

## Cartesian Coordinates and Electronic Energies:

### Optimized Cartesian coordinates (in Å) of $\alpha$ -phenylnaphthalene:

- BP86-D/SDD,  $E_{el} = -98.380521$  a.u.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.171716  | 0.693600  | -0.018805 |
| C | -0.060707 | 1.289714  | -0.412225 |
| H | -0.090574 | 2.362647  | -0.610786 |
| C | -1.205691 | 0.527966  | -0.567669 |
| H | -2.138083 | 1.008216  | -0.876542 |
| C | -1.177992 | -0.871204 | -0.342589 |
| H | -2.090920 | -1.460442 | -0.463664 |
| C | 0.007335  | -1.488519 | 0.010013  |
| H | 0.048103  | -2.571168 | 0.164773  |
| C | 1.205425  | -0.737613 | 0.168814  |
| C | 2.433494  | -1.377802 | 0.488320  |
| H | 2.438567  | -2.462822 | 0.629960  |
| C | 3.596263  | -0.641072 | 0.609524  |
| H | 4.540920  | -1.135723 | 0.850840  |
| C | 3.567331  | 0.763382  | 0.446339  |
| H | 4.484638  | 1.342401  | 0.584576  |
| C | 2.387002  | 1.443519  | 0.156382  |
| C | 2.426950  | 2.922576  | 0.050645  |
| C | 3.418434  | 3.547959  | -0.731117 |
| H | 4.116469  | 2.924179  | -1.296400 |
| C | 3.499522  | 4.942596  | -0.802154 |
| H | 4.270289  | 5.410531  | -1.420809 |
| C | 2.591649  | 5.737822  | -0.090887 |
| H | 2.653570  | 6.827872  | -0.147162 |
| C | 1.604640  | 5.127861  | 0.695010  |
| H | 0.900424  | 5.741564  | 1.263487  |
| C | 1.522509  | 3.733633  | 0.766072  |
| H | 0.766115  | 3.257627  | 1.395253  |

- RI-MP2/def2-TZVP,  $E_{el} = 615.578616$  a.u.

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.196561  | 0.698758  | -0.015849 |
| C | -0.009405 | 1.311378  | -0.438700 |
| H | -0.025296 | 2.380127  | -0.621009 |
| C | -1.149348 | 0.562357  | -0.637205 |
| H | -2.060544 | 1.049583  | -0.967448 |
| C | -1.138914 | -0.831413 | -0.425842 |
| H | -2.043932 | -1.408849 | -0.580264 |
| C | 0.022868  | -1.459674 | -0.037017 |
| H | 0.044162  | -2.535390 | 0.111265  |
| C | 1.214028  | -0.722876 | 0.164534  |
| C | 2.419620  | -1.366134 | 0.527672  |
| H | 2.419660  | -2.443599 | 0.663672  |
| C | 3.575502  | -0.637428 | 0.697077  |
| H | 4.498668  | -1.135862 | 0.972632  |
| C | 3.560978  | 0.760433  | 0.534410  |
| H | 4.468043  | 1.333381  | 0.702050  |
| C | 2.398601  | 1.436151  | 0.198792  |
| C | 2.429042  | 2.906949  | 0.076995  |
| C | 3.312843  | 3.522974  | -0.817168 |
| H | 3.943194  | 2.902984  | -1.447020 |
| C | 3.370627  | 4.911859  | -0.913014 |
| H | 4.055217  | 5.376049  | -1.614946 |
| C | 2.548498  | 5.703450  | -0.113127 |
| H | 2.593895  | 6.784653  | -0.187067 |
| C | 1.668247  | 5.099154  | 0.784253  |
| H | 1.033219  | 5.709616  | 1.417205  |
| C | 1.607559  | 3.711153  | 0.877669  |
| H | 0.933807  | 3.239515  | 1.586648  |

