$comment

1-acene singlet

$end

$molecule

0 1

C 2.43475960 -0.69611929 0.00000000

C 2.43475960 0.69611929 0.00000000

C 1.22913336 -1.39226340 0.00000000

C 1.22913336 1.39226340 0.00000000

C 0.02350703 -0.69611925 0.00000000

C 0.02350703 0.69611924 0.00000000

H 3.38539202 -1.24490060 0.00000000

H 3.38539202 1.24490060 0.00000000

H 1.22913324 -2.48992283 0.00000000

H 1.22913324 2.48992283 0.00000000

H -0.92712527 -1.24490076 0.00000000

H -0.92712527 1.24490076 0.00000000

$end

$comment

1-acene triplet

$end

$molecule

0 3

C 2.44027355 -0.74548087 0.00000000

C 2.44028649 0.74543110 0.00000000

C 1.22918284 -1.43051828 0.00000000

C 1.22908392 1.43051827 0.00000000

C 0.01798014 -0.74543127 0.00000000

C 0.01799305 0.74548097 0.00000000

H 3.39386460 -1.28363960 0.00000000

H 3.39386709 1.28360144 0.00000000

H 1.22916782 -2.52851675 0.00000000

H 1.22909897 2.52851674 0.00000000

H -0.93560051 -1.28360148 0.00000000

H -0.93559799 1.28363971 0.00000000

$end

$comment

2-acene singlet

$end

$molecule

0 1

C 2.42398048 -0.70477355 0.00000000

C 2.42398047 0.70477355 0.00000000

C 1.23599344 -1.39775201 0.00000000

C 1.23599343 1.39775201 0.00000000

C 0.00000000 -0.71495553 0.00000000

C 0.00000000 0.71495554 0.00000000

C -1.23599344 -1.39775201 0.00000000

C -1.23599343 1.39775202 0.00000000

C -2.42398047 -0.70477355 0.00000000

C -2.42398047 0.70477356 0.00000000

H 1.22707212 -2.49677029 0.00000000

H 1.22707212 2.49677029 0.00000000

H -1.22707212 -2.49677029 0.00000000

H -1.22707212 2.49677030 0.00000000

H 3.37722463 1.24838306 0.00000000

H 3.37722465 -1.24838307 0.00000000

H -3.37722464 1.24838307 0.00000000

H -3.37722464 -1.24838307 0.00000000

$end

$comment

2-acene triplet

$end

$molecule

0 3

C 2.47345093 -0.68473334 0.00000000

C 2.47345104 0.68473333 0.00000000

C 1.23419909 -1.39383337 0.00000000

C 1.23419924 1.39383349 0.00000000

C 0.00000000 -0.71837193 0.00000000

C -0.00000000 0.71837196 0.00000000

C -1.23419917 -1.39383345 0.00000000

C -1.23419917 1.39383343 0.00000000

C -2.47345097 -0.68473339 0.00000000

C -2.47345099 0.68473327 0.00000000

H 1.23202477 -2.49206718 0.00000000

H 1.23202503 2.49206735 0.00000000

H -1.23202489 -2.49206726 0.00000000

H -1.23202490 2.49206727 0.00000000

H 3.41530541 1.24655255 0.00000000

H 3.41530524 -1.24655261 0.00000000

H -3.41530535 1.24655251 0.00000000

H -3.41530528 -1.24655264 0.00000000

$end

$comment

3-acene singlet

$end

$molecule

0 1

C 4.87112782 -0.70824352 0.00000000

C 4.87112789 0.70824341 0.00000000

C 3.68909893 -1.40166621 0.00000000

C 3.68909905 1.40166621 0.00000000

C 2.44507179 -0.72022074 0.00000000

C 2.44507184 0.72022079 0.00000000

C 1.22590001 -1.39916042 0.00000000

C 1.22590001 1.39916058 0.00000000

C 0.00672822 -0.72022075 0.00000000

C 0.00672818 0.72022080 0.00000000

C -1.23729894 -1.40166618 0.00000000

C -1.23729907 1.40166620 0.00000000

C -2.41932784 -0.70824352 0.00000000

C -2.41932791 0.70824341 0.00000000

H 3.68053801 -2.50053668 0.00000000

H 3.68053817 2.50053672 0.00000000

H 1.22590006 -2.49953292 0.00000000

H 1.22590006 2.49953313 0.00000000

H -1.22873804 -2.50053666 0.00000000

H -1.22873821 2.50053671 0.00000000

H 5.82568925 -1.24940384 0.00000000

H 5.82568938 1.24940367 0.00000000

H -3.37388926 -1.24940385 0.00000000

H -3.37388940 1.24940368 0.00000000

$end

$comment

3-acene triplet

$end

$molecule

0 3

C 4.91227840 -0.69182595 0.00000000

C 4.91227836 0.69182592 0.00000000

C 3.69300590 -1.39195515 0.00000000

C 3.69300582 1.39195507 0.00000000

C 2.46797152 -0.71718126 0.00000000

C 2.46797156 0.71718120 0.00000000

C 1.22590004 -1.39587120 0.00000000

C 1.22589996 1.39587120 0.00000000

C -0.01617156 -0.71718119 0.00000000

C -0.01617153 0.71718128 0.00000000

C -1.24120582 -1.39195505 0.00000000

C -1.24120592 1.39195515 0.00000000

C -2.46047836 -0.69182592 0.00000000

C -2.46047842 0.69182594 0.00000000

H 3.68772648 -2.49072437 0.00000000

H 3.68772639 2.49072425 0.00000000

H 1.22590006 -2.49585138 0.00000000

H 1.22590004 2.49585139 0.00000000

H -1.23592641 -2.49072423 0.00000000

H -1.23592653 2.49072435 0.00000000

H 5.85798365 -1.24749726 0.00000000

H 5.85798360 1.24749728 0.00000000

H -3.40618356 -1.24749731 0.00000000

H -3.40618367 1.24749727 0.00000000

$end

$comment

4-acene singlet

$end

$molecule

0 1

C 4.86849527 0.70960485 0.00000000

C 4.86849540 -0.70960454 0.00000000

C 3.68839532 -1.40304795 0.00000000

C 2.44124772 -0.72252508 0.00000000

C 2.44124761 0.72252500 0.00000000

C 3.68839508 1.40304803 0.00000000

C 1.22790726 -1.40160612 0.00000000

C 0.00000000 -0.72406617 0.00000000

C 0.00000000 0.72406597 0.00000000

C 1.22790714 1.40160582 0.00000000

C -1.22790726 -1.40160612 0.00000000

C -2.44124772 -0.72252508 0.00000000

C -2.44124761 0.72252500 0.00000000

C -1.22790714 1.40160582 0.00000000

C -3.68839532 -1.40304794 0.00000000

C -4.86849540 -0.70960454 0.00000000

C -4.86849527 0.70960485 0.00000000

C -3.68839508 1.40304803 0.00000000

H 5.82352308 1.24991683 0.00000000

H 5.82352331 -1.24991640 0.00000000

H 3.68033563 -2.50188311 0.00000000

H 3.68033524 2.50188313 0.00000000

H 1.22831614 -2.50181909 0.00000000

H 1.22831600 2.50181871 0.00000000

H -1.22831614 -2.50181908 0.00000000

H -1.22831600 2.50181873 0.00000000

H -3.68033563 -2.50188309 0.00000000

H -5.82352331 -1.24991640 0.00000000

H -5.82352308 1.24991683 0.00000000

H -3.68033524 2.50188313 0.00000000

$end

$comment

4-acene triplet

$end

$molecule

0 3

C 4.90183926 0.69707562 0.00000000

C 4.90183927 -0.69707562 0.00000000

C 3.69558126 -1.39384213 0.00000000

C 2.46826884 -0.71640447 0.00000000

C 2.46826883 0.71640446 0.00000000

C 3.69558125 1.39384213 0.00000000

C 1.22738211 -1.39651115 0.00000000

C -0.00000004 -0.72352973 0.00000000

C -0.00000004 0.72352972 0.00000000

C 1.22738211 1.39651114 0.00000000

C -1.22738203 -1.39651116 0.00000000

C -2.46826875 -0.71640451 0.00000000

C -2.46826875 0.71640452 0.00000000

C -1.22738203 1.39651115 0.00000000

C -3.69558133 -1.39384221 0.00000000

C -4.90183931 -0.69707568 0.00000000

C -4.90183931 0.69707569 0.00000000

C -3.69558132 1.39384222 0.00000000

H 5.85045966 1.24803201 0.00000000

H 5.85045969 -1.24803201 0.00000000

H 3.68868555 -2.49271337 0.00000000

H 3.68868554 2.49271337 0.00000000

H 1.22900478 -2.49663800 0.00000000

H 1.22900477 2.49663799 0.00000000

H -1.22900466 -2.49663802 0.00000000

H -1.22900465 2.49663801 0.00000000

H -3.68868565 -2.49271349 0.00000000

H -5.85045970 -1.24803210 0.00000000

H -5.85045971 1.24803212 0.00000000

H -3.68868564 2.49271350 0.00000000

$end

$comment

5-acene singlet

$end

$molecule

0 1

C 7.31114719 -0.70969377 0.00000000

C 7.31114717 0.70969382 0.00000000

C 6.13089932 -1.40330814 0.00000000

C 6.13089928 1.40330815 0.00000000

C 4.88348555 -0.72321752 0.00000000

C 4.88348554 0.72321750 0.00000000

C 3.67108847 -1.40236559 0.00000000

C 3.67108848 1.40236555 0.00000000

C 2.44037950 -0.72588296 0.00000000

C 2.44037951 0.72588295 0.00000000

C 1.21786109 -1.40357867 0.00000000

C 1.21786110 1.40357862 0.00000000

C -0.00465730 -0.72588296 0.00000000

C -0.00465729 0.72588293 0.00000000

C -1.23536625 -1.40236559 0.00000000

C -1.23536625 1.40236556 0.00000000

C -2.44776332 -0.72321750 0.00000000

C -2.44776331 0.72321751 0.00000000

C -3.69517707 -1.40330814 0.00000000

C -3.69517707 1.40330816 0.00000000

C -4.87542495 -0.70969378 0.00000000

C -4.87542495 0.70969382 0.00000000

H 8.26608569 -1.25012563 0.00000000

H 8.26608565 1.25012569 0.00000000

H 6.12322356 -2.50212615 0.00000000

H 6.12322351 2.50212616 0.00000000

H 3.67209401 -2.50254092 0.00000000

H 3.67209403 2.50254089 0.00000000

H 1.21786108 -2.50362011 0.00000000

H 1.21786109 2.50362007 0.00000000

H -1.23637179 -2.50254092 0.00000000

H -1.23637179 2.50254090 0.00000000

H -3.68750131 -2.50212615 0.00000000

H -3.68750130 2.50212618 0.00000000

H -5.83036345 -1.25012565 0.00000000

H -5.83036344 1.25012567 0.00000000

$end

$comment

5-acene triplet

$end

$molecule

0 3

C 7.33746248 -0.70073359 0.00000000

C 7.33746248 0.70073359 0.00000000

C 6.13948944 -1.39605758 0.00000000

C 6.13948944 1.39605757 0.00000000

C 4.90790596 -0.71710729 0.00000000

C 4.90790597 0.71710728 0.00000000

C 3.67213820 -1.39703655 0.00000000

C 3.67213821 1.39703654 0.00000000

C 2.45081901 -0.72398235 0.00000000

C 2.45081902 0.72398236 0.00000000

C 1.21786124 -1.39901528 0.00000000

C 1.21786124 1.39901530 0.00000000

C -0.01509677 -0.72398239 0.00000000

C -0.01509677 0.72398240 0.00000000

C -1.23641600 -1.39703661 0.00000000

C -1.23641600 1.39703661 0.00000000

C -2.47218374 -0.71710735 0.00000000

C -2.47218375 0.71710736 0.00000000

C -3.70376726 -1.39605776 0.00000000

C -3.70376726 1.39605776 0.00000000

C -4.90174031 -0.70073375 0.00000000

C -4.90174032 0.70073374 0.00000000

H 8.28806419 -1.24842723 0.00000000

H 8.28806419 1.24842723 0.00000000

H 6.13189477 -2.49493576 0.00000000

H 6.13189477 2.49493575 0.00000000

H 3.67356978 -2.49726203 0.00000000

H 3.67356979 2.49726202 0.00000000

H 1.21786125 -2.49908913 0.00000000

H 1.21786125 2.49908915 0.00000000

H -1.23784752 -2.49726209 0.00000000

H -1.23784752 2.49726210 0.00000000

H -3.69617263 -2.49493597 0.00000000

H -3.69617264 2.49493597 0.00000000

H -5.85234211 -1.24842740 0.00000000

H -5.85234212 1.24842738 0.00000000

$end

$comment

6-acene singlet

$end

$molecule

0 1

C 7.31933057 -0.70921399 0.00000000

C 7.31933046 0.70921438 0.00000000

C 6.13800170 -1.40287706 0.00000000

C 6.13800148 1.40287727 0.00000000

C 4.89164682 -0.72295763 0.00000000

C 4.89164674 0.72295768 0.00000000

C 3.67785671 -1.40217524 0.00000000

C 3.67785656 1.40217509 0.00000000

C 2.44759589 -0.72627305 0.00000000

C 2.44759584 0.72627281 0.00000000

C 1.22529256 -1.40384887 0.00000000

C 1.22529251 1.40384853 0.00000000

C -0.00000001 -0.72740813 0.00000000

C -0.00000000 0.72740782 0.00000000

C -1.22529257 -1.40384886 0.00000000

C -1.22529252 1.40384854 0.00000000

C -2.44759590 -0.72627304 0.00000000

C -2.44759584 0.72627282 0.00000000

C -3.67785671 -1.40217522 0.00000000

C -3.67785657 1.40217510 0.00000000

C -4.89164682 -0.72295761 0.00000000

C -4.89164674 0.72295769 0.00000000

C -6.13800168 -1.40287705 0.00000000

C -6.13800148 1.40287727 0.00000000

C -7.31933056 -0.70921400 0.00000000

C -7.31933046 0.70921437 0.00000000

H 8.27409532 -1.24986004 0.00000000

H 8.27409515 1.24986056 0.00000000

H 6.13003265 -2.50170465 0.00000000

H 6.13003228 2.50170484 0.00000000

H 3.67874047 -2.50236185 0.00000000

H 3.67874019 2.50236169 0.00000000

H 1.22568039 -2.50388303 0.00000000

H 1.22568033 2.50388267 0.00000000

H -1.22568041 -2.50388303 0.00000000

H -1.22568033 2.50388268 0.00000000

H -3.67874047 -2.50236183 0.00000000

H -3.67874020 2.50236170 0.00000000

H -6.13003262 -2.50170464 0.00000000

H -6.13003228 2.50170485 0.00000000

H -8.27409531 -1.24986006 0.00000000

H -8.27409515 1.24986055 0.00000000

$end

$comment

6-acene triplet

$end

$molecule

0 3

C 7.33906748 -0.70324463 0.00000000

C 7.33906747 0.70324462 0.00000000

C 6.14642981 -1.39787415 0.00000000

C 6.14642981 1.39787417 0.00000000

C 4.91101817 -0.71822698 0.00000000

C 4.91101816 0.71822698 0.00000000

C 3.68054646 -1.39791931 0.00000000

C 3.68054646 1.39791931 0.00000000

C 2.46010370 -0.72386755 0.00000000

C 2.46010370 0.72386755 0.00000000

C 1.22562047 -1.39986582 0.00000000

C 1.22562047 1.39986581 0.00000000

C -0.00000007 -0.72602238 0.00000000

C -0.00000007 0.72602239 0.00000000

C -1.22562034 -1.39986584 0.00000000

C -1.22562034 1.39986584 0.00000000

C -2.46010367 -0.72386759 0.00000000

C -2.46010367 0.72386759 0.00000000

C -3.68054646 -1.39791941 0.00000000

C -3.68054646 1.39791941 0.00000000

C -4.91101805 -0.71822708 0.00000000

C -4.91101806 0.71822710 0.00000000

C -6.14642989 -1.39787435 0.00000000

C -6.14642990 1.39787436 0.00000000

C -7.33906752 -0.70324478 0.00000000

C -7.33906751 0.70324477 0.00000000

H 8.29097226 -1.24877040 0.00000000

H 8.29097226 1.24877039 0.00000000

H 6.13858400 -2.49674029 0.00000000

H 6.13858401 2.49674030 0.00000000

H 3.68163886 -2.49816873 0.00000000

H 3.68163887 2.49816873 0.00000000

H 1.22600709 -2.49997894 0.00000000

H 1.22600709 2.49997893 0.00000000

H -1.22600688 -2.49997894 0.00000000

H -1.22600689 2.49997895 0.00000000

H -3.68163888 -2.49816884 0.00000000

H -3.68163888 2.49816884 0.00000000

H -6.13858414 -2.49674053 0.00000000

H -6.13858417 2.49674054 0.00000000

H -8.29097237 -1.24877057 0.00000000

H -8.29097237 1.24877056 0.00000000

$end

$comment

7-acene singlet

$end

$molecule

0 1

C 9.76677107 -0.70863710 0.00000000

C 9.76677088 0.70863779 0.00000000

C 8.58434667 -1.40225493 0.00000000

C 8.58434637 1.40225528 0.00000000

C 7.33921267 -0.72237910 0.00000000

C 7.33921259 0.72237930 0.00000000

C 6.12338964 -1.40158137 0.00000000

C 6.12338951 1.40158131 0.00000000

C 4.89487460 -0.72601404 0.00000000

C 4.89487458 0.72601383 0.00000000

C 3.67051665 -1.40342565 0.00000000

C 3.67051659 1.40342532 0.00000000

C 2.44592681 -0.72779453 0.00000000

C 2.44592679 0.72779419 0.00000000

C 1.22065889 -1.40379781 0.00000000

C 1.22065894 1.40379741 0.00000000

C -0.00464010 -0.72779072 0.00000000

C -0.00464002 0.72779043 0.00000000

C -1.22921533 -1.40341091 0.00000000

C -1.22921524 1.40341068 0.00000000

C -2.45358320 -0.72598977 0.00000000

C -2.45358317 0.72598959 0.00000000

C -3.68206771 -1.40162664 0.00000000

C -3.68206764 1.40162658 0.00000000

C -4.89794841 -0.72234842 0.00000000

C -4.89794840 0.72234850 0.00000000

C -6.14293298 -1.40231167 0.00000000

C -6.14293278 1.40231186 0.00000000

C -7.32543939 -0.70858134 0.00000000

C -7.32543928 0.70858179 0.00000000

H 10.72128335 -1.24968219 0.00000000

H 10.72128305 1.24968303 0.00000000

H 8.57568311 -2.50110775 0.00000000

H 8.57568260 2.50110806 0.00000000

H 6.12427888 -2.50180883 0.00000000

H 6.12427851 2.50180877 0.00000000

H 3.67086442 -2.50346645 0.00000000

H 3.67086432 2.50346617 0.00000000

H 1.22059604 -2.50382917 0.00000000

H 1.22059610 2.50382881 0.00000000

H -1.22968668 -2.50345596 0.00000000

H -1.22968658 2.50345579 0.00000000

H -3.68281426 -2.50182065 0.00000000

H -3.68281402 2.50182062 0.00000000

H -6.13475253 -2.50114164 0.00000000

H -6.13475214 2.50114181 0.00000000

H -8.27998818 -1.24957620 0.00000000

H -8.27998800 1.24957674 0.00000000

$end

$comment

7-acene triplet

$end

$molecule

0 3

C 9.78037499 -0.70501778 0.00000000

C 9.78037501 0.70501791 0.00000000

C 8.59131832 -1.39919571 0.00000000

C 8.59131833 1.39919582 0.00000000

C 7.35291774 -0.71926674 0.00000000

C 7.35291773 0.71926686 0.00000000

C 6.12674807 -1.39883212 0.00000000

C 6.12674805 1.39883223 0.00000000

C 4.90527227 -0.72401792 0.00000000

C 4.90527228 0.72401799 0.00000000

C 3.67170129 -1.40059409 0.00000000

C 3.67170128 1.40059413 0.00000000

C 2.44978621 -0.72640119 0.00000000

C 2.44978621 0.72640121 0.00000000

C 1.22063715 -1.40082401 0.00000000

C 1.22063714 1.40082404 0.00000000

C -0.00847828 -0.72640189 0.00000000

C -0.00847829 0.72640191 0.00000000

C -1.23043862 -1.40057116 0.00000000

C -1.23043864 1.40057114 0.00000000

C -2.46397222 -0.72400192 0.00000000

C -2.46397223 0.72400188 0.00000000

C -3.68542591 -1.39887926 0.00000000

C -3.68542592 1.39887924 0.00000000

C -4.91164185 -0.71924092 0.00000000

C -4.91164185 0.71924089 0.00000000

C -6.14990072 -1.39926628 0.00000000

C -6.14990072 1.39926626 0.00000000

C -7.33906694 -0.70496702 0.00000000

C -7.33906695 0.70496701 0.00000000

H 10.73319827 -1.24894890 0.00000000

H 10.73319828 1.24894902 0.00000000

H 8.58267977 -2.49807023 0.00000000

H 8.58267978 2.49807034 0.00000000

H 6.12789952 -2.49910313 0.00000000

H 6.12789947 2.49910324 0.00000000

H 3.67219724 -2.50071015 0.00000000

H 3.67219720 2.50071020 0.00000000

H 1.22061741 -2.50094942 0.00000000

H 1.22061740 2.50094944 0.00000000

H -1.23099939 -2.50069133 0.00000000

H -1.23099943 2.50069131 0.00000000

H -3.68640543 -2.49911336 0.00000000

H -3.68640543 2.49911334 0.00000000

H -6.14175083 -2.49811589 0.00000000

H -6.14175082 2.49811586 0.00000000

H -8.29193416 -1.24884166 0.00000000

H -8.29193417 1.24884165 0.00000000

$end

$comment

8-acene singlet

$end

$molecule

0 1

C 9.77260935 -0.70813249 0.00000000

C 9.77260944 0.70813206 0.00000000

C 8.58934436 -1.40191348 0.00000000

C 8.58934452 1.40191319 0.00000000

C 7.34532808 -0.72184489 0.00000000

C 7.34532816 0.72184473 0.00000000

C 6.12790040 -1.40116398 0.00000000

C 6.12790054 1.40116397 0.00000000

C 4.90109755 -0.72556090 0.00000000

C 4.90109761 0.72556100 0.00000000

C 3.67451333 -1.40284356 0.00000000

C 3.67451343 1.40284378 0.00000000

C 2.45182965 -0.72765555 0.00000000

C 2.45182968 0.72765583 0.00000000

C 1.22450804 -1.40324845 0.00000000

C 1.22450807 1.40324879 0.00000000

C 0.00000005 -0.72830371 0.00000000

C 0.00000006 0.72830404 0.00000000

C -1.22450795 -1.40324845 0.00000000

C -1.22450797 1.40324880 0.00000000

C -2.45182957 -0.72765556 0.00000000

C -2.45182960 0.72765584 0.00000000

C -3.67451329 -1.40284356 0.00000000

C -3.67451339 1.40284379 0.00000000

C -4.90109754 -0.72556090 0.00000000

C -4.90109760 0.72556101 0.00000000

C -6.12790042 -1.40116400 0.00000000

C -6.12790057 1.40116399 0.00000000

C -7.34532813 -0.72184490 0.00000000

C -7.34532821 0.72184474 0.00000000

C -8.58934443 -1.40191349 0.00000000

C -8.58934460 1.40191319 0.00000000

C -9.77260945 -0.70813251 0.00000000

C -9.77260953 0.70813205 0.00000000

H 10.72690391 -1.24957387 0.00000000

H 10.72690406 1.24957332 0.00000000

H 8.58129254 -2.50074445 0.00000000

H 8.58129284 2.50074416 0.00000000

H 6.12881821 -2.50137087 0.00000000

H 6.12881847 2.50137087 0.00000000

H 3.67515031 -2.50291630 0.00000000

H 3.67515051 2.50291653 0.00000000

H 1.22470470 -2.50331663 0.00000000

H 1.22470476 2.50331700 0.00000000

H -1.22470463 -2.50331664 0.00000000

H -1.22470468 2.50331701 0.00000000

H -3.67515028 -2.50291630 0.00000000

H -3.67515046 2.50291655 0.00000000

H -6.12881822 -2.50137089 0.00000000

H -6.12881849 2.50137090 0.00000000

H -8.58129261 -2.50074446 0.00000000

H -8.58129290 2.50074418 0.00000000

H -10.72690400 -1.24957389 0.00000000

H -10.72690414 1.24957333 0.00000000

$end

$comment

8-acene triplet

$end

$molecule

0 3

C 9.78174855 -0.70606741 0.00000000

C 9.78174855 0.70606739 0.00000000

C 8.59475307 -1.40017757 0.00000000

C 8.59475306 1.40017755 0.00000000

C 7.35444274 -0.72010286 0.00000000

C 7.35444274 0.72010285 0.00000000

C 6.13127981 -1.39955100 0.00000000

C 6.13127981 1.39955099 0.00000000

C 4.90833302 -0.72433059 0.00000000

C 4.90833303 0.72433058 0.00000000

C 3.67649709 -1.40114363 0.00000000

C 3.67649710 1.40114364 0.00000000

C 2.45565207 -0.72647414 0.00000000

C 2.45565208 0.72647415 0.00000000

C 1.22521022 -1.40140908 0.00000000

C 1.22521022 1.40140911 0.00000000

C 0.00000021 -0.72701301 0.00000000

C 0.00000021 0.72701303 0.00000000

C -1.22521007 -1.40140908 0.00000000

C -1.22521007 1.40140910 0.00000000

C -2.45565180 -0.72647415 0.00000000

C -2.45565179 0.72647417 0.00000000

C -3.67649696 -1.40114361 0.00000000

C -3.67649697 1.40114364 0.00000000

C -4.90833308 -0.72433058 0.00000000

C -4.90833309 0.72433060 0.00000000

C -6.13127982 -1.39955094 0.00000000

C -6.13127984 1.39955096 0.00000000

C -7.35444298 -0.72010279 0.00000000

C -7.35444299 0.72010279 0.00000000

C -8.59475318 -1.40017751 0.00000000

C -8.59475321 1.40017750 0.00000000

C -9.78174883 -0.70606736 0.00000000

C -9.78174884 0.70606732 0.00000000

H 10.73502780 -1.24928857 0.00000000

H 10.73502780 1.24928855 0.00000000

H 8.58690810 -2.49901869 0.00000000

H 8.58690810 2.49901867 0.00000000

H 6.13222689 -2.49978233 0.00000000

H 6.13222690 2.49978231 0.00000000

H 3.67674907 -2.50125952 0.00000000

H 3.67674909 2.50125952 0.00000000

H 1.22514296 -2.50153020 0.00000000

H 1.22514297 2.50153022 0.00000000

H -1.22514272 -2.50153021 0.00000000

H -1.22514272 2.50153023 0.00000000

H -3.67674893 -2.50125952 0.00000000

H -3.67674895 2.50125954 0.00000000

H -6.13222688 -2.49978227 0.00000000

H -6.13222690 2.49978228 0.00000000

H -8.58690823 -2.49901863 0.00000000

H -8.58690828 2.49901861 0.00000000

H -10.73502807 -1.24928855 0.00000000

H -10.73502809 1.24928850 0.00000000

$end

$comment

9-acene singlet

$end

$molecule

0 1

C 12.22037878 -0.70810588 0.00000000

C 12.22037912 0.70810380 0.00000000

C 11.03706770 -1.40175543 0.00000000

C 11.03706833 1.40175390 0.00000000

C 9.79310639 -0.72175547 0.00000000

C 9.79310667 0.72175445 0.00000000

C 8.57512085 -1.40090313 0.00000000

C 8.57512139 1.40090271 0.00000000

C 7.34906205 -0.72519775 0.00000000

C 7.34906230 0.72519778 0.00000000

C 6.12133002 -1.40254417 0.00000000

C 6.12133039 1.40254464 0.00000000

C 4.90004563 -0.72728710 0.00000000

C 4.90004578 0.72728781 0.00000000

C 3.67089394 -1.40281350 0.00000000

C 3.67089413 1.40281450 0.00000000

C 2.44821785 -0.72818558 0.00000000

C 2.44821790 0.72818667 0.00000000

