# Supporting Information: Embedded mean-field theory with block-orthogonalized partitioning

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## I. Comparison of EMFT using the three exact exchange schemes.

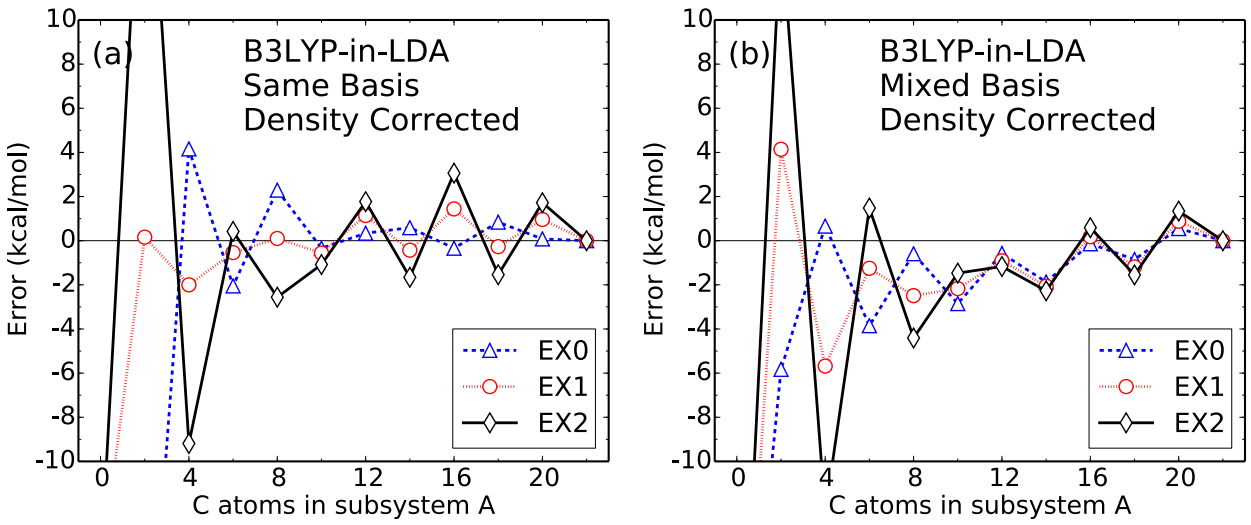


Figure S1. Performance of EMFT using EX0 (dashed blue lines), EX1 (dotted red lines) and EX2 (solid black lines) exact exchange schemes for the terminal hydrogenation of pentacene. Results are shown in terms of the error in the reaction energy, as a function of the size of

subsystem A. (a) B3LYP-in-LDA with same-basis embedding; (b) B3LYP-in-LDA with mixed-basis embedding. All calculations are carried out using the density-corrected implementation of EMFT. All errors are plotted relative to the high-level DFT results: 32.5 kcal/mol for B3LYP/6-31G*.

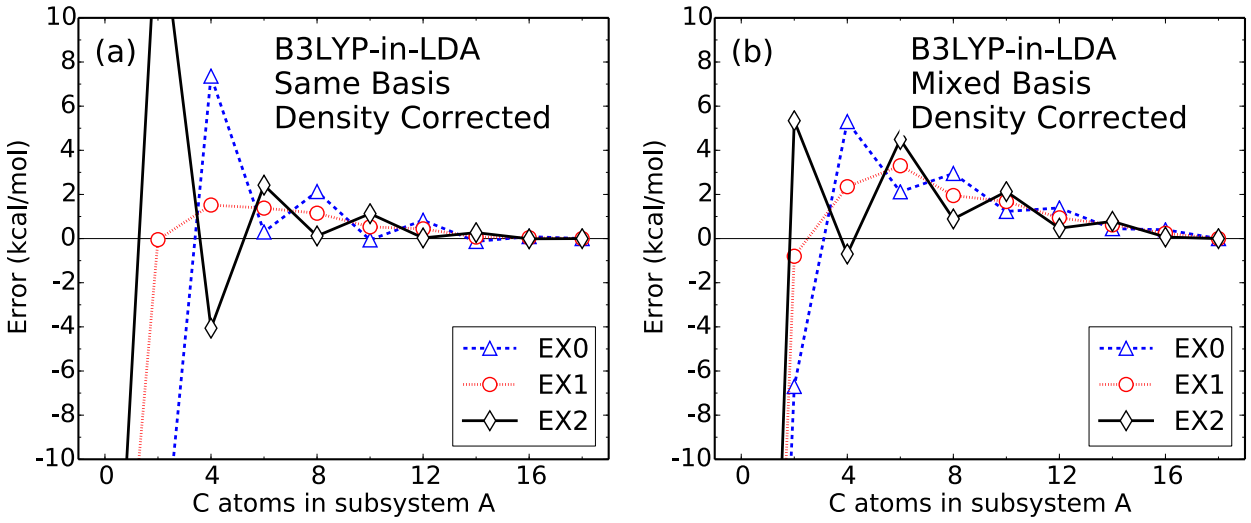


Figure S2. Performance of EMFT using EX0 (dashed blue lines), EX1 (dotted red lines) and EX2 (solid black lines) exact exchange schemes for the Diels-Alder reaction between the 1,3-butadiene and conjugated octadecanonene. Results are shown in terms of the error in the reaction energy, as a function of the size of subsystem A. (a) B3LYP-in-LDA with same-basis embedding; (b) B3LYP-in-LDA with mixed-basis embedding. All calculations are carried out using the density-corrected implementation of EMFT. All errors are plotted relative to the high-level DFT results: 21.1 kcal/mol for B3LYP/6-31G*.