## Optimized Cartesian coordinates (in Å) of 11's derivative (CH<sub>3</sub> groups substitute *iso*-butyl groups):

- BP86/SDD, E<sub>el</sub> = -1173.835811

|   |            |           |           |
|---|------------|-----------|-----------|
| C | 3.400507   | 3.419650  | 1.714164  |
| C | 1.924193   | 3.585878  | 1.902971  |
| C | 1.383757   | 3.075978  | -0.503181 |
| H | 2.447396   | 2.977404  | -0.738693 |
| C | 0.978049   | 3.397664  | 0.811070  |
| C | -0.447391  | 3.516011  | 1.088223  |
| H | -1.966117  | 3.949190  | 2.601410  |
| C | 0.032645   | 4.018246  | 3.429128  |
| H | -0.299703  | 4.266600  | 4.442973  |
| C | -1.390220  | 3.276930  | 0.060101  |
| H | -2.455327  | 3.374571  | 0.291756  |
| C | -0.891174  | 3.847657  | 2.414069  |
| C | 1.431342   | 3.876038  | 3.174972  |
| C | -0.982911  | 2.926686  | -1.246485 |
| H | 2.139575   | 4.021144  | 3.998559  |
| C | 0.886465   | 2.599724  | -2.877573 |
| C | -1.440464  | 2.429588  | -3.604642 |
| C | 0.442149   | 2.864390  | -1.537110 |
| C | -1.931276  | 2.649452  | -2.316052 |
| H | 0.291215   | 2.222355  | -4.913214 |
| H | 1.962680   | 2.555440  | -3.079191 |
| H | -2.147467  | 2.210667  | -4.412642 |
| C | -0.040652  | 2.415073  | -3.887151 |
| H | -11.344866 | -5.415136 | 4.426498  |
| H | -12.598244 | -6.574773 | 3.843965  |
| H | -11.901151 | -3.180607 | 4.860959  |
| C | -12.383763 | -5.521553 | 4.064397  |
| H | -7.454617  | 2.748682  | 1.585156  |
| O | -12.568807 | -4.826827 | 2.791768  |
| H | -7.577716  | 1.906662  | 3.188622  |
| H | -10.982489 | -0.323924 | 6.865810  |
| C | -11.998230 | -2.688300 | 3.892959  |
| H | -10.413881 | -1.860874 | 6.111425  |
| C | -8.129974  | 2.408899  | 2.383898  |
| O | -11.490052 | -0.488883 | 4.896624  |
| C | -11.248804 | -1.140340 | 6.182950  |
| H | -13.089206 | -5.148595 | 4.829475  |
| H | -8.705900  | 3.259482  | 2.788572  |
| C | -12.324756 | -3.437784 | 2.746586  |
| C | -11.804885 | -1.298824 | 3.784413  |
| H | -8.623700  | -5.556968 | -0.923870 |
| O | -8.458201  | -3.528179 | -2.197245 |
| C | -12.618891 | 0.304351  | -8.237841 |
| H | -12.499937 | -0.515187 | -8.957527 |
| H | -11.773384 | 1.010551  | -8.325977 |
| H | -13.571826 | 0.832252  | -8.426072 |
| O | -10.052546 | -4.294987 | 0.042000  |
| H | -14.098047 | 4.342490  | -6.567162 |
| C | -9.490313  | -5.636407 | -0.247264 |
| H | -9.193436  | -6.033095 | 0.732233  |
| O | -9.058593  | 1.374157  | 1.868625  |
| H | -12.157880 | -1.652339 | 6.548485  |
| H | -9.522771  | -4.139223 | -5.366125 |
| C | -10.633130 | -3.620513 | -1.055886 |
| C | -9.850345  | -3.259152 | -2.173908 |
| H | -12.975040 | 2.352946  | -6.818935 |
| C | -12.436740 | -2.814697 | 1.483734  |
| H | -8.060445  | -3.613504 | -4.439723 |
| C | -13.254803 | 4.700479  | -5.948373 |
| O | -8.250625  | 2.639283  | -0.547874 |
| C | -11.937437 | -0.636673 | 2.538650  |
| C | -8.881474  | -3.283280 | -5.092348 |
| O | -12.624201 | -0.345288 | -6.928194 |
| H | -12.304418 | 4.575649  | -6.498784 |
| H | -12.528021 | -4.691981 | 0.501392  |
| C | -10.008196 | 1.769291  | 0.909517  |
| C | -12.895146 | 1.860586  | -5.849389 |
| C | -12.001594 | -3.268651 | -0.992652 |
| H | -10.265095 | -6.278322 | -0.699921 |
| C | -12.809129 | -3.653708 | 0.250783  |
| C | -9.625650  | 2.391562  | -0.302686 |
| H | -10.988733 | 1.139170  | 3.210712  |