C 1.22181585 -1.40279138 0.00000000

C 1.22181586 1.40279258 0.00000000

C -0.00453272 -0.72821629 0.00000000

C -0.00453273 0.72821739 0.00000000

C -1.22724482 -1.40278473 0.00000000

C -1.22724497 1.40278583 0.00000000

C -2.45642325 -0.72734722 0.00000000

C -2.45642339 0.72734803 0.00000000

C -3.67764995 -1.40250706 0.00000000

C -3.67765031 1.40250766 0.00000000

C -4.90545171 -0.72525336 0.00000000

C -4.90545194 0.72525352 0.00000000

C -6.13141789 -1.40094871 0.00000000

C -6.13141834 1.40094852 0.00000000

C -7.34944252 -0.72161408 0.00000000

C -7.34944276 0.72161347 0.00000000

C -8.59309864 -1.40177458 0.00000000

C -8.59309917 1.40177353 0.00000000

C -9.77658187 -0.70798043 0.00000000

C -9.77658213 0.70797892 0.00000000

H 13.17478272 -1.24936969 0.00000000

H 13.17478331 1.24936721 0.00000000

H 11.02831703 -2.50060301 0.00000000

H 11.02831812 2.50060150 0.00000000

H 8.57546468 -2.50112800 0.00000000

H 8.57546568 2.50112763 0.00000000

H 6.12145074 -2.50261576 0.00000000

H 6.12145141 2.50261629 0.00000000

H 3.67104243 -2.50290020 0.00000000

H 3.67104279 2.50290126 0.00000000

H 1.22192911 -2.50289121 0.00000000

H 1.22192912 2.50289248 0.00000000

H -1.22734411 -2.50287896 0.00000000

H -1.22734439 2.50288014 0.00000000

H -3.67815611 -2.50259468 0.00000000

H -3.67815672 2.50259533 0.00000000

H -6.13225041 -2.50116025 0.00000000

H -6.13225118 2.50116008 0.00000000

H -8.58500599 -2.50060439 0.00000000

H -8.58500693 2.50060334 0.00000000

H -10.73082227 -1.24951218 0.00000000

H -10.73082274 1.24951032 0.00000000

$end

$comment

9-acene triplet

$end

$molecule

0 3

C 12.22660613 -0.70691321 0.00000000

C 12.22660613 0.70691302 0.00000000

C 11.04113026 -1.40073931 0.00000000

C 11.04113025 1.40073908 0.00000000

C 9.79926773 -0.72079467 0.00000000

C 9.79926772 0.72079442 0.00000000

C 8.57807435 -1.40001978 0.00000000

C 8.57807436 1.40001956 0.00000000

C 7.35391634 -0.72452418 0.00000000

C 7.35391634 0.72452401 0.00000000

C 6.12361543 -1.40166496 0.00000000

C 6.12361541 1.40166476 0.00000000

C 4.90280275 -0.72651963 0.00000000

C 4.90280274 0.72651941 0.00000000

C 3.67230567 -1.40178666 0.00000000

C 3.67230567 1.40178644 0.00000000

C 2.44905487 -0.72711528 0.00000000

C 2.44905486 0.72711507 0.00000000

C 1.22180306 -1.40167292 0.00000000

C 1.22180305 1.40167270 0.00000000

C -0.00533973 -0.72715012 0.00000000

C -0.00533973 0.72714988 0.00000000

C -1.22867507 -1.40175257 0.00000000

C -1.22867504 1.40175235 0.00000000

C -2.45917197 -0.72658450 0.00000000

C -2.45917194 0.72658433 0.00000000

C -3.67994580 -1.40162611 0.00000000

C -3.67994572 1.40162599 0.00000000

C -4.91030889 -0.72457326 0.00000000

C -4.91030883 0.72457321 0.00000000

C -6.13438195 -1.40008204 0.00000000

C -6.13438183 1.40008211 0.00000000

C -7.35559468 -0.72062112 0.00000000

C -7.35559462 0.72062130 0.00000000

C -8.59714820 -1.40076879 0.00000000

C -8.59714809 1.40076906 0.00000000

C -9.78281738 -0.70678775 0.00000000

C -9.78281732 0.70678811 0.00000000

H 13.18049393 -1.24906065 0.00000000

H 13.18049392 1.24906047 0.00000000

H 11.03229430 -2.49959662 0.00000000

H 11.03229425 2.49959637 0.00000000

H 8.57840804 -2.50025774 0.00000000

H 8.57840809 2.50025754 0.00000000

H 6.12364370 -2.50175105 0.00000000

H 6.12364366 2.50175085 0.00000000

H 3.67237381 -2.50190108 0.00000000

H 3.67237382 2.50190085 0.00000000

H 1.22194521 -2.50180799 0.00000000

H 1.22194518 2.50180777 0.00000000

H -1.22866164 -2.50187476 0.00000000

H -1.22866159 2.50187453 0.00000000

H -3.68036906 -2.50172724 0.00000000

H -3.68036893 2.50172711 0.00000000

H -6.13519023 -2.50029906 0.00000000

H -6.13518999 2.50029911 0.00000000

H -8.58898094 -2.49960374 0.00000000

H -8.58898075 2.49960400 0.00000000

H -10.73654654 -1.24919203 0.00000000

H -10.73654644 1.24919247 0.00000000

$end

$comment

10-acene singlet

$end

$molecule

0 1

C 12.22378638 -0.70795687 0.00000000

C 12.22378719 0.70795388 0.00000000

C 11.04032854 -1.40179688 0.00000000

C 11.04033004 1.40179529 0.00000000

C 9.79671779 -0.72157235 0.00000000

C 9.79671844 0.72157179 0.00000000

C 8.57859931 -1.40092216 0.00000000

C 8.57860015 1.40092282 0.00000000

C 7.35291911 -0.72513585 0.00000000

C 7.35291928 0.72513676 0.00000000

C 6.12463410 -1.40240705 0.00000000

C 6.12463413 1.40240851 0.00000000

C 4.90423003 -0.72713187 0.00000000

C 4.90422979 0.72713314 0.00000000

C 3.67388584 -1.40258251 0.00000000

C 3.67388544 1.40258358 0.00000000

C 2.45270789 -0.72799667 0.00000000

C 2.45270761 0.72799766 0.00000000

C 1.22450132 -1.40246359 0.00000000

C 1.22450109 1.40246410 0.00000000

C 0.00000009 -0.72822430 0.00000000

C 0.00000007 0.72822508 0.00000000

C -1.22450116 -1.40246359 0.00000000

C -1.22450094 1.40246410 0.00000000

C -2.45270773 -0.72799666 0.00000000

C -2.45270745 0.72799767 0.00000000

C -3.67388565 -1.40258250 0.00000000

C -3.67388527 1.40258359 0.00000000

C -4.90422983 -0.72713185 0.00000000

C -4.90422960 0.72713315 0.00000000

C -6.12463390 -1.40240705 0.00000000

C -6.12463394 1.40240851 0.00000000

C -7.35291891 -0.72513586 0.00000000

C -7.35291909 0.72513675 0.00000000

C -8.57859911 -1.40092217 0.00000000

C -8.57859997 1.40092280 0.00000000

C -9.79671760 -0.72157237 0.00000000

C -9.79671825 0.72157177 0.00000000

C -11.04032835 -1.40179691 0.00000000

C -11.04032985 1.40179526 0.00000000

C -12.22378619 -0.70795690 0.00000000

C -12.22378700 0.70795384 0.00000000

H 13.17797516 -1.24962867 0.00000000

H 13.17797654 1.24962472 0.00000000

H 11.03243487 -2.50063110 0.00000000

H 11.03243738 2.50062967 0.00000000

H 8.57955195 -2.50113859 0.00000000

H 8.57955342 2.50113950 0.00000000

H 6.12508969 -2.50250544 0.00000000

H 6.12509003 2.50250709 0.00000000

H 3.67389764 -2.50269330 0.00000000

H 3.67389732 2.50269435 0.00000000

H 1.22445150 -2.50259005 0.00000000

H 1.22445127 2.50259034 0.00000000

H -1.22445134 -2.50259005 0.00000000

H -1.22445111 2.50259035 0.00000000

H -3.67389745 -2.50269329 0.00000000

H -3.67389715 2.50269435 0.00000000

H -6.12508948 -2.50250543 0.00000000

H -6.12508985 2.50250708 0.00000000

H -8.57955174 -2.50113859 0.00000000

H -8.57955324 2.50113948 0.00000000

H -11.03243467 -2.50063112 0.00000000

H -11.03243720 2.50062964 0.00000000

H -13.17797497 -1.24962870 0.00000000

H -13.17797635 1.24962469 0.00000000

$end

$comment

10-acene triplet

$end

$molecule

0 3

C 12.22844482 -0.70714593 0.00000000

C 12.22844410 0.70714897 0.00000000

C 11.04349615 -1.40113939 0.00000000

C 11.04349477 1.40114121 0.00000000

C 9.80124219 -0.72099574 0.00000000

C 9.80124153 0.72099649 0.00000000

C 8.58113059 -1.40040528 0.00000000

C 8.58112956 1.40040493 0.00000000

C 7.35634244 -0.72485514 0.00000000

C 7.35634204 0.72485418 0.00000000

C 6.12693630 -1.40194473 0.00000000

C 6.12693580 1.40194302 0.00000000

C 4.90596383 -0.72675523 0.00000000

C 4.90596373 0.72675341 0.00000000

C 3.67578924 -1.40208554 0.00000000

C 3.67578926 1.40208342 0.00000000

C 2.45319069 -0.72719665 0.00000000

C 2.45319082 0.72719480 0.00000000

C 1.22527857 -1.40190967 0.00000000

C 1.22527897 1.40190799 0.00000000

C 0.00000029 -0.72718286 0.00000000

C 0.00000057 0.72718162 0.00000000

C -1.22527861 -1.40190924 0.00000000

C -1.22527806 1.40190842 0.00000000

C -2.45319028 -0.72719593 0.00000000

C -2.45318999 0.72719557 0.00000000

C -3.67578919 -1.40208442 0.00000000

C -3.67578872 1.40208452 0.00000000

C -4.90596379 -0.72675415 0.00000000

C -4.90596358 0.72675454 0.00000000

C -6.12693611 -1.40194348 0.00000000

C -6.12693586 1.40194425 0.00000000

C -7.35634251 -0.72485421 0.00000000

C -7.35634245 0.72485506 0.00000000

C -8.58113019 -1.40040457 0.00000000

C -8.58113019 1.40040557 0.00000000

C -9.80124225 -0.72099561 0.00000000

C -9.80124231 0.72099650 0.00000000

C -11.04349575 -1.40113985 0.00000000

C -11.04349590 1.40114066 0.00000000

C -12.22844499 -0.70714706 0.00000000

C -12.22844508 0.70714772 0.00000000

H 13.18221535 -1.24954413 0.00000000

H 13.18221408 1.24954809 0.00000000

H 11.03574635 -2.49997557 0.00000000

H 11.03574397 2.49997730 0.00000000

H 8.58219261 -2.50062419 0.00000000

H 8.58219086 2.50062367 0.00000000

H 6.12728033 -2.50204698 0.00000000

H 6.12727944 2.50204506 0.00000000

H 3.67556115 -2.50220080 0.00000000

H 3.67556113 2.50219850 0.00000000

H 1.22510803 -2.50204137 0.00000000

H 1.22510867 2.50203958 0.00000000

H -1.22510833 -2.50204092 0.00000000

H -1.22510742 2.50204009 0.00000000

H -3.67556122 -2.50219961 0.00000000

H -3.67556044 2.50219977 0.00000000

H -6.12728004 -2.50204561 0.00000000

H -6.12727957 2.50204647 0.00000000

H -8.58219190 -2.50062338 0.00000000

H -8.58219188 2.50062446 0.00000000

H -11.03574542 -2.49997599 0.00000000

H -11.03574568 2.49997684 0.00000000

H -13.18221520 -1.24954585 0.00000000

H -13.18221534 1.24954639 0.00000000

$end

$comment

11-acene singlet

$end

$molecule

0 1

C 14.66843295 -0.70814150 0.00000000

C 14.66843301 0.70814093 0.00000000

C 13.48537174 -1.40183316 0.00000000

C 13.48537191 1.40183268 0.00000000

C 12.24128697 -0.72171469 0.00000000

C 12.24128711 0.72171449 0.00000000

C 11.02356031 -1.40090024 0.00000000

C 11.02356057 1.40090016 0.00000000

C 9.79764726 -0.72503702 0.00000000

C 9.79764744 0.72503712 0.00000000

C 8.56956211 -1.40242682 0.00000000

C 8.56956238 1.40242719 0.00000000

C 7.34922561 -0.72693373 0.00000000

C 7.34922571 0.72693424 0.00000000

C 6.11861637 -1.40251126 0.00000000

C 6.11861651 1.40251200 0.00000000

C 4.89818851 -0.72775318 0.00000000

C 4.89818855 0.72775394 0.00000000

C 3.66889327 -1.40224559 0.00000000

C 3.66889332 1.40224648 0.00000000

C 2.44595244 -0.72802860 0.00000000

C 2.44595245 0.72802948 0.00000000

C 1.21959119 -1.40209821 0.00000000

C 1.21959118 1.40209912 0.00000000

C -0.00663443 -0.72804740 0.00000000

C -0.00663442 0.72804823 0.00000000

C -1.22968949 -1.40223607 0.00000000

C -1.22968953 1.40223696 0.00000000

C -2.45892851 -0.72780937 0.00000000

C -2.45892856 0.72781009 0.00000000

C -3.67935954 -1.40249691 0.00000000

C -3.67935974 1.40249765 0.00000000

C -4.91003788 -0.72700125 0.00000000

C -4.91003805 0.72700167 0.00000000

C -6.13025150 -1.40240659 0.00000000

C -6.13025189 1.40240685 0.00000000

C -7.35843500 -0.72507827 0.00000000

C -7.35843526 0.72507811 0.00000000

C -8.58421276 -1.40095243 0.00000000

C -8.58421318 1.40095194 0.00000000

C -9.80209988 -0.72159801 0.00000000

C -9.80210010 0.72159730 0.00000000

C -11.04585251 -1.40184068 0.00000000

C -11.04585280 1.40183961 0.00000000

C -12.22915212 -0.70804272 0.00000000

C -12.22915225 0.70804147 0.00000000

H 15.62278617 -1.24949332 0.00000000

H 15.62278632 1.24949262 0.00000000

H 13.47683609 -2.50065989 0.00000000

H 13.47683647 2.50065938 0.00000000

H 11.02396459 -2.50111291 0.00000000

H 11.02396491 2.50111281 0.00000000

H 8.56958179 -2.50249413 0.00000000

H 8.56958222 2.50249455 0.00000000

H 6.11865683 -2.50261264 0.00000000

H 6.11865708 2.50261342 0.00000000

H 3.66898555 -2.50237955 0.00000000

H 3.66898566 2.50238046 0.00000000

H 1.21971663 -2.50224598 0.00000000

H 1.21971657 2.50224690 0.00000000

H -1.22959160 -2.50237339 0.00000000

H -1.22959172 2.50237432 0.00000000

H -3.67944456 -2.50260649 0.00000000

H -3.67944489 2.50260731 0.00000000

H -6.13073960 -2.50249612 0.00000000

H -6.13074020 2.50249644 0.00000000

H -8.58504242 -2.50115925 0.00000000

H -8.58504301 2.50115877 0.00000000

H -11.03778419 -2.50066388 0.00000000

H -11.03778474 2.50066278 0.00000000

H -13.18342424 -1.24951897 0.00000000

H -13.18342450 1.24951750 0.00000000

$end

$comment

11-acene triplet

$end

$molecule

0 3

C 14.67240769 -0.70749938 0.00000000

C 14.67240760 0.70750010 0.00000000

C 13.48814095 -1.40130304 0.00000000

C 13.48814071 1.40130365 0.00000000

C 12.24516200 -0.72126388 0.00000000

C 12.24516183 0.72126423 0.00000000

C 11.02584722 -1.40051215 0.00000000

C 11.02584681 1.40051229 0.00000000

C 9.80056074 -0.72486958 0.00000000

C 9.80056059 0.72486954 0.00000000

C 8.57178620 -1.40214419 0.00000000

C 8.57178572 1.40214398 0.00000000

C 7.35059724 -0.72675803 0.00000000

C 7.35059721 0.72675776 0.00000000

C 6.12074012 -1.40224616 0.00000000

C 6.12073960 1.40224584 0.00000000

C 4.89836968 -0.72722776 0.00000000

C 4.89836976 0.72722753 0.00000000

C 3.67028243 -1.40195915 0.00000000

C 3.67028192 1.40195895 0.00000000

C 2.44585425 -0.72715043 0.00000000

C 2.44585440 0.72715044 0.00000000

C 1.21959577 -1.40180278 0.00000000

C 1.21959526 1.40180291 0.00000000

C -0.00653380 -0.72716703 0.00000000

C -0.00653367 0.72716731 0.00000000

C -1.23107051 -1.40195324 0.00000000

C -1.23107106 1.40195366 0.00000000

C -2.45910554 -0.72727948 0.00000000

C -2.45910549 0.72728001 0.00000000

C -3.68147689 -1.40223219 0.00000000

C -3.68147740 1.40223274 0.00000000

C -4.91140113 -0.72682194 0.00000000

C -4.91140113 0.72682255 0.00000000

C -6.13247356 -1.40212276 0.00000000

C -6.13247398 1.40212328 0.00000000

C -7.36133496 -0.72490832 0.00000000

C -7.36133507 0.72490877 0.00000000

C -8.58650620 -1.40056843 0.00000000

C -8.58650662 1.40056864 0.00000000

C -9.80596763 -0.72114707 0.00000000

C -9.80596781 0.72114702 0.00000000

C -11.04863865 -1.40131534 0.00000000

C -11.04863902 1.40131497 0.00000000

C -12.23314291 -0.70741034 0.00000000

C -12.23314309 0.70740979 0.00000000

H 15.62647317 -1.24933623 0.00000000

H 15.62647299 1.24933713 0.00000000

H 13.47957716 -2.50013352 0.00000000

H 13.47957676 2.50013415 0.00000000

H 11.02626903 -2.50072649 0.00000000

H 11.02626842 2.50072665 0.00000000

H 8.57182469 -2.50220796 0.00000000

H 8.57182411 2.50220774 0.00000000

H 6.12078860 -2.50234282 0.00000000

H 6.12078812 2.50234246 0.00000000

H 3.67037321 -2.50208866 0.00000000

H 3.67037284 2.50208842 0.00000000

H 1.21971847 -2.50194566 0.00000000

H 1.21971810 2.50194578 0.00000000

H -1.23097186 -2.50208528 0.00000000

H -1.23097225 2.50208571 0.00000000

H -3.68156603 -2.50233650 0.00000000

H -3.68156648 2.50233704 0.00000000

H -6.13298005 -2.50220837 0.00000000

H -6.13298057 2.50220889 0.00000000

H -8.58734771 -2.50077534 0.00000000

H -8.58734836 2.50077554 0.00000000

H -11.04052851 -2.50014218 0.00000000

H -11.04052911 2.50014179 0.00000000

H -13.18714165 -1.24934798 0.00000000

H -13.18714196 1.24934715 0.00000000

$end

$comment

12-acene singlet

$end

$molecule

0 1

C 14.67386978 -0.70809290 0.00000000

C 14.67386851 0.70810065 0.00000000

C 13.49069852 -1.40192860 0.00000000

C 13.49069624 1.40193417 0.00000000

C 12.24679977 -0.72167960 0.00000000

C 12.24679888 0.72168352 0.00000000

C 11.02912088 -1.40103009 0.00000000

C 11.02911939 1.40103223 0.00000000

C 9.80315275 -0.72515155 0.00000000

C 9.80315215 0.72515247 0.00000000

C 8.57518404 -1.40248106 0.00000000

C 8.57518283 1.40248088 0.00000000

C 7.35486605 -0.72701206 0.00000000

C 7.35486543 0.72701071 0.00000000

C 6.12423917 -1.40256455 0.00000000

C 6.12423804 1.40256230 0.00000000

C 4.90402278 -0.72771528 0.00000000

C 4.90402222 0.72771203 0.00000000

C 3.67438449 -1.40224937 0.00000000

C 3.67438365 1.40224535 0.00000000

C 2.45215262 -0.72785536 0.00000000

C 2.45215229 0.72785070 0.00000000

C 1.22479026 -1.40198411 0.00000000

C 1.22478992 1.40197904 0.00000000

C 0.00000002 -0.72785024 0.00000000

C 0.00000000 0.72784501 0.00000000

C -1.22479020 -1.40198416 0.00000000

C -1.22478996 1.40197900 0.00000000

C -2.45215258 -0.72785544 0.00000000

C -2.45215230 0.72785061 0.00000000

C -3.67438446 -1.40224949 0.00000000

C -3.67438367 1.40224522 0.00000000

C -4.90402277 -0.72771542 0.00000000

C -4.90402223 0.72771189 0.00000000

C -6.12423917 -1.40256471 0.00000000

C -6.12423804 1.40256216 0.00000000

C -7.35486606 -0.72701220 0.00000000

C -7.35486542 0.72701056 0.00000000

C -8.57518407 -1.40248119 0.00000000

C -8.57518281 1.40248075 0.00000000

C -9.80315278 -0.72515167 0.00000000

C -9.80315213 0.72515236 0.00000000

C -11.02912096 -1.40103017 0.00000000

C -11.02911934 1.40103218 0.00000000

C -12.24679982 -0.72167961 0.00000000

C -12.24679885 0.72168351 0.00000000

C -13.49069860 -1.40192855 0.00000000

C -13.49069617 1.40193422 0.00000000

C -14.67386983 -0.70809279 0.00000000

C -14.67386848 0.70810075 0.00000000

H 15.62812940 -1.24964943 0.00000000

H 15.62812723 1.24965877 0.00000000

H 13.48284322 -2.50075916 0.00000000

H 13.48283922 2.50076454 0.00000000

H 11.03008851 -2.50124250 0.00000000

H 11.03008561 2.50124452 0.00000000

H 8.57560058 -2.50257735 0.00000000

H 8.57559833 2.50257717 0.00000000

H 6.12410427 -2.50267897 0.00000000

H 6.12410231 2.50267669 0.00000000

H 3.67409210 -2.50239148 0.00000000

H 3.67409064 2.50238733 0.00000000

H 1.22465338 -2.50214353 0.00000000

H 1.22465278 2.50213826 0.00000000

H -1.22465327 -2.50214359 0.00000000

H -1.22465286 2.50213822 0.00000000

H -3.67409204 -2.50239160 0.00000000

H -3.67409069 2.50238718 0.00000000

H -6.12410427 -2.50267914 0.00000000

H -6.12410231 2.50267654 0.00000000

H -8.57560063 -2.50257750 0.00000000

H -8.57559830 2.50257703 0.00000000

H -11.03008863 -2.50124260 0.00000000

H -11.03008551 2.50124444 0.00000000

H -13.48284335 -2.50075914 0.00000000

H -13.48283910 2.50076458 0.00000000

H -15.62812948 -1.24964928 0.00000000

H -15.62812716 1.24965893 0.00000000

$end

$comment

12-acene triplet

$end

$molecule

0 3

C 14.67749723 -0.70750213 0.00000000

C 14.67749737 0.70749996 0.00000000

C 13.49320928 -1.40146060 0.00000000

C 13.49320966 1.40145868 0.00000000

C 12.25036181 -0.72127702 0.00000000

C 12.25036207 0.72127550 0.00000000

C 11.03118984 -1.40068919 0.00000000

C 11.03119038 1.40068802 0.00000000

C 9.80587809 -0.72504337 0.00000000

C 9.80587839 0.72504261 0.00000000

C 8.57723225 -1.40224104 0.00000000

C 8.57723292 1.40224068 0.00000000

C 7.35614355 -0.72696160 0.00000000

C 7.35614390 0.72696172 0.00000000

C 6.12636150 -1.40239161 0.00000000

C 6.12636239 1.40239211 0.00000000

C 4.90404852 -0.72739892 0.00000000

C 4.90404894 0.72739987 0.00000000

C 3.67612128 -1.40211394 0.00000000

C 3.67612225 1.40211529 0.00000000

C 2.45178541 -0.72717383 0.00000000

C 2.45178576 0.72717546 0.00000000

C 1.22547137 -1.40186509 0.00000000

C 1.22547223 1.40186697 0.00000000

C -0.00000018 -0.72700526 0.00000000

C 0.00000007 0.72700727 0.00000000

C -1.22547223 -1.40186498 0.00000000

C -1.22547153 1.40186712 0.00000000

C -2.45178578 -0.72717357 0.00000000

C -2.45178560 0.72717573 0.00000000

C -3.67612205 -1.40211353 0.00000000

C -3.67612160 1.40211568 0.00000000

C -4.90404881 -0.72739841 0.00000000

C -4.90404876 0.72740035 0.00000000

C -6.12636198 -1.40239097 0.00000000

C -6.12636196 1.40239273 0.00000000

C -7.35614362 -0.72696105 0.00000000

C -7.35614379 0.72696228 0.00000000

C -8.57723230 -1.40224050 0.00000000

C -8.57723283 1.40224123 0.00000000

C -9.80587799 -0.72504300 0.00000000

C -9.80587839 0.72504297 0.00000000

C -11.03118959 -1.40068901 0.00000000

C -11.03119053 1.40068817 0.00000000

C -12.25036160 -0.72127716 0.00000000

C -12.25036215 0.72127536 0.00000000

C -13.49320878 -1.40146104 0.00000000

C -13.49321003 1.40145823 0.00000000

C -14.67749689 -0.70750304 0.00000000

C -14.67749756 0.70749906 0.00000000

H 15.63144081 -1.24959932 0.00000000

H 15.63144107 1.24959690 0.00000000

H 13.48545072 -2.50029284 0.00000000

H 13.48545137 2.50029085 0.00000000

H 11.03227353 -2.50090228 0.00000000

H 11.03227445 2.50090104 0.00000000

H 8.57767651 -2.50233530 0.00000000

H 8.57767769 2.50233487 0.00000000

H 6.12619900 -2.50249827 0.00000000

H 6.12620044 2.50249870 0.00000000

H 3.67581532 -2.50224241 0.00000000

H 3.67581683 2.50224376 0.00000000

H 1.22533656 -2.50200743 0.00000000

H 1.22533788 2.50200937 0.00000000

H -1.22533782 -2.50200729 0.00000000

H -1.22533676 2.50200951 0.00000000

H -3.67581644 -2.50224193 0.00000000

H -3.67581583 2.50224421 0.00000000

H -6.12619969 -2.50249750 0.00000000

H -6.12619980 2.50249943 0.00000000

H -8.57767661 -2.50233463 0.00000000

H -8.57767758 2.50233554 0.00000000

H -11.03227311 -2.50090198 0.00000000

H -11.03227477 2.50090130 0.00000000

H -13.48544987 -2.50029319 0.00000000

H -13.48545208 2.50029048 0.00000000

H -15.63144027 -1.24960052 0.00000000

H -15.63144146 1.24959569 0.00000000

$end

$comment

13-acene singlet

$end

$molecule

0 1

C 17.11935798 -0.70823849 0.00000000

C 17.11935902 0.70822994 0.00000000

C 15.93647187 -1.40194073 0.00000000

C 15.93647378 1.40193382 0.00000000

C 14.69220205 -0.72181232 0.00000000

C 14.69220294 0.72180692 0.00000000

C 13.47481431 -1.40101449 0.00000000

C 13.47481590 1.40101074 0.00000000

C 12.24859085 -0.72510866 0.00000000

C 12.24859148 0.72510619 0.00000000

C 11.02093920 -1.40254598 0.00000000

C 11.02094037 1.40254466 0.00000000

C 9.80033127 -0.72693067 0.00000000

C 9.80033180 0.72693042 0.00000000

C 8.57000482 -1.40261144 0.00000000

C 8.57000579 1.40261201 0.00000000

C 7.34967959 -0.72761414 0.00000000

C 7.34968007 0.72761560 0.00000000

C 6.12007054 -1.40225387 0.00000000

C 6.12007130 1.40225593 0.00000000

