**Supplementary materials**

Table S1 : B3LYP/6-311+G(d,p) and B3LYP/6-311++G(3df,2p) energies (E1 and E2), Zero point energy (ZPE), thermal correction to energy, thermal correction to enthalpy (TCH) and thermal correction to free energy (TCG). All values are in hartree.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | E1 | E2 | ZPE | TCE | TCH | TCG |
|  | R =H | | | | | |
| **A** | -719.669361 | -719.699228 | 0.064687 | 0.070735 | 0.071679 | 0.033998 |
| B | -719.640256 | -719.671173 | 0.064298 | 0.070295 | 0.071239 | 0.033813 |
| C | -719.646056 | -719.676348 | 0.064496 | 0.070489 | 0.071434 | 0.034075 |
| D | -719.635741 | -719.667627 | 0.063770 | 0.070175 | 0.071120 | 0.033284 |
| E | -719.623977 | -719.657069 | 0.063858 | 0.070096 | 0.071040 | 0.033641 |
|  | R= CH3 | | | | | |
| A | -758.996641 | -759.028404 | 0.092718 | 0.100239 | 0.101183 | 0.060117 |
| B | -758.967388 | -759.000165 | 0.092321 | 0.099808 | 0.100752 | 0.059909 |
| C | -758.972572 | -759.004634 | 0.092643 | 0.100086 | 0.101030 | 0.060404 |
| D | -758.953097 | -758.987976 | 0.091535 | 0.099639 | 0.100583 | 0.058910 |
| E | -758.962194 | -758.995810 | 0.091229 | 0.099455 | 0.100399 | 0.058464 |
|  | R= Cl | | | | | |
| A | -1179.280558 | -1179.315281 | 0.055335 | 0.062522 | 0.063466 | 0.022239 |
| B | -1179.251787 | -1179.287519 | 0.054956 | 0.062105 | 0.063049 | 0.022006 |
| C | -1179.257532 | -1179.292691 | 0.055174 | 0.062320 | 0.063264 | 0.022361 |
| D | -1179.237247 | -1179.276009 | 0.054697 | 0.062227 | 0.063171 | 0.022132 |
| E | -1179.250885 | -1179.288712 | 0.054695 | 0.062357 | 0.063301 | 0.021849 |
|  | R= CN | | | | | |
| A | -811.916997 | -811.952953 | 0.063080 | 0.070900 | 0.071844 | 0.029428 |
| B | -811.889964 | -811.927058 | 0.062665 | 0.070438 | 0.071383 | 0.029250 |
| C | -811.893939 | -811.930312 | 0.062932 | 0.070699 | 0.071643 | 0.029650 |
| D | -811.895435 | -811.933689 | 0.062320 | 0.070606 | 0.071551 | 0.028913 |
| E | -811.890598 | -811.929988 | 0.062963 | 0.070911 | 0.071856 | 0.030031 |
|  | R= F | | | | | |
| A | -818.924929 | -818.960700 | 0.056797 | 0.063657 | 0.064601 | 0.024582 |
| B | -818.895735 | -818.932453 | 0.056454 | 0.063270 | 0.064214 | 0.024410 |
| C | -818.901588 | -818.937700 | 0.056653 | 0.063463 | 0.064408 | 0.024749 |
| D | -818.886274 | -818.924285 | 0.055692 | 0.063201 | 0.064146 | 0.023559 |
| E | -818.873252 | -818.912504 | 0.055800 | 0.063097 | 0.064146 | 0.023559 |
|  | R = NO2 | | | | | |
| A | -924.214597 | -924.259123 | 0.066988 | 0.075626 | 0.076571 | 0.031595 |
| B | -924.186267 | -924.231889 | 0.066547 | 0.075158 | 0.076102 | 0.031180 |
| C | -924.191755 | -924.236498 | 0.066754 | 0.075373 | 0.076317 | 0.031596 |
| D | -924.180523 | -924.229676 | 0.066729 | 0.075390 | 0.076334 | 0.032480 |
| E | -924.180523 | -924.232616 | 0.065957 | 0.075073 | 0.076017 | 0.031038 |
|  | R = NH2 | | | | | |
| A | -775.036155 | -775.069258 | 0.081743 | 0.089223 | 0.090167 | 0.049149 |
| B | -775.007359 | -775.041315 | 0.081329 | 0.088864 | 0.089808 | 0.048702 |
| C | -775.008017 | -775.041458 | 0.081416 | 0.088902 | 0.089846 | 0.049012 |
| D | -775.011432 | -775.045754 | 0.081529 | 0.089150 | 0.090095 | 0.049534 |
| E | -774.992088 | -775.028094 | 0.080594 | 0.088442 | 0.089386 | 0.048544 |

Table S2 : B3LYP/6-311+G(d,p) and B3LYP/6-311++G(3df,2p) energies (E1 and E2), Zero point energy (ZPE) and thermal correction to enthalpy (TCH). All values are in hartree.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | E1 | E2 | ZPE | TCH |
|  | R=-H | | | |
| neutral | -719.669361 | -719.699228 | 0.064687 | 0.071679 |
| O2 | -719.950646 | -719.982426 | 0.073568 | 0.081182 |
| O2 | -719.981265 | -720.014456 | 0.076733 | 0.083943 |
| O4 | -719.977550 | -720.010951 | 0.076811 | 0.084008 |
| N3 | -719.945002 | -719.975777 | 0.075982 | 0.083556 |
|  | R=-CH3 | | | |
| neutral | -758.996641 | -759.028404 | 0.092718 | 0.101183 |
| O2 | -759.313466 | -759.348513 | 0.104704 | 0.113422 |
| O4 | -759.308687 | -759.343898 | 0.104876 | 0.113554 |
| N3 | -759.277853 | -759.310588 | 0.103930 | 0.112973 |
|  | R=Cl | | | |
| neutral | -1179.280558 | -1179.315281 | 0.055335 | 0.063466 |
| O2 | -1179.584060 | -1179.622787 | 0.067289 | 0.075656 |
| O4 | -1179.582628 | -1179.621700 | 0.067476 | 0.075795 |
| N3 | -1179.546928 | -1179.583552 | 0.066500 | 0.075158 |
|  | R = CN | | | |
| neutral | -811.916997 | -811.952953 | 0.063080 | 0.071844 |
| O2 | -812.212319 | -812.251620 | 0.074955 | 0.083991 |
| O4 | -812.208853 | -812.248009 | 0.075115 | 0.084112 |
| N3 | -812.174269 | -812.211027 | 0.074200 | 0.083558 |
|  | R=F | | | |
| neutral | -818.924929 | -818.960700 | 0.056797 | 0.064601 |
| O2 | -819.225048 | -819.264859 | 0.068858 | 0.076908 |
| O4 | -819.223100 | -819.262771 | 0.069006 | 0.077011 |
| N3 | -819.188429 | -819.226074 | 0.068111 | 0.076444 |
|  | R=NO2 | | | |
| neutral | -924.214597 | -924.259123 | 0.066988 | 0.076571 |
| O2 | -924.507240 | -924.556043 | 0.078644 | 0.088499 |
| O4 | -924.511978 | -924.560784 | 0.079018 | 0.088506 |
| N3 | -924.479534 | -924.519534 | 0.078415 | 0.088365 |
|  | R=NH2 | | | |
| neutral | -775.036155 | -775.069258 | 0.081743 | 0.090167 |
| O2 | -775.361030 | -775.395583 | 0.093843 | 0.102703 |
| O4 | -775.358082 | -775.393153 | 0.094770 | 0.103015 |
| N3 | was not converged | | | |