|   |            |           |           |
|---|------------|-----------|-----------|
| C | -12.237088 | -1.420972 | 1.407298  |
| C | -10.447280 | -2.628893 | -3.291890 |
| H | -13.404512 | 5.756957  | -5.692793 |
| C | -12.708303 | 0.467812  | -5.777700 |
| O | -13.210618 | 4.006235  | -4.662885 |
| H | -8.501323  | -2.788817 | -5.995533 |
| C | -11.797494 | 0.894373  | 2.500649  |
| C | -11.373104 | 1.475154  | 1.149385  |
| C | -12.985917 | 2.613181  | -4.662837 |
| O | -9.694113  | -2.244174 | -4.414798 |
| C | -12.572631 | -2.613499 | -2.103463 |
| C | -11.828841 | -2.315768 | -3.268017 |
| C | -10.601356 | 2.765710  | -1.252109 |
| C | -12.320406 | 1.785183  | 0.146987  |
| C | -12.613179 | -0.194313 | -4.528583 |
| H | -12.298784 | -0.934119 | 0.427884  |
| O | -10.230921 | 3.431221  | -2.442179 |
| C | -14.344510 | -3.631332 | 0.029981  |
| C | -11.961795 | 2.433642  | -1.053088 |
| H | -13.638188 | -2.371009 | -2.084637 |
| C | -12.867206 | 1.989593  | -3.400821 |
| C | -13.100714 | 1.559024  | 3.036599  |
| C | -12.494016 | -1.727413 | -4.514874 |
| H | -14.848118 | -4.010825 | 0.935126  |
| H | -8.614711  | 4.660379  | -1.775970 |
| H | -11.839803 | -1.985324 | -5.365583 |
| H | -13.292084 | 1.211109  | 4.065012  |
| C | -12.679877 | 0.592624  | -3.361959 |
| H | -13.373454 | 1.557789  | 0.331328  |
| H | -14.635470 | -4.268648 | -0.824665 |
| C | -9.594607  | 4.759901  | -2.270549 |
| C | -12.985533 | 2.832219  | -2.120671 |
| H | -14.716648 | -2.607069 | -0.153251 |
| H | -13.002201 | 2.659454  | 3.047951  |
| H | -13.978648 | 1.294635  | 2.420655  |
| H | -12.741604 | 3.866495  | -2.421677 |
| H | -9.486177  | 5.152238  | -3.289939 |
| H | -12.562611 | 0.104506  | -2.388269 |
| H | -10.253024 | 5.416706  | -1.676989 |
| C | -13.886451 | -2.369606 | -4.790336 |
| H | -13.810281 | -3.471526 | -4.817344 |
| H | -14.626191 | -2.090726 | -4.018888 |
| C | -14.450901 | 2.832308  | -1.611406 |
| H | -14.796609 | 1.813358  | -1.359616 |
| H | -14.264844 | -2.017982 | -5.764253 |
| H | -14.564267 | 3.472308  | -0.717646 |
| H | -15.112050 | 3.220875  | -2.404396 |
| C | 4.109566   | 2.501510  | 2.528962  |
| C | -3.404483  | 2.532780  | -2.086508 |
| C | 7.671732   | 2.758950  | 1.158779  |
| H | 8.060445   | 3.613504  | 4.439723  |
| O | 8.458201   | 3.528179  | 2.197245  |
| H | 8.623700   | 5.556968  | 0.923870  |
| H | 9.193436   | 6.033095  | -0.732233 |
| C | 9.490313   | 5.636407  | 0.247264  |
| C | 8.881474   | 3.283280  | 5.092348  |
| H | 9.522771   | 4.139223  | 5.366125  |
| O | 10.052546  | 4.294987  | -0.042000 |
| C | 9.850345   | 3.259152  | 2.173908  |
| H | 8.501323   | 2.788817  | 5.995533  |
| O | 9.694113   | 2.244174  | 4.414798  |
| H | 10.265095  | 6.278322  | 0.699921  |
| C | 10.633130  | 3.620513  | 1.055886  |
| C | 10.447280  | 2.628893  | 3.291890  |
| H | 12.499937  | 0.515187  | 8.957527  |
| H | 11.344866  | 5.415136  | -4.426498 |
| H | 11.773384  | -1.010551 | 8.325977  |
| C | 12.618891  | -0.304351 | 8.237841  |
| C | 12.383763  | 5.521553  | -4.064397 |
| H | 12.598244  | 6.574773  | -3.843965 |
| C | 12.001594  | 3.268651  | 0.992652  |
| C | 11.828841  | 2.315768  | 3.268017  |
| H | 12.528021  | 4.691981  | -0.501392 |
| O | 12.624201  | 0.345288  | 6.928194  |
| O | 12.568807  | 4.826827  | -2.791768 |
| H | 11.839803  | 1.985324  | 5.365583  |
| C | 12.809129  | 3.653708  | -0.250783 |
| C | 12.572631  | 2.613499  | 2.103463  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 13.089206 | 5.148595  | -4.829475 |
| H | 14.635470 | 4.268648  | 0.824665  |
| H | 13.571826 | -0.832252 | 8.426072  |
| C | 12.494016 | 1.727413  | 4.514874  |
| C | 12.708303 | -0.467812 | 5.777700  |
| C | 14.344510 | 3.631332  | -0.029981 |
| C | 12.324756 | 3.437784  | -2.746586 |
| H | 13.810281 | 3.471526  | 4.817344  |
| C | 12.613179 | 0.194313  | 4.528583  |
| C | 12.436740 | 2.814697  | -1.483734 |
| H | 12.975040 | -2.352946 | 6.818935  |
| C | 13.886451 | 2.369606  | 4.790336  |
| C | 12.895146 | -1.860586 | 5.849389  |
| H | 14.848118 | 4.010825  | -0.935126 |
| H | 13.638188 | 2.371009  | 2.084637  |
| C | 11.998230 | 2.688300  | -3.892959 |
| H | 14.716648 | 2.607069  | 0.153251  |
| H | 11.901151 | 3.180607  | -4.860959 |
| H | 14.264844 | 2.017982  | 5.764253  |
| C | 12.679877 | -0.592624 | 3.361959  |
| C | 12.237088 | 1.420972  | -1.407298 |
| H | 14.626191 | 2.090726  | 4.018888  |
| C | 12.985917 | -2.613181 | 4.662837  |
| H | 12.562611 | -0.104506 | 2.388269  |
| H | 12.298784 | 0.934119  | -0.427884 |
| C | 12.867206 | -1.989593 | 3.400821  |
| C | 11.804885 | 1.298824  | -3.784413 |
| H | 12.304418 | -4.575649 | 6.498784  |