C 4.89810820 -0.72772056 0.00000000

C 4.89810856 0.72772324 0.00000000

C 3.67028583 -1.40190141 0.00000000

C 3.67028628 1.40190453 0.00000000

C 2.44635109 -0.72765620 0.00000000

C 2.44635123 0.72765960 0.00000000

C 1.22040983 -1.40176317 0.00000000

C 1.22040990 1.40176673 0.00000000

C -0.00540718 -0.72766132 0.00000000

C -0.00540726 0.72766488 0.00000000

C -1.22945621 -1.40189697 0.00000000

C -1.22945648 1.40190039 0.00000000

C -2.45719123 -0.72774143 0.00000000

C -2.45719148 0.72774466 0.00000000

C -3.67921002 -1.40224584 0.00000000

C -3.67921053 1.40224862 0.00000000

C -4.90881819 -0.72766196 0.00000000

C -4.90881850 0.72766442 0.00000000

C -6.12909748 -1.40259883 0.00000000

C -6.12909815 1.40260058 0.00000000

C -7.35952910 -0.72698908 0.00000000

C -7.35952945 0.72699028 0.00000000

C -8.57998876 -1.40252484 0.00000000

C -8.57998960 1.40252526 0.00000000

C -9.80775417 -0.72514582 0.00000000

C -9.80775464 0.72514536 0.00000000

C -11.03383469 -1.40106153 0.00000000

C -11.03383595 1.40106013 0.00000000

C -12.25138482 -0.72169965 0.00000000

C -12.25138556 0.72169680 0.00000000

C -13.49533077 -1.40194647 0.00000000

C -13.49533247 1.40194232 0.00000000

C -14.67844725 -0.70814071 0.00000000

C -14.67844815 0.70813502 0.00000000

H 18.07375275 -1.24951458 0.00000000

H 18.07375454 1.24950474 0.00000000

H 15.92797282 -2.50076168 0.00000000

H 15.92797600 2.50075489 0.00000000

H 13.47521849 -2.50121901 0.00000000

H 13.47522148 2.50121538 0.00000000

H 11.02095161 -2.50260567 0.00000000

H 11.02095385 2.50260444 0.00000000

H 8.56999530 -2.50270540 0.00000000

H 8.56999702 2.50270604 0.00000000

H 6.12005984 -2.50238520 0.00000000

H 6.12006110 2.50238738 0.00000000

H 3.67029307 -2.50205897 0.00000000

H 3.67029379 2.50206228 0.00000000

H 1.22048403 -2.50193018 0.00000000

H 1.22048420 2.50193395 0.00000000

H -1.22931466 -2.50205547 0.00000000

H -1.22931500 2.50205905 0.00000000

H -3.67908840 -2.50238012 0.00000000

H -3.67908920 2.50238299 0.00000000

H -6.12916889 -2.50270059 0.00000000

H -6.12917014 2.50270239 0.00000000

H -8.58047685 -2.50260695 0.00000000

H -8.58047852 2.50260745 0.00000000

H -11.03467307 -2.50126261 0.00000000

H -11.03467547 2.50126134 0.00000000

H -13.48728195 -2.50076539 0.00000000

H -13.48728487 2.50076135 0.00000000

H -15.63276323 -1.24953744 0.00000000

H -15.63276476 1.24953065 0.00000000

$end

$comment

13-acene triplet

$end

$molecule

0 3

C 17.12278899 -0.70772556 0.00000000

C 17.12278857 0.70772561 0.00000000

C 15.93894937 -1.40150301 0.00000000

C 15.93894852 1.40150230 0.00000000

C 14.69559343 -0.72143066 0.00000000

C 14.69559297 0.72142915 0.00000000

C 13.47685153 -1.40067022 0.00000000

C 13.47685071 1.40066803 0.00000000

C 12.25130385 -0.72496587 0.00000000

C 12.25130329 0.72496294 0.00000000

C 11.02289438 -1.40229681 0.00000000

C 11.02289339 1.40229315 0.00000000

C 9.80178791 -0.72688784 0.00000000

C 9.80178754 0.72688381 0.00000000

C 8.57202662 -1.40242826 0.00000000

C 8.57202562 1.40242390 0.00000000

C 7.34990581 -0.72742470 0.00000000

C 7.34990574 0.72742055 0.00000000

C 6.12188762 -1.40213064 0.00000000

C 6.12188663 1.40212680 0.00000000

C 4.89773136 -0.72725387 0.00000000

C 4.89773148 0.72725075 0.00000000

C 3.67138661 -1.40183776 0.00000000

C 3.67138570 1.40183536 0.00000000

C 2.44611084 -0.72698565 0.00000000

C 2.44611112 0.72698434 0.00000000

C 1.22041675 -1.40172751 0.00000000

C 1.22041596 1.40172718 0.00000000

C -0.00518971 -0.72698586 0.00000000

C -0.00518937 0.72698674 0.00000000

C -1.23054824 -1.40183612 0.00000000

C -1.23054896 1.40183803 0.00000000

C -2.45682465 -0.72726333 0.00000000

C -2.45682440 0.72726624 0.00000000

C -3.68102825 -1.40212464 0.00000000

C -3.68102902 1.40212828 0.00000000

C -4.90903886 -0.72746183 0.00000000

C -4.90903879 0.72746595 0.00000000

C -6.13112592 -1.40241319 0.00000000

C -6.13112687 1.40241757 0.00000000

C -7.36096812 -0.72694105 0.00000000

C -7.36096849 0.72694501 0.00000000

C -8.58195150 -1.40227375 0.00000000

C -8.58195284 1.40227724 0.00000000

C -9.81044393 -0.72500180 0.00000000

C -9.81044474 0.72500406 0.00000000

C -11.03587959 -1.40072422 0.00000000

C -11.03588129 1.40072524 0.00000000

C -12.25476088 -0.72131716 0.00000000

C -12.25476187 0.72131659 0.00000000

C -13.49781085 -1.40151615 0.00000000

C -13.49781283 1.40151391 0.00000000

C -14.68188064 -0.70763956 0.00000000

C -14.68188168 0.70763562 0.00000000

H 18.07695967 -1.24937981 0.00000000

H 18.07695896 1.24938041 0.00000000

H 15.93040023 -2.50032939 0.00000000

H 15.93039860 2.50032868 0.00000000

H 13.47727054 -2.50088096 0.00000000

H 13.47726910 2.50087878 0.00000000

H 11.02293972 -2.50235714 0.00000000

H 11.02293816 2.50235345 0.00000000

H 8.57207677 -2.50251857 0.00000000

H 8.57207542 2.50251413 0.00000000

H 6.12194429 -2.50225270 0.00000000

H 6.12194333 2.50224876 0.00000000

H 3.67143441 -2.50197973 0.00000000

H 3.67143377 2.50197722 0.00000000

H 1.22047737 -2.50187569 0.00000000

H 1.22047698 2.50187529 0.00000000

H -1.23046364 -2.50197804 0.00000000

H -1.23046399 2.50197995 0.00000000

H -3.68096830 -2.50224824 0.00000000

H -3.68096900 2.50225195 0.00000000

H -6.13123946 -2.50251023 0.00000000

H -6.13124082 2.50251477 0.00000000

H -8.58245859 -2.50235558 0.00000000

H -8.58246079 2.50235925 0.00000000

H -11.03671046 -2.50092829 0.00000000

H -11.03671340 2.50092943 0.00000000

H -13.48971282 -2.50033918 0.00000000

H -13.48971625 2.50033702 0.00000000

H -15.63598270 -1.24939757 0.00000000

H -15.63598448 1.24939228 0.00000000

$end

$comment

14-acene singlet

$end

$molecule

0 1

C 17.12416403 -0.70813977 0.00000000

C 17.12416349 0.70814100 0.00000000

C 15.94107369 -1.40199130 0.00000000

C 15.94107257 1.40199164 0.00000000

C 14.69709068 -0.72174107 0.00000000

C 14.69709003 0.72174037 0.00000000

C 13.47958120 -1.40110626 0.00000000

C 13.47958010 1.40110453 0.00000000

C 12.25343029 -0.72522031 0.00000000

C 12.25342978 0.72521795 0.00000000

C 11.02575150 -1.40258075 0.00000000

C 11.02575094 1.40257750 0.00000000

C 9.80515843 -0.72706651 0.00000000

C 9.80515831 0.72706331 0.00000000

C 8.57489721 -1.40268017 0.00000000

C 8.57489733 1.40267659 0.00000000

C 7.35443229 -0.72770463 0.00000000

C 7.35443254 0.72770167 0.00000000

C 6.12502831 -1.40234101 0.00000000

C 6.12502908 1.40233832 0.00000000

C 4.90289138 -0.72770897 0.00000000

C 4.90289192 0.72770738 0.00000000

C 3.67520083 -1.40196721 0.00000000

C 3.67520201 1.40196635 0.00000000

C 2.45135496 -0.72752532 0.00000000

C 2.45135566 0.72752572 0.00000000

C 1.22511210 -1.40175066 0.00000000

C 1.22511342 1.40175209 0.00000000

C -0.00000033 -0.72743278 0.00000000

C 0.00000035 0.72743536 0.00000000

C -1.22511329 -1.40174956 0.00000000

C -1.22511218 1.40175319 0.00000000

C -2.45135555 -0.72752330 0.00000000

C -2.45135504 0.72752774 0.00000000

C -3.67520173 -1.40196418 0.00000000

C -3.67520109 1.40196940 0.00000000

C -4.90289175 -0.72770547 0.00000000

C -4.90289155 0.72771089 0.00000000

C -6.12502867 -1.40233678 0.00000000

C -6.12502872 1.40234254 0.00000000

C -7.35443231 -0.72770052 0.00000000

C -7.35443254 0.72770579 0.00000000

C -8.57489682 -1.40267588 0.00000000

C -8.57489772 1.40268088 0.00000000

C -9.80515801 -0.72706301 0.00000000

C -9.80515872 0.72706681 0.00000000

C -11.02575035 -1.40257776 0.00000000

C -11.02575209 1.40258048 0.00000000

C -12.25342950 -0.72521874 0.00000000

C -12.25343059 0.72521953 0.00000000

C -13.47957942 -1.40110592 0.00000000

C -13.47958189 1.40110486 0.00000000

C -14.69708966 -0.72174252 0.00000000

C -14.69709109 0.72173891 0.00000000

C -15.94107160 -1.40199451 0.00000000

C -15.94107469 1.40198843 0.00000000

C -17.12416297 -0.70814481 0.00000000

C -17.12416458 0.70813596 0.00000000

H 18.07843941 -1.24966972 0.00000000

H 18.07843843 1.24967168 0.00000000

H 15.93325014 -2.50081994 0.00000000

H 15.93324818 2.50082025 0.00000000

H 13.48058837 -2.50131522 0.00000000

H 13.48058666 2.50131336 0.00000000

H 11.02621024 -2.50267218 0.00000000

H 11.02620938 2.50266864 0.00000000

H 8.57477774 -2.50278849 0.00000000

H 8.57477795 2.50278461 0.00000000

H 6.12467827 -2.50247810 0.00000000

H 6.12467958 2.50247518 0.00000000

H 3.67489511 -2.50212754 0.00000000

H 3.67489708 2.50212653 0.00000000

H 1.22499673 -2.50192333 0.00000000

H 1.22499892 2.50192474 0.00000000

H -1.22499873 -2.50192217 0.00000000

H -1.22499689 2.50192593 0.00000000

H -3.67489657 -2.50212433 0.00000000

H -3.67489559 2.50212977 0.00000000

H -6.12467884 -2.50247361 0.00000000

H -6.12467900 2.50247967 0.00000000

H -8.57477708 -2.50278389 0.00000000

H -8.57477862 2.50278921 0.00000000

H -11.02620828 -2.50266891 0.00000000

H -11.02621134 2.50267191 0.00000000

H -13.48058532 -2.50131470 0.00000000

H -13.48058972 2.50131387 0.00000000

H -15.93324648 -2.50082304 0.00000000

H -15.93325186 2.50081714 0.00000000

H -18.07843755 -1.24967616 0.00000000

H -18.07844034 1.24966525 0.00000000

$end

$comment

14-acene triplet

$end

$molecule

0 3

C 17.12728720 -0.70765419 0.00000000

C 17.12728615 0.70767600 0.00000000

C 15.94331802 -1.40159292 0.00000000

C 15.94331502 1.40161260 0.00000000

C 14.70020707 -0.72137605 0.00000000

C 14.70020708 0.72139416 0.00000000

C 13.48143660 -1.40078583 0.00000000

C 13.48143317 1.40080173 0.00000000

C 12.25599124 -0.72507255 0.00000000

C 12.25599239 0.72508681 0.00000000

C 11.02752065 -1.40232477 0.00000000

C 11.02751688 1.40233770 0.00000000

C 9.80664430 -0.72701499 0.00000000

C 9.80664604 0.72702622 0.00000000

C 8.57673680 -1.40249096 0.00000000

C 8.57673317 1.40250171 0.00000000

C 7.35480186 -0.72755544 0.00000000

C 7.35480404 0.72756525 0.00000000

C 6.12676797 -1.40222850 0.00000000

C 6.12676489 1.40223780 0.00000000

C 4.90260011 -0.72736246 0.00000000

C 4.90260248 0.72737111 0.00000000

C 3.67646192 -1.40193224 0.00000000

C 3.67645876 1.40194041 0.00000000

C 2.45101305 -0.72701989 0.00000000

C 2.45101494 0.72702737 0.00000000

C 1.22557360 -1.40176921 0.00000000

C 1.22556941 1.40177577 0.00000000

C -0.00000073 -0.72687240 0.00000000

C 0.00000096 0.72687847 0.00000000

C -1.22556819 -1.40177029 0.00000000

C -1.22557346 1.40177454 0.00000000

C -2.45101476 -0.72702227 0.00000000

C -2.45101272 0.72702544 0.00000000

C -3.67645709 -1.40193525 0.00000000

C -3.67646302 1.40193601 0.00000000

C -4.90260218 -0.72736800 0.00000000

C -4.90259991 0.72736672 0.00000000

C -6.12676309 -1.40223422 0.00000000

C -6.12676925 1.40223029 0.00000000

C -7.35480366 -0.72756397 0.00000000

C -7.35480179 0.72755741 0.00000000

C -8.57673213 -1.40250122 0.00000000

C -8.57673811 1.40249189 0.00000000

C -9.80664557 -0.72702662 0.00000000

C -9.80664470 0.72701423 0.00000000

C -11.02751665 -1.40233975 0.00000000

C -11.02752224 1.40232434 0.00000000

C -12.25599170 -0.72508890 0.00000000

C -12.25599194 0.72507003 0.00000000

C -13.48143302 -1.40080513 0.00000000

C -13.48143824 1.40078322 0.00000000

C -14.70020664 -0.72139815 0.00000000

C -14.70020810 0.72137232 0.00000000

C -15.94331493 -1.40161773 0.00000000

C -15.94331998 1.40158830 0.00000000

C -17.12728619 -0.70768222 0.00000000

C -17.12728839 0.70764873 0.00000000

H 18.08131551 -1.24960054 0.00000000

H 18.08131322 1.24962427 0.00000000

H 15.93554039 -2.50042227 0.00000000

H 15.93553719 2.50044195 0.00000000

H 13.48248970 -2.50099676 0.00000000

H 13.48248751 2.50101267 0.00000000

H 11.02796843 -2.50241707 0.00000000

H 11.02796785 2.50242999 0.00000000

H 8.57661349 -2.50259484 0.00000000

H 8.57661445 2.50260550 0.00000000

H 6.12649628 -2.50235362 0.00000000

H 6.12649694 2.50236290 0.00000000

H 3.67628354 -2.50207400 0.00000000

H 3.67628378 2.50208227 0.00000000

H 1.22552214 -2.50191951 0.00000000

H 1.22552216 2.50192617 0.00000000

H -1.22551327 -2.50192072 0.00000000

H -1.22551415 2.50192491 0.00000000

H -3.67627817 -2.50207733 0.00000000

H -3.67627993 2.50207801 0.00000000

H -6.12649734 -2.50235965 0.00000000

H -6.12649988 2.50235573 0.00000000

H -8.57661800 -2.50260512 0.00000000

H -8.57662157 2.50259587 0.00000000

H -11.02796911 -2.50243194 0.00000000

H -11.02797422 2.50241662 0.00000000

H -13.48248514 -2.50101606 0.00000000

H -13.48249157 2.50099424 0.00000000

H -15.93553421 -2.50044715 0.00000000

H -15.93554194 2.50041779 0.00000000

H -18.08131365 -1.24962988 0.00000000

H -18.08131780 1.24959315 0.00000000

$end

$comment

15-acene singlet

$end

$molecule

0 1

C 19.57043294 -0.70823895 0.00000000

C 19.57043258 0.70824443 0.00000000

C 18.38755869 -1.40195539 0.00000000

C 18.38755807 1.40196038 0.00000000

C 17.14327728 -0.72182358 0.00000000

C 17.14327699 0.72182812 0.00000000

C 15.92594030 -1.40104225 0.00000000

C 15.92593977 1.40104618 0.00000000

C 14.69963688 -0.72514043 0.00000000

C 14.69963669 0.72514394 0.00000000

C 13.47212869 -1.40259228 0.00000000

C 13.47212829 1.40259540 0.00000000

C 12.25133387 -0.72697531 0.00000000

C 12.25133367 0.72697801 0.00000000

C 11.02128084 -1.40268306 0.00000000

C 11.02128039 1.40268540 0.00000000

C 9.80066287 -0.72764390 0.00000000

C 9.80066261 0.72764575 0.00000000

C 8.57141131 -1.40234388 0.00000000

C 8.57141073 1.40234532 0.00000000

C 7.34918088 -0.72768084 0.00000000

C 7.34918054 0.72768169 0.00000000

C 6.12157973 -1.40197116 0.00000000

C 6.12157909 1.40197153 0.00000000

C 4.89773414 -0.72747767 0.00000000

C 4.89773379 0.72747749 0.00000000

C 3.67143676 -1.40172913 0.00000000

C 3.67143622 1.40172846 0.00000000

C 2.44657481 -0.72730876 0.00000000

C 2.44657457 0.72730774 0.00000000

C 1.22103611 -1.40165052 0.00000000

C 1.22103578 1.40164911 0.00000000

C -0.00443930 -0.72730592 0.00000000

C -0.00443939 0.72730433 0.00000000

C -1.22936544 -1.40173079 0.00000000

C -1.22936552 1.40172901 0.00000000

C -2.45559537 -0.72747509 0.00000000

C -2.45559534 0.72747325 0.00000000

C -3.67950501 -1.40197065 0.00000000

C -3.67950492 1.40196883 0.00000000

C -4.90705308 -0.72769373 0.00000000

C -4.90705300 0.72769191 0.00000000

C -6.12931596 -1.40233981 0.00000000

C -6.12931577 1.40233818 0.00000000

C -7.35857492 -0.72768819 0.00000000

C -7.35857481 0.72768671 0.00000000

C -8.57914420 -1.40267328 0.00000000

C -8.57914391 1.40267207 0.00000000

C -9.80929548 -0.72703535 0.00000000

C -9.80929531 0.72703446 0.00000000

C -11.02994747 -1.40257347 0.00000000

C -11.02994705 1.40257285 0.00000000

C -12.25756093 -0.72518331 0.00000000

C -12.25756066 0.72518320 0.00000000

C -13.48372485 -1.40109017 0.00000000

C -13.48372413 1.40109052 0.00000000

C -14.70121943 -0.72172008 0.00000000

C -14.70121901 0.72172130 0.00000000

C -15.94518351 -1.40196432 0.00000000

C -15.94518255 1.40196625 0.00000000

C -17.12828155 -0.70814628 0.00000000

C -17.12828105 0.70814908 0.00000000

H 20.52483201 -1.24950419 0.00000000

H 20.52483139 1.24951013 0.00000000

H 18.37908132 -2.50077346 0.00000000

H 18.37908041 2.50077839 0.00000000

H 15.92634397 -2.50124293 0.00000000

H 15.92634293 2.50124681 0.00000000

H 13.47215713 -2.50264832 0.00000000

H 13.47215633 2.50265143 0.00000000

H 11.02128655 -2.50277124 0.00000000

H 11.02128570 2.50277360 0.00000000

H 8.57139433 -2.50246748 0.00000000

H 8.57139332 2.50246893 0.00000000

H 6.12153561 -2.50212120 0.00000000

H 6.12153455 2.50212152 0.00000000

H 3.67140672 -2.50189390 0.00000000

H 3.67140585 2.50189312 0.00000000

H 1.22105927 -2.50181959 0.00000000

H 1.22105869 2.50181803 0.00000000

H -1.22926616 -2.50189512 0.00000000

H -1.22926640 2.50189321 0.00000000

H -3.67934750 -2.50212073 0.00000000

H -3.67934744 2.50211882 0.00000000

H -6.12919174 -2.50246550 0.00000000

H -6.12919138 2.50246382 0.00000000

H -8.57922173 -2.50276858 0.00000000

H -8.57922115 2.50276731 0.00000000

H -11.03044465 -2.50265135 0.00000000

H -11.03044386 2.50265065 0.00000000

H -13.48457223 -2.50128832 0.00000000

H -13.48457091 2.50128858 0.00000000

H -15.93714556 -2.50078087 0.00000000

H -15.93714393 2.50078272 0.00000000

H -18.08260263 -1.24953012 0.00000000

H -18.08260177 1.24953354 0.00000000

$end

$comment

15-acene triplet

$end

$molecule

0 3

C 19.57329195 -0.70786250 0.00000000

C 19.57329240 0.70786234 0.00000000

C 18.38971858 -1.40162444 0.00000000

C 18.38971949 1.40162514 0.00000000

C 17.14613478 -0.72152122 0.00000000

C 17.14613532 0.72152281 0.00000000

C 15.92773656 -1.40075550 0.00000000

C 15.92773742 1.40075794 0.00000000

C 14.70206924 -0.72498896 0.00000000

C 14.70206986 0.72499221 0.00000000

C 13.47380045 -1.40235791 0.00000000

C 13.47380145 1.40236207 0.00000000

C 12.25290217 -0.72691139 0.00000000

C 12.25290264 0.72691607 0.00000000

C 11.02296122 -1.40249029 0.00000000

C 11.02296226 1.40249560 0.00000000

C 9.80127388 -0.72753141 0.00000000

C 9.80127405 0.72753672 0.00000000

C 8.57300089 -1.40220746 0.00000000

C 8.57300189 1.40221282 0.00000000

C 7.34912950 -0.72743736 0.00000000

C 7.34912937 0.72744220 0.00000000

C 6.12282691 -1.40191643 0.00000000

C 6.12282783 1.40192077 0.00000000

C 4.89746935 -0.72711859 0.00000000

C 4.89746904 0.72712211 0.00000000

C 3.67211806 -1.40175358 0.00000000

C 3.67211890 1.40175620 0.00000000

C 2.44643874 -0.72689309 0.00000000

C 2.44643836 0.72689480 0.00000000

C 1.22104236 -1.40170908 0.00000000

C 1.22104321 1.40170973 0.00000000

C -0.00432328 -0.72688827 0.00000000

C -0.00432363 0.72688801 0.00000000

C -1.23003767 -1.40175895 0.00000000

C -1.23003675 1.40175766 0.00000000

C -2.45533993 -0.72711137 0.00000000

C -2.45534018 0.72710932 0.00000000

C -3.68075134 -1.40192258 0.00000000

C -3.68075034 1.40191972 0.00000000

C -4.90699693 -0.72744627 0.00000000

C -4.90699701 0.72744295 0.00000000

C -6.13091213 -1.40221010 0.00000000

C -6.13091106 1.40220631 0.00000000

C -7.35917218 -0.72757540 0.00000000

C -7.35917199 0.72757163 0.00000000

C -8.58083356 -1.40248432 0.00000000

C -8.58083245 1.40248067 0.00000000

C -9.81084774 -0.72697371 0.00000000

C -9.81084729 0.72697063 0.00000000

C -11.03162904 -1.40234227 0.00000000

C -11.03162794 1.40233983 0.00000000

C -12.25997820 -0.72503160 0.00000000

C -12.25997760 0.72503009 0.00000000

C -13.48553290 -1.40081195 0.00000000

C -13.48553183 1.40081142 0.00000000

C -14.70407130 -0.72140988 0.00000000

C -14.70407071 0.72141035 0.00000000

C -15.94734619 -1.40163574 0.00000000

C -15.94734512 1.40163725 0.00000000

C -17.13114817 -0.70777148 0.00000000

C -17.13114761 0.70777390 0.00000000

H 20.52752623 -1.24940637 0.00000000

H 20.52752698 1.24940566 0.00000000

H 18.38118051 -2.50044768 0.00000000

H 18.38118229 2.50044836 0.00000000

H 15.92814949 -2.50096386 0.00000000

H 15.92815104 2.50096626 0.00000000

H 13.47383834 -2.50241747 0.00000000

H 13.47384004 2.50242162 0.00000000

H 11.02300603 -2.50257981 0.00000000

H 11.02300758 2.50258514 0.00000000

H 8.57305209 -2.50232786 0.00000000

H 8.57305324 2.50233328 0.00000000

H 6.12285749 -2.50205622 0.00000000

H 6.12285826 2.50206060 0.00000000

H 3.67213273 -2.50190134 0.00000000

H 3.67213322 2.50190398 0.00000000

H 1.22105433 -2.50185820 0.00000000

H 1.22105471 2.50185882 0.00000000

H -1.22999935 -2.50190575 0.00000000

H -1.22999886 2.50190441 0.00000000

H -3.68066968 -2.50206156 0.00000000

H -3.68066890 2.50205863 0.00000000

H -6.13084322 -2.50233181 0.00000000

H -6.13084209 2.50232798 0.00000000

H -8.58093531 -2.50258067 0.00000000

H -8.58093376 2.50257699 0.00000000

H -11.03212566 -2.50242350 0.00000000

H -11.03212384 2.50242105 0.00000000

H -13.48636047 -2.50101416 0.00000000

H -13.48635853 2.50101365 0.00000000

H -15.93926345 -2.50045579 0.00000000

H -15.93926153 2.50045729 0.00000000

H -18.08531149 -1.24942279 0.00000000

H -18.08531052 1.24942596 0.00000000

$end

$comment

16-acene singlet

$end

$molecule

0 1

C 19.57470823 -0.70813190 0.00000000

C 19.57470970 0.70811637 0.00000000

C 18.39159076 -1.40199839 0.00000000

C 18.39159355 1.40198528 0.00000000

C 17.14765169 -0.72174025 0.00000000

C 17.14765301 0.72172945 0.00000000

C 15.93010717 -1.40111664 0.00000000

C 15.93010960 1.40110813 0.00000000

C 14.70397548 -0.72523256 0.00000000

C 14.70397664 0.72522620 0.00000000

C 13.47631362 -1.40259927 0.00000000

C 13.47631591 1.40259482 0.00000000

C 12.25565820 -0.72709219 0.00000000

C 12.25565937 0.72708989 0.00000000

C 11.02552510 -1.40271498 0.00000000

C 11.02552728 1.40271445 0.00000000

C 9.80487242 -0.72773749 0.00000000

C 9.80487350 0.72773896 0.00000000

C 8.57573864 -1.40240021 0.00000000

C 8.57574060 1.40240330 0.00000000

C 7.35329695 -0.72772523 0.00000000

C 7.35329792 0.72773019 0.00000000

C 6.12596663 -1.40204226 0.00000000

C 6.12596839 1.40204864 0.00000000

C 4.90183246 -0.72747291 0.00000000

C 4.90183337 0.72748095 0.00000000

C 3.67582164 -1.40179791 0.00000000

C 3.67582314 1.40180721 0.00000000

C 2.45076944 -0.72724115 0.00000000

C 2.45077016 0.72725163 0.00000000

C 1.22531970 -1.40168413 0.00000000

C 1.22532060 1.40169561 0.00000000

C 0.00000000 -0.72715244 0.00000000

C 0.00000026 0.72716434 0.00000000

C -1.22531988 -1.40168366 0.00000000

