329487 |
| 1 | 3.496527  | -2.395333 | -0.264580 |
| 6 | -3.654391 | -1.956094 | -0.178249 |
| 6 | -5.513970 | 0.104688  | 0.044307  |
| 6 | -5.007269 | -2.239428 | -0.192515 |
| 6 | -5.944553 | -1.207914 | -0.081033 |
| 8 | -4.548249 | 2.748910  | 0.291931  |
| 8 | -0.084161 | 1.363861  | 0.128825  |
| 7 | -0.904756 | -1.352636 | -0.146683 |
| 1 | -2.912682 | -2.740646 | -0.263152 |
| 1 | -5.341098 | -3.266596 | -0.290971 |
| 1 | -7.005215 | -1.432686 | -0.092701 |
| 1 | -6.216544 | 0.925660  | 0.132669  |
| 7 | 4.493123  | 0.084374  | -0.002350 |
| 6 | 4.927004  | 1.443124  | 0.279320  |
| 6 | 5.031197  | 2.316753  | -0.968065 |
| 1 | 5.903652  | 1.375441  | 0.766018  |
| 1 | 4.251176  | 1.890272  | 1.011705  |
| 1 | 5.381796  | 3.315149  | -0.695475 |
| 1 | 5.739110  | 1.892206  | -1.683754 |
| 1 | 4.064449  | 2.415665  | -1.465258 |
| 6 | 5.546090  | -0.890407 | -0.241155 |
| 6 | 5.985371  | -1.630789 | 1.019158  |
| 1 | 6.394358  | -0.347218 | -0.666185 |
| 1 | 5.220145  | -1.592679 | -1.011189 |
| 1 | 6.793457  | -2.326655 | 0.780634  |
| 1 | 6.351267  | -0.933127 | 1.775950  |

1 5.159386 -2.197568 1.453306

PBE0

6 3.166711 -0.251521 -0.043518  
6 2.158126 0.727902 0.063951  
6 0.830141 0.365990 0.030947  
6 0.402449 -0.982672 -0.112163  
6 1.427241 -1.948776 -0.221040  
6 2.756490 -1.609116 -0.190135  
6 -1.789815 -0.343850 -0.034007  
6 -1.410048 1.023995 0.102202  
6 -2.303365 2.054366 0.211604  
1 -1.947429 3.073369 0.311653  
6 -3.733135 1.823552 0.197589  
6 -4.152411 0.413756 0.060541  
6 -3.200459 -0.628074 -0.051591  
1 2.384873 1.781660 0.154714  
1 1.122084 -2.983975 -0.324534  
1 3.495224 -2.396238 -0.259226  
6 -3.652296 -1.955185 -0.180630  
6 -5.511873 0.105453 0.042107  
6 -5.005073 -2.237780 -0.196698  
6 -5.942715 -1.206484 -0.085148  
8 -4.543680 2.747839 0.294025  
8 -0.084448 1.362016 0.131079  
7 -0.901428 -1.352932 -0.144869  
1 -2.910741 -2.740858 -0.265688  
1 -5.339096 -3.265553 -0.296639  
1 -7.004075 -1.431369 -0.098195  
1 -6.214728 0.927119 0.130759  
7 4.489305 0.084132 -0.002757  
6 4.924268 1.442072 0.274166  
6 5.026352 2.311160 -0.975245  
1 5.902448 1.374995 0.759585  
1 4.250857 1.892433 1.007925  
1 5.378151 3.311050 -0.707106  
1 5.733055 1.883390 -1.691414  
1 4.058103 2.408586 -1.471494  
6 5.541808 -0.889543 -0.240288  
6 5.983435 -1.624569 1.020939  
1 6.389356 -0.346435 -0.668827  
1 5.216662 -1.594745 -1.009006  
1 6.792953 -2.320522 0.784520  
1 6.348994 -0.922967 1.775387  
1 5.158207 -2.191227 1.458646