| H | 14.098047 | -4.342490 | 6.567162  |
| O | 13.210618 | -4.006235 | 4.662885  |
| C | 11.937437 | 0.636673  | -2.538650 |
| C | 13.254803 | -4.700479 | 5.948373  |
| H | 12.157880 | 1.652339  | -6.548485 |
| C | 11.248804 | 1.140340  | -6.182950 |
| O | 11.490052 | 0.488883  | -4.896624 |
| C | 12.985533 | -2.832219 | 2.120671  |
| H | 10.982489 | 0.323924  | -6.865810 |
| C | 12.320406 | -1.785183 | -0.146987 |
| C | 11.961795 | -2.433642 | 1.053088  |
| H | 13.373454 | -1.557789 | -0.331328 |
| C | 10.601356 | -2.765710 | 1.252109  |
| C | 11.373104 | -1.475154 | -1.149385 |
| O | 10.230921 | -3.431221 | 2.442179  |
| C | 11.797494 | -0.894373 | -2.500649 |
| H | 13.404512 | -5.756957 | 5.692793  |
| H | 12.741604 | -3.866495 | 2.421677  |
| C | 9.625650  | -2.391562 | 0.302686  |
| C | 10.008196 | -1.769291 | -0.909517 |
| O | 8.250625  | -2.639283 | 0.547874  |
| H | 13.978648 | -1.294635 | -2.420655 |
| H | 10.413881 | 1.860874  | -6.111425 |
| O | 9.058593  | -1.374157 | -1.868625 |
| C | 14.450901 | -2.832308 | 1.611406  |
| C | 13.100714 | -1.559024 | -3.036599 |
| H | 14.796609 | -1.813358 | 1.359616  |
| H | 10.988733 | -1.139170 | -3.210712 |
| H | 15.112050 | -3.220875 | 2.404396  |
| C | 9.594607  | -4.759901 | 2.270549  |
| H | 8.614711  | -4.660379 | 1.775970  |
| H | 13.292084 | -1.211109 | -4.065012 |
| H | 9.486177  | -5.152238 | 3.289939  |
| C | 8.129974  | -2.408899 | -2.383898 |
| H | 14.564267 | -3.472308 | 0.717646  |
| H | 13.002201 | -2.659454 | -3.047951 |
| H | 10.253024 | -5.416706 | 1.676989  |
| H | 7.577716  | -1.906662 | -3.188622 |
| H | 8.705900  | -3.259482 | -2.788572 |
| H | 7.454617  | -2.748682 | -1.585156 |
| C | 5.487538  | 2.301008  | 2.358830  |
| C | 6.205320  | 3.013566  | 1.374025  |
| C | 5.510479  | 3.955126  | 0.583691  |
| C | 4.129691  | 4.155530  | 0.747342  |
| H | 3.560047  | 1.914845  | 3.272891  |
| H | 6.012601  | 1.569407  | 2.982667  |
| H | 6.057546  | 4.529922  | -0.172322 |
| H | 3.611425  | 4.897631  | 0.130613  |
| C | -5.300868 | 1.478943  | -0.941094 |
| C | -3.919986 | 1.687195  | -1.069270 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -4.326283 | 3.178340  | -2.946779 |
| H | -3.227689 | 1.153218  | -0.410527 |
| C | -5.708887 | 2.972116  | -2.809823 |
| C | -6.215232 | 2.108958  | -1.814138 |
| H | -5.678477 | 0.800165  | -0.168592 |
| H | -3.949241 | 3.851103  | -3.725212 |
| H | -6.405164 | 3.475686  | -3.490126 |
| H | 6.405164  | -3.475686 | 3.490126  |
| C | 5.708887  | -2.972116 | 2.809823  |
| C | 6.215232  | -2.108958 | 1.814138  |
| C | 5.300868  | -1.478943 | 0.941094  |
| H | 5.678477  | -0.800165 | 0.168592  |
| C | 4.326283  | -3.178340 | 2.946779  |
| H | 3.949241  | -3.851103 | 3.725212  |
| C | 3.919986  | -1.687195 | 1.069270  |
| H | 3.227689  | -1.153218 | 0.410527  |
| C | 3.404483  | -2.532780 | 2.086508  |
| H | 2.147467  | -2.210667 | 4.412642  |
| C | 1.931276  | -2.649452 | 2.316052  |
| C | 1.440464  | -2.429588 | 3.604642  |
| C | 1.390220  | -3.276930 | -0.060101 |
| H | 2.455327  | -3.374571 | -0.291756 |
| C | 0.982911  | -2.926686 | 1.246485  |
| C | 0.040652  | -2.415073 | 3.887151  |
| H | 1.966117  | -3.949190 | -2.601410 |
| H | -0.291215 | -2.222355 | 4.913214  |
| C | 0.891174  | -3.847657 | -2.414069 |
| C | 0.447391  | -3.516011 | -1.088223 |
| C | -0.442149 | -2.864390 | 1.537110  |
| C | -0.886465 | -2.599724 | 2.877573  |
| C | -0.032645 | -4.018246 | -3.429128 |
| C | -0.978049 | -3.397664 | -0.811070 |
| C | -1.383757 | -3.075978 | 0.503181  |
| H | -2.447396 | -2.977404 | 0.738693  |
| H | 0.299703  | -4.266600 | -4.442973 |
| H | -1.962680 | -2.555440 | 3.079191  |
| C | -1.431342 | -3.876038 | -3.174972 |
| C | -1.924193 | -3.585878 | -1.902971 |
| C | -4.109566 | -2.501510 | -2.528962 |
| H | -3.560047 | -1.914845 | -3.272891 |
| C | -7.671732 | -2.758950 | -1.158779 |
| C | -5.487538 | -2.301008 | -2.358830 |
| C | -6.205320 | -3.013566 | -1.374025 |
| C | -3.400507 | -3.419650 | -1.714164 |
| H | -2.139575 | -4.021144 | -3.998559 |
| H | -6.012601 | -1.569407 | -2.982667 |
| H | -3.611425 | -4.897631 | -0.130613 |
| C | -4.129691 | -4.155530 | -0.747342 |
| C | -5.510479 | -3.955126 | -0.583691 |
| H | -6.057546 | -4.529922 | 0.172322  |
| C | -7.690943 | 1.841679  | -1.705415 |
| H | -8.235906 | 2.136892  | -2.616497 |
| H | -7.897430 | 0.779927  | -1.484643 |
| H | 7.923760  | 1.693185  | 1.295762  |
| H | 8.011983  | 3.087166  | 0.163462  |
| C | 7.690943  | -1.841679 | 1.705415  |
| H | 7.897430  | -0.779927 | 1.484643  |
| H | 8.235906  | -2.136892 | 2.616497  |
| H | -7.923760 | -1.693185 | -1.295762 |
| H | -8.011983 | -3.087166 | -0.163462 |