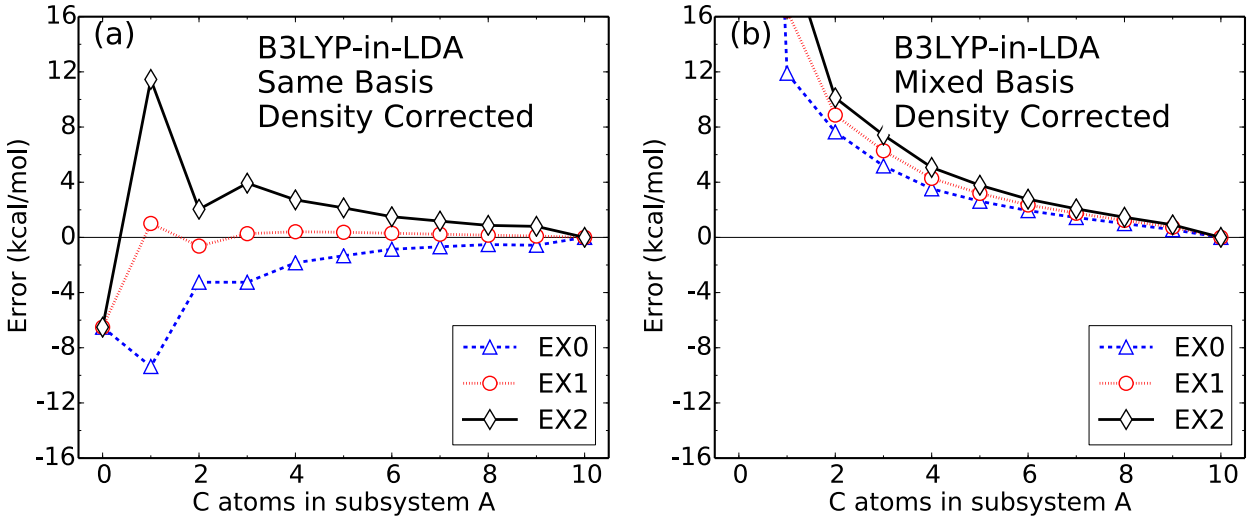

Figure S3. Performance of EMFT using EX0 (dashed blue lines), EX1 (dotted red lines) and EX2 (solid black lines) exact exchange schemes for the deprotonation of decanoic acid. Results are shown in terms of the error in the reaction energy, as a function of the size of subsystem A. (a) B3LYP-in-LDA with same-basis embedding; (b) B3LYP-in-LDA with mixed-basis embedding. All calculations are carried out using the density-corrected implementation of EMFT. All errors are plotted relative to the high-level DFT results: 363.4 kcal/mol for B3LYP/6-31G*.

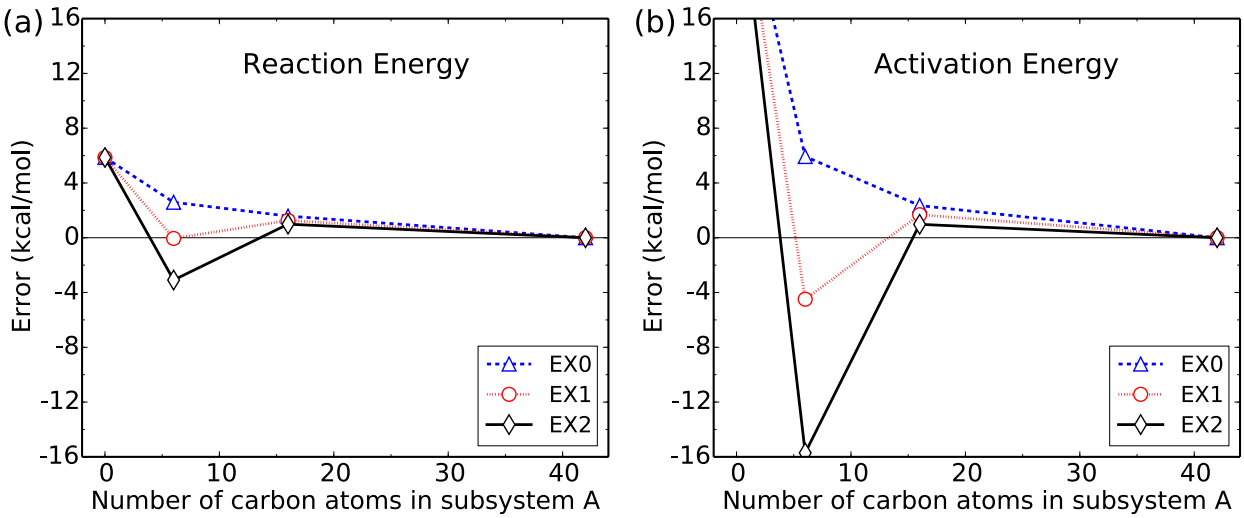


Figure S4. Performance of EMFT using EX0 (dashed blue lines), EX1 (dotted red lines) and EX2 (solid black lines) exact exchange schemes for the defect formation in a graphene sheet. Results are shown in terms of the error in the reaction energy, as a function of the size of subsystem A. (a) Error in the reaction energy; (b) error in the activation energy. All calculations are carried out using the density-corrected implementation of EMFT within the framework of B3LYP-in-LDA with mixed-basis embedding. 6-31G* is used as the high-level AO basis and STO-3G is employed as the low-level AO basis. All errors are plotted relative to the high-level (B3LYP/6-31G*) DFT results: 71.7 kcal/mol for the reaction energy, and 215.1 kcal/mol for the activation energy.

## II. Zoomed-in comparison of EMFT with AO partitioning, BO partitioning, and the density-corrected implementation for the three benchmark reactions.