C -1.22531984 1.40169604 0.00000000

C -2.45076931 -0.72724031 0.00000000

C -2.45076952 0.72725242 0.00000000

C -3.67582151 -1.40179661 0.00000000

C -3.67582226 1.40180844 0.00000000

C -4.90183200 -0.72747139 0.00000000

C -4.90183256 0.72748240 0.00000000

C -6.12596610 -1.40204041 0.00000000

C -6.12596747 1.40205046 0.00000000

C -7.35329626 -0.72772341 0.00000000

C -7.35329710 0.72773203 0.00000000

C -8.57573790 -1.40239819 0.00000000

C -8.57573991 1.40240538 0.00000000

C -9.80487177 -0.72773575 0.00000000

C -9.80487298 0.72774080 0.00000000

C -11.02552444 -1.40271328 0.00000000

C -11.02552719 1.40271633 0.00000000

C -12.25565787 -0.72709098 0.00000000

C -12.25565947 0.72709126 0.00000000

C -13.47631324 -1.40259836 0.00000000

C -13.47631662 1.40259597 0.00000000

C -14.70397558 -0.72523232 0.00000000

C -14.70397744 0.72522661 0.00000000

C -15.93010711 -1.40111696 0.00000000

C -15.93011106 1.40110805 0.00000000

C -17.14765216 -0.72174128 0.00000000

C -17.14765436 0.72172857 0.00000000

C -18.39159098 -1.40200016 0.00000000

C -18.39159553 1.40198368 0.00000000

C -19.57470900 -0.70813443 0.00000000

C -19.57471135 0.70811392 0.00000000

H 20.52897344 -1.24967399 0.00000000

H 20.52897603 1.24965654 0.00000000

H 18.38377259 -2.50082504 0.00000000

H 18.38377754 2.50081203 0.00000000

H 15.93112049 -2.50132354 0.00000000

H 15.93112501 2.50131508 0.00000000

H 13.47678454 -2.50268809 0.00000000

H 13.47678872 2.50268364 0.00000000

H 11.02543140 -2.50281917 0.00000000

H 11.02543529 2.50281865 0.00000000

H 8.57542332 -2.50253110 0.00000000

H 8.57542681 2.50253426 0.00000000

H 6.12567574 -2.50219499 0.00000000

H 6.12567881 2.50220147 0.00000000

H 3.67565110 -2.50196418 0.00000000

H 3.67565356 2.50197369 0.00000000

H 1.22526715 -2.50185644 0.00000000

H 1.22526856 2.50186826 0.00000000

H -1.22526758 -2.50185594 0.00000000

H -1.22526749 2.50186869 0.00000000

H -3.67565119 -2.50196280 0.00000000

H -3.67565244 2.50197495 0.00000000

H -6.12567534 -2.50219304 0.00000000

H -6.12567782 2.50220338 0.00000000

H -8.57542257 -2.50252902 0.00000000

H -8.57542622 2.50253649 0.00000000

H -11.02543056 -2.50281744 0.00000000

H -11.02543543 2.50282075 0.00000000

H -13.47678379 -2.50268719 0.00000000

H -13.47678982 2.50268500 0.00000000

H -15.93111991 -2.50132389 0.00000000

H -15.93112695 2.50131518 0.00000000

H -18.38377216 -2.50082685 0.00000000

H -18.38378016 2.50081055 0.00000000

H -20.52897394 -1.24967711 0.00000000

H -20.52897804 1.24965356 0.00000000

$end

$comment

16-acene triplet

$end

$molecule

0 3

C 19.57724124 -0.70777952 0.00000000

C 19.57724004 0.70779004 0.00000000

C 18.39350461 -1.40170487 0.00000000

C 18.39350137 1.40171313 0.00000000

C 17.15018895 -0.72146475 0.00000000

C 17.15018881 0.72147119 0.00000000

C 15.93172838 -1.40087069 0.00000000

C 15.93172462 1.40087464 0.00000000

C 14.70615237 -0.72510016 0.00000000

C 14.70615333 0.72510225 0.00000000

C 13.47783239 -1.40238938 0.00000000

C 13.47782803 1.40238998 0.00000000

C 12.25711105 -0.72702793 0.00000000

C 12.25711320 0.72702735 0.00000000

C 11.02704587 -1.40254512 0.00000000

C 11.02704115 1.40254444 0.00000000

C 9.80553214 -0.72762373 0.00000000

C 9.80553540 0.72762310 0.00000000

C 8.57717263 -1.40228446 0.00000000

C 8.57716785 1.40228444 0.00000000

C 7.35340234 -0.72751116 0.00000000

C 7.35340639 0.72751205 0.00000000

C 6.12711514 -1.40199656 0.00000000

C 6.12711002 1.40199884 0.00000000

C 4.90171955 -0.72719483 0.00000000

C 4.90172357 0.72719855 0.00000000

C 3.67653941 -1.40182698 0.00000000

C 3.67653323 1.40183240 0.00000000

C 2.45066777 -0.72695200 0.00000000

C 2.45067163 0.72695924 0.00000000

C 1.22556237 -1.40176410 0.00000000

C 1.22555503 1.40177248 0.00000000

C -0.00000202 -0.72686725 0.00000000

C 0.00000198 0.72687680 0.00000000

C -1.22555413 -1.40176388 0.00000000

C -1.22556220 1.40177379 0.00000000

C -2.45067200 -0.72695030 0.00000000

C -2.45066795 0.72696027 0.00000000

C -3.67653232 -1.40182587 0.00000000

C -3.67654069 1.40183562 0.00000000

C -4.90172438 -0.72719220 0.00000000

C -4.90172084 0.72720109 0.00000000

C -6.12711010 -1.40199365 0.00000000

C -6.12711837 1.40200185 0.00000000

C -7.35340754 -0.72750888 0.00000000

C -7.35340511 0.72751546 0.00000000

C -8.57716872 -1.40228092 0.00000000

C -8.57717658 1.40228608 0.00000000

C -9.80553626 -0.72762242 0.00000000

C -9.80553535 0.72762509 0.00000000

C -11.02704196 -1.40254436 0.00000000

C -11.02704921 1.40254456 0.00000000

C -12.25711281 -0.72702891 0.00000000

C -12.25711348 0.72702553 0.00000000

C -13.47782763 -1.40239336 0.00000000

C -13.47783433 1.40238636 0.00000000

C -14.70615099 -0.72510632 0.00000000

C -14.70615293 0.72509481 0.00000000

C -15.93172221 -1.40088052 0.00000000

C -15.93172852 1.40086438 0.00000000

C -17.15018529 -0.72147828 0.00000000

C -17.15018785 0.72145713 0.00000000

C -18.39349751 -1.40172197 0.00000000

C -18.39350366 1.40169579 0.00000000

C -19.57723606 -0.70780062 0.00000000

C -19.57723899 0.70776943 0.00000000

H 20.53133197 -1.24961616 0.00000000

H 20.53132951 1.24962879 0.00000000

H 18.38571920 -2.50053184 0.00000000

H 18.38571566 2.50054013 0.00000000

H 15.93276527 -2.50107967 0.00000000

H 15.93276245 2.50108375 0.00000000

H 13.47827303 -2.50248060 0.00000000

H 13.47827213 2.50248129 0.00000000

H 11.02692050 -2.50264859 0.00000000

H 11.02692111 2.50264794 0.00000000

H 8.57690111 -2.50240913 0.00000000

H 8.57690174 2.50240921 0.00000000

H 6.12694726 -2.50213729 0.00000000

H 6.12694809 2.50213980 0.00000000

H 3.67649564 -2.50197641 0.00000000

H 3.67649665 2.50198208 0.00000000

H 1.22555915 -2.50191676 0.00000000

H 1.22555925 2.50192522 0.00000000

H -1.22555977 -2.50191655 0.00000000

H -1.22556091 2.50192644 0.00000000

H -3.67649192 -2.50197544 0.00000000

H -3.67649431 2.50198520 0.00000000

H -6.12694211 -2.50213472 0.00000000

H -6.12694572 2.50214299 0.00000000

H -8.57690074 -2.50240585 0.00000000

H -8.57690577 2.50241111 0.00000000

H -11.02692359 -2.50264762 0.00000000

H -11.02693031 2.50264788 0.00000000

H -13.47827178 -2.50248410 0.00000000

H -13.47828010 2.50247710 0.00000000

H -15.93275694 -2.50108917 0.00000000

H -15.93276667 2.50107300 0.00000000

H -18.38570797 -2.50054870 0.00000000

H -18.38571825 2.50052257 0.00000000

H -20.53132576 -1.24963862 0.00000000

H -20.53133103 1.24960331 0.00000000

$end

$comment

17-acene singlet

$end

$molecule

0 1

C 22.02349233 -0.70818732 0.00000000

C 22.02349183 0.70819331 0.00000000

C 20.84041810 -1.40196784 0.00000000

C 20.84041715 1.40197306 0.00000000

C 19.59627512 -0.72178695 0.00000000

C 19.59627465 0.72179144 0.00000000

C 18.37873308 -1.40100508 0.00000000

C 18.37873222 1.40100870 0.00000000

C 17.15249212 -0.72514714 0.00000000

C 17.15249174 0.72515012 0.00000000

C 15.92494129 -1.40262126 0.00000000

C 15.92494067 1.40262359 0.00000000

C 14.70419481 -0.72700701 0.00000000

C 14.70419456 0.72700892 0.00000000

C 13.47416058 -1.40270582 0.00000000

C 13.47416016 1.40270725 0.00000000

C 12.25347782 -0.72767700 0.00000000

C 12.25347767 0.72767811 0.00000000

C 11.02436717 -1.40237305 0.00000000

C 11.02436686 1.40237386 0.00000000

C 9.80192864 -0.72771626 0.00000000

C 9.80192849 0.72771679 0.00000000

C 8.57461456 -1.40202590 0.00000000

C 8.57461427 1.40202623 0.00000000

C 7.35044517 -0.72749242 0.00000000

C 7.35044501 0.72749249 0.00000000

C 6.12451796 -1.40180127 0.00000000

C 6.12451765 1.40180111 0.00000000

C 4.89936253 -0.72725015 0.00000000

C 4.89936236 0.72724972 0.00000000

C 3.67405017 -1.40169782 0.00000000

C 3.67404984 1.40169712 0.00000000

C 2.44864982 -0.72710624 0.00000000

C 2.44864964 0.72710527 0.00000000

C 1.22336449 -1.40167100 0.00000000

C 1.22336414 1.40166967 0.00000000

C -0.00191489 -0.72710172 0.00000000

C -0.00191508 0.72710015 0.00000000

C -1.22732468 -1.40170038 0.00000000

C -1.22732498 1.40169848 0.00000000

C -2.45261294 -0.72723990 0.00000000

C -2.45261308 0.72723787 0.00000000

C -3.67779933 -1.40180558 0.00000000

C -3.67779950 1.40180324 0.00000000

C -4.90367906 -0.72748579 0.00000000

C -4.90367910 0.72748350 0.00000000

C -6.12789689 -1.40202809 0.00000000

C -6.12789685 1.40202564 0.00000000

C -7.35516509 -0.72772651 0.00000000

C -7.35516500 0.72772425 0.00000000

C -8.57763442 -1.40237093 0.00000000

C -8.57763411 1.40236877 0.00000000

C -9.80674712 -0.72771438 0.00000000

C -9.80674688 0.72771268 0.00000000

C -11.02740173 -1.40268582 0.00000000

C -11.02740113 1.40268448 0.00000000

C -12.25751611 -0.72704725 0.00000000

C -12.25751570 0.72704655 0.00000000

C -13.47816850 -1.40257737 0.00000000

C -13.47816767 1.40257727 0.00000000

C -14.70580589 -0.72518242 0.00000000

C -14.70580540 0.72518306 0.00000000

C -15.93193029 -1.40109043 0.00000000

C -15.93192930 1.40109191 0.00000000

C -17.14946506 -0.72170957 0.00000000

C -17.14946453 0.72171195 0.00000000

C -18.39338771 -1.40196288 0.00000000

C -18.39338666 1.40196618 0.00000000

C -19.57650806 -0.70813103 0.00000000

C -19.57650752 0.70813521 0.00000000

H 22.97777696 -1.24967657 0.00000000

H 22.97777608 1.24968322 0.00000000

H 20.83241790 -2.50077383 0.00000000

H 20.83241641 2.50077900 0.00000000

H 18.37920414 -2.50120693 0.00000000

H 18.37920262 2.50121047 0.00000000

H 15.92500437 -2.50268442 0.00000000

H 15.92500328 2.50268665 0.00000000

H 13.47416082 -2.50279394 0.00000000

H 13.47416000 2.50279528 0.00000000

H 11.02434494 -2.50249423 0.00000000

H 11.02434435 2.50249499 0.00000000

H 8.57456835 -2.50217117 0.00000000

H 8.57456787 2.50217149 0.00000000

H 6.12447295 -2.50195937 0.00000000

H 6.12447244 2.50195920 0.00000000

H 3.67401985 -2.50186059 0.00000000

H 3.67401930 2.50185990 0.00000000

H 1.22336022 -2.50183442 0.00000000

H 1.22335964 2.50183309 0.00000000

H -1.22728462 -2.50186230 0.00000000

H -1.22728508 2.50186035 0.00000000

H -3.67769692 -2.50196259 0.00000000

H -3.67769718 2.50196016 0.00000000

H -6.12774419 -2.50217324 0.00000000

H -6.12774414 2.50217066 0.00000000

H -8.57751511 -2.50249435 0.00000000

H -8.57751458 2.50249204 0.00000000

H -11.02748067 -2.50278062 0.00000000

H -11.02747967 2.50277913 0.00000000

H -13.47866570 -2.50265536 0.00000000

H -13.47866433 2.50265515 0.00000000

H -15.93278036 -2.50128842 0.00000000

H -15.93277860 2.50128985 0.00000000

H -18.38535544 -2.50077892 0.00000000

H -18.38535358 2.50078218 0.00000000

H -20.53082161 -1.24952532 0.00000000

H -20.53082066 1.24953023 0.00000000

$end

$comment

17-acene triplet

$end

$molecule

0 3

C 22.02580526 -0.70791946 0.00000000

C 22.02580490 0.70792595 0.00000000

C 20.84223510 -1.40173196 0.00000000

C 20.84223451 1.40173794 0.00000000

C 19.59857917 -0.72156541 0.00000000

C 19.59857879 0.72157077 0.00000000

C 18.38029037 -1.40079622 0.00000000

C 18.38028969 1.40080082 0.00000000

C 17.15450125 -0.72502618 0.00000000

C 17.15450069 0.72502971 0.00000000

C 15.92639231 -1.40244420 0.00000000

C 15.92639116 1.40244687 0.00000000

C 14.70561230 -0.72694104 0.00000000

C 14.70561153 0.72694254 0.00000000

C 13.47558413 -1.40255385 0.00000000

C 13.47558234 1.40255436 0.00000000

C 12.25423516 -0.72757653 0.00000000

C 12.25423439 0.72757609 0.00000000

C 11.02568885 -1.40225493 0.00000000

C 11.02568670 1.40225345 0.00000000

C 9.80220735 -0.72753789 0.00000000

C 9.80220689 0.72753598 0.00000000

C 8.57567819 -1.40196377 0.00000000

C 8.57567611 1.40196112 0.00000000

C 7.35050444 -0.72726624 0.00000000

C 7.35050437 0.72726360 0.00000000

C 6.12522119 -1.40180816 0.00000000

C 6.12521918 1.40180525 0.00000000

C 4.89936823 -0.72702750 0.00000000

C 4.89936828 0.72702468 0.00000000

C 3.67438831 -1.40176213 0.00000000

C 3.67438626 1.40175946 0.00000000

C 2.44864876 -0.72690403 0.00000000

C 2.44864875 0.72690153 0.00000000

C 1.22336794 -1.40175759 0.00000000

C 1.22336593 1.40175530 0.00000000

C -0.00192180 -0.72689823 0.00000000

C -0.00192169 0.72689646 0.00000000

C -1.22765836 -1.40176443 0.00000000

C -1.22765996 1.40176293 0.00000000

C -2.45262512 -0.72701358 0.00000000

C -2.45262469 0.72701293 0.00000000

C -3.67850325 -1.40181154 0.00000000

C -3.67850434 1.40181148 0.00000000

C -4.90374077 -0.72725437 0.00000000

C -4.90374021 0.72725510 0.00000000

C -6.12896478 -1.40196417 0.00000000

C -6.12896564 1.40196578 0.00000000

C -7.35544164 -0.72754323 0.00000000

C -7.35544129 0.72754526 0.00000000

C -8.57896024 -1.40225004 0.00000000

C -8.57896107 1.40225276 0.00000000

C -9.80750048 -0.72761103 0.00000000

C -9.80750047 0.72761372 0.00000000

C -11.02882620 -1.40253066 0.00000000

C -11.02882696 1.40253356 0.00000000

C -12.25892934 -0.72697996 0.00000000

C -12.25892960 0.72698236 0.00000000

C -13.47961832 -1.40240018 0.00000000

C -13.47961894 1.40240234 0.00000000

C -14.70780976 -0.72505996 0.00000000

C -14.70781017 0.72506134 0.00000000

C -15.93348715 -1.40088712 0.00000000

C -15.93348780 1.40088792 0.00000000

C -17.15176407 -0.72148568 0.00000000

C -17.15176452 0.72148552 0.00000000

C -18.39520035 -1.40173052 0.00000000

C -18.39520121 1.40172960 0.00000000

C -19.57881575 -0.70786891 0.00000000

C -19.57881621 0.70786709 0.00000000

H 22.97997193 -1.24961025 0.00000000

H 22.97997135 1.24961718 0.00000000

H 20.83420354 -2.50054040 0.00000000

H 20.83420256 2.50054641 0.00000000

H 18.38074822 -2.50100215 0.00000000

H 18.38074667 2.50100689 0.00000000

H 15.92644677 -2.50251038 0.00000000

H 15.92644474 2.50251325 0.00000000

H 13.47559834 -2.50264393 0.00000000

H 13.47559575 2.50264458 0.00000000

H 11.02570867 -2.50237558 0.00000000

H 11.02570587 2.50237407 0.00000000

H 8.57569280 -2.50210396 0.00000000

H 8.57569020 2.50210118 0.00000000

H 6.12523391 -2.50195578 0.00000000

H 6.12523151 2.50195278 0.00000000

H 3.67439052 -2.50191031 0.00000000

H 3.67438840 2.50190759 0.00000000

H 1.22335960 -2.50190500 0.00000000

H 1.22335779 2.50190259 0.00000000

H -1.22765718 -2.50191188 0.00000000

H -1.22765848 2.50191020 0.00000000

H -3.67845983 -2.50195797 0.00000000

H -3.67846062 2.50195779 0.00000000

H -6.12886810 -2.50210373 0.00000000

H -6.12886865 2.50210534 0.00000000

H -8.57887562 -2.50237233 0.00000000

H -8.57887628 2.50237510 0.00000000

H -11.02891604 -2.50262702 0.00000000

H -11.02891695 2.50262993 0.00000000

H -13.48010905 -2.50248070 0.00000000

H -13.48011007 2.50248287 0.00000000

H -15.93431826 -2.50108780 0.00000000

H -15.93431953 2.50108863 0.00000000

H -18.38713347 -2.50054872 0.00000000

H -18.38713498 2.50054784 0.00000000

H -20.53301875 -1.24945086 0.00000000

H -20.53301952 1.24944849 0.00000000

$end

$comment

18-acene singlet

$end

$molecule

0 1

C 22.02527054 -0.70810811 0.00000000

C 22.02526934 0.70811984 0.00000000

C 20.84214056 -1.40198407 0.00000000

C 20.84213823 1.40199375 0.00000000

C 19.59823288 -0.72171947 0.00000000

C 19.59823176 0.72172717 0.00000000

C 18.38065891 -1.40110702 0.00000000

C 18.38065680 1.40111277 0.00000000

C 17.15456269 -0.72521812 0.00000000

C 17.15456166 0.72522212 0.00000000

C 15.92687161 -1.40258962 0.00000000

C 15.92686978 1.40259183 0.00000000

C 14.70624110 -0.72708572 0.00000000

C 14.70624025 0.72708655 0.00000000

C 13.47609569 -1.40271142 0.00000000

C 13.47609428 1.40271073 0.00000000

C 12.25543824 -0.72774455 0.00000000

C 12.25543766 0.72774285 0.00000000

C 11.02633694 -1.40240890 0.00000000

C 11.02633594 1.40240614 0.00000000

C 9.80382272 -0.72774996 0.00000000

C 9.80382228 0.72774645 0.00000000

C 8.57661743 -1.40207362 0.00000000

C 8.57661671 1.40206940 0.00000000

C 7.35229968 -0.72751198 0.00000000

C 7.35229937 0.72750729 0.00000000

C 6.12654298 -1.40185837 0.00000000

C 6.12654259 1.40185316 0.00000000

C 4.90119607 -0.72726900 0.00000000

C 4.90119597 0.72726371 0.00000000

C 3.67608916 -1.40176116 0.00000000

C 3.67608908 1.40175555 0.00000000

C 2.45048827 -0.72711395 0.00000000

C 2.45048834 0.72710835 0.00000000

C 1.22538991 -1.40173172 0.00000000

C 1.22538997 1.40172611 0.00000000

C -0.00000009 -0.72706286 0.00000000

C -0.00000005 0.72705724 0.00000000

C -1.22538999 -1.40173153 0.00000000

C -1.22538992 1.40172603 0.00000000

C -2.45048800 -0.72711369 0.00000000

C -2.45048799 0.72710829 0.00000000

C -3.67608840 -1.40176069 0.00000000

C -3.67608820 1.40175542 0.00000000

C -4.90119470 -0.72726858 0.00000000

C -4.90119454 0.72726369 0.00000000

C -6.12654104 -1.40185785 0.00000000

C -6.12654058 1.40185312 0.00000000

C -7.35229725 -0.72751160 0.00000000

C -7.35229690 0.72750739 0.00000000

C -8.57661473 -1.40207329 0.00000000

C -8.57661400 1.40206959 0.00000000

C -9.80381999 -0.72774978 0.00000000

C -9.80381956 0.72774674 0.00000000

C -11.02633450 -1.40240888 0.00000000

C -11.02633353 1.40240663 0.00000000

C -12.25543633 -0.72774458 0.00000000

C -12.25543577 0.72774331 0.00000000

C -13.47609452 -1.40271174 0.00000000

C -13.47609322 1.40271140 0.00000000

C -14.70624084 -0.72708598 0.00000000

C -14.70624004 0.72708701 0.00000000

C -15.92687226 -1.40259015 0.00000000

C -15.92687058 1.40259246 0.00000000

C -17.15456429 -0.72521853 0.00000000

C -17.15456334 0.72522244 0.00000000

C -18.38066126 -1.40110769 0.00000000

C -18.38065931 1.40111324 0.00000000

C -19.59823592 -0.72171995 0.00000000

C -19.59823488 0.72172730 0.00000000

C -20.84214413 -1.40198471 0.00000000

C -20.84214199 1.40199390 0.00000000

C -22.02527450 -0.70810858 0.00000000

C -22.02527340 0.70811965 0.00000000

H 22.97953890 -1.24964292 0.00000000

H 22.97953681 1.24965619 0.00000000

H 20.83431363 -2.50080891 0.00000000

H 20.83430951 2.50081850 0.00000000

H 18.38166572 -2.50131166 0.00000000

H 18.38166197 2.50131732 0.00000000

H 15.92734039 -2.50267738 0.00000000

H 15.92733722 2.50267941 0.00000000

H 13.47600459 -2.50281433 0.00000000

H 13.47600201 2.50281344 0.00000000

H 11.02603667 -2.50253778 0.00000000

H 11.02603481 2.50253485 0.00000000

H 8.57635893 -2.50222288 0.00000000

H 8.57635771 2.50221851 0.00000000

H 6.12641375 -2.50201945 0.00000000

H 6.12641310 2.50201409 0.00000000

H 3.67605598 -2.50192734 0.00000000

H 3.67605566 2.50192163 0.00000000

H 1.22538858 -2.50189934 0.00000000

H 1.22538856 2.50189371 0.00000000

H -1.22538847 -2.50189905 0.00000000

H -1.22538824 2.50189353 0.00000000

H -3.67605516 -2.50192665 0.00000000

H -3.67605465 2.50192129 0.00000000

H -6.12641194 -2.50201871 0.00000000

H -6.12641121 2.50201387 0.00000000

H -8.57635650 -2.50222254 0.00000000

H -8.57635530 2.50221873 0.00000000

H -11.02603452 -2.50253799 0.00000000

H -11.02603272 2.50253561 0.00000000

H -13.47600353 -2.50281508 0.00000000

H -13.47600117 2.50281458 0.00000000

H -15.92734095 -2.50267840 0.00000000

H -15.92733805 2.50268056 0.00000000

H -18.38166789 -2.50131276 0.00000000

H -18.38166439 2.50131823 0.00000000

H -20.83431712 -2.50080986 0.00000000

H -20.83431332 2.50081897 0.00000000

H -22.97954302 -1.24964363 0.00000000

H -22.97954110 1.24965613 0.00000000

$end

$comment

18-acene triplet

$end

$molecule

0 3

C 22.02731440 -0.70788961 0.00000000

C 22.02731684 0.70785387 0.00000000

C 20.84374033 -1.40180351 0.00000000

C 20.84374524 1.40177178 0.00000000

C 19.60027903 -0.72154524 0.00000000

C 19.60028143 0.72151747 0.00000000

C 18.38204874 -1.40095087 0.00000000

C 18.38205340 1.40092703 0.00000000

C 17.15635053 -0.72513657 0.00000000

C 17.15635261 0.72511611 0.00000000

C 15.92818562 -1.40245144 0.00000000

C 15.92818974 1.40243449 0.00000000

C 14.70751073 -0.72704161 0.00000000

C 14.70751265 0.72702801 0.00000000

C 13.47740087 -1.40259249 0.00000000

C 13.47740467 1.40258235 0.00000000

C 12.25614639 -0.72765090 0.00000000

C 12.25614843 0.72764461 0.00000000

C 11.02755571 -1.40231654 0.00000000

C 11.02755927 1.40231421 0.00000000

C 9.80414887 -0.72757276 0.00000000

C 9.80415090 0.72757458 0.00000000

C 8.57759661 -1.40201953 0.00000000

C 8.57759962 1.40202572 0.00000000

C 7.35247480 -0.72729172 0.00000000

C 7.35247656 0.72730199 0.00000000

C 6.12719194 -1.40185281 0.00000000

C 6.12719419 1.40186746 0.00000000

C 4.90133771 -0.72706709 0.00000000

C 4.90133908 0.72708549 0.00000000

C 3.67642877 -1.40180189 0.00000000

C 3.67643017 1.40182417 0.00000000

C 2.45058386 -0.72695543 0.00000000

C 2.45058482 0.72698080 0.00000000

C 1.22549153 -1.40179993 0.00000000

C 1.22549198 1.40182854 0.00000000

C 0.00000018 -0.72692440 0.00000000

C 0.00000060 0.72695510 0.00000000

C -1.22549063 -1.40179774 0.00000000

C -1.22549145 1.40183085 0.00000000

C -2.45058365 -0.72695127 0.00000000

C -2.45058397 0.72698515 0.00000000

C -3.67642801 -1.40179565 0.00000000

C -3.67643035 1.40183079 0.00000000

C -4.90133782 -0.72705919 0.00000000

C -4.90133901 0.72709363 0.00000000

C -6.12719142 -1.40184326 0.00000000

C -6.12719539 1.40187739 0.00000000

C -7.35247528 -0.72728106 0.00000000

C -7.35247733 0.72731285 0.00000000

C -8.57759617 -1.40200786 0.00000000

C -8.57760179 1.40203761 0.00000000

C -9.80414933 -0.72756104 0.00000000

C -9.80415237 0.72758635 0.00000000

C -11.02755478 -1.40230469 0.00000000

C -11.02756218 1.40232597 0.00000000