• BP86-D/SDD,  $E_{el} = -1174.078365326$  a.u.

|   |           |          |           |
|---|-----------|----------|-----------|
| C | 3.432247  | 2.693514 | 0.532081  |
| C | 1.987234  | 3.037913 | 0.533709  |
| C | 1.305539  | 1.082324 | -0.896669 |
| H | 2.326943  | 0.700669 | -0.887604 |
| C | 1.000408  | 2.264445 | -0.195873 |
| C | -0.385875 | 2.711946 | -0.191669 |
| H | -1.796191 | 4.195450 | 0.550698  |
| C | 0.201065  | 4.560050 | 1.293886  |
| H | -0.078141 | 5.443685 | 1.873877  |
| C | -1.359158 | 1.989741 | -0.912448 |
| H | -2.382505 | 2.370898 | -0.919627 |
| C | -0.750801 | 3.873088 | 0.563341  |

|   |            |           |           |
|---|------------|-----------|-----------|
| C | 1.564861   | 4.144785  | 1.268933  |
| C | -1.047490  | 0.816213  | -1.626305 |
| H | 2.313197   | 4.730006  | 1.809985  |
| C | 0.693710   | -0.816395 | -2.350770 |
| C | -1.598726  | -1.031514 | -3.135946 |
| C | 0.334168   | 0.358282  | -1.615964 |
| C | -2.025887  | 0.062480  | -2.388357 |
| H | 0.028218   | -2.379396 | -3.670423 |
| H | 1.725305   | -1.172956 | -2.290827 |
| H | -2.339198  | -1.591335 | -3.711383 |
| C | -0.246674  | -1.480829 | -3.114604 |
| H | -11.273118 | -5.904746 | 3.902866  |
| H | -12.531349 | -7.009274 | 3.218017  |
| H | -11.814005 | -3.744369 | 4.541715  |
| C | -12.309603 | -5.981031 | 3.527357  |
| H | -7.289395  | 1.963568  | 1.326762  |
| O | -12.477010 | -5.178800 | 2.315824  |
| H | -7.094936  | 0.702763  | 2.613873  |
| H | -10.758247 | -1.136994 | 6.774960  |
| C | -11.873422 | -3.168719 | 3.619109  |
| H | -10.281465 | -2.630456 | 5.872623  |
| C | -7.801668  | 1.363289  | 2.095494  |
| O | -11.258543 | -1.086803 | 4.796297  |
| C | -11.067492 | -1.867811 | 6.018325  |
| H | -13.016529 | -5.656646 | 4.312347  |
| H | -8.318255  | 2.018746  | 2.818217  |
| C | -12.204232 | -3.798039 | 2.404091  |
| C | -11.613420 | -1.786207 | 3.622465  |
| H | -7.861571  | -4.312044 | -0.978871 |
| O | -8.225202  | -2.142057 | -1.955451 |
| C | -12.834571 | 1.095708  | -8.114742 |
| H | -12.711887 | 0.367624  | -8.925359 |
| H | -12.045333 | 1.867401  | -8.164940 |
| H | -13.828886 | 1.574081  | -8.176921 |
| O | -9.743303  | -3.775485 | -0.110348 |
| H | -14.356097 | 4.861231  | -5.971652 |
| C | -8.749685  | -4.792791 | -0.537839 |
| H | -8.486922  | -5.326386 | 0.383582  |
| O | -8.782806  | 0.454245  | 1.458009  |
| H | -12.010949 | -2.356882 | 6.321410  |
| H | -8.383211  | -2.590927 | -4.811085 |
| C | -10.366092 | -3.074785 | -1.168044 |
| C | -9.612527  | -2.306485 | -2.078977 |
| H | -13.213977 | 2.967195  | -6.497252 |
| C | -12.262572 | -3.075049 | 1.197335  |
| H | -7.447534  | -1.246311 | -4.058672 |
| C | -13.481730 | 5.197215  | -5.385317 |
| O | -8.080806  | 1.752130  | -0.904526 |
| C | -11.693265 | -1.016689 | 2.440540  |
| C | -8.301543  | -1.496554 | -4.704478 |
| O | -12.711844 | 0.314072  | -6.884760 |
| H | -12.569601 | 5.134524  | -6.006106 |
| H | -12.153493 | -4.815803 | -0.012481 |
| C | -9.775128  | 1.110699  | 0.697909  |
| C | -13.043715 | 2.390703  | -5.589037 |
| C | -11.773486 | -3.118563 | -1.253420 |
| H | -9.214310  | -5.476806 | -1.267611 |
| C | -12.543840 | -3.789190 | -0.125347 |
| C | -9.429619  | 1.743890  | -0.517655 |
| H | -10.581006 | 0.642026  | 3.158292  |
| C | -12.018249 | -1.691194 | 1.252163  |
| C | -10.254696 | -1.717526 | -3.193102 |
| H | -13.634451 | 6.223068  | -5.029529 |
| C | -12.779131 | 1.010223  | -5.658728 |
| O | -13.333088 | 4.395177  | -4.171469 |
| H | -8.209022  | -1.017946 | -5.688979 |
| C | -11.454358 | 0.491064  | 2.499793  |
| C | -11.109812 | 1.104913  | 1.149766  |
| C | -13.077866 | 3.016189  | -4.328321 |
| O | -9.551920  | -0.945115 | -4.134168 |
| C | -12.387856 | -2.493574 | -2.351974 |
| C | -11.650382 | -1.842926 | -3.363046 |
| C | -10.420908 | 2.392647  | -1.275851 |
| C | -12.092704 | 1.687464  | 0.320301  |
| C | -12.562842 | 0.240656  | -4.495022 |
| H | -12.037096 | -1.120965 | 0.319393  |
| O | -10.085253 | 3.083067  | -2.459390 |
| C | -14.065091 | -3.883819 | -0.376358 |