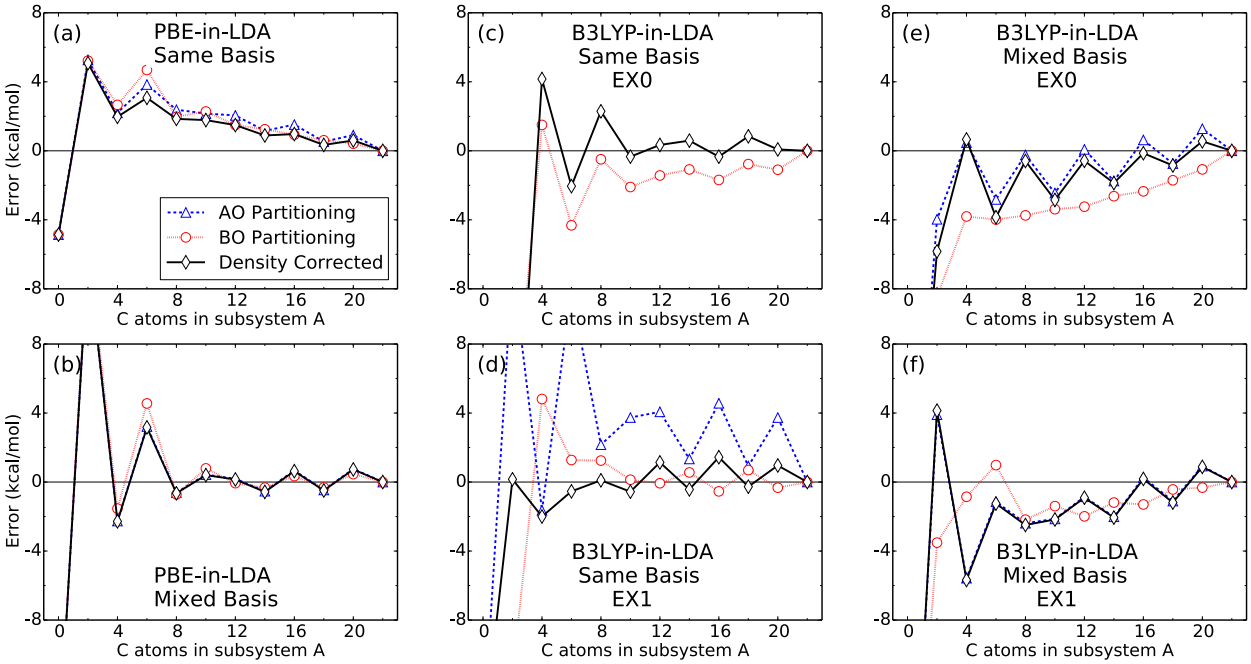


Figure S5. Zoomed-in plot of Figure 4 in the main text.

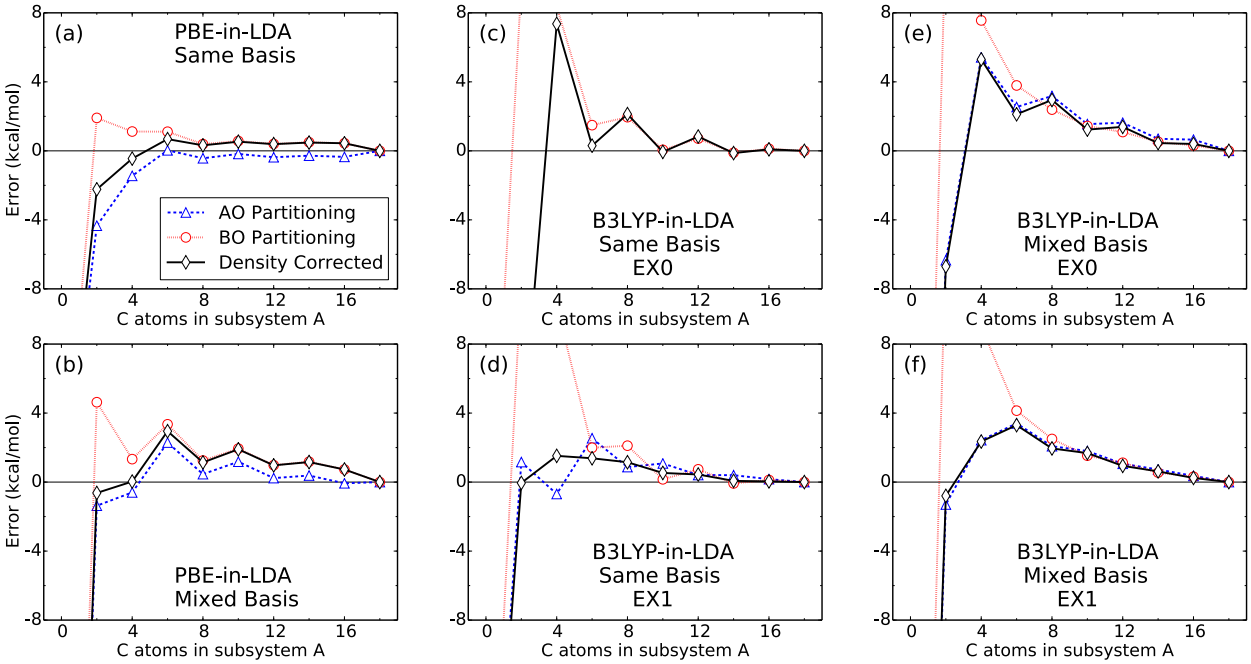


Figure S6. Zoomed-in version of Figure 5 from the main text.