C -12.25614617 -0.72764048 0.00000000

C -12.25615043 0.72765488 0.00000000

C -13.47739877 -1.40258325 0.00000000

C -13.47740813 1.40259127 0.00000000

C -14.70750938 -0.72703526 0.00000000

C -14.70751484 0.72703410 0.00000000

C -15.92818231 -1.40244769 0.00000000

C -15.92819324 1.40243777 0.00000000

C -17.15634827 -0.72513640 0.00000000

C -17.15635442 0.72511600 0.00000000

C -18.38204471 -1.40095406 0.00000000

C -18.38205645 1.40092336 0.00000000

C -19.60027637 -0.72155198 0.00000000

C -19.60028268 0.72151050 0.00000000

C -20.84373579 -1.40181372 0.00000000

C -20.84374797 1.40176124 0.00000000

C -22.02731150 -0.70790318 0.00000000

C -22.02731772 0.70784017 0.00000000

H 22.98145711 -1.24963888 0.00000000

H 22.98146137 1.24959995 0.00000000

H 20.83593380 -2.50062912 0.00000000

H 20.83594238 2.50059750 0.00000000

H 18.38307340 -2.50115753 0.00000000

H 18.38308160 2.50113384 0.00000000

H 15.92863363 -2.50254150 0.00000000

H 15.92864099 2.50252467 0.00000000

H 13.47728101 -2.50269586 0.00000000

H 13.47728786 2.50268577 0.00000000

H 11.02726830 -2.50244247 0.00000000

H 11.02727478 2.50244023 0.00000000

H 8.57740411 -2.50216197 0.00000000

H 8.57740982 2.50216836 0.00000000

H 6.12714886 -2.50200333 0.00000000

H 6.12715347 2.50201825 0.00000000

H 3.67646169 -2.50195456 0.00000000

H 3.67646475 2.50197717 0.00000000

H 1.22551395 -2.50195242 0.00000000

H 1.22551518 2.50198148 0.00000000

H -1.22551345 -2.50195021 0.00000000

H -1.22551445 2.50198393 0.00000000

H -3.67646120 -2.50194825 0.00000000

H -3.67646477 2.50198411 0.00000000

H -6.12714823 -2.50199366 0.00000000

H -6.12715470 2.50202856 0.00000000

H -8.57740293 -2.50215007 0.00000000

H -8.57741255 2.50218062 0.00000000

H -11.02726594 -2.50243020 0.00000000

H -11.02727890 2.50245233 0.00000000

H -13.47727678 -2.50268611 0.00000000

H -13.47729326 2.50269492 0.00000000

H -15.92862776 -2.50253736 0.00000000

H -15.92864702 2.50252798 0.00000000

H -18.38306665 -2.50116051 0.00000000

H -18.38308744 2.50113008 0.00000000

H -20.83592631 -2.50063916 0.00000000

H -20.83594806 2.50058689 0.00000000

H -22.98145267 -1.24965501 0.00000000

H -22.98146367 1.24958361 0.00000000

$end

$comment

19-acene singlet

$end

$molecule

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C 24.47412603 -0.70843798 0.00000000

C 24.47412472 0.70844884 0.00000000

C 23.29132302 -1.40203887 0.00000000

C 23.29132041 1.40204745 0.00000000

C 22.04688242 -0.72173409 0.00000000

C 22.04688114 0.72174044 0.00000000

C 20.82947100 -1.40089147 0.00000000

C 20.82946866 1.40089559 0.00000000

C 19.60324197 -0.72513021 0.00000000

C 19.60324086 0.72513260 0.00000000

C 18.37573177 -1.40264274 0.00000000

C 18.37572992 1.40264322 0.00000000

C 17.15500304 -0.72699027 0.00000000

C 17.15500225 0.72698948 0.00000000

C 15.92494094 -1.40269788 0.00000000

C 15.92493971 1.40269564 0.00000000

C 14.70429576 -0.72767113 0.00000000

C 14.70429530 0.72766812 0.00000000

C 13.47514136 -1.40237128 0.00000000

C 13.47514068 1.40236741 0.00000000

C 12.25273288 -0.72773242 0.00000000

C 12.25273267 0.72772809 0.00000000

C 11.02541293 -1.40203314 0.00000000

C 11.02541260 1.40202839 0.00000000

C 9.80119831 -0.72752961 0.00000000

C 9.80119821 0.72752464 0.00000000

C 8.57537342 -1.40182735 0.00000000

C 8.57537331 1.40182226 0.00000000

C 7.35004095 -0.72729832 0.00000000

C 7.35004091 0.72729319 0.00000000

C 6.12498025 -1.40174949 0.00000000

C 6.12498024 1.40174433 0.00000000

C 4.89927736 -0.72713516 0.00000000

C 4.89927737 0.72713004 0.00000000

C 3.67434069 -1.40173786 0.00000000

C 3.67434078 1.40173277 0.00000000

C 2.44877531 -0.72705543 0.00000000

C 2.44877540 0.72705050 0.00000000

C 1.22358359 -1.40174061 0.00000000

C 1.22358384 1.40173583 0.00000000

C -0.00163282 -0.72705040 0.00000000

C -0.00163266 0.72704596 0.00000000

C -1.22717850 -1.40173866 0.00000000

C -1.22717811 1.40173447 0.00000000

C -2.45211792 -0.72712142 0.00000000

C -2.45211767 0.72711768 0.00000000

C -3.67783131 -1.40175136 0.00000000

C -3.67783074 1.40174800 0.00000000

C -4.90285470 -0.72728066 0.00000000

C -4.90285438 0.72727790 0.00000000

C -6.12823919 -1.40182962 0.00000000

C -6.12823851 1.40182735 0.00000000

C -7.35399034 -0.72751805 0.00000000

C -7.35398994 0.72751643 0.00000000

C -8.57828270 -1.40203174 0.00000000

C -8.57828189 1.40203074 0.00000000

C -9.80553018 -0.72774168 0.00000000

C -9.80552971 0.72774141 0.00000000

C -11.02799111 -1.40236484 0.00000000

C -11.02799022 1.40236530 0.00000000

C -12.25713689 -0.72771502 0.00000000

C -12.25713638 0.72771623 0.00000000

C -13.47775093 -1.40267745 0.00000000

C -13.47775000 1.40267949 0.00000000

C -14.70790520 -0.72703855 0.00000000

C -14.70790471 0.72704133 0.00000000

C -15.92852303 -1.40256871 0.00000000

C -15.92852223 1.40257229 0.00000000

C -17.15618125 -0.72517126 0.00000000

C -17.15618089 0.72517538 0.00000000

C -18.38229315 -1.40108465 0.00000000

C -18.38229258 1.40108942 0.00000000

C -19.59982736 -0.72170371 0.00000000

C -19.59982712 0.72170887 0.00000000

C -20.84375492 -1.40196350 0.00000000

C -20.84375453 1.40196904 0.00000000

C -22.02686642 -0.70813266 0.00000000

C -22.02686622 0.70813850 0.00000000

H 25.42887046 -1.24950528 0.00000000

H 25.42886817 1.24951788 0.00000000

H 23.28217417 -2.50082923 0.00000000

H 23.28216954 2.50083771 0.00000000

H 20.83001146 -2.50111376 0.00000000

H 20.83000739 2.50111773 0.00000000

H 18.37573679 -2.50270047 0.00000000

H 18.37573354 2.50270072 0.00000000

H 15.92494803 -2.50278460 0.00000000

H 15.92494576 2.50278212 0.00000000

H 13.47514736 -2.50249218 0.00000000

H 13.47514602 2.50248811 0.00000000

H 11.02539659 -2.50217804 0.00000000

H 11.02539593 2.50217316 0.00000000

H 8.57535510 -2.50198392 0.00000000

H 8.57535491 2.50197877 0.00000000

H 6.12496734 -2.50190887 0.00000000

H 6.12496734 2.50190368 0.00000000

H 3.67432904 -2.50189627 0.00000000

H 3.67432922 2.50189117 0.00000000

H 1.22357013 -2.50189799 0.00000000

H 1.22357062 2.50189318 0.00000000

H -1.22718309 -2.50189630 0.00000000

H -1.22718239 2.50189205 0.00000000

H -3.67780039 -2.50190936 0.00000000

H -3.67779939 2.50190594 0.00000000

H -6.12814564 -2.50198474 0.00000000

H -6.12814447 2.50198241 0.00000000

H -8.57813406 -2.50217623 0.00000000

H -8.57813268 2.50217517 0.00000000

H -11.02787159 -2.50248797 0.00000000

H -11.02787006 2.50248838 0.00000000

H -13.47782854 -2.50277184 0.00000000

H -13.47782693 2.50277387 0.00000000

H -15.92902029 -2.50264613 0.00000000

H -15.92901892 2.50264977 0.00000000

H -18.38314255 -2.50128156 0.00000000

H -18.38314148 2.50128640 0.00000000

H -20.83572398 -2.50077849 0.00000000

H -20.83572326 2.50078407 0.00000000

H -22.98118779 -1.24951517 0.00000000

H -22.98118742 1.24952130 0.00000000

$end

$comment

19-acene triplet

$end

$molecule

0 3

C 24.47603503 -0.70823581 0.00000000

C 24.47603356 0.70824716 0.00000000

C 23.29285905 -1.40185692 0.00000000

C 23.29285617 1.40186567 0.00000000

C 22.04878451 -0.72156965 0.00000000

C 22.04878296 0.72157558 0.00000000

C 20.83081182 -1.40073631 0.00000000

C 20.83080894 1.40073948 0.00000000

C 19.60492412 -0.72504285 0.00000000

C 19.60492242 0.72504301 0.00000000

C 18.37700179 -1.40251674 0.00000000

C 18.37699884 1.40251411 0.00000000

C 17.15623834 -0.72694368 0.00000000

C 17.15623668 0.72693842 0.00000000

C 15.92619722 -1.40259193 0.00000000

C 15.92619439 1.40258411 0.00000000

C 14.70503861 -0.72759293 0.00000000

C 14.70503734 0.72758343 0.00000000

C 13.47631487 -1.40228878 0.00000000

C 13.47631248 1.40227746 0.00000000

C 12.25313421 -0.72758601 0.00000000

C 12.25313355 0.72757415 0.00000000

C 11.02636747 -1.40198644 0.00000000

C 11.02636576 1.40197375 0.00000000

C 9.80146398 -0.72734232 0.00000000

C 9.80146391 0.72733015 0.00000000

C 8.57602280 -1.40182414 0.00000000

C 8.57602184 1.40181223 0.00000000

C 7.35028082 -0.72712435 0.00000000

C 7.35028125 0.72711381 0.00000000

C 6.12534078 -1.40178540 0.00000000

C 6.12534044 1.40177604 0.00000000

C 4.89947289 -0.72700663 0.00000000

C 4.89947361 0.72699927 0.00000000

C 3.67448953 -1.40179905 0.00000000

C 3.67448961 1.40179359 0.00000000

C 2.44885188 -0.72696333 0.00000000

C 2.44885276 0.72696023 0.00000000

C 1.22358421 -1.40180914 0.00000000

C 1.22358456 1.40180832 0.00000000

C -0.00171407 -0.72695670 0.00000000

C -0.00171308 0.72695849 0.00000000

C -1.22732587 -1.40179566 0.00000000

C -1.22732536 1.40179989 0.00000000

C -2.45231979 -0.72698746 0.00000000

C -2.45231876 0.72699427 0.00000000

C -3.67818994 -1.40177931 0.00000000

C -3.67818953 1.40178852 0.00000000

C -4.90310106 -0.72709669 0.00000000

C -4.90310021 0.72710800 0.00000000

C -6.12888699 -1.40181617 0.00000000

C -6.12888710 1.40182947 0.00000000

C -7.35425857 -0.72731703 0.00000000

C -7.35425822 0.72733139 0.00000000

C -8.57923722 -1.40197446 0.00000000

C -8.57923828 1.40198994 0.00000000

C -9.80592800 -0.72758106 0.00000000

C -9.80592843 0.72759608 0.00000000

C -11.02916622 -1.40227274 0.00000000

C -11.02916847 1.40228755 0.00000000

C -12.25787190 -0.72762620 0.00000000

C -12.25787327 0.72763882 0.00000000

C -13.47900839 -1.40256435 0.00000000

C -13.47901182 1.40257513 0.00000000

C -14.70913115 -0.72698727 0.00000000

C -14.70913334 0.72699445 0.00000000

C -15.92979373 -1.40244155 0.00000000

C -15.92979807 1.40244534 0.00000000

C -17.15785429 -0.72508424 0.00000000

C -17.15785694 0.72508357 0.00000000

C -18.38363503 -1.40093946 0.00000000

C -18.38364000 1.40093434 0.00000000

C -19.60172455 -0.72154288 0.00000000

C -19.60172734 0.72153294 0.00000000

C -20.84528316 -1.40179829 0.00000000

C -20.84528847 1.40178348 0.00000000

C -22.02876840 -0.70794533 0.00000000

C -22.02877113 0.70792586 0.00000000

H 25.43067936 -1.24946940 0.00000000

H 25.43067673 1.24948279 0.00000000

H 23.28367707 -2.50064979 0.00000000

H 23.28367177 2.50065852 0.00000000

H 20.83135516 -2.50096258 0.00000000

H 20.83134982 2.50096574 0.00000000

H 18.37700884 -2.50257642 0.00000000

H 18.37700367 2.50257369 0.00000000

H 15.92622000 -2.50268005 0.00000000

H 15.92621536 2.50267196 0.00000000

H 13.47635019 -2.50240970 0.00000000

H 13.47634655 2.50239795 0.00000000

H 11.02638674 -2.50212858 0.00000000

H 11.02638443 2.50211538 0.00000000

H 8.57603632 -2.50197444 0.00000000

H 8.57603542 2.50196205 0.00000000

H 6.12534880 -2.50193546 0.00000000

H 6.12534909 2.50192573 0.00000000

H 3.67448701 -2.50194627 0.00000000

H 3.67448816 2.50194056 0.00000000

H 1.22356948 -2.50195473 0.00000000

H 1.22357119 2.50195378 0.00000000

H -1.22734317 -2.50194200 0.00000000

H -1.22734127 2.50194625 0.00000000

H -3.67818510 -2.50192762 0.00000000

H -3.67818354 2.50193704 0.00000000

H -6.12882935 -2.50196424 0.00000000

H -6.12882889 2.50197796 0.00000000

H -8.57912288 -2.50211509 0.00000000

H -8.57912429 2.50213115 0.00000000

H -11.02906830 -2.50239481 0.00000000

H -11.02907199 2.50241024 0.00000000

H -13.47909297 -2.50265940 0.00000000

H -13.47909885 2.50267072 0.00000000

H -15.93028646 -2.50252040 0.00000000

H -15.93029410 2.50252456 0.00000000

H -18.38447009 -2.50113815 0.00000000

H -18.38447903 2.50113324 0.00000000

H -20.83722515 -2.50061484 0.00000000

H -20.83723466 2.50060016 0.00000000

H -22.98300477 -1.24947160 0.00000000

H -22.98300958 1.24944848 0.00000000

$end

$comment

20-acene singlet

$end

$molecule

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C 24.47578610 -0.70811182 0.00000000

C 24.47578576 0.70811572 0.00000000

C 23.29265965 -1.40199309 0.00000000

C 23.29265897 1.40199639 0.00000000

C 22.04875857 -0.72172047 0.00000000

C 22.04875826 0.72172312 0.00000000

C 20.83118480 -1.40111250 0.00000000

C 20.83118406 1.40111455 0.00000000

C 19.60509866 -0.72521666 0.00000000

C 19.60509821 0.72521797 0.00000000

C 18.37740232 -1.40259343 0.00000000

C 18.37740156 1.40259416 0.00000000

C 17.15679072 -0.72708141 0.00000000

C 17.15679030 0.72708172 0.00000000

C 15.92662946 -1.40271144 0.00000000

C 15.92662895 1.40271103 0.00000000

C 14.70599960 -0.72773925 0.00000000

C 14.70599948 0.72773874 0.00000000

C 13.47687469 -1.40240645 0.00000000

C 13.47687455 1.40240551 0.00000000

C 12.25439034 -0.72774934 0.00000000

C 12.25439039 0.72774833 0.00000000

C 11.02716661 -1.40207249 0.00000000

C 11.02716657 1.40207142 0.00000000

C 9.80285629 -0.72752188 0.00000000

C 9.80285625 0.72752071 0.00000000

C 8.57712297 -1.40186615 0.00000000

C 8.57712290 1.40186501 0.00000000

C 7.35171565 -0.72729532 0.00000000

C 7.35171557 0.72729418 0.00000000

C 6.12672637 -1.40178929 0.00000000

C 6.12672629 1.40178805 0.00000000

C 4.90095054 -0.72715242 0.00000000

C 4.90095051 0.72715128 0.00000000

C 3.67610304 -1.40178602 0.00000000

C 3.67610301 1.40178474 0.00000000

C 2.45042332 -0.72708791 0.00000000

C 2.45042335 0.72708668 0.00000000

C 1.22537663 -1.40180060 0.00000000

C 1.22537663 1.40179930 0.00000000

C 0.00000014 -0.72707136 0.00000000

C 0.00000014 0.72707006 0.00000000

C -1.22537638 -1.40180065 0.00000000

C -1.22537640 1.40179930 0.00000000

C -2.45042314 -0.72708796 0.00000000

C -2.45042317 0.72708667 0.00000000

C -3.67610294 -1.40178610 0.00000000

C -3.67610292 1.40178475 0.00000000

C -4.90095056 -0.72715249 0.00000000

C -4.90095053 0.72715128 0.00000000

C -6.12672652 -1.40178936 0.00000000

C -6.12672643 1.40178809 0.00000000

C -7.35171592 -0.72729538 0.00000000

C -7.35171583 0.72729421 0.00000000

C -8.57712335 -1.40186619 0.00000000

C -8.57712325 1.40186506 0.00000000

C -9.80285673 -0.72752189 0.00000000

C -9.80285670 0.72752075 0.00000000

C -11.02716709 -1.40207249 0.00000000

C -11.02716705 1.40207143 0.00000000

C -12.25439081 -0.72774932 0.00000000

C -12.25439085 0.72774832 0.00000000

C -13.47687510 -1.40240639 0.00000000

C -13.47687494 1.40240548 0.00000000

C -14.70599991 -0.72773918 0.00000000

C -14.70599980 0.72773874 0.00000000

C -15.92662965 -1.40271133 0.00000000

C -15.92662916 1.40271101 0.00000000

C -17.15679078 -0.72708131 0.00000000

C -17.15679036 0.72708171 0.00000000

C -18.37740222 -1.40259332 0.00000000

C -18.37740149 1.40259411 0.00000000

C -19.60509844 -0.72521660 0.00000000

C -19.60509800 0.72521794 0.00000000

C -20.83118444 -1.40111244 0.00000000

C -20.83118375 1.40111449 0.00000000

C -22.04875812 -0.72172047 0.00000000

C -22.04875783 0.72172303 0.00000000

C -23.29265911 -1.40199309 0.00000000

C -23.29265846 1.40199628 0.00000000

C -24.47578550 -0.70811187 0.00000000

C -24.47578518 0.70811563 0.00000000

H 25.43005520 -1.24964453 0.00000000

H 25.43005460 1.24964888 0.00000000

H 23.28483524 -2.50081694 0.00000000

H 23.28483395 2.50082023 0.00000000

H 20.83219181 -2.50131646 0.00000000

H 20.83219048 2.50131853 0.00000000

H 18.37786666 -2.50268082 0.00000000

H 18.37786566 2.50268148 0.00000000

H 15.92653366 -2.50281424 0.00000000

H 15.92653283 2.50281365 0.00000000

H 13.47656910 -2.50253496 0.00000000

H 13.47656859 2.50253388 0.00000000

H 11.02690904 -2.50222095 0.00000000

H 11.02690885 2.50221982 0.00000000

H 8.57700823 -2.50202560 0.00000000

H 8.57700823 2.50202443 0.00000000

H 6.12672533 -2.50195247 0.00000000

H 6.12672530 2.50195119 0.00000000

H 3.67614287 -2.50194913 0.00000000

H 3.67614276 2.50194780 0.00000000

H 1.22539728 -2.50196281 0.00000000

H 1.22539721 2.50196149 0.00000000

H -1.22539703 -2.50196287 0.00000000

H -1.22539702 2.50196150 0.00000000

H -3.67614279 -2.50194925 0.00000000

H -3.67614269 2.50194786 0.00000000

H -6.12672549 -2.50195260 0.00000000

H -6.12672541 2.50195127 0.00000000

H -8.57700861 -2.50202568 0.00000000

H -8.57700855 2.50202451 0.00000000

H -11.02690949 -2.50222095 0.00000000

H -11.02690931 2.50221983 0.00000000

H -13.47656951 -2.50253488 0.00000000

H -13.47656894 2.50253382 0.00000000

H -15.92653384 -2.50281407 0.00000000

H -15.92653302 2.50281358 0.00000000

H -18.37786654 -2.50268065 0.00000000

H -18.37786560 2.50268137 0.00000000

H -20.83219144 -2.50131635 0.00000000

H -20.83219021 2.50131842 0.00000000

H -23.28483467 -2.50081690 0.00000000

H -23.28483345 2.50082009 0.00000000

H -25.43005462 -1.24964460 0.00000000

H -25.43005404 1.24964877 0.00000000

$end

$comment

20-acene triplet

$end

$molecule

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C 23.29405704 1.40182651 0.00000000

C 22.05050141 -0.72158425 0.00000000

C 22.05050302 0.72156248 0.00000000

C 20.83241802 -1.40099243 0.00000000

C 20.83242100 1.40097344 0.00000000

C 19.60663610 -0.72515637 0.00000000

C 19.60663711 0.72513910 0.00000000

C 18.37858276 -1.40249096 0.00000000

C 18.37858501 1.40247609 0.00000000

C 17.15791725 -0.72705230 0.00000000

C 17.15791798 0.72703919 0.00000000

C 15.92780953 -1.40262777 0.00000000

C 15.92781142 1.40261644 0.00000000

C 14.70668478 -0.72766970 0.00000000

C 14.70668598 0.72766077 0.00000000

C 13.47798756 -1.40234523 0.00000000

C 13.47798947 1.40233825 0.00000000

C 12.25478691 -0.72760786 0.00000000

C 12.25478860 0.72760365 0.00000000

C 11.02807919 -1.40203870 0.00000000

C 11.02808103 1.40203719 0.00000000

C 9.80316288 -0.72733847 0.00000000

C 9.80316474 0.72733984 0.00000000

C 8.57774954 -1.40186260 0.00000000

C 8.57775119 1.40186721 0.00000000

C 7.35203313 -0.72712345 0.00000000

C 7.35203498 0.72713111 0.00000000

C 6.12708042 -1.40181248 0.00000000

C 6.12708181 1.40182344 0.00000000

C 4.90125005 -0.72702583 0.00000000

C 4.90125192 0.72703978 0.00000000

C 3.67626264 -1.40182665 0.00000000

C 3.67626373 1.40184380 0.00000000

C 2.45061053 -0.72700538 0.00000000

C 2.45061228 0.72702526 0.00000000

C 1.22542025 -1.40184819 0.00000000

C 1.22542077 1.40187103 0.00000000

C 0.00000076 -0.72700523 0.00000000

C 0.00000220 0.72703012 0.00000000

C -1.22541763 -1.40184614 0.00000000

C -1.22541791 1.40187351 0.00000000

C -2.45060973 -0.72700133 0.00000000

C -2.45060882 0.72702988 0.00000000

C -3.67626130 -1.40182069 0.00000000

C -3.67626268 1.40185092 0.00000000

C -4.90125106 -0.72701813 0.00000000

C -4.90125087 0.72704838 0.00000000

C -6.12708102 -1.40180324 0.00000000

C -6.12708368 1.40183406 0.00000000

C -7.35203622 -0.72711294 0.00000000

C -7.35203684 0.72714247 0.00000000

C -8.57775195 -1.40185104 0.00000000

C -8.57775591 1.40187979 0.00000000

C -9.80316741 -0.72732637 0.00000000

C -9.80316889 0.72735237 0.00000000

C -11.02808220 -1.40202621 0.00000000

C -11.02808752 1.40204985 0.00000000

C -12.25479123 -0.72759616 0.00000000

C -12.25479369 0.72761516 0.00000000

C -13.47798930 -1.40233383 0.00000000

C -13.47799615 1.40234892 0.00000000

C -14.70668684 -0.72766070 0.00000000

C -14.70669060 0.72766904 0.00000000

C -15.92780843 -1.40262005 0.00000000

C -15.92781676 1.40262278 0.00000000

C -17.15791592 -0.72704792 0.00000000

C -17.15792086 0.72704254 0.00000000

C -18.37857861 -1.40248915 0.00000000

C -18.37858782 1.40247628 0.00000000

C -19.60663197 -0.72515780 0.00000000

C -19.60663718 0.72513662 0.00000000

C -20.83241158 -1.40099709 0.00000000

C -20.83242102 1.40096720 0.00000000

C -22.05049554 -0.72159208 0.00000000

C -22.05050050 0.72155378 0.00000000

C -23.29404554 -1.40186165 0.00000000

C -23.29405508 1.40181463 0.00000000

C -24.47752011 -0.70795174 0.00000000

C -24.47752497 0.70789650 0.00000000

H 25.43169762 -1.24963921 0.00000000

H 25.43170052 1.24960983 0.00000000

H 23.28624814 -2.50067533 0.00000000

H 23.28625380 2.50065108 0.00000000

H 20.83344360 -2.50119779 0.00000000

H 20.83344843 2.50117904 0.00000000

H 18.37903552 -2.50257986 0.00000000

H 18.37903994 2.50256517 0.00000000

H 15.92769443 -2.50273062 0.00000000

H 15.92769837 2.50271925 0.00000000

H 13.47769143 -2.50247122 0.00000000

H 13.47769521 2.50246413 0.00000000

H 11.02786475 -2.50218183 0.00000000

H 11.02786882 2.50218027 0.00000000

H 8.57768534 -2.50201420 0.00000000

H 8.57768970 2.50201881 0.00000000

H 6.12711206 -2.50196588 0.00000000

H 6.12711618 2.50197689 0.00000000

H 3.67631368 -2.50197885 0.00000000

H 3.67631728 2.50199615 0.00000000

H 1.22544168 -2.50199906 0.00000000

H 1.22544425 2.50202221 0.00000000

H -1.22544112 -2.50199710 0.00000000

H -1.22543995 2.50202495 0.00000000

H -3.67631406 -2.50197309 0.00000000

H -3.67631485 2.50200396 0.00000000

H -6.12711379 -2.50195683 0.00000000

H -6.12711687 2.50198837 0.00000000

H -8.57768803 -2.50200263 0.00000000

H -8.57769368 2.50203213 0.00000000

H -11.02786684 -2.50216895 0.00000000

H -11.02787553 2.50219338 0.00000000

H -13.47769131 -2.50245901 0.00000000

H -13.47770311 2.50247492 0.00000000

H -15.92769126 -2.50272193 0.00000000

H -15.92770546 2.50272530 0.00000000

H -18.37902917 -2.50257729 0.00000000

H -18.37904503 2.50256472 0.00000000

H -20.83343437 -2.50120193 0.00000000

H -20.83345152 2.50117211 0.00000000

H -23.28623729 -2.50068566 0.00000000

H -23.28625454 2.50063875 0.00000000

H -25.43168895 -1.24965499 0.00000000

H -25.43169752 1.24959324 0.00000000

$end

$comment

21-acene singlet

$end

$molecule

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C 26.92385770 0.70828104 0.00000000