|   |            |           |           |
|---|------------|-----------|-----------|
| C | -11.775801 | 2.344430  | -0.881722 |
| H | -13.472721 | -2.545992 | -2.446584 |
| C | -12.840108 | 2.289945  | -3.146363 |
| C | -12.668633 | 1.185859  | 3.172186  |
| C | -12.318086 | -1.262513 | -4.601521 |
| H | -14.535423 | -4.414371 | 0.466558  |
| H | -8.198171  | 3.915512  | -1.904394 |
| H | -11.619517 | -1.406684 | -5.444536 |
| H | -12.778756 | 0.796092  | 4.195659  |
| C | -12.601496 | 0.910641  | -3.262584 |
| H | -13.132932 | 1.663162  | 0.646287  |
| H | -14.279132 | -4.433279 | -1.309993 |
| C | -9.188102  | 4.247337  | -2.258741 |
| C | -12.816503 | 2.986986  | -1.788422 |
| H | -14.510486 | -2.876344 | -0.449254 |
| H | -12.519356 | 2.278788  | 3.210479  |
| H | -13.599046 | 0.975074  | 2.617991  |
| H | -12.497056 | 4.027178  | -1.976536 |
| H | -9.117592  | 4.718767  | -3.246539 |
| H | -12.390903 | 0.339852  | -2.354173 |
| H | -9.638476  | 4.941389  | -1.528969 |
| C | -13.642835 | -1.984103 | -4.962251 |
| H | -13.487282 | -3.074991 | -5.024764 |
| H | -14.421079 | -1.780008 | -4.207014 |
| C | -14.235485 | 3.029486  | -1.178927 |
| H | -14.621324 | 2.007273  | -1.021239 |
| H | -13.997027 | -1.609447 | -5.934794 |
| H | -14.236793 | 3.561715  | -0.211332 |
| H | -14.909002 | 3.552505  | -1.876088 |
| C | 4.155432   | 2.722806  | 1.745737  |
| C | -3.470635  | 0.402648  | -2.359372 |
| C | 7.678041   | 1.740031  | 0.627716  |
| H | 7.447047   | 1.246061  | 4.056836  |
| O | 8.221564   | 2.131405  | 1.962129  |
| H | 7.854943   | 4.307874  | 0.999654  |
| H | 8.475810   | 5.328683  | -0.359922 |
| C | 8.741259   | 4.792477  | 0.559212  |
| C | 8.300888   | 1.476445  | 4.710283  |
| H | 8.392151   | 2.567793  | 4.838920  |
| O | 9.736849   | 3.779224  | 0.126689  |
| C | 9.608145   | 2.299071  | 2.087235  |
| H | 8.201131   | 0.979623  | 5.684952  |
| O | 9.548646   | 0.925613  | 4.133552  |
| H | 9.205244   | 5.475037  | 1.290760  |
| C | 10.360503  | 3.074350  | 1.181179  |
| C | 10.251147  | 1.705869  | 3.198506  |
| H | 12.704535  | -0.401531 | 8.923258  |
| H | 11.268698  | 5.932417  | -3.875770 |
| H | 12.040609  | -1.898335 | 8.154718  |
| C | 12.828976  | -1.125461 | 8.109194  |
| C | 12.304355  | 6.008951  | -3.498028 |
| H | 12.523452  | 7.036113  | -3.183251 |
| C | 11.767743  | 3.121432  | 1.268093  |
| C | 11.646160  | 1.834686  | 3.370911  |
| H | 12.143778  | 4.825816  | 0.035751  |
| O | 12.706665  | -0.337922 | 6.882939  |
| O | 12.471226  | 5.201123  | -2.290134 |
| H | 11.615028  | 1.388754  | 5.450428  |
| C | 12.537211  | 3.799887  | 0.144082  |
| C | 12.382940  | 2.492761  | 2.364099  |
| H | 13.013346  | 5.689846  | -4.283321 |
| H | 14.269133  | 4.443664  | 1.333807  |
| H | 13.823794  | -1.602950 | 8.170100  |
| C | 12.314043  | 1.249379  | 4.606976  |
| C | 12.776255  | -1.027983 | 5.653569  |
| C | 14.057876  | 3.898106  | 0.397250  |
| C | 12.201538  | 3.820256  | -2.385681 |
| H | 13.481062  | 3.061086  | 5.039561  |
| C | 12.560443  | -0.252957 | 4.493391  |
| C | 12.259461  | 3.091457  | -1.182395 |
| H | 13.212300  | -2.988572 | 6.482985  |
| C | 13.637824  | 1.970687  | 4.971616  |
| C | 13.042493  | -2.407811 | 5.577406  |
| H | 14.527387  | 4.434288  | -0.442544 |
| H | 13.467557  | 2.547888  | 2.460015  |
| C | 11.873984  | 3.196296  | -3.604304 |
| H | 14.506380  | 2.891701  | 0.465716  |