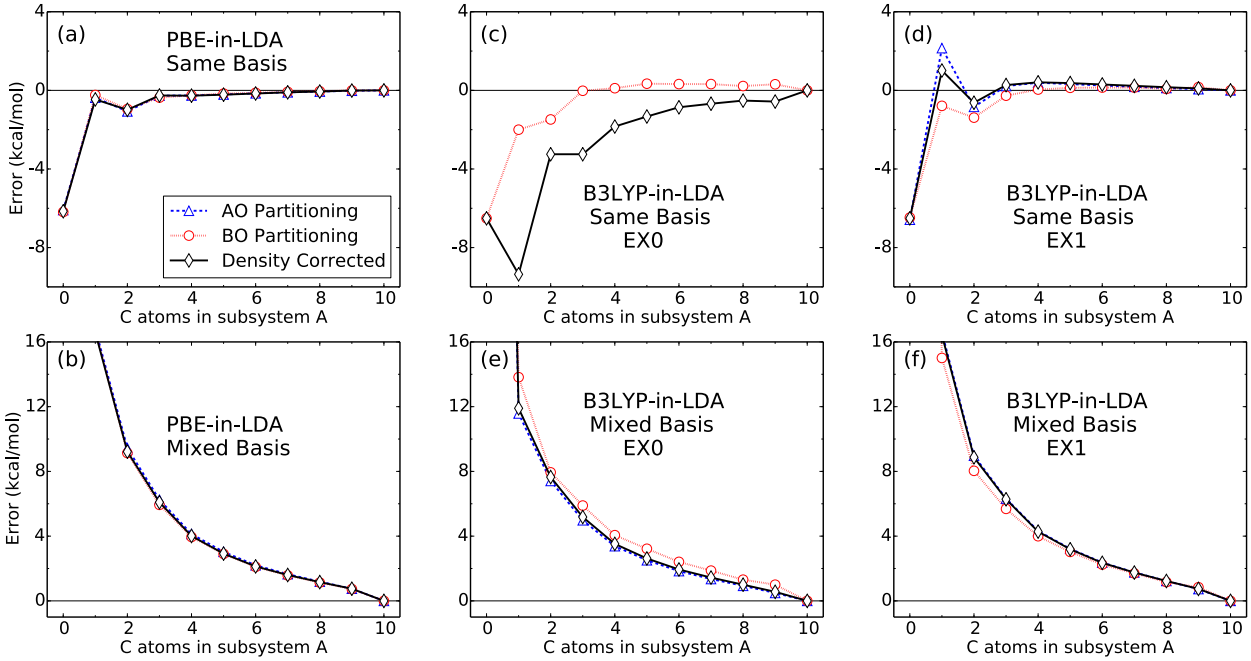


Figure S7. Zoomed-in version of Figure 6 from the main text.

## III. Cartesian coordinates for the test molecules

Pentacene

| | | | |
|---|---|---|---|
| C | -0.715841 | -6.107749 | 0.000000 |
| C | 0.715842 | -6.107749 | 0.000000 |
| H | -1.245672 | -7.053626 | 0.000000 |
| H | 1.245673 | -7.053625 | 0.000000 |
| C | 1.408460 | -4.934989 | 0.000000 |
| C | -1.408460 | -4.934990 | 0.000000 |
| H | 2.493485 | -4.935051 | 0.000000 |
| H | -2.493485 | -4.935052 | 0.000000 |
| C | 0.726859 | -3.672425 | 0.000000 |
| C | -0.726860 | -3.672425 | 0.000000 |
| C | 1.406111 | -2.464080 | 0.000000 |
| C | -1.406112 | -2.464081 | 0.000000 |
| H | 2.491875 | -2.465022 | 0.000000 |
| H | -2.491877 | -2.465022 | 0.000000 |
| C | 0.727673 | -1.224439 | 0.000000 |
| C | -0.727673 | -1.224439 | 0.000000 |
| C | 1.406586 | 0.000000 | 0.000000 |
| C | -1.406587 | 0.000000 | 0.000000 |
| H | 2.492262 | 0.000000 | 0.000000 |
| H | -2.492264 | 0.000000 | 0.000000 |
| C | 0.727673 | 1.224439 | 0.000000 |

| | | | |
|---|---|---|---|
| C | -0.727673 | 1.224439 | 0.000000 |
| C | 1.406111 | 2.464080 | 0.000000 |
| C | -1.406112 | 2.464081 | 0.000000 |
| H | 2.491875 | 2.465022 | 0.000000 |
| H | -2.491876 | 2.465023 | 0.000000 |
| C | 0.726859 | 3.672425 | 0.000000 |
| C | -0.726859 | 3.672425 | 0.000000 |
| C | 1.408461 | 4.934989 | 0.000000 |
| C | -1.408460 | 4.934990 | 0.000000 |
| H | 2.493485 | 4.935050 | 0.000000 |
| H | -2.493485 | 4.935052 | 0.000000 |
| C | 0.715842 | 6.107749 | 0.000000 |
| C | -0.715841 | 6.107749 | 0.000000 |
| H | 1.245674 | 7.053625 | 0.000000 |
| H | -1.245672 | 7.053626 | 0.000000 |

Hydrogenated pentacene

| | | | |
|---|---|---|---|
| C | -6.093712 | 0.621473 | 0.443128 |
| C | -6.093753 | -0.621492 | -0.443000 |
| H | -6.998689 | 1.226372 | 0.276700 |
| H | -6.093697 | -0.298386 | -1.512652 |
| H | -6.093564 | 0.298350 | 1.512776 |
| H | -6.998704 | -1.226408 | -0.276487 |
| C | -4.846849 | -1.419514 | -0.181912 |
| C | -4.846841 | 1.419518 | 0.181946 |
| H | -4.841011 | -2.510477 | -0.288386 |
| H | -4.841010 | 2.510479 | 0.288434 |
| C | -3.632982 | -0.743670 | -0.005379 |
| C | -3.632971 | 0.743704 | 0.005307 |
| C | -2.390344 | -1.430648 | 0.068529 |
| C | -2.390321 | 1.430668 | -0.068656 |
| H | -2.383303 | -2.527657 | 0.086452 |
| H | -2.383263 | 2.527675 | -0.086599 |
| C | -1.151815 | -0.735152 | 0.045954 |
| C | -1.151786 | 0.735170 | -0.046057 |
| C | 0.077654 | -1.422598 | 0.080690 |
| C | 0.077687 | 1.422596 | -0.080707 |
| H | 0.082467 | -2.518221 | 0.140311 |
| H | 0.082524 | 2.518220 | -0.140288 |
| C | 1.321971 | -0.729572 | 0.041325 |
| C | 1.321993 | 0.729557 | -0.041324 |
| C | 2.554122 | -1.417287 | 0.080549 |
| C | 2.554130 | 1.417299 | -0.080538 |
| H | 2.559098 | -2.512713 | 0.142385 |
| H | 2.559101 | 2.512724 | -0.142376 |