C 25.74098720 -1.40199051 0.00000000

C 25.74099095 1.40196963 0.00000000

C 24.49669617 -0.72178021 0.00000000

C 24.49669810 0.72176263 0.00000000

C 23.27932044 -1.40099765 0.00000000

C 23.27932405 1.40098327 0.00000000

C 22.05305674 -0.72513801 0.00000000

C 22.05305858 0.72512662 0.00000000

C 20.82550693 -1.40261180 0.00000000

C 20.82551035 1.40260354 0.00000000

C 19.60477670 -0.72698207 0.00000000

C 19.60477840 0.72697665 0.00000000

C 18.37470323 -1.40269262 0.00000000

C 18.37470643 1.40269010 0.00000000

C 17.15407615 -0.72766570 0.00000000

C 17.15407774 0.72766587 0.00000000

C 15.92490638 -1.40236805 0.00000000

C 15.92490928 1.40237085 0.00000000

C 14.70252610 -0.72772358 0.00000000

C 14.70252750 0.72772874 0.00000000

C 13.47518402 -1.40202510 0.00000000

C 13.47518649 1.40203258 0.00000000

C 12.25099829 -0.72752315 0.00000000

C 12.25099943 0.72753258 0.00000000

C 11.02515823 -1.40181864 0.00000000

C 11.02516015 1.40182996 0.00000000

C 9.79982941 -0.72730233 0.00000000

C 9.79983023 0.72731515 0.00000000

C 8.57479831 -1.40174877 0.00000000

C 8.57479965 1.40176294 0.00000000

C 7.34902666 -0.72715528 0.00000000

C 7.34902720 0.72717049 0.00000000

C 6.12421924 -1.40175622 0.00000000

C 6.12422002 1.40177223 0.00000000

C 4.89846579 -0.72708577 0.00000000

C 4.89846604 0.72710240 0.00000000

C 3.67354033 -1.40178459 0.00000000

C 3.67354058 1.40180147 0.00000000

C 2.44802185 -0.72706308 0.00000000

C 2.44802184 0.72708016 0.00000000

C 1.22283063 -1.40179847 0.00000000

C 1.22283037 1.40181530 0.00000000

C -0.00238778 -0.72706134 0.00000000

C -0.00238805 0.72707793 0.00000000

C -1.22788166 -1.40178611 0.00000000

C -1.22788244 1.40180196 0.00000000

C -2.45282363 -0.72708000 0.00000000

C -2.45282415 0.72709514 0.00000000

C -3.67856837 -1.40175931 0.00000000

C -3.67856960 1.40177334 0.00000000

C -4.90336764 -0.72714493 0.00000000

C -4.90336843 0.72715788 0.00000000

C -6.12915936 -1.40175350 0.00000000

C -6.12916107 1.40176493 0.00000000

C -7.35414752 -0.72728999 0.00000000

C -7.35414855 0.72729993 0.00000000

C -8.57953075 -1.40182383 0.00000000

C -8.57953288 1.40183185 0.00000000

C -9.80529857 -0.72751669 0.00000000

C -9.80529981 0.72752293 0.00000000

C -11.02955806 -1.40202651 0.00000000

C -11.02956050 1.40203052 0.00000000

C -12.25683280 -0.72773632 0.00000000

C -12.25683418 0.72773839 0.00000000

C -13.47926106 -1.40236450 0.00000000

C -13.47926375 1.40236401 0.00000000

C -14.70842423 -0.72771050 0.00000000

C -14.70842568 0.72770794 0.00000000

C -15.92901774 -1.40268280 0.00000000

C -15.92902060 1.40267751 0.00000000

C -17.15917673 -0.72703822 0.00000000

C -17.15917822 0.72703065 0.00000000

C -18.37978435 -1.40257957 0.00000000

C -18.37978744 1.40256915 0.00000000

C -19.60744022 -0.72517641 0.00000000

C -19.60744184 0.72516335 0.00000000

C -20.83354600 -1.40109910 0.00000000

C -20.83354932 1.40108317 0.00000000

C -22.05107791 -0.72171459 0.00000000

C -22.05107967 0.72169580 0.00000000

C -23.29499869 -1.40198238 0.00000000

C -23.29500214 1.40196057 0.00000000

C -24.47810708 -0.70814859 0.00000000

C -24.47810885 0.70812394 0.00000000

H 27.87840121 -1.24942445 0.00000000

H 27.87840451 1.24939787 0.00000000

H 25.73226081 -2.50079967 0.00000000

H 25.73226754 2.50077883 0.00000000

H 23.27982156 -2.50120745 0.00000000

H 23.27982790 2.50119312 0.00000000

H 20.82554915 -2.50266644 0.00000000

H 20.82555527 2.50265823 0.00000000

H 18.37471670 -2.50277869 0.00000000

H 18.37472243 2.50277621 0.00000000

H 15.92490618 -2.50248801 0.00000000

H 15.92491133 2.50249086 0.00000000

H 13.47516214 -2.50216886 0.00000000

H 13.47516654 2.50217644 0.00000000

H 11.02514028 -2.50197383 0.00000000

H 11.02514377 2.50198526 0.00000000

H 8.57479407 -2.50190604 0.00000000

H 8.57479653 2.50192032 0.00000000

H 6.12422387 -2.50191111 0.00000000

H 6.12422533 2.50192723 0.00000000

H 3.67354216 -2.50193653 0.00000000

H 3.67354264 2.50195351 0.00000000

H 1.22282078 -2.50194909 0.00000000

H 1.22282032 2.50196601 0.00000000

H -1.22790092 -2.50193770 0.00000000

H -1.22790233 2.50195362 0.00000000

H -3.67857922 -2.50191343 0.00000000

H -3.67858138 2.50192752 0.00000000

H -6.12913166 -2.50190959 0.00000000

H -6.12913466 2.50192105 0.00000000

H -8.57943863 -2.50197785 0.00000000

H -8.57944235 2.50198586 0.00000000

H -11.02941223 -2.50217014 0.00000000

H -11.02941645 2.50217409 0.00000000

H -13.47914692 -2.50248672 0.00000000

H -13.47915164 2.50248616 0.00000000

H -15.92910098 -2.50277616 0.00000000

H -15.92910616 2.50277082 0.00000000

H -18.38028060 -2.50265581 0.00000000

H -18.38028631 2.50264541 0.00000000

H -20.83438718 -2.50129477 0.00000000

H -20.83439318 2.50127888 0.00000000

H -23.28695911 -2.50079577 0.00000000

H -23.28696527 2.50077400 0.00000000

H -25.43242993 -1.24952327 0.00000000

H -25.43243308 1.24949619 0.00000000

$end

$comment

21-acene triplet

$end

$molecule

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C 25.74235699 1.40183164 0.00000000

C 24.49835848 -0.72164541 0.00000000

C 24.49835909 0.72163517 0.00000000

C 23.28053619 -1.40087264 0.00000000

C 23.28053762 1.40086334 0.00000000

C 22.05453946 -0.72506815 0.00000000

C 22.05454004 0.72505973 0.00000000

C 20.82666720 -1.40251164 0.00000000

C 20.82666864 1.40250424 0.00000000

C 19.60589559 -0.72694731 0.00000000

C 19.60589615 0.72694077 0.00000000

C 18.37585655 -1.40261104 0.00000000

C 18.37585767 1.40260553 0.00000000

C 17.15479572 -0.72760603 0.00000000

C 17.15479625 0.72760135 0.00000000

C 15.92599825 -1.40230784 0.00000000

C 15.92599898 1.40230434 0.00000000

C 14.70297416 -0.72760603 0.00000000

C 14.70297470 0.72760365 0.00000000

C 13.47609894 -1.40199443 0.00000000

C 13.47609928 1.40199327 0.00000000

C 12.25135340 -0.72736623 0.00000000

C 12.25135399 0.72736636 0.00000000

C 11.02581417 -1.40181992 0.00000000

C 11.02581433 1.40182130 0.00000000

C 9.80019465 -0.72714962 0.00000000

C 9.80019539 0.72715257 0.00000000

C 8.57519591 -1.40177425 0.00000000

C 8.57519601 1.40177858 0.00000000

C 7.34939007 -0.72703941 0.00000000

C 7.34939092 0.72704545 0.00000000

C 6.12441994 -1.40179358 0.00000000

C 6.12441996 1.40180115 0.00000000

C 4.89874353 -0.72701306 0.00000000

C 4.89874440 0.72702235 0.00000000

C 3.67361759 -1.40182430 0.00000000

C 3.67361746 1.40183527 0.00000000

C 2.44812768 -0.72701731 0.00000000

C 2.44812847 0.72702989 0.00000000

C 1.22283121 -1.40183683 0.00000000

C 1.22283081 1.40185097 0.00000000

C -0.00248995 -0.72701469 0.00000000

C -0.00248932 0.72703016 0.00000000

C -1.22795699 -1.40182233 0.00000000

C -1.22795775 1.40183910 0.00000000

C -2.45310062 -0.72700425 0.00000000

C -2.45310020 0.72702189 0.00000000

C -3.67876551 -1.40179015 0.00000000

C -3.67876673 1.40180873 0.00000000

C -4.90373412 -0.72702316 0.00000000

C -4.90373406 0.72704196 0.00000000

C -6.12955249 -1.40177045 0.00000000

C -6.12955439 1.40178959 0.00000000

C -7.35451747 -0.72712816 0.00000000

C -7.35451791 0.72714660 0.00000000

C -8.58018298 -1.40181604 0.00000000

C -8.58018568 1.40183403 0.00000000

C -9.80565600 -0.72734842 0.00000000

C -9.80565709 0.72736467 0.00000000

C -11.03047146 -1.40198776 0.00000000

C -11.03047498 1.40200247 0.00000000

C -12.25727882 -0.72760788 0.00000000

C -12.25728051 0.72761986 0.00000000

C -13.48035378 -1.40229763 0.00000000

C -13.48035803 1.40230700 0.00000000

C -14.70913891 -0.72764318 0.00000000

C -14.70914120 0.72764879 0.00000000

C -15.93017266 -1.40259647 0.00000000

C -15.93017763 1.40259833 0.00000000

C -17.16028979 -0.72700053 0.00000000

C -17.16029265 0.72699756 0.00000000

C -18.38094622 -1.40247895 0.00000000

C -18.38095196 1.40247121 0.00000000

C -19.60891699 -0.72510767 0.00000000

C -19.60892034 0.72509423 0.00000000

C -20.83476345 -1.40098176 0.00000000

C -20.83476995 1.40096268 0.00000000

C -22.05273795 -0.72158433 0.00000000

C -22.05274159 0.72155904 0.00000000

C -23.29636559 -1.40184745 0.00000000

C -23.29637263 1.40181593 0.00000000

C -24.47977303 -0.70799532 0.00000000

C -24.47977666 0.70795768 0.00000000

H 27.87999308 -1.24938019 0.00000000

H 27.87999415 1.24936700 0.00000000

H 25.73360665 -2.50065412 0.00000000

H 25.73360906 2.50064279 0.00000000

H 23.28104152 -2.50108544 0.00000000

H 23.28104373 2.50107614 0.00000000

H 20.82671366 -2.50256764 0.00000000

H 20.82671594 2.50256029 0.00000000

H 18.37588414 -2.50269758 0.00000000

H 18.37588608 2.50269217 0.00000000

H 15.92602088 -2.50242674 0.00000000

H 15.92602261 2.50242333 0.00000000

H 13.47610235 -2.50213481 0.00000000

H 13.47610378 2.50213366 0.00000000

H 11.02581551 -2.50196926 0.00000000

H 11.02581680 2.50197057 0.00000000

H 8.57519986 -2.50192394 0.00000000

H 8.57520107 2.50192820 0.00000000

H 6.12442406 -2.50194023 0.00000000

H 6.12442519 2.50194776 0.00000000

H 3.67361710 -2.50196803 0.00000000

H 3.67361806 2.50197902 0.00000000

H 1.22282213 -2.50197936 0.00000000

H 1.22282264 2.50199361 0.00000000

H -1.22797379 -2.50196579 0.00000000

H -1.22797398 2.50198274 0.00000000

H -3.67877890 -2.50193612 0.00000000

H -3.67877999 2.50195498 0.00000000

H -6.12953852 -2.50191892 0.00000000

H -6.12954091 2.50193843 0.00000000

H -8.58011474 -2.50196392 0.00000000

H -8.58011863 2.50198232 0.00000000

H -11.03035045 -2.50212756 0.00000000

H -11.03035597 2.50214266 0.00000000

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H -13.48026348 2.50242812 0.00000000

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H -15.93027164 2.50269225 0.00000000

H -18.38144157 -2.50255627 0.00000000

H -18.38145194 2.50254883 0.00000000

H -20.83559614 -2.50117887 0.00000000

H -20.83560789 2.50116003 0.00000000

H -23.28830661 -2.50066214 0.00000000

H -23.28831913 2.50063080 0.00000000

H -25.43402795 -1.24948542 0.00000000

H -25.43403431 1.24944295 0.00000000

$end

$comment

22-acene singlet

$end

$molecule

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C 25.74316111 1.40200486 0.00000000

C 24.49926488 -0.72171936 0.00000000

C 24.49926424 0.72172549 0.00000000

C 23.28169579 -1.40111619 0.00000000

C 23.28169449 1.40112123 0.00000000

C 22.05561179 -0.72521540 0.00000000

C 22.05561108 0.72521926 0.00000000

C 20.82792268 -1.40259766 0.00000000

C 20.82792136 1.40260040 0.00000000

C 19.60731323 -0.72707987 0.00000000

C 19.60731255 0.72708158 0.00000000

C 18.37715766 -1.40271658 0.00000000

C 18.37715656 1.40271720 0.00000000

C 17.15653587 -0.72773651 0.00000000

C 17.15653540 0.72773641 0.00000000

C 15.92740818 -1.40240987 0.00000000

C 15.92740748 1.40240892 0.00000000

C 14.70494063 -0.72774518 0.00000000

C 14.70494037 0.72774380 0.00000000

C 13.47770320 -1.40207379 0.00000000

C 13.47770281 1.40207193 0.00000000

C 12.25342081 -0.72751916 0.00000000

C 12.25342066 0.72751701 0.00000000

C 11.02766242 -1.40186623 0.00000000

C 11.02766216 1.40186383 0.00000000

C 9.80228645 -0.72729752 0.00000000

C 9.80228632 0.72729488 0.00000000

C 8.57727726 -1.40179125 0.00000000

C 8.57727700 1.40178839 0.00000000

C 7.35150964 -0.72716641 0.00000000

C 7.35150949 0.72716331 0.00000000

C 6.12668392 -1.40179834 0.00000000

C 6.12668362 1.40179499 0.00000000

C 4.90094427 -0.72711887 0.00000000

C 4.90094410 0.72711530 0.00000000

C 3.67601405 -1.40183330 0.00000000

C 3.67601377 1.40182945 0.00000000

C 2.45046259 -0.72711467 0.00000000

C 2.45046246 0.72711069 0.00000000

C 1.22533652 -1.40185955 0.00000000

C 1.22533641 1.40185536 0.00000000

C 0.00000006 -0.72711782 0.00000000

C 0.00000006 0.72711370 0.00000000

C -1.22533643 -1.40185953 0.00000000

C -1.22533630 1.40185538 0.00000000

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C -2.45046238 0.72711074 0.00000000

C -3.67601400 -1.40183326 0.00000000

C -3.67601371 1.40182952 0.00000000

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C -4.90094407 0.72711538 0.00000000

C -6.12668394 -1.40179829 0.00000000

C -6.12668363 1.40179509 0.00000000

C -7.35150968 -0.72716636 0.00000000

C -7.35150952 0.72716339 0.00000000

C -8.57727732 -1.40179118 0.00000000

C -8.57727706 1.40178849 0.00000000

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C -12.25342073 0.72751707 0.00000000

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C -13.47770288 1.40207197 0.00000000

C -14.70494065 -0.72774511 0.00000000

C -14.70494043 0.72774383 0.00000000

C -15.92740819 -1.40240979 0.00000000

C -15.92740752 1.40240895 0.00000000

C -17.15653588 -0.72773646 0.00000000

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C -18.37715764 -1.40271653 0.00000000

C -18.37715658 1.40271722 0.00000000

C -19.60731322 -0.72707985 0.00000000

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C -25.74316114 1.40200476 0.00000000

C -26.92628390 -0.70811046 0.00000000

C -26.92628330 0.70811856 0.00000000

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H 27.88055379 1.24964885 0.00000000

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H 25.73533904 2.50082775 0.00000000

H 23.28270541 -2.50131942 0.00000000

H 23.28270309 2.50132446 0.00000000

H 20.82838730 -2.50268434 0.00000000

H 20.82838506 2.50268703 0.00000000

H 18.37705901 -2.50281868 0.00000000

H 18.37705713 2.50281913 0.00000000

H 15.92709955 -2.50253780 0.00000000

H 15.92709826 2.50253667 0.00000000

H 13.47744014 -2.50222170 0.00000000

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H 11.02754252 2.50202270 0.00000000

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H 6.12673845 2.50195668 0.00000000

H 3.67606772 -2.50199287 0.00000000

H 3.67606727 2.50198896 0.00000000

H 1.22535753 -2.50201757 0.00000000

H 1.22535738 2.50201329 0.00000000

H -1.22535747 -2.50201756 0.00000000

H -1.22535724 2.50201332 0.00000000

H -3.67606767 -2.50199284 0.00000000

H -3.67606720 2.50198905 0.00000000

H -6.12673897 -2.50196001 0.00000000

H -6.12673845 2.50195679 0.00000000

H -8.57727775 -2.50195370 0.00000000

H -8.57727728 2.50195098 0.00000000

H -11.02754307 -2.50202509 0.00000000

H -11.02754260 2.50202278 0.00000000

H -13.47744017 -2.50222162 0.00000000

H -13.47743945 2.50221974 0.00000000

H -15.92709956 -2.50253770 0.00000000

H -15.92709828 2.50253669 0.00000000

H -18.37705899 -2.50281861 0.00000000

H -18.37705716 2.50281915 0.00000000

H -20.82838724 -2.50268432 0.00000000

H -20.82838509 2.50268701 0.00000000

H -23.28270535 -2.50131943 0.00000000

H -23.28270311 2.50132439 0.00000000

H -25.73534126 -2.50082056 0.00000000

H -25.73533910 2.50082764 0.00000000

H -27.88055486 -1.24963974 0.00000000

H -27.88055380 1.24964867 0.00000000

$end

$comment

22-acene triplet

$end

$molecule

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C 26.92783024 -0.70795734 0.00000000

C 26.92783023 0.70796176 0.00000000

C 25.74442563 -1.40187276 0.00000000

C 25.74442559 1.40187712 0.00000000

C 24.50081416 -0.72159796 0.00000000

C 24.50081415 0.72160225 0.00000000

C 23.28282560 -1.40100882 0.00000000

C 23.28282554 1.40101310 0.00000000

C 22.05699114 -0.72515867 0.00000000

C 22.05699107 0.72516286 0.00000000

C 20.82900959 -1.40250689 0.00000000

C 20.82900940 1.40251097 0.00000000

C 19.60835261 -0.72705070 0.00000000

C 19.60835247 0.72705455 0.00000000

C 18.37824755 -1.40264347 0.00000000

C 18.37824722 1.40264711 0.00000000

C 17.15720745 -0.72767734 0.00000000

C 17.15720722 0.72768064 0.00000000

C 15.92844905 -1.40235828 0.00000000

C 15.92844857 1.40236121 0.00000000

C 14.70537413 -0.72762874 0.00000000

C 14.70537383 0.72763118 0.00000000

C 13.47858404 -1.40204926 0.00000000

C 13.47858340 1.40205117 0.00000000

C 12.25378092 -0.72736610 0.00000000

C 12.25378055 0.72736739 0.00000000

C 11.02830565 -1.40186875 0.00000000

C 11.02830491 1.40186940 0.00000000

C 9.80266861 -0.72715036 0.00000000

C 9.80266821 0.72715030 0.00000000

C 8.57768058 -1.40181424 0.00000000

C 8.57767978 1.40181346 0.00000000

C 7.35190388 -0.72705281 0.00000000

C 7.35190343 0.72705131 0.00000000

C 6.12690111 -1.40183022 0.00000000

C 6.12690029 1.40182797 0.00000000

C 4.90127591 -0.72704325 0.00000000

C 4.90127545 0.72704032 0.00000000

C 3.67611042 -1.40186482 0.00000000

C 3.67610961 1.40186109 0.00000000

C 2.45065002 -0.72706579 0.00000000

C 2.45064959 0.72706143 0.00000000

C 1.22535921 -1.40188829 0.00000000

C 1.22535848 1.40188320 0.00000000

C -0.00000592 -0.72707855 0.00000000

C -0.00000627 0.72707295 0.00000000

C -1.22537069 -1.40188879 0.00000000

C -1.22537127 1.40188255 0.00000000

C -2.45066157 -0.72706677 0.00000000

C -2.45066179 0.72706025 0.00000000

C -3.67612138 -1.40186620 0.00000000

C -3.67612175 1.40185924 0.00000000

C -4.90128654 -0.72704512 0.00000000

C -4.90128665 0.72703806 0.00000000

C -6.12691081 -1.40183235 0.00000000

C -6.12691091 1.40182502 0.00000000

C -7.35191272 -0.72705532 0.00000000

C -7.35191270 0.72704814 0.00000000

C -8.57768804 -1.40181685 0.00000000

C -8.57768783 1.40180962 0.00000000

C -9.80267475 -0.72715327 0.00000000

C -9.80267455 0.72714647 0.00000000

C -11.02831006 -1.40187159 0.00000000

C -11.02830948 1.40186502 0.00000000

C -12.25378371 -0.72736909 0.00000000

C -12.25378330 0.72736331 0.00000000

C -13.47858512 -1.40205201 0.00000000

C -13.47858414 1.40204680 0.00000000

C -14.70537362 -0.72763149 0.00000000

C -14.70537300 0.72762740 0.00000000

C -15.92844723 -1.40236057 0.00000000

C -15.92844578 1.40235746 0.00000000

C -17.15720411 -0.72767931 0.00000000

C -17.15720323 0.72767777 0.00000000

C -18.37824328 -1.40264471 0.00000000

C -18.37824137 1.40264453 0.00000000

C -19.60834661 -0.72705130 0.00000000

C -19.60834552 0.72705307 0.00000000

C -20.82900271 -1.40250650 0.00000000

C -20.82900044 1.40250998 0.00000000

C -22.05698224 -0.72515744 0.00000000

C -22.05698096 0.72516310 0.00000000

C -23.28281597 -1.40100637 0.00000000

C -23.28281339 1.40101410 0.00000000

C -24.50080270 -0.72159463 0.00000000

C -24.50080131 0.72160471 0.00000000

C -25.74441383 -1.40186821 0.00000000

C -25.74441109 1.40188069 0.00000000

C -26.92781730 -0.70795198 0.00000000

C -26.92781591 0.70796680 0.00000000

H 27.88202673 -1.24962228 0.00000000

H 27.88202671 1.24962673 0.00000000

H 25.73661770 -2.50069651 0.00000000

H 25.73661759 2.50070088 0.00000000

H 23.28385218 -2.50121360 0.00000000

H 23.28385206 2.50121792 0.00000000

H 20.82946590 -2.50259505 0.00000000

H 20.82946556 2.50259917 0.00000000

H 18.37813673 -2.50274546 0.00000000

H 18.37813616 2.50274915 0.00000000

H 15.92814874 -2.50248398 0.00000000

H 15.92814788 2.50248696 0.00000000

H 13.47835379 -2.50219265 0.00000000

H 13.47835264 2.50219461 0.00000000

H 11.02822623 -2.50202158 0.00000000

H 11.02822489 2.50202226 0.00000000

H 8.57770243 -2.50196948 0.00000000

H 8.57770098 2.50196869 0.00000000

H 6.12695338 -2.50198417 0.00000000

H 6.12695194 2.50198189 0.00000000

H 3.67615045 -2.50201657 0.00000000

H 3.67614903 2.50201279 0.00000000

H 1.22537330 -2.50203855 0.00000000

H 1.22537203 2.50203338 0.00000000

H -1.22538427 -2.50203896 0.00000000

H -1.22538525 2.50203261 0.00000000

H -3.67616094 -2.50201768 0.00000000

H -3.67616155 2.50201059 0.00000000

H -6.12696269 -2.50198582 0.00000000

H -6.12696282 2.50197833 0.00000000

H -8.57770959 -2.50197142 0.00000000

H -8.57770920 2.50196401 0.00000000

H -11.02823051 -2.50202365 0.00000000

H -11.02822946 2.50201689 0.00000000

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H -13.47835322 2.50218922 0.00000000

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H -15.92814471 2.50248224 0.00000000

H -18.37813306 -2.50274601 0.00000000

H -18.37812969 2.50274565 0.00000000

H -20.82945980 -2.50259399 0.00000000

H -20.82945583 2.50259733 0.00000000

H -23.28384356 -2.50121056 0.00000000

H -23.28383903 2.50121819 0.00000000

H -25.73660690 -2.50069150 0.00000000

H -25.73660204 2.50070391 0.00000000

H -27.88201403 -1.24961583 0.00000000

H -27.88201158 1.24963250 0.00000000

$end

$comment

23-acene singlet

$end

$molecule

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C 29.37398728 0.70823476 0.00000000