| H | 11.814784  | 3.776386  | -4.524138 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 13.992227 | 1.591595  | 5.942357  |
| C | 12.601377 | -0.916771 | 3.257713  |
| C | 12.018211 | 1.707381  | -1.244435 |
| H | 14.416443 | 1.771247  | 4.215518  |
| C | 13.078925 | -3.027010 | 4.313663  |
| H | 12.391217 | -0.341766 | 2.351843  |
| H | 12.036834 | 1.132510  | -0.314498 |
| C | 12.841825 | -2.295188 | 3.135003  |
| C | 11.616854 | 1.813290  | -3.614908 |
| H | 12.571066 | -5.154283 | 5.980229  |
| H | 14.357279 | -4.878605 | 5.949544  |
| O | 13.336089 | -4.404860 | 4.150329  |
| C | 11.696506 | 1.038134  | -2.436643 |
| C | 13.484112 | -5.212752 | 5.360376  |
| H | 12.017607 | 2.397985  | -6.310353 |
| C | 11.074662 | 1.905462  | -6.011280 |
| O | 11.265259 | 1.118929  | -4.792732 |
| C | 12.820827 | -2.985549 | 1.773626  |
| H | 10.768263 | 1.177682  | -6.771996 |
| C | 12.098265 | -1.675974 | -0.329329 |
| C | 11.780615 | -2.339524 | 0.868857  |
| H | 13.138866 | -1.648734 | -0.653911 |
| C | 10.425394 | -2.391155 | 1.261169  |
| C | 11.115557 | -1.090750 | -1.157124 |
| O | 10.089191 | -3.088167 | 2.440798  |
| C | 11.461073 | -0.469752 | -2.503616 |
| H | 13.638595 | -6.236627 | 4.999682  |
| H | 12.502165 | -4.026948 | 1.956278  |
| C | 9.434069  | -1.739635 | 0.505302  |
| C | 9.780244  | -1.100461 | -0.706984 |
| O | 8.084841  | -1.750941 | 0.890740  |
| H | 13.607081 | -0.948236 | -2.620314 |
| H | 10.286773 | 2.665737  | -5.863245 |
| O | 8.788124  | -0.441935 | -1.465465 |
| C | 14.240642 | -3.023729 | 1.165737  |
| C | 12.678128 | -1.158554 | -3.177149 |
| H | 14.625825 | -2.000400 | 1.013758  |
| H | 10.589218 | -0.619513 | -3.164375 |
| H | 14.913708 | -3.549727 | 1.861093  |
| C | 9.194545  | -4.252963 | 2.231995  |
| H | 8.205337  | -3.920947 | 1.875694  |
| H | 12.789135 | -0.763669 | -4.198566 |
| H | 9.121150  | -4.728819 | 3.217468  |
| C | 7.807107  | -1.349019 | -2.105748 |
| H | 14.243616 | -3.551004 | 0.195430  |
| H | 12.531482 | -2.251642 | -3.220908 |
| H | 9.648540  | -4.943167 | 1.500811  |
| H | 7.100550  | -0.686948 | -2.622418 |
| H | 8.323761  | -2.002519 | -2.830215 |
| H | 7.294543  | -1.951448 | -1.338857 |
| C | 5.522883  | 2.432242  | 1.787670  |
| C | 6.220874  | 2.114689  | 0.607183  |
| C | 5.518859  | 2.111478  | -0.616488 |
| C | 4.144042  | 2.390712  | -0.654814 |
| H | 3.618910  | 2.949211  | 2.669149  |
| H | 6.057672  | 2.429190  | 2.736994  |
| H | 6.058870  | 1.893099  | -1.543437 |
| H | 3.617285  | 2.408638  | -1.612001 |
| C | -5.513936 | 0.863618  | -1.090481 |
| C | -4.139506 | 0.609535  | -1.132750 |
| C | -4.233332 | 0.462025  | -3.549322 |
| H | -3.576656 | 0.529784  | -0.202005 |
| C | -5.609457 | 0.739479  | -3.509045 |
| C | -6.267629 | 0.941305  | -2.277424 |
| H | -6.018924 | 0.990187  | -0.133690 |
| H | -3.729400 | 0.316226  | -4.508822 |
| H | -6.177313 | 0.813644  | -4.441900 |
| H | 6.183437  | -0.819962 | 4.432847  |
| C | 5.613849  | -0.746917 | 3.500964  |
| C | 6.270018  | -0.949452 | 2.268315  |
| C | 5.514458  | -0.872128 | 1.082662  |
| H | 6.017946  | -0.998498 | 0.125014  |
| C | 4.237694  | -0.470370 | 3.543475  |
| H | 3.735301  | -0.324393 | 4.503785  |
| C | 4.139978  | -0.617816 | 1.127068  |
| H | 3.575865  | -0.537451 | 0.197022  |
| C | 3.472786  | -0.411664 | 2.354749  |
| H | 2.342991  | 1.581387  | 3.709588  |