BMK

6 3.167683 -0.252962 -0.044923  
6 2.160347 0.727190 0.062820  
6 0.831296 0.364784 0.028621  
6 0.405155 -0.981407 -0.114673  
6 1.427019 -1.947284 -0.224637  
6 2.758591 -1.608756 -0.193637  
6 -1.791132 -0.344548 -0.035311  
6 -1.412488 1.025797 0.100346  
6 -2.306454 2.055286 0.209491  
1 -1.951702 3.074014 0.308698  
6 -3.734974 1.823928 0.196176  
6 -4.154654 0.413718 0.060979  
6 -3.202726 -0.628754 -0.051104  
1 2.388092 1.779779 0.155435  
1 1.121686 -2.981562 -0.329487  
1 3.496527 -2.395333 -0.264580  
6 -3.654391 -1.956094 -0.178249  
6 -5.513970 0.104688 0.044307  
6 -5.007269 -2.239428 -0.192515  
6 -5.944553 -1.207914 -0.081033  
8 -4.548249 2.748910 0.291931  
8 -0.084161 1.363861 0.128825  
7 -0.904756 -1.352636 -0.146683  
1 -2.912682 -2.740646 -0.263152  
1 -5.341098 -3.266596 -0.290971  
1 -7.005215 -1.432686 -0.092701  
1 -6.216544 0.925660 0.132669  
7 4.493123 0.084374 -0.002350  
6 4.927004 1.443124 0.279320

|   |          |           |           |
|---|----------|-----------|-----------|
| 6 | 5.031197 | 2.316753  | -0.968065 |
| 1 | 5.903652 | 1.375441  | 0.766018  |
| 1 | 4.251176 | 1.890272  | 1.011705  |
| 1 | 5.381796 | 3.315149  | -0.695475 |
| 1 | 5.739110 | 1.892206  | -1.683754 |
| 1 | 4.064449 | 2.415665  | -1.465258 |
| 6 | 5.546090 | -0.890407 | -0.241155 |
| 6 | 5.985371 | -1.630789 | 1.019158  |
| 1 | 6.394358 | -0.347218 | -0.666185 |
| 1 | 5.220145 | -1.592679 | -1.011189 |
| 1 | 6.793457 | -2.326655 | 0.780634  |
| 1 | 6.351267 | -0.933127 | 1.775950  |
| 1 | 5.159386 | -2.197568 | 1.453306  |

BHandHLYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.155764  | -0.249607 | -0.042748 |
| 6 | 2.146896  | 0.726451  | 0.065727  |
| 6 | 0.828188  | 0.371714  | 0.032966  |
| 6 | 0.395958  | -0.978946 | -0.111987 |
| 6 | 1.424906  | -1.945890 | -0.222255 |
| 6 | 2.740940  | -1.607200 | -0.190721 |
| 6 | -1.787496 | -0.334410 | -0.032715 |
| 6 | -1.409910 | 1.024071  | 0.104137  |
| 6 | -2.294837 | 2.048904  | 0.213686  |
| 1 | -1.942451 | 3.059534  | 0.314695  |
| 6 | -3.721962 | 1.816098  | 0.198791  |
| 6 | -4.140800 | 0.409680  | 0.060521  |
| 6 | -3.190053 | -0.625458 | -0.051820 |
| 1 | 2.373833  | 1.770276  | 0.157914  |
| 1 | 1.123152  | -2.972845 | -0.326101 |
| 1 | 3.473697  | -2.386884 | -0.261321 |
| 6 | -3.639290 | -1.948748 | -0.182358 |
| 6 | -5.494393 | 0.101774  | 0.041208  |
| 6 | -4.985146 | -2.230026 | -0.199187 |
| 6 | -5.920866 | -1.204514 | -0.087226 |
| 8 | -4.525309 | 2.731731  | 0.295479  |
| 8 | -0.085825 | 1.356599  | 0.133045  |
| 7 | -0.888250 | -1.337549 | -0.144104 |
| 1 | -2.907279 | -2.730344 | -0.267915 |
| 1 | -5.315808 | -3.249764 | -0.299777 |
| 1 | -6.973298 | -1.429592 | -0.100920 |
| 1 | -6.196291 | 0.911864  | 0.129436  |
| 7 | 4.468161  | 0.081235  | -0.003045 |
| 6 | 4.907934  | 1.440403  | 0.269685  |
| 6 | 5.012428  | 2.305699  | -0.979085 |
| 1 | 5.878474  | 1.372104  | 0.749513  |
| 1 | 4.243423  | 1.892454  | 0.996510  |
| 1 | 5.365855  | 3.297581  | -0.714026 |
| 1 | 5.712122  | 1.877061  | -1.689723 |
| 1 | 4.051690  | 2.406328  | -1.471818 |
| 6 | 5.523640  | -0.892310 | -0.237849 |
| 6 | 5.968048  | -1.621566 | 1.022685  |
| 1 | 6.363222  | -0.353327 | -0.663735 |
| 1 | 5.204333  | -1.595453 | -0.997583 |
| 1 | 6.774481  | -2.310057 | 0.788646  |
| 1 | 6.328739  | -0.921290 | 1.769399  |
| 1 | 5.152111  | -2.186787 | 1.459933  |