C 28.19110970 -1.40196218 0.00000000

C 28.19110721 1.40197048 0.00000000

C 26.94687139 -0.72180941 0.00000000

C 26.94687015 0.72181552 0.00000000

C 25.72949940 -1.40104281 0.00000000

C 25.72949709 1.40104687 0.00000000

C 24.50325735 -0.72512664 0.00000000

C 24.50325619 0.72512877 0.00000000

C 23.27571088 -1.40259715 0.00000000

C 23.27570877 1.40259731 0.00000000

C 22.05496450 -0.72697416 0.00000000

C 22.05496348 0.72697267 0.00000000

C 20.82490574 -1.40269597 0.00000000

C 20.82490408 1.40269279 0.00000000

C 19.60427293 -0.72766445 0.00000000

C 19.60427219 0.72766015 0.00000000

C 18.37511004 -1.40237544 0.00000000

C 18.37510896 1.40236987 0.00000000

C 17.15273404 -0.72772473 0.00000000

C 17.15273364 0.72771852 0.00000000

C 15.92538705 -1.40203399 0.00000000

C 15.92538657 1.40202708 0.00000000

C 14.70121888 -0.72752593 0.00000000

C 14.70121875 0.72751887 0.00000000

C 13.47535937 -1.40182736 0.00000000

C 13.47535934 1.40182006 0.00000000

C 12.25006137 -0.72730817 0.00000000

C 12.25006145 0.72730099 0.00000000

C 11.02499962 -1.40175688 0.00000000

C 11.02499988 1.40174980 0.00000000

C 9.79926090 -0.72716801 0.00000000

C 9.79926108 0.72716125 0.00000000

C 8.57443009 -1.40176671 0.00000000

C 8.57443051 1.40176029 0.00000000

C 7.34868190 -0.72711165 0.00000000

C 7.34868214 0.72710568 0.00000000

C 6.12378014 -1.40180478 0.00000000

C 6.12378068 1.40179923 0.00000000

C 4.89819163 -0.72710587 0.00000000

C 4.89819193 0.72710096 0.00000000

C 3.67312584 -1.40183772 0.00000000

C 3.67312660 1.40183332 0.00000000

C 2.44771624 -0.72711372 0.00000000

C 2.44771669 0.72711023 0.00000000

C 1.22248616 -1.40184978 0.00000000

C 1.22248717 1.40184693 0.00000000

C -0.00276134 -0.72711279 0.00000000

C -0.00276073 0.72711101 0.00000000

C -1.22815367 -1.40183658 0.00000000

C -1.22815248 1.40183567 0.00000000

C -2.45323504 -0.72710202 0.00000000

C -2.45323438 0.72710216 0.00000000

C -3.67880952 -1.40180266 0.00000000

C -3.67880841 1.40180379 0.00000000

C -4.90371881 -0.72710265 0.00000000

C -4.90371828 0.72710455 0.00000000

C -6.12946485 -1.40176424 0.00000000

C -6.12946405 1.40176705 0.00000000

C -7.35428305 -0.72715260 0.00000000

C -7.35428275 0.72715583 0.00000000

C -8.58004445 -1.40175456 0.00000000

C -8.58004405 1.40175843 0.00000000

C -9.80506210 -0.72728906 0.00000000

C -9.80506202 0.72729303 0.00000000

C -11.03041474 -1.40182497 0.00000000

C -11.03041467 1.40182924 0.00000000

C -12.25620207 -0.72751234 0.00000000

C -12.25620213 0.72751651 0.00000000

C -13.48044334 -1.40202822 0.00000000

C -13.48044349 1.40203242 0.00000000

C -14.70772310 -0.72773088 0.00000000

C -14.70772323 0.72773486 0.00000000

C -15.93014532 -1.40236543 0.00000000

C -15.93014562 1.40236925 0.00000000

C -17.15930342 -0.72770486 0.00000000

C -17.15930360 0.72770835 0.00000000

C -18.37989746 -1.40268175 0.00000000

C -18.37989789 1.40268495 0.00000000

C -19.61004771 -0.72703196 0.00000000

C -19.61004797 0.72703467 0.00000000

C -20.83065664 -1.40257558 0.00000000

C -20.83065735 1.40257777 0.00000000

C -22.05830605 -0.72516876 0.00000000

C -22.05830648 0.72517014 0.00000000

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C -23.28441115 1.40109358 0.00000000

C -24.50193986 -0.72170467 0.00000000

C -24.50194042 0.72170440 0.00000000

C -25.74585669 -1.40197532 0.00000000

C -25.74585779 1.40197412 0.00000000

C -26.92896270 -0.70813597 0.00000000

C -26.92896327 0.70813383 0.00000000

H 30.32838928 -1.24947859 0.00000000

H 30.32838709 1.24949070 0.00000000

H 28.18263308 -2.50077593 0.00000000

H 28.18262860 2.50078417 0.00000000

H 25.72990618 -2.50124026 0.00000000

H 25.72990210 2.50124425 0.00000000

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H 20.82491637 2.50277731 0.00000000

H 18.37511082 -2.50249430 0.00000000

H 18.37510889 2.50248845 0.00000000

H 15.92536560 -2.50217684 0.00000000

H 15.92536473 2.50216967 0.00000000

H 13.47534011 -2.50198178 0.00000000

H 13.47533999 2.50197426 0.00000000

H 11.02499493 -2.50191349 0.00000000

H 11.02499535 2.50190628 0.00000000

H 8.57443838 -2.50192091 0.00000000

H 8.57443917 2.50191440 0.00000000

H 6.12379276 -2.50195549 0.00000000

H 6.12379380 2.50194986 0.00000000

H 3.67313317 -2.50198584 0.00000000

H 3.67313459 2.50198134 0.00000000

H 1.22248134 -2.50199692 0.00000000

H 1.22248307 2.50199400 0.00000000

H -1.22817232 -2.50198449 0.00000000

H -1.22817036 2.50198358 0.00000000

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H -3.67883328 2.50195409 0.00000000

H -6.12947841 -2.50191748 0.00000000

H -6.12947705 2.50192043 0.00000000

H -8.58001682 -2.50190978 0.00000000

H -8.58001607 2.50191378 0.00000000

H -11.03032108 -2.50197790 0.00000000

H -11.03032088 2.50198225 0.00000000

H -13.48029468 -2.50217053 0.00000000

H -13.48029487 2.50217476 0.00000000

H -15.93002819 -2.50248619 0.00000000

H -15.93002869 2.50249002 0.00000000

H -18.37997812 -2.50277359 0.00000000

H -18.37997892 2.50277684 0.00000000

H -20.83115363 -2.50265032 0.00000000

H -20.83115496 2.50265262 0.00000000

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H -23.28525824 2.50128775 0.00000000

H -25.73782405 -2.50078711 0.00000000

H -25.73782598 2.50078595 0.00000000

H -27.88328545 -1.24950916 0.00000000

H -27.88328645 1.24950627 0.00000000

$end

$comment

23-acene triplet

$end

$molecule

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C 28.19235782 1.40183269 0.00000000

C 26.94835869 -0.72171988 0.00000000

C 26.94836151 0.72168891 0.00000000

C 25.73061573 -1.40095812 0.00000000

C 25.73062111 1.40093193 0.00000000

C 24.50459520 -0.72508220 0.00000000

C 24.50459791 0.72506057 0.00000000

C 23.27677842 -1.40252427 0.00000000

C 23.27678345 1.40250720 0.00000000

C 22.05599993 -0.72695176 0.00000000

C 22.05600242 0.72693884 0.00000000

C 20.82596547 -1.40263156 0.00000000

C 20.82597003 1.40262290 0.00000000

C 19.60497381 -0.72761631 0.00000000

C 19.60497602 0.72761136 0.00000000

C 18.37612084 -1.40232338 0.00000000

C 18.37612482 1.40232221 0.00000000

C 17.15320373 -0.72762438 0.00000000

C 17.15320565 0.72762637 0.00000000

C 15.92625666 -1.40200279 0.00000000

C 15.92626006 1.40200806 0.00000000

C 14.70160705 -0.72738769 0.00000000

C 14.70160866 0.72739564 0.00000000

C 13.47601917 -1.40182002 0.00000000

C 13.47602197 1.40183072 0.00000000

C 12.25046184 -0.72716642 0.00000000

C 12.25046314 0.72717925 0.00000000

C 11.02544336 -1.40176670 0.00000000

C 11.02544554 1.40178171 0.00000000

C 9.79967651 -0.72704881 0.00000000

C 9.79967750 0.72706541 0.00000000

C 8.57469761 -1.40178153 0.00000000

C 8.57469922 1.40179986 0.00000000

C 7.34905460 -0.72702207 0.00000000

C 7.34905530 0.72704153 0.00000000

C 6.12392328 -1.40181450 0.00000000

C 6.12392430 1.40183517 0.00000000

C 4.89845000 -0.72703963 0.00000000

C 4.89845039 0.72706094 0.00000000

C 3.67318506 -1.40183966 0.00000000

C 3.67318549 1.40186164 0.00000000

C 2.44780788 -0.72706010 0.00000000

C 2.44780795 0.72708214 0.00000000

C 1.22248202 -1.40184884 0.00000000

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C -2.45350073 0.72706087 0.00000000

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C -3.67896195 1.40183592 0.00000000

C -4.90410303 -0.72701932 0.00000000

C -4.90410380 0.72703770 0.00000000

C -6.12973984 -1.40178418 0.00000000

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C -7.35471344 -0.72703988 0.00000000

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C -8.58049519 -1.40177042 0.00000000

C -8.58049742 1.40178405 0.00000000

C -9.80547703 -0.72715278 0.00000000

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C -11.03108169 -1.40182419 0.00000000

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C -12.25660013 -0.72737798 0.00000000

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C -20.83171773 -1.40250134 0.00000000

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C -22.05962764 -0.72512126 0.00000000

C -22.05962989 0.72510212 0.00000000

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C -25.74708277 -1.40187420 0.00000000

C -25.74708732 1.40184332 0.00000000

C -26.93043436 -0.70802045 0.00000000

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H 28.18386368 2.50064866 0.00000000

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H 25.73102793 2.50113251 0.00000000

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H 23.27681611 2.50256200 0.00000000

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H 18.37614778 2.50244076 0.00000000

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H 15.92626341 2.50214834 0.00000000

H 13.47601642 -2.50196933 0.00000000

H 13.47602141 2.50198028 0.00000000

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H 11.02544753 2.50193204 0.00000000

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H 8.57470320 2.50194746 0.00000000

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H 6.12392811 2.50197977 0.00000000

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H 3.67318713 2.50200432 0.00000000

H 1.22247912 -2.50199073 0.00000000

H 1.22247885 2.50201313 0.00000000

H -1.22823090 -2.50198314 0.00000000

H -1.22823208 2.50200478 0.00000000

H -3.67897625 -2.50196045 0.00000000

H -3.67897843 2.50198040 0.00000000

H -6.12975035 -2.50193086 0.00000000

H -6.12975342 2.50194816 0.00000000

H -8.58047693 -2.50191901 0.00000000

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H -11.03100800 -2.50197141 0.00000000

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H -15.93105910 -2.50243663 0.00000000

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H -18.38104401 -2.50270988 0.00000000

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H -25.73904109 2.50065578 0.00000000

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$end

$comment

24-acene singlet

$end

$molecule

0 1

C 29.37679052 -0.70812044 0.00000000

C 29.37679151 0.70810458 0.00000000

C 28.19366881 -1.40201216 0.00000000

C 28.19367081 1.40199795 0.00000000

C 26.94977830 -0.72172838 0.00000000

C 26.94977936 0.72171604 0.00000000

C 25.73220735 -1.40112811 0.00000000

C 25.73220950 1.40111753 0.00000000

C 24.50612888 -0.72522218 0.00000000

C 24.50613004 0.72521355 0.00000000

C 23.27844189 -1.40260658 0.00000000

C 23.27844413 1.40259986 0.00000000

C 22.05783351 -0.72708317 0.00000000

C 22.05783468 0.72707827 0.00000000

C 20.82768526 -1.40272280 0.00000000

C 20.82768726 1.40271980 0.00000000

C 19.60706185 -0.72773666 0.00000000

C 19.60706277 0.72773513 0.00000000

C 18.37794281 -1.40241473 0.00000000

C 18.37794432 1.40241481 0.00000000

C 17.15547599 -0.72774217 0.00000000

C 17.15547663 0.72774335 0.00000000

C 15.92824317 -1.40207539 0.00000000

C 15.92824427 1.40207774 0.00000000

C 14.70396605 -0.72751277 0.00000000

C 14.70396653 0.72751601 0.00000000

C 13.47820462 -1.40186507 0.00000000

C 13.47820551 1.40186915 0.00000000

C 12.25284450 -0.72728891 0.00000000

C 12.25284493 0.72729376 0.00000000

C 11.02781942 -1.40178703 0.00000000

C 11.02782017 1.40179254 0.00000000

C 9.80208044 -0.72715707 0.00000000

C 9.80208081 0.72716319 0.00000000

C 8.57722763 -1.40179116 0.00000000

C 8.57722825 1.40179785 0.00000000

C 7.35152008 -0.72711384 0.00000000

C 7.35152037 0.72712098 0.00000000

C 6.12656749 -1.40182760 0.00000000

C 6.12656794 1.40183520 0.00000000

C 4.90102517 -0.72712087 0.00000000

C 4.90102537 0.72712878 0.00000000

C 3.67591868 -1.40186304 0.00000000

C 3.67591897 1.40187127 0.00000000

C 2.45052264 -0.72714062 0.00000000

C 2.45052276 0.72714901 0.00000000

C 1.22530140 -1.40188301 0.00000000

C 1.22530152 1.40189159 0.00000000

C 0.00000005 -0.72714973 0.00000000

C 0.00000007 0.72715833 0.00000000

C -1.22530132 -1.40188298 0.00000000

C -1.22530137 1.40189162 0.00000000

C -2.45052255 -0.72714058 0.00000000

C -2.45052262 0.72714906 0.00000000

C -3.67591861 -1.40186297 0.00000000

C -3.67591882 1.40187136 0.00000000

C -4.90102509 -0.72712077 0.00000000

C -4.90102525 0.72712889 0.00000000

C -6.12656744 -1.40182745 0.00000000

C -6.12656783 1.40183533 0.00000000

C -7.35152002 -0.72711367 0.00000000

C -7.35152029 0.72712114 0.00000000

C -8.57722758 -1.40179097 0.00000000

C -8.57722816 1.40179803 0.00000000

C -9.80208037 -0.72715686 0.00000000

C -9.80208073 0.72716338 0.00000000

C -11.02781935 -1.40178679 0.00000000

C -11.02782008 1.40179274 0.00000000

C -12.25284442 -0.72728868 0.00000000

C -12.25284484 0.72729398 0.00000000

C -13.47820452 -1.40186483 0.00000000

C -13.47820541 1.40186937 0.00000000

C -14.70396593 -0.72751255 0.00000000

C -14.70396642 0.72751623 0.00000000

C -15.92824305 -1.40207519 0.00000000

C -15.92824418 1.40207796 0.00000000

C -17.15547589 -0.72774198 0.00000000

C -17.15547654 0.72774355 0.00000000

C -18.37794270 -1.40241457 0.00000000

C -18.37794427 1.40241501 0.00000000

C -19.60706179 -0.72773654 0.00000000

C -19.60706275 0.72773528 0.00000000

C -20.82768521 -1.40272273 0.00000000

C -20.82768732 1.40271992 0.00000000

C -22.05783354 -0.72708315 0.00000000

C -22.05783477 0.72707833 0.00000000

C -23.27844192 -1.40260664 0.00000000

C -23.27844431 1.40259986 0.00000000

C -24.50612899 -0.72522229 0.00000000

C -24.50613025 0.72521348 0.00000000

C -25.73220747 -1.40112830 0.00000000

C -25.73220977 1.40111742 0.00000000

C -26.94977849 -0.72172860 0.00000000

C -26.94977963 0.72171585 0.00000000

C -28.19366899 -1.40201245 0.00000000

C -28.19367114 1.40199771 0.00000000

C -29.37679076 -0.70812080 0.00000000

C -29.37679183 0.70810424 0.00000000

H 30.33105972 -1.24965159 0.00000000

H 30.33106150 1.24963436 0.00000000

H 28.18585192 -2.50083437 0.00000000

H 28.18585552 2.50082015 0.00000000

H 25.73321953 -2.50133070 0.00000000

H 25.73322335 2.50132009 0.00000000

H 23.27890685 -2.50269263 0.00000000

H 23.27891072 2.50268596 0.00000000

H 20.82758510 -2.50282402 0.00000000

H 20.82758858 2.50282121 0.00000000

H 18.37763113 -2.50254167 0.00000000

H 18.37763388 2.50254198 0.00000000

H 15.92797753 -2.50222244 0.00000000

H 15.92797960 2.50222497 0.00000000

H 13.47807927 -2.50202318 0.00000000

H 13.47808089 2.50202737 0.00000000

H 11.02781357 -2.50194879 0.00000000

H 11.02781489 2.50195438 0.00000000

H 8.57727826 -2.50195224 0.00000000

H 8.57727932 2.50195900 0.00000000

H 6.12662410 -2.50198629 0.00000000

H 6.12662487 2.50199396 0.00000000

H 3.67595663 -2.50201949 0.00000000

H 3.67595712 2.50202779 0.00000000

H 1.22531421 -2.50203819 0.00000000

H 1.22531442 2.50204683 0.00000000

H -1.22531416 -2.50203816 0.00000000

H -1.22531426 2.50204686 0.00000000

H -3.67595659 -2.50201943 0.00000000

H -3.67595696 2.50202789 0.00000000

H -6.12662407 -2.50198614 0.00000000

H -6.12662474 2.50199409 0.00000000

H -8.57727821 -2.50195204 0.00000000

H -8.57727921 2.50195918 0.00000000

H -11.02781350 -2.50194855 0.00000000

H -11.02781477 2.50195459 0.00000000

H -13.47807916 -2.50202294 0.00000000

H -13.47808079 2.50202760 0.00000000

H -15.92797741 -2.50222224 0.00000000

H -15.92797953 2.50222520 0.00000000

H -18.37763101 -2.50254152 0.00000000

H -18.37763387 2.50254221 0.00000000

H -20.82758502 -2.50282397 0.00000000

H -20.82758869 2.50282136 0.00000000

H -23.27890684 -2.50269271 0.00000000

H -23.27891095 2.50268601 0.00000000

H -25.73321960 -2.50133091 0.00000000

H -25.73322366 2.50132001 0.00000000

H -28.18585204 -2.50083469 0.00000000

H -28.18585591 2.50081992 0.00000000

H -30.33105995 -1.24965202 0.00000000

H -30.33106186 1.24963398 0.00000000

$end

$comment

24-acene triplet

$end

$molecule

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C 29.37817001 0.70798295 0.00000000

C 28.19481149 -1.40189706 0.00000000

C 28.19481165 1.40189870 0.00000000

C 26.95116096 -0.72161897 0.00000000

C 26.95116105 0.72162091 0.00000000

C 25.73324175 -1.40103167 0.00000000

C 25.73324177 1.40103409 0.00000000

C 24.50737295 -0.72516850 0.00000000

C 24.50737299 0.72517123 0.00000000

C 23.27944255 -1.40252585 0.00000000

C 23.27944256 1.40252916 0.00000000

C 22.05879769 -0.72705513 0.00000000

C 22.05879772 0.72705870 0.00000000

C 20.82868999 -1.40265930 0.00000000

C 20.82869004 1.40266310 0.00000000

C 19.60772145 -0.72768648 0.00000000

C 19.60772152 0.72769026 0.00000000

C 18.37890874 -1.40237234 0.00000000

C 18.37890886 1.40237590 0.00000000

C 17.15593162 -0.72764763 0.00000000

C 17.15593176 0.72765084 0.00000000

C 15.92907990 -1.40205787 0.00000000

C 15.92908009 1.40206060 0.00000000

C 14.70435672 -0.72739070 0.00000000

C 14.70435693 0.72739282 0.00000000

C 13.47884844 -1.40187286 0.00000000

C 13.47884870 1.40187440 0.00000000

C 12.25325222 -0.72717144 0.00000000

C 12.25325247 0.72717225 0.00000000

C 11.02826769 -1.40181397 0.00000000

C 11.02826801 1.40181419 0.00000000

C 9.80250402 -0.72706485 0.00000000

C 9.80250428 0.72706435 0.00000000

C 8.57751923 -1.40182547 0.00000000

C 8.57751961 1.40182444 0.00000000

C 7.35190803 -0.72704835 0.00000000

C 7.35190827 0.72704665 0.00000000

C 6.12674770 -1.40185818 0.00000000

C 6.12674816 1.40185599 0.00000000

C 4.90131882 -0.72707285 0.00000000

C 4.90131905 0.72707016 0.00000000

C 3.67601834 -1.40188485 0.00000000

C 3.67601885 1.40188163 0.00000000

C 2.45068017 -0.72710036 0.00000000

C 2.45068044 0.72709680 0.00000000

C 1.22533435 -1.40189833 0.00000000

C 1.22533498 1.40189423 0.00000000

C 0.00000139 -0.72711159 0.00000000

C 0.00000174 0.72710735 0.00000000

C -1.22533201 -1.40189873 0.00000000

C -1.22533120 1.40189401 0.00000000

C -2.45067782 -0.72710102 0.00000000

C -2.45067736 0.72709640 0.00000000

C -3.67601684 -1.40188596 0.00000000

C -3.67601578 1.40188099 0.00000000

C -4.90131752 -0.72707399 0.00000000

C -4.90131689 0.72706937 0.00000000

C -6.12674741 -1.40185976 0.00000000

C -6.12674611 1.40185491 0.00000000

C -7.35190783 -0.72704977 0.00000000

C -7.35190706 0.72704551 0.00000000

C -8.57751982 -1.40182724 0.00000000

C -8.57751835 1.40182294 0.00000000

C -9.80250442 -0.72706646 0.00000000

C -9.80250352 0.72706282 0.00000000

C -11.02826847 -1.40181585 0.00000000

C -11.02826694 1.40181230 0.00000000

C -12.25325250 -0.72717326 0.00000000

C -12.25325156 0.72717034 0.00000000

C -13.47884880 -1.40187488 0.00000000

C -13.47884730 1.40187220 0.00000000

C -14.70435650 -0.72739277 0.00000000

C -14.70435560 0.72739062 0.00000000

C -15.92907972 -1.40206008 0.00000000

C -15.92907833 1.40205835 0.00000000

C -17.15593110 -0.72764985 0.00000000

C -17.15593030 0.72764867 0.00000000

C -18.37890850 -1.40237448 0.00000000

C -18.37890731 1.40237399 0.00000000

C -19.60772128 -0.72768843 0.00000000

C -19.60772065 0.72768859 0.00000000

C -20.82869044 -1.40266092 0.00000000

C -20.82868948 1.40266204 0.00000000

C -22.05879853 -0.72705613 0.00000000

C -22.05879807 0.72705814 0.00000000

C -23.27944420 -1.40252633 0.00000000

C -23.27944347 1.40252940 0.00000000

C -24.50737513 -0.72516804 0.00000000

C -24.50737476 0.72517217 0.00000000

C -25.73324466 -1.40103072 0.00000000

C -25.73324405 1.40103578 0.00000000

C -26.95116427 -0.72161716 0.00000000

C -26.95116393 0.72162316 0.00000000

C -28.19481546 -1.40189477 0.00000000

C -28.19481479 1.40190157 0.00000000

C -29.37817393 -0.70797865 0.00000000

C -29.37817358 0.70798621 0.00000000

H 30.33237199 -1.24962576 0.00000000

H 30.33237219 1.24962695 0.00000000

H 28.18700789 -2.50071909 0.00000000

H 28.18700813 2.50072074 0.00000000

H 25.73426757 -2.50123465 0.00000000

H 25.73426762 2.50123707 0.00000000

H 23.27990130 -2.50261235 0.00000000

H 23.27990155 2.50261564 0.00000000

H 20.82858008 -2.50275997 0.00000000

H 20.82858035 2.50276372 0.00000000

H 18.37860864 -2.50249696 0.00000000

H 18.37860890 2.50250047 0.00000000

H 15.92884950 -2.50220067 0.00000000

H 15.92884985 2.50220336 0.00000000

H 13.47876126 -2.50202501 0.00000000

H 13.47876173 2.50202651 0.00000000

H 11.02828099 -2.50196862 0.00000000

H 11.02828163 2.50196881 0.00000000

H 8.57756435 -2.50197908 0.00000000

H 8.57756515 2.50197801 0.00000000

H 6.12678361 -2.50200967 0.00000000

H 6.12678463 2.50200743 0.00000000

H 3.67603554 -2.50203468 0.00000000

H 3.67603664 2.50203137 0.00000000

H 1.22533854 -2.50204735 0.00000000

H 1.22533978 2.50204312 0.00000000

H -1.22533690 -2.50204785 0.00000000

H -1.22533535 2.50204296 0.00000000

H -3.67603482 -2.50203602 0.00000000

H -3.67603282 2.50203086 0.00000000

H -6.12678414 -2.50201151 0.00000000

H -6.12678175 2.50200647 0.00000000

H -8.57756571 -2.50198104 0.00000000

H -8.57756311 2.50197657 0.00000000

H -11.02828249 -2.50197056 0.00000000

H -11.02827984 2.50196691 0.00000000

H -13.47876225 -2.50202700 0.00000000

H -13.47875969 2.50202429 0.00000000

H -15.92884990 -2.50220286 0.00000000

H -15.92884752 2.50220117 0.00000000

H -18.37860894 -2.50249919 0.00000000

H -18.37860682 2.50249877 0.00000000

H -20.82858111 -2.50276179 0.00000000

H -20.82857922 2.50276299 0.00000000

H -23.27990348 -2.50261309 0.00000000

H -23.27990193 2.50261622 0.00000000

H -25.73427077 -2.50123396 0.00000000

H -25.73426960 2.50123906 0.00000000

H -28.18701220 -2.50071702 0.00000000

H -28.18701100 2.50072381 0.00000000

H -30.33237636 -1.24962252 0.00000000

H -30.33237571 1.24963056 0.00000000

$end

$comment

25-acene singlet

$end

$molecule

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C 30.64183734 1.40195943 0.00000000

C 29.39759959 -0.72182038 0.00000000

C 29.39760181 0.72180335 0.00000000

C 28.18022772 -1.40105425 0.00000000

C 28.18023199 1.40104098 0.00000000

C 26.95398961 -0.72513186 0.00000000

C 26.95399180 0.72512230 0.00000000

C 25.72644524 -1.40260313 0.00000000

C 25.72644930 1.40259725 0.00000000

C 24.50570199 -0.72697427 0.00000000

C 24.50570401 0.72697161 0.00000000

C 23.27564710 -1.40269735 0.00000000

C 23.27565052 1.40269807 0.00000000

C 22.05501606 -0.72766035 0.00000000

C 22.05501761 0.72766348 0.00000000

C 20.82585844 -1.40237348 0.00000000

C 20.82586089 1.40237933 0.00000000

C 19.60348315 -0.72771740 0.00000000

C 19.60348414 0.72772476 0.00000000

C 18.37614123 -1.40202998 0.00000000

C 18.37614263 1.40203916 0.00000000

C 17.15197530 -0.72751592 0.00000000

C 17.15197575 0.72752587 0.00000000

C 15.92611750 -1.40182130 0.00000000

C 15.92611800 1.40183213 0.00000000

C 14.70082753 -0.72729583 0.00000000

C 14.70082759 0.72730675 0.00000000

C 13.47575958 -1.40174904 0.00000000

C 13.47575946 1.40176014 0.00000000

C 12.25003965 -0.72715455 0.00000000

C 12.25003946 0.72716535 0.00000000

C 11.02518997 -1.40175701 0.00000000

C 11.02518946 1.40176752 0.00000000

C 9.79947252 -0.72709973 0.00000000

C 9.79947217 0.72710968 0.00000000

C 8.57454142 -1.40179421 0.00000000

C 8.57454069 1.40180360 0.00000000

C 7.34898530 -0.72710105 0.00000000

C 7.34898489 0.72710966 0.00000000

C 6.12389770 -1.40183045 0.00000000

C 6.12389675 1.40183833 0.00000000

C 4.89849320 -0.72712329 0.00000000

C 4.89849267 0.72713010 0.00000000

C 3.67328829 -1.40185377 0.00000000

C 3.67328710 1.40185975 0.00000000

C 2.44797085 -0.72714156 0.00000000

C 2.44797017 0.72714617 0.00000000

C 1.22270527 -1.40186244 0.00000000

C 1.22270381 1.40186606 0.00000000

C -0.00256725 -0.72714368 0.00000000

C -0.00256810 0.72714579 0.00000000

C -1.22787707 -1.40185672 0.00000000

C -1.22787870 1.40185763 0.00000000

C -2.45309224 -0.72712868 0.00000000

C -2.45309313 0.72712812 0.00000000

C -3.67848538 -1.40183613 0.00000000

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C -6.12912998 -1.40180240 0.00000000