| | | | |
|---|---|---|---|
| C | 3.787589 | -0.723776 | 0.040281 |
| C | 3.787601 | 0.723786 | -0.040259 |
| C | 5.042065 | -1.415618 | 0.079451 |
| C | 5.042090 | 1.415608 | -0.079420 |
| H | 5.042721 | -2.509422 | 0.140878 |
| H | 5.042767 | 2.509411 | -0.140850 |
| C | 6.239410 | -0.714554 | 0.040169 |
| C | 6.239420 | 0.714519 | -0.040133 |
| H | 7.189197 | -1.256988 | 0.070646 |
| H | 7.189216 | 1.256938 | -0.070606 |

1,3-Butadiene

| | | | |
|---|---|---|---|
| H | 0.700454 | 2.513208 | -0.414085 |
| H | -0.700454 | -2.513208 | -0.414085 |
| C | 0.268358 | 1.522251 | -0.489554 |
| H | -0.175244 | 1.250498 | -1.441656 |
| C | 0.268358 | 0.683720 | 0.549286 |
| H | 0.675752 | 1.029586 | 1.497344 |
| C | -0.268358 | -0.683720 | 0.549286 |
| H | -0.675752 | -1.029586 | 1.497344 |
| H | 0.175244 | -1.250498 | -1.441656 |
| C | -0.268358 | -1.522251 | -0.489554 |

Octadecanonene

| | | | |
|---|---|---|---|
| H | 0.604592 | -1.428605 | -0.000052 |
| C | 0.605178 | -0.329731 | -0.000053 |
| H | -0.604599 | 1.428772 | -0.000051 |
| C | -0.605178 | 0.329899 | -0.000053 |
| H | 1.880240 | 1.436878 | -0.000049 |
| C | 1.879829 | 0.337995 | -0.000049 |
| H | -1.880213 | -1.436726 | -0.000048 |
| C | -1.879823 | -0.337842 | -0.000049 |
| H | 3.090066 | -1.420013 | -0.000033 |
| C | 3.089846 | -0.321159 | -0.000038 |
| H | -3.090107 | 1.420136 | -0.000034 |
| C | -3.089856 | 0.321283 | -0.000037 |
| H | 4.364413 | 1.446715 | -0.000030 |
| C | 4.365376 | 0.347846 | -0.000024 |
| H | -4.364357 | -1.446634 | -0.000030 |
| C | -4.365364 | -0.347765 | -0.000025 |
| H | 5.576644 | -1.408293 | 0.000000 |
| C | 5.574287 | -0.309537 | -0.000009 |
| H | -5.576712 | 1.408321 | -0.000001 |
| C | -5.574303 | 0.309565 | -0.000009 |
| H | 6.848464 | 1.461318 | 0.000004 |
| C | 6.852255 | 0.362548 | 0.000010 |

| | | | |
|---|---|---|---|
| H | -6.848392 | -1.461348 | 0.000004 |
| C | -6.852237 | -0.362580 | 0.000009 |
| H | 8.067149 | -1.389590 | 0.000036 |
| C | 8.058647 | -0.290939 | 0.000031 |
| H | -8.067222 | 1.389495 | 0.000035 |
| C | -8.058662 | 0.290845 | 0.000030 |
| H | 9.324316 | 1.488983 | 0.000044 |
| C | 9.342242 | 0.391708 | 0.000049 |
| H | -9.324235 | -1.489142 | 0.000045 |
| C | -9.342221 | -0.391870 | 0.000049 |
| H | 10.591084 | -1.346176 | 0.000074 |
| H | 11.482353 | 0.299740 | 0.000079 |
| C | 10.540330 | -0.253059 | 0.000070 |
| H | -11.482337 | -0.300020 | 0.000083 |
| H | -10.591159 | 1.345946 | 0.000072 |
| C | -10.540344 | 0.252832 | 0.000073 |

C22H30 (Product of Diels-Alder reaction between 1,3-butadiene and octadecanonene)

| | | | |
|---|---|---|---|
| H | 0.939454 | 2.340273 | -1.974596 |
| H | 0.165656 | 0.272009 | 1.173960 |
| H | 0.026080 | 4.647057 | 1.275029 |
| H | 0.764877 | 2.507396 | 2.351165 |
| H | -0.014499 | 4.706728 | -1.137606 |
| H | -0.185010 | 0.332876 | -1.252436 |
| H | -0.947293 | 2.248182 | 1.992475 |
| H | -0.771391 | 2.628216 | -2.316816 |
| C | 0.016612 | 3.699878 | 0.722977 |
| C | 0.040044 | 2.417755 | 1.522734 |
| C | -0.012711 | 3.733435 | -0.632935 |
| C | -0.045998 | 2.492590 | -1.495114 |
| C | -0.427322 | 1.243095 | -0.674226 |
| C | 0.414680 | 1.207843 | 0.641229 |
| H | 2.327582 | 2.171365 | 0.016451 |
| C | 1.885834 | 1.215925 | 0.332978 |
| H | -2.334949 | 2.188677 | -0.006889 |
| C | -1.897492 | 1.244266 | -0.360362 |
| H | 2.258975 | -0.834664 | 0.751935 |
| C | 2.693268 | 0.121085 | 0.426424 |
| H | -2.275502 | -0.791744 | -0.840993 |
| C | -2.706256 | 0.153078 | -0.480715 |
| H | 4.544956 | 1.102213 | -0.194529 |
| C | 4.114126 | 0.144309 | 0.128221 |
| H | -4.550453 | 1.111763 | 0.195498 |
| C | -4.122448 | 0.164457 | -0.160536 |
| H | 4.506913 | -1.904206 | 0.557995 |
| C | 4.936980 | -0.946708 | 0.233760 |