CAM-B3LYP

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | 3.167492  | -0.247872 | -0.040456 |
| 6 | 2.157356  | 0.730057  | 0.072192  |
| 6 | 0.834192  | 0.371613  | 0.041184  |
| 6 | 0.400956  | -0.983142 | -0.106448 |
| 6 | 1.433772  | -1.951957 | -0.217652 |
| 6 | 2.752920  | -1.610462 | -0.187260 |
| 6 | -1.791987 | -0.337637 | -0.028190 |
| 6 | -1.415145 | 1.022197  | 0.115245  |
| 6 | -2.302684 | 2.051998  | 0.228551  |
| 1 | -1.947849 | 3.069899  | 0.335791  |
| 6 | -3.733283 | 1.818788  | 0.209478  |
| 6 | -4.152592 | 0.409455  | 0.060544  |
| 6 | -3.200127 | -0.628359 | -0.053722 |
| 1 | 2.381871  | 1.781682  | 0.169910  |
| 1 | 1.128178  | -2.986354 | -0.322813 |
| 1 | 3.490929  | -2.395356 | -0.261516 |
| 6 | -3.651709 | -1.953249 | -0.193405 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| 6 | -5.510944 | 0.102696  | 0.032808  |
| 6 | -5.001741 | -2.233857 | -0.218217 |
| 6 | -5.939774 | -1.205015 | -0.105083 |
| 8 | -4.542578 | 2.740851  | 0.311585  |
| 8 | -0.083863 | 1.361525  | 0.147640  |
| 7 | -0.888935 | -1.346658 | -0.140886 |
| 1 | -2.913839 | -2.740287 | -0.280142 |
| 1 | -5.335181 | -3.260361 | -0.326532 |
| 1 | -7.000225 | -1.430406 | -0.125429 |
| 1 | -6.214699 | 0.921812  | 0.122511  |
| 7 | 4.485823  | 0.083856  | -0.006078 |
| 6 | 4.926622  | 1.452160  | 0.243173  |
| 6 | 5.013629  | 2.297336  | -1.024847 |
| 1 | 5.908531  | 1.393153  | 0.717025  |
| 1 | 4.264585  | 1.916405  | 0.975389  |
| 1 | 5.364957  | 3.302555  | -0.782453 |
| 1 | 5.712605  | 1.857483  | -1.739124 |
| 1 | 4.041428  | 2.382722  | -1.512182 |
| 6 | 5.544406  | -0.897099 | -0.226083 |
| 6 | 5.977929  | -1.613383 | 1.049716  |
| 1 | 6.392695  | -0.360502 | -0.655834 |
| 1 | 5.226753  | -1.611919 | -0.985845 |
| 1 | 6.787388  | -2.313393 | 0.831671  |
| 1 | 6.338422  | -0.900474 | 1.793949  |
| 1 | 5.151042  | -2.171665 | 1.491401  |