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.027879  | -0.071936 | 2.386391  |
| C | 1.601726  | 1.021940  | 3.134846  |
| C | 1.357902  | -1.999943 | 0.912311  |
| H | 2.380787  | -2.382458 | 0.919104  |
| C | 1.048077  | -0.825519 | 1.625726  |
| C | 0.249920  | 1.471995  | 3.114808  |
| H | 1.791408  | -4.206804 | -0.550570 |
| H | -0.023937 | 2.370649  | 3.670990  |
| C | 0.746438  | -3.882914 | -0.562942 |
| C | 0.383345  | -2.721230 | 0.192205  |
| C | -0.333266 | -0.366505 | 1.616513  |
| C | -0.691435 | 0.808404  | 2.351507  |
| C | -0.206567 | -4.568290 | -1.293576 |
| C | -1.002294 | -2.271880 | 0.196796  |
| C | -1.305733 | -1.089677 | 0.897985  |
| H | -2.326741 | -0.707242 | 0.889990  |
| H | 0.071282  | -5.452143 | -1.873895 |
| H | -1.722751 | 1.165705  | 2.292297  |
| C | -1.569720 | -4.150902 | -1.268473 |
| C | -1.990273 | -3.043647 | -0.532846 |
| C | -4.158426 | -2.725587 | -1.744182 |
| H | -3.622537 | -2.952247 | -2.667924 |
| C | -7.680299 | -1.743191 | -0.623856 |
| C | -5.525822 | -2.434792 | -1.785140 |
| C | -6.222979 | -2.117294 | -0.604075 |
| C | -3.434610 | -2.696892 | -0.530904 |
| H | -2.318991 | -4.734684 | -1.809783 |
| H | -6.061482 | -2.432094 | -2.733970 |
| H | -3.617927 | -2.411613 | 1.613176  |
| C | -4.145329 | -2.393357 | 0.656388  |
| C | -5.520094 | -2.113798 | 0.619062  |
| H | -6.059474 | -1.895539 | 1.546382  |
| C | -7.752427 | 1.205156  | -2.253439 |
| H | -8.055520 | 1.929954  | -3.026186 |
| H | -8.345163 | 0.286542  | -2.410690 |
| H | 7.824634  | 0.654970  | 0.503103  |
| H | 8.247247  | 2.246906  | -0.166886 |
| C | 7.754743  | -1.213936 | 2.243281  |
| H | 8.347584  | -0.296828 | 2.408892  |
| H | 8.056335  | -1.945088 | 3.010575  |
| H | -7.827192 | -0.657567 | -0.504275 |
| H | -8.248001 | -2.246294 | 0.174206  |

### Computational details for obtaining the RI-MP2/def2-TZVP optimized structure of $\alpha$ -phenylnaphthalene:

The structure optimization was performed with the ORCA programme using the def2-TZVP basis set from the programme's internal basis set database in combination with the QZVP/C basis set for the resolution-of-identity procedure. In addition to the charge density fitting of the Coulomb energy contributions also the RIJCOSX charge density fitting for the exchange energy contribution was activated with a grid accuracy of "GRIDX6". "scfconv7" SCF convergence criteria and standard convergence criteria in structure optimization result in a relative accuracy of the electronic energy of  $5 \times 10^{-7}$  a.u.