| | | | |
|---|---|---|---|
| H | -4.514711 | -1.874639 | -0.632974 |
| C | -4.942577 | -0.927513 | -0.276955 |
| H | 6.782260 | 0.046058 | -0.380485 |
| C | 6.355427 | -0.913034 | -0.056038 |
| H | -6.779502 | 0.039363 | 0.400845 |
| C | -6.353988 | -0.909775 | 0.046753 |
| H | 6.764259 | -2.958803 | 0.378688 |
| C | 7.185156 | -1.997384 | 0.054042 |
| H | -6.757166 | -2.950588 | -0.415025 |
| C | -7.177461 | -1.999047 | -0.061740 |
| H | 9.021949 | -0.985365 | -0.558353 |
| C | 8.610717 | -1.950062 | -0.234976 |
| H | -9.005726 | -1.015696 | 0.619322 |
| C | -8.594540 | -1.970746 | 0.268420 |
| H | 10.505574 | -2.940681 | -0.351541 |
| H | 9.060743 | -3.997097 | 0.195462 |
| C | 9.440204 | -3.022052 | -0.124944 |
| H | -9.035961 | -4.015635 | -0.180441 |
| H | -10.474884 | -2.983394 | 0.425144 |
| C | -9.415961 | -3.049672 | 0.165791 |

Decanoic acid

| | | | |
|---|---|---|---|
| O | -4.948361 | 1.342597 | -0.000731 |
| O | -5.890651 | -0.729041 | -0.017629 |
| H | -6.682665 | -0.161116 | -0.022450 |
| C | -4.815839 | 0.128576 | -0.004071 |
| H | -3.516974 | -1.294029 | 0.895855 |
| H | -3.510364 | -1.312853 | -0.866177 |
| C | -3.507328 | -0.638128 | 0.007669 |
| H | -2.304362 | 0.925329 | -0.884875 |
| H | -2.307476 | 0.938863 | 0.880661 |
| C | -2.272305 | 0.271464 | 0.003068 |
| H | -0.937369 | -1.189510 | 0.901278 |
| H | -0.934245 | -1.200899 | -0.870891 |
| C | -0.961911 | -0.533552 | 0.010908 |
| H | 0.262641 | 1.019182 | -0.881438 |
| H | 0.263463 | 1.026113 | 0.890356 |
| C | 0.288978 | 0.361359 | 0.007053 |
| H | 1.629362 | -1.095061 | 0.898012 |
| H | 1.627247 | -1.102598 | -0.874041 |
| C | 1.603676 | -0.437174 | 0.009210 |
| H | 2.828592 | 1.116513 | -0.883144 |
| H | 2.834599 | 1.119274 | 0.888699 |
| C | 2.855989 | 0.456134 | 0.003736 |
| H | 4.198052 | -1.003686 | 0.887474 |
| H | 4.191324 | -1.006812 | -0.884571 |

| | | | |
|---|---|---|---|
| C | 4.170123 | -0.343095 | 0.000376 |
| H | 5.393340 | 1.208888 | -0.891433 |
| H | 5.401533 | 1.210074 | 0.878865 |
| C | 5.422997 | 0.548684 | -0.005949 |
| H | 7.612748 | 0.396879 | -0.015292 |
| H | 6.785709 | -0.909114 | -0.902400 |
| H | 6.793434 | -0.909042 | 0.879056 |
| C | 6.729537 | -0.261741 | -0.011445 |

Decanoate

| | | | |
|---|---|---|---|
| O | -4.836598 | 1.357615 | 0.353344 |
| O | -5.983821 | -0.510685 | -0.221336 |
| C | -4.957218 | 0.144955 | 0.056608 |
| H | -3.541900 | -1.150674 | 1.068652 |
| H | -3.722761 | -1.521436 | -0.641079 |
| C | -3.617649 | -0.693764 | 0.069807 |
| H | -2.370337 | 0.469512 | -1.248520 |
| H | -2.440681 | 1.041119 | 0.400371 |
| C | -2.360195 | 0.130981 | -0.202918 |
| H | -1.022904 | -0.917648 | 1.128724 |
| H | -0.982775 | -1.513336 | -0.520519 |
| C | -1.037809 | -0.592990 | 0.078602 |
| H | 0.199396 | 0.575722 | -1.250697 |
| H | 0.146136 | 1.182278 | 0.392658 |
| C | 0.207282 | 0.259380 | -0.198891 |
| H | 1.542415 | -0.762443 | 1.156322 |
| H | 1.590627 | -1.374649 | -0.486015 |
| C | 1.532739 | -0.449712 | 0.103577 |
| H | 2.765875 | 0.716701 | -1.231371 |
| H | 2.715670 | 1.330321 | 0.410002 |
| C | 2.774037 | 0.405216 | -0.178449 |
| H | 4.108153 | -0.614619 | 1.180124 |
| H | 4.157946 | -1.229205 | -0.461247 |
| C | 4.098541 | -0.303687 | 0.126945 |
| H | 5.330741 | 0.861585 | -1.207793 |
| H | 5.280572 | 1.475886 | 0.432157 |
| C | 5.339132 | 0.551542 | -0.155576 |
| H | 7.521651 | 0.470846 | -0.058626 |
| H | 6.760353 | -1.076612 | -0.444920 |
| H | 6.709788 | -0.457402 | 1.207272 |
| C | 6.657038 | -0.165486 | 0.153367 |

Graphene sheet (Figure 6), reactant

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.000000 | 0.705999 |
| C | 0.000000 | 0.000000 | -0.705999 |
| C | 0.000000 | 1.237229 | 1.420917 |

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.237229 | -1.420917 |
| C | 0.000000 | -1.237229 | -1.420917 |
| C | 0.000000 | -1.237229 | 1.420917 |
| C | 0.000000 | 0.000000 | 3.556305 |
| C | 0.000000 | 1.236310 | 2.842298 |
| C | 0.000000 | 2.466458 | 0.710849 |
| C | 0.000000 | 2.466458 | -0.710849 |
| C | 0.000000 | 1.236310 | -2.842298 |
| C | 0.000000 | 0.000000 | -3.556305 |
| C | 0.000000 | -1.236310 | -2.842298 |
| C | 0.000000 | -2.466458 | -0.710849 |
| C | 0.000000 | -2.466458 | 0.710849 |
| C | 0.000000 | -1.236310 | 2.842298 |
| C | 0.000000 | 0.000000 | 4.976723 |
| C | 0.000000 | 1.249223 | 5.663016 |
| C | 0.000000 | 2.438614 | 4.981172 |
| C | 0.000000 | 2.474637 | 3.553806 |
| C | 0.000000 | 3.684150 | 2.826743 |
| C | 0.000000 | 3.706570 | 1.434942 |
| C | 0.000000 | 4.934996 | 0.679710 |
| C | 0.000000 | 4.934996 | -0.679710 |
| C | 0.000000 | 3.706570 | -1.434942 |
| C | 0.000000 | 3.684150 | -2.826743 |
| C | 0.000000 | 2.474637 | -3.553806 |
| C | 0.000000 | 2.438614 | -4.981172 |
| C | 0.000000 | 1.249223 | -5.663016 |
| C | 0.000000 | 0.000000 | -4.976723 |
| C | 0.000000 | -1.249223 | -5.663016 |
| C | 0.000000 | -2.438614 | -4.981172 |
| C | 0.000000 | -2.474637 | -3.553806 |
| C | 0.000000 | -3.684150 | -2.826743 |
| C | 0.000000 | -3.706570 | -1.434942 |
| C | 0.000000 | -4.934996 | -0.679710 |
| C | 0.000000 | -4.934996 | 0.679710 |
| C | 0.000000 | -3.706570 | 1.434942 |
| C | 0.000000 | -3.684150 | 2.826743 |
| C | 0.000000 | -2.474637 | 3.553806 |
| C | 0.000000 | -2.438614 | 4.981172 |
| C | 0.000000 | -1.249223 | 5.663016 |
| H | 0.000000 | 1.244193 | 6.750415 |
| H | 0.000000 | 3.380469 | 5.524346 |
| H | 0.000000 | 4.624855 | 3.373527 |
| H | 0.000000 | 5.873642 | 1.228582 |
| H | 0.000000 | 5.873642 | -1.228582 |
| H | 0.000000 | 4.624855 | -3.373527 |
| H | 0.000000 | 3.380469 | -5.524346 |

| | | | |
|---|---|---|---|
| H | 0.000000 | 1.244193 | -6.750415 |
| H | 0.000000 | -1.244193 | -6.750415 |
| H | 0.000000 | -3.380469 | -5.524346 |
| H | 0.000000 | -4.624855 | -3.373527 |
| H | 0.000000 | -5.873642 | -1.228582 |
| H | 0.000000 | -5.873642 | 1.228582 |
| H | 0.000000 | -4.624855 | 3.373527 |
| H | 0.000000 | -3.380469 | 5.524346 |
| H | 0.000000 | -1.244193 | 6.750415 |

Graphene sheet (Figure 6), transition structure

| | | | |
|---|---|---|---|
| C | 0.405926 | 0.395551 | 0.273042 |
| C | -0.405927 | -0.395552 | -0.273065 |
| C | 1.394265 | -1.431084 | -0.210849 |
| C | -1.317659 | -1.449700 | -0.147297 |
| C | -1.394264 | 1.431083 | 0.210839 |
| C | 1.317659 | 1.449699 | 0.147282 |
| C | 3.428275 | 0.041098 | -0.013887 |
| C | 2.771651 | -1.262888 | -0.060706 |
| C | 0.773001 | -2.669272 | -0.133886 |
| C | -0.659116 | -2.696408 | -0.128263 |
| C | -2.728206 | -1.310272 | -0.043065 |
| C | -3.428275 | -0.041099 | 0.013881 |
| C | -2.771650 | 1.262888 | 0.060701 |
| C | -0.773001 | 2.669272 | 0.133881 |
| C | 0.659116 | 2.696408 | 0.128257 |
| C | 2.728206 | 1.310271 | 0.043057 |
| C | 4.847188 | 0.067415 | -0.004400 |
| C | 5.587662 | -1.155425 | 0.020141 |
| C | 4.974131 | -2.375909 | 0.047016 |
| C | 3.550893 | -2.482497 | 0.018424 |
| C | 2.910899 | -3.747390 | 0.037508 |
| C | 1.521110 | -3.877589 | -0.015985 |
| C | 0.763985 | -5.109632 | 0.054204 |
| C | -0.603785 | -5.123634 | 0.052676 |
| C | -1.385474 | -3.905633 | -0.015484 |
| C | -2.778895 | -3.802391 | 0.021975 |
| C | -3.453679 | -2.555756 | 0.006955 |
| C | -4.881414 | -2.508006 | 0.042798 |
| C | -5.544012 | -1.315679 | 0.023040 |
| C | -4.847189 | -0.067414 | 0.004401 |
| C | -5.587662 | 1.155425 | -0.020135 |
| C | -4.974131 | 2.375910 | -0.047008 |
| C | -3.550893 | 2.482498 | -0.018421 |
| C | -2.910899 | 3.747391 | -0.037500 |
| C | -1.521110 | 3.877589 | 0.015990 |

| | | | |
|---|---|---|---|
| C | -0.763984 | 5.109633 | -0.054194 |
| C | 0.603786 | 5.123635 | -0.052667 |
| C | 1.385474 | 3.905632 | 0.015485 |
| C | 2.778895 | 3.802391 | -0.021972 |
| C | 3.453678 | 2.555756 | -0.006957 |
| C | 4.881413 | 2.508006 | -0.042795 |
| C | 5.544012 | 1.315680 | -0.023037 |
| H | 6.673202 | -1.092654 | 0.025417 |
| H | 5.567356 | -3.287210 | 0.073965 |
| H | 3.534774 | -4.636140 | 0.109655 |
| H | 1.308045 | -6.049533 | 0.118281 |
| H | -1.132082 | -6.071994 | 0.115917 |
| H | -3.382884 | -4.705899 | 0.074488 |
| H | -5.432129 | -3.444716 | 0.074131 |
| H | -6.631063 | -1.295097 | 0.031273 |
| H | -6.673202 | 1.092655 | -0.025407 |
| H | -5.567356 | 3.287211 | -0.073952 |
| H | -3.534774 | 4.636142 | -0.109641 |
| H | -1.308044 | 6.049535 | -0.118264 |
| H | 1.132082 | 6.071994 | -0.115903 |
| H | 3.382884 | 4.705898 | -0.074480 |
| H | 5.432129 | 3.444716 | -0.074124 |
| H | 6.631062 | 1.295097 | -0.031266 |

Graphene sheet (Figure 6), product

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.673284 | 0.000000 |
| C | 0.000000 | -0.673284 | 0.000000 |
| C | 0.000000 | -1.526265 | 1.197170 |
| C | 0.000000 | -1.526265 | -1.197170 |
| C | 0.000000 | 1.526265 | -1.197170 |
| C | 0.000000 | 1.526265 | 1.197170 |
| C | 0.000000 | 0.000000 | 3.270740 |
| C | 0.000000 | -1.296963 | 2.595755 |
| C | 0.000000 | -2.836216 | 0.705581 |
| C | 0.000000 | -2.836216 | -0.705581 |
| C | 0.000000 | -1.296963 | -2.595755 |
| C | 0.000000 | 0.000000 | -3.270740 |
| C | 0.000000 | 1.296963 | -2.595755 |
| C | 0.000000 | 2.836216 | -0.705581 |
| C | 0.000000 | 2.836216 | 0.705581 |
| C | 0.000000 | 1.296963 | 2.595755 |
| C | 0.000000 | 0.000000 | 4.695689 |
| C | 0.000000 | -1.216882 | 5.438013 |
| C | 0.000000 | -2.425764 | 4.818368 |
| C | 0.000000 | -2.522446 | 3.396385 |
| C | 0.000000 | -3.823750 | 2.832859 |

| | | | |
|---|---|---|---|
| C | 0.000000 | -4.021041 | 1.453672 |
| C | 0.000000 | -5.252385 | 0.685948 |
| C | 0.000000 | -5.252385 | -0.685948 |
| C | 0.000000 | -4.021041 | -1.453672 |
| C | 0.000000 | -3.823750 | -2.832859 |
| C | 0.000000 | -2.522446 | -3.396385 |
| C | 0.000000 | -2.425764 | -4.818368 |
| C | 0.000000 | -1.216882 | -5.438013 |
| C | 0.000000 | 0.000000 | -4.695689 |
| C | 0.000000 | 1.216882 | -5.438013 |
| C | 0.000000 | 2.425764 | -4.818368 |
| C | 0.000000 | 2.522446 | -3.396385 |
| C | 0.000000 | 3.823750 | -2.832859 |
| C | 0.000000 | 4.021041 | -1.453672 |
| C | 0.000000 | 5.252385 | -0.685948 |
| C | 0.000000 | 5.252385 | 0.685948 |
| C | 0.000000 | 4.021041 | 1.453672 |
| C | 0.000000 | 3.823750 | 2.832859 |
| C | 0.000000 | 2.522446 | 3.396385 |
| C | 0.000000 | 2.425764 | 4.818368 |
| C | 0.000000 | 1.216882 | 5.438013 |
| H | 0.000000 | -1.153145 | 6.523038 |
| H | 0.000000 | -3.345288 | 5.397990 |
| H | 0.000000 | -4.670484 | 3.515815 |
| H | 0.000000 | -6.200163 | 1.218997 |
| H | 0.000000 | -6.200163 | -1.218997 |
| H | 0.000000 | -4.670484 | -3.515815 |
| H | 0.000000 | -3.345288 | -5.397990 |
| H | 0.000000 | -1.153145 | -6.523038 |
| H | 0.000000 | 1.153145 | -6.523038 |
| H | 0.000000 | 3.345288 | -5.397990 |
| H | 0.000000 | 4.670484 | -3.515815 |
| H | 0.000000 | 6.200163 | -1.218997 |
| H | 0.000000 | 6.200163 | 1.218997 |
| H | 0.000000 | 4.670484 | 3.515815 |
| H | 0.000000 | 3.345288 | 5.397990 |
| H | 0.000000 | 1.153145 | 6.523038 |