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C -7.35406992 -0.72710290 0.00000000

C -7.35407039 0.72709788 0.00000000

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C -9.80462382 -0.72715261 0.00000000

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C -11.03036475 -1.40176104 0.00000000

C -11.03036491 1.40175446 0.00000000

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C -14.70652057 -0.72751572 0.00000000

C -14.70652038 0.72750950 0.00000000

C -15.93076004 -1.40203716 0.00000000

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C -17.15803462 -0.72773507 0.00000000

C -17.15803437 0.72772947 0.00000000

C -18.38045746 -1.40237407 0.00000000

C -18.38045693 1.40236887 0.00000000

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C -19.60960924 0.72770404 0.00000000

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C -20.83020349 1.40268482 0.00000000

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C -23.28095687 1.40257858 0.00000000

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C -29.37925261 -0.70813146 0.00000000

C -29.37925142 0.70813794 0.00000000

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H 32.77911516 1.24946868 0.00000000

H 30.63335732 -2.50079305 0.00000000

H 30.63336484 2.50077228 0.00000000

H 28.18063263 -2.50125080 0.00000000

H 28.18064021 2.50123759 0.00000000

H 25.72647394 -2.50265500 0.00000000

H 25.72648099 2.50264934 0.00000000

H 23.27565963 -2.50278111 0.00000000

H 23.27566555 2.50278222 0.00000000

H 20.82585799 -2.50249125 0.00000000

H 20.82586232 2.50249761 0.00000000

H 18.37611851 -2.50217171 0.00000000

H 18.37612112 2.50218139 0.00000000

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H 15.92609769 2.50198592 0.00000000

H 13.47575179 -2.50190473 0.00000000

H 13.47575166 2.50191615 0.00000000

H 11.02519534 -2.50191048 0.00000000

H 11.02519448 2.50192120 0.00000000

H 8.57455329 -2.50194438 0.00000000

H 8.57455195 2.50195390 0.00000000

H 6.12390959 -2.50197796 0.00000000

H 6.12390780 2.50198595 0.00000000

H 3.67329586 -2.50199979 0.00000000

H 3.67329365 2.50200589 0.00000000

H 1.22270552 -2.50200805 0.00000000

H 1.22270298 2.50201176 0.00000000

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H -1.22788939 2.50200380 0.00000000

H -3.67850533 -2.50198378 0.00000000

H -3.67850792 2.50198176 0.00000000

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H -8.57979541 -2.50192020 0.00000000

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$end

$comment

25-acene triplet

$end

$molecule

0 3

C 31.82605368 -0.70812088 0.00000000

C 31.82605335 0.70811604 0.00000000

C 30.64297324 -1.40187533 0.00000000

C 30.64297271 1.40186989 0.00000000

C 29.39894253 -0.72172389 0.00000000

C 29.39894214 0.72171787 0.00000000

C 28.18126344 -1.40096644 0.00000000

C 28.18126311 1.40095989 0.00000000

C 26.95521028 -0.72508251 0.00000000

C 26.95520992 0.72507557 0.00000000

C 25.72744070 -1.40253464 0.00000000

C 25.72744063 1.40252732 0.00000000

C 24.50667190 -0.72695246 0.00000000

C 24.50667174 0.72694501 0.00000000

C 23.27663635 -1.40264435 0.00000000

C 23.27663639 1.40263681 0.00000000

C 22.05570620 -0.72762519 0.00000000

C 22.05570626 0.72761786 0.00000000

C 20.82680762 -1.40233764 0.00000000

C 20.82680758 1.40233055 0.00000000

C 19.60397722 -0.72764508 0.00000000

C 19.60397747 0.72763842 0.00000000

C 18.37697433 -1.40201690 0.00000000

C 18.37697416 1.40201071 0.00000000

C 17.15239647 -0.72741640 0.00000000

C 17.15239685 0.72741089 0.00000000

C 15.92677682 -1.40183241 0.00000000

C 15.92677659 1.40182750 0.00000000

C 14.70125300 -0.72719558 0.00000000

C 14.70125348 0.72719154 0.00000000

C 13.47623816 -1.40177736 0.00000000

C 13.47623796 1.40177400 0.00000000

C 12.25047378 -0.72707255 0.00000000

C 12.25047436 0.72707021 0.00000000

C 11.02551861 -1.40179035 0.00000000

C 11.02551856 1.40178886 0.00000000

C 9.79987332 -0.72703865 0.00000000

C 9.79987401 0.72703839 0.00000000

C 8.57475869 -1.40182121 0.00000000

C 8.57475883 1.40182199 0.00000000

C 7.34930265 -0.72705293 0.00000000

C 7.34930343 0.72705506 0.00000000

C 6.12403005 -1.40184509 0.00000000

C 6.12403032 1.40184844 0.00000000

C 4.89869137 -0.72707876 0.00000000

C 4.89869214 0.72708354 0.00000000

C 3.67334716 -1.40185652 0.00000000

C 3.67334740 1.40186261 0.00000000

C 2.44803238 -0.72709556 0.00000000

C 2.44803306 0.72710297 0.00000000

C 1.22269383 -1.40185879 0.00000000

C 1.22269386 1.40186743 0.00000000

C -0.00264679 -0.72709537 0.00000000

C -0.00264630 0.72710510 0.00000000

C -1.22795742 -1.40185420 0.00000000

C -1.22795784 1.40186485 0.00000000

C -2.45330759 -0.72707757 0.00000000

C -2.45330736 0.72708881 0.00000000

C -3.67863538 -1.40184087 0.00000000

C -3.67863638 1.40185264 0.00000000

C -4.90391955 -0.72704883 0.00000000

C -4.90391965 0.72706060 0.00000000

C -6.12935940 -1.40181614 0.00000000

C -6.12936105 1.40182791 0.00000000

C -7.35448457 -0.72702912 0.00000000

C -7.35448500 0.72704031 0.00000000

C -8.58011886 -1.40178545 0.00000000

C -8.58012105 1.40179616 0.00000000

C -9.80506862 -0.72705606 0.00000000

C -9.80506931 0.72706574 0.00000000

C -11.03084384 -1.40177390 0.00000000

C -11.03084636 1.40178269 0.00000000

C -12.25582157 -0.72717505 0.00000000

C -12.25582242 0.72718258 0.00000000

C -13.48139033 -1.40183034 0.00000000

C -13.48139294 1.40183669 0.00000000

C -14.70694037 -0.72740096 0.00000000

C -14.70694127 0.72740591 0.00000000

C -15.93158749 -1.40201231 0.00000000

C -15.93158997 1.40201591 0.00000000

C -17.15852046 -0.72764994 0.00000000

C -17.15852139 0.72765209 0.00000000

C -18.38139885 -1.40232932 0.00000000

C -18.38140106 1.40233003 0.00000000

C -19.61028607 -0.72766540 0.00000000

C -19.61028706 0.72766453 0.00000000

C -20.83118215 -1.40263072 0.00000000

C -20.83118414 1.40262821 0.00000000

C -22.06130226 -0.72701079 0.00000000

C -22.06130337 0.72700645 0.00000000

C -23.28193866 -1.40251351 0.00000000

C -23.28194059 1.40250731 0.00000000

C -24.50980544 -0.72512476 0.00000000

C -24.50980664 0.72511652 0.00000000

C -25.73572553 -1.40101843 0.00000000

C -25.73572757 1.40100818 0.00000000

C -26.95355910 -0.72161795 0.00000000

C -26.95356030 0.72160562 0.00000000

C -28.19727057 -1.40188878 0.00000000

C -28.19727278 1.40187433 0.00000000

C -29.38057932 -0.70803286 0.00000000

C -29.38058048 0.70801640 0.00000000

H 32.78040678 -1.24945467 0.00000000

H 32.78040624 1.24945021 0.00000000

H 30.63448352 -2.50068961 0.00000000

H 30.63448237 2.50068413 0.00000000

H 28.18166910 -2.50116519 0.00000000

H 28.18166826 2.50115859 0.00000000

H 25.72747224 -2.50258789 0.00000000

H 25.72747184 2.50258054 0.00000000

H 23.27666030 -2.50272891 0.00000000

H 23.27666029 2.50272141 0.00000000

H 20.82682584 -2.50245505 0.00000000

H 20.82682607 2.50244804 0.00000000

H 18.37697248 -2.50215650 0.00000000

H 18.37697287 2.50215037 0.00000000

H 15.92677205 -2.50198187 0.00000000

H 15.92677253 2.50197698 0.00000000

H 13.47623639 -2.50192801 0.00000000

H 13.47623696 2.50192461 0.00000000

H 11.02551987 -2.50193849 0.00000000

H 11.02552074 2.50193692 0.00000000

H 8.57476060 -2.50196642 0.00000000

H 8.57476172 2.50196711 0.00000000

H 6.12403157 -2.50198829 0.00000000

H 6.12403290 2.50199160 0.00000000

H 3.67334830 -2.50199873 0.00000000

H 3.67334957 2.50200486 0.00000000

H 1.22269388 -2.50200067 0.00000000

H 1.22269477 2.50200943 0.00000000

H -1.22796106 -2.50199619 0.00000000

H -1.22796103 2.50200704 0.00000000

H -3.67864594 -2.50198358 0.00000000

H -3.67864696 2.50199559 0.00000000

H -6.12937585 -2.50196045 0.00000000

H -6.12937801 2.50197246 0.00000000

H -8.58012950 -2.50193218 0.00000000

H -8.58013260 2.50194307 0.00000000

H -11.03082398 -2.50192265 0.00000000

H -11.03082766 2.50193152 0.00000000

H -13.48131327 -2.50197782 0.00000000

H -13.48131720 2.50198412 0.00000000

H -15.93145768 -2.50215093 0.00000000

H -15.93146152 2.50215441 0.00000000

H -18.38129464 -2.50244826 0.00000000

H -18.38129827 2.50244883 0.00000000

H -20.83126826 -2.50272218 0.00000000

H -20.83127183 2.50271957 0.00000000

H -23.28243540 -2.50258857 0.00000000

H -23.28243905 2.50258234 0.00000000

H -25.73656685 -2.50121291 0.00000000

H -25.73657069 2.50120267 0.00000000

H -28.18922707 -2.50070064 0.00000000

H -28.18923113 2.50068622 0.00000000

H -30.33485587 -1.24948308 0.00000000

H -30.33485792 1.24946507 0.00000000

$end

$comment

26-acene singlet

$end

$molecule

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C 31.82728718 -0.70812585 0.00000000

C 31.82728857 0.70810222 0.00000000

C 30.64416413 -1.40202083 0.00000000

C 30.64416695 1.40199953 0.00000000

C 29.40027876 -0.72173048 0.00000000

C 29.40028026 0.72171177 0.00000000

C 28.18270985 -1.40113381 0.00000000

C 28.18271286 1.40111761 0.00000000

C 26.95663389 -0.72522325 0.00000000

C 26.95663550 0.72520972 0.00000000

C 25.72895262 -1.40261116 0.00000000

C 25.72895566 1.40260027 0.00000000

C 24.50834216 -0.72708276 0.00000000

C 24.50834372 0.72707440 0.00000000

C 23.27820340 -1.40272623 0.00000000

C 23.27820618 1.40272046 0.00000000

C 22.05757592 -0.72773501 0.00000000

C 22.05757726 0.72773140 0.00000000

C 20.82846739 -1.40241825 0.00000000

C 20.82846966 1.40241691 0.00000000

C 19.60599784 -0.72774016 0.00000000

C 19.60599886 0.72774054 0.00000000

C 18.37877239 -1.40207924 0.00000000

C 18.37877417 1.40208145 0.00000000

C 17.15449738 -0.72750956 0.00000000

C 17.15449817 0.72751318 0.00000000

C 15.92873920 -1.40186679 0.00000000

C 15.92874060 1.40187177 0.00000000

C 14.70338306 -0.72728442 0.00000000

C 14.70338369 0.72729058 0.00000000

C 13.47836154 -1.40178794 0.00000000

C 13.47836270 1.40179518 0.00000000

C 12.25263022 -0.72715292 0.00000000

C 12.25263076 0.72716112 0.00000000

C 11.02777130 -1.40179158 0.00000000

C 11.02777222 1.40180066 0.00000000

C 9.80208099 -0.72710751 0.00000000

C 9.80208140 0.72711730 0.00000000

C 8.57711179 -1.40182521 0.00000000

C 8.57711244 1.40183570 0.00000000

C 7.35159719 -0.72711437 0.00000000

C 7.35159746 0.72712531 0.00000000

C 6.12646449 -1.40185938 0.00000000

C 6.12646488 1.40187079 0.00000000

C 4.90109891 -0.72713870 0.00000000

C 4.90109905 0.72715036 0.00000000

C 3.67585645 -1.40188115 0.00000000

C 3.67585662 1.40189305 0.00000000

C 2.45056256 -0.72715928 0.00000000

C 2.45056263 0.72717124 0.00000000

C 1.22528142 -1.40189092 0.00000000

C 1.22528147 1.40190297 0.00000000

C 0.00000004 -0.72716694 0.00000000

C 0.00000004 0.72717898 0.00000000

C -1.22528135 -1.40189092 0.00000000

C -1.22528142 1.40190296 0.00000000

C -2.45056251 -0.72715930 0.00000000

C -2.45056256 0.72717122 0.00000000

C -3.67585638 -1.40188121 0.00000000

C -3.67585657 1.40189301 0.00000000

C -4.90109884 -0.72713876 0.00000000

C -4.90109898 0.72715030 0.00000000

C -6.12646440 -1.40185947 0.00000000

C -6.12646479 1.40187074 0.00000000

C -7.35159710 -0.72711443 0.00000000

C -7.35159737 0.72712526 0.00000000

C -8.57711169 -1.40182529 0.00000000

C -8.57711235 1.40183564 0.00000000

C -9.80208090 -0.72710758 0.00000000

C -9.80208132 0.72711723 0.00000000

C -11.02777123 -1.40179165 0.00000000

C -11.02777214 1.40180061 0.00000000

C -12.25263018 -0.72715298 0.00000000

C -12.25263072 0.72716107 0.00000000

C -13.47836152 -1.40178800 0.00000000

C -13.47836268 1.40179513 0.00000000

C -14.70338306 -0.72728448 0.00000000

C -14.70338370 0.72729053 0.00000000

C -15.92873923 -1.40186685 0.00000000

C -15.92874064 1.40187172 0.00000000

C -17.15449744 -0.72750964 0.00000000

C -17.15449823 0.72751310 0.00000000

C -18.37877248 -1.40207932 0.00000000

C -18.37877424 1.40208137 0.00000000

C -19.60599793 -0.72774024 0.00000000

C -19.60599896 0.72774047 0.00000000

C -20.82846751 -1.40241831 0.00000000

C -20.82846975 1.40241685 0.00000000

C -22.05757603 -0.72773505 0.00000000

C -22.05757735 0.72773135 0.00000000

C -23.27820351 -1.40272623 0.00000000

C -23.27820626 1.40272044 0.00000000

C -24.50834224 -0.72708274 0.00000000

C -24.50834380 0.72707441 0.00000000

C -25.72895269 -1.40261111 0.00000000

C -25.72895571 1.40260030 0.00000000

C -26.95663394 -0.72522320 0.00000000

C -26.95663553 0.72520975 0.00000000

C -28.18270987 -1.40113375 0.00000000

C -28.18271287 1.40111765 0.00000000

C -29.40027876 -0.72173042 0.00000000

C -29.40028028 0.72171183 0.00000000

C -30.64416413 -1.40202077 0.00000000

C -30.64416695 1.40199958 0.00000000

C -31.82728717 -0.70812579 0.00000000

C -31.82728856 0.70810227 0.00000000

H 32.78156133 -1.24964783 0.00000000

H 32.78156382 1.24962228 0.00000000

H 30.63633610 -2.50084104 0.00000000

H 30.63634115 2.50081971 0.00000000

H 28.18371369 -2.50133457 0.00000000

H 28.18371902 2.50131836 0.00000000

H 25.72941243 -2.50269552 0.00000000

H 25.72941774 2.50268470 0.00000000

H 23.27810242 -2.50282588 0.00000000

H 23.27810729 2.50282029 0.00000000

H 20.82815649 -2.50254331 0.00000000

H 20.82816055 2.50254222 0.00000000

H 18.37850699 -2.50222452 0.00000000

H 18.37851025 2.50222695 0.00000000

H 15.92861808 -2.50202287 0.00000000

H 15.92862066 2.50202802 0.00000000

H 13.47835930 -2.50194784 0.00000000

H 13.47836138 2.50195521 0.00000000

H 11.02781858 -2.50195071 0.00000000

H 11.02782021 2.50195992 0.00000000

H 8.57716063 -2.50198214 0.00000000

H 8.57716179 2.50199275 0.00000000

H 6.12649609 -2.50201406 0.00000000

H 6.12649680 2.50202556 0.00000000

H 3.67587106 -2.50203439 0.00000000

H 3.67587138 2.50204636 0.00000000

H 1.22528530 -2.50204350 0.00000000

H 1.22528538 2.50205560 0.00000000

H -1.22528523 -2.50204351 0.00000000

H -1.22528535 2.50205559 0.00000000

H -3.67587099 -2.50203445 0.00000000

H -3.67587135 2.50204632 0.00000000

H -6.12649600 -2.50201414 0.00000000

H -6.12649671 2.50202552 0.00000000

H -8.57716053 -2.50198223 0.00000000

H -8.57716171 2.50199270 0.00000000

H -11.02781851 -2.50195079 0.00000000

H -11.02782012 2.50195987 0.00000000

H -13.47835928 -2.50194791 0.00000000

H -13.47836137 2.50195518 0.00000000

H -15.92861811 -2.50202294 0.00000000

H -15.92862071 2.50202798 0.00000000

H -18.37850708 -2.50222460 0.00000000

H -18.37851032 2.50222688 0.00000000

H -20.82815663 -2.50254336 0.00000000

H -20.82816064 2.50254216 0.00000000

H -23.27810256 -2.50282587 0.00000000

H -23.27810734 2.50282027 0.00000000

H -25.72941251 -2.50269548 0.00000000

H -25.72941778 2.50268473 0.00000000

H -28.18371373 -2.50133452 0.00000000

H -28.18371901 2.50131839 0.00000000

H -30.63633610 -2.50084097 0.00000000

H -30.63634115 2.50081976 0.00000000

H -32.78156130 -1.24964777 0.00000000

H -32.78156379 1.24962232 0.00000000

$end

$comment

26-acene triplet

$end

$molecule

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C 31.82853289 -0.70802185 0.00000000

C 31.82853536 0.70798741 0.00000000

C 30.64521038 -1.40193514 0.00000000

C 30.64521518 1.40190499 0.00000000

C 29.40152730 -0.72164792 0.00000000

C 29.40152977 0.72162215 0.00000000

C 28.18366489 -1.40106067 0.00000000

C 28.18366940 1.40103938 0.00000000

C 26.95776649 -0.72518442 0.00000000

C 26.95776889 0.72516733 0.00000000

C 25.72987876 -1.40254814 0.00000000

C 25.72988303 1.40253551 0.00000000

C 24.50923988 -0.72706278 0.00000000

C 24.50924213 0.72705393 0.00000000

C 23.27913256 -1.40267492 0.00000000

C 23.27913658 1.40267006 0.00000000

C 22.05821744 -0.72769417 0.00000000

C 22.05821942 0.72769254 0.00000000

C 20.82936429 -1.40238232 0.00000000

C 20.82936807 1.40238400 0.00000000

C 19.60646691 -0.72765990 0.00000000

C 19.60646868 0.72766419 0.00000000

C 18.37956178 -1.40206215 0.00000000

C 18.37956531 1.40206905 0.00000000

C 17.15490990 -0.72740462 0.00000000

C 17.15491147 0.72741359 0.00000000

C 15.92936775 -1.40186989 0.00000000

C 15.92937097 1.40188097 0.00000000

C 14.70380744 -0.72718242 0.00000000

C 14.70380883 0.72719504 0.00000000

C 13.47882733 -1.40180658 0.00000000

C 13.47883011 1.40182091 0.00000000

C 12.25306487 -0.72707104 0.00000000

C 12.25306598 0.72708637 0.00000000

C 11.02810741 -1.40181680 0.00000000

C 11.02810964 1.40183341 0.00000000

C 9.80248422 -0.72704652 0.00000000

C 9.80248501 0.72706357 0.00000000

C 8.57735500 -1.40184722 0.00000000

C 8.57735661 1.40186508 0.00000000

C 7.35192464 -0.72706493 0.00000000

C 7.35192509 0.72708269 0.00000000

C 6.12663672 -1.40187257 0.00000000

C 6.12663768 1.40189062 0.00000000

C 4.90132372 -0.72709122 0.00000000

C 4.90132386 0.72710870 0.00000000

C 3.67596272 -1.40188524 0.00000000

C 3.67596309 1.40190250 0.00000000

C 2.45067561 -0.72710948 0.00000000

C 2.45067548 0.72712583 0.00000000

C 1.22531811 -1.40188992 0.00000000

C 1.22531804 1.40190557 0.00000000

C 0.00000066 -0.72711633 0.00000000

C 0.00000029 0.72713082 0.00000000

C -1.22531693 -1.40189112 0.00000000

C -1.22531730 1.40190443 0.00000000

C -2.45067447 -0.72711169 0.00000000

C -2.45067494 0.72712370 0.00000000

C -3.67596194 -1.40188866 0.00000000

C -3.67596243 1.40189920 0.00000000

C -4.90132299 -0.72709540 0.00000000

C -4.90132347 0.72710463 0.00000000

C -6.12663663 -1.40187785 0.00000000

C -6.12663708 1.40188549 0.00000000

C -7.35192446 -0.72707064 0.00000000

C -7.35192489 0.72707708 0.00000000

C -8.57735559 -1.40185377 0.00000000

C -8.57735595 1.40185863 0.00000000

C -9.80248448 -0.72705321 0.00000000

C -9.80248484 0.72705692 0.00000000

C -11.02810846 -1.40182402 0.00000000

C -11.02810875 1.40182619 0.00000000

C -12.25306530 -0.72707821 0.00000000

C -12.25306564 0.72707918 0.00000000

C -13.47882857 -1.40181395 0.00000000

C -13.47882884 1.40181345 0.00000000

C -14.70380785 -0.72718958 0.00000000

C -14.70380820 0.72718782 0.00000000

C -15.92936897 -1.40187698 0.00000000

C -15.92936929 1.40187380 0.00000000

C -17.15491018 -0.72741130 0.00000000

C -17.15491058 0.72740686 0.00000000

C -18.37956292 -1.40206846 0.00000000

C -18.37956340 1.40206271 0.00000000

C -19.60646718 -0.72766553 0.00000000

C -19.60646765 0.72765857 0.00000000

C -20.82936551 -1.40238725 0.00000000

C -20.82936619 1.40237911 0.00000000

C -22.05821800 -0.72769790 0.00000000

C -22.05821844 0.72768889 0.00000000

C -23.27913412 -1.40267751 0.00000000

C -23.27913495 1.40266762 0.00000000

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C -24.50924135 0.72705327 0.00000000

C -25.72988085 -1.40254734 0.00000000

C -25.72988173 1.40253649 0.00000000

C -26.95776815 -0.72518146 0.00000000

C -26.95776845 0.72517042 0.00000000

C -28.18366754 -1.40105583 0.00000000

C -28.18366836 1.40104440 0.00000000

C -29.40152935 -0.72164093 0.00000000

C -29.40152965 0.72162925 0.00000000

C -30.64521357 -1.40192618 0.00000000

C -30.64521419 1.40191409 0.00000000

C -31.82853518 -0.70801086 0.00000000

C -31.82853545 0.70799846 0.00000000

H 32.78274983 -1.24964026 0.00000000

H 32.78275417 1.24960256 0.00000000

H 30.63739130 -2.50075526 0.00000000

H 30.63739987 2.50072521 0.00000000

H 28.18467847 -2.50126186 0.00000000

H 28.18468661 2.50124066 0.00000000

H 25.73033192 -2.50263297 0.00000000

H 25.73033967 2.50262045 0.00000000

H 23.27902215 -2.50277414 0.00000000

H 23.27902943 2.50276940 0.00000000

H 20.82906217 -2.50250540 0.00000000

H 20.82906889 2.50250719 0.00000000

H 18.37932586 -2.50220378 0.00000000

H 18.37933193 2.50221081 0.00000000

H 15.92927937 -2.50202090 0.00000000

H 15.92928475 2.50203214 0.00000000

H 13.47884330 -2.50196044 0.00000000

H 13.47884783 2.50197498 0.00000000

H 11.02815223 -2.50196951 0.00000000

H 11.02815581 2.50198638 0.00000000

H 8.57738776 -2.50199795 0.00000000

H 8.57739029 2.50201608 0.00000000

H 6.12664918 -2.50202156 0.00000000

H 6.12665065 2.50203986 0.00000000

H 3.67596319 -2.50203336 0.00000000

H 3.67596371 2.50205082 0.00000000

H 1.22531698 -2.50203776 0.00000000

H 1.22531677 2.50205355 0.00000000

H -1.22531554 -2.50203902 0.00000000

H -1.22531633 2.50205238 0.00000000

H -3.67596222 -2.50203694 0.00000000

H -3.67596327 2.50204746 0.00000000

H -6.12664904 -2.50202705 0.00000000

H -6.12665008 2.50203462 0.00000000

H -8.57738848 -2.50200472 0.00000000

H -8.57738943 2.50200949 0.00000000

H -11.02815361 -2.50197691 0.00000000

H -11.02815453 2.50197899 0.00000000

H -13.47884508 -2.50196792 0.00000000

H -13.47884601 2.50196737 0.00000000

H -15.92928135 -2.50202805 0.00000000

H -15.92928233 2.50202485 0.00000000

H -18.37932797 -2.50221015 0.00000000

H -18.37932910 2.50220442 0.00000000

H -20.82906460 -2.50251041 0.00000000

H -20.82906588 2.50250230 0.00000000

H -23.27902511 -2.50277686 0.00000000

H -23.27902646 2.50276698 0.00000000

H -25.73033549 -2.50263232 0.00000000

H -25.73033690 2.50262145 0.00000000

H -28.18468265 -2.50125715 0.00000000

H -28.18468402 2.50124569 0.00000000

H -30.63739614 -2.50074642 0.00000000

H -30.63739724 2.50073429 0.00000000

H -32.78275305 -1.24962792 0.00000000

H -32.78275354 1.24961509 0.00000000

$end

$comment

27-acene singlet

$end

$molecule

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C 34.27600533 -0.70829256 0.00000000

C 34.27600310 0.70831710 0.00000000

C 33.09315170 -1.40198213 0.00000000

C 33.09314742 1.40200297 0.00000000

C 31.84885337 -0.72175865 0.00000000

C 31.84885125 0.72177589 0.00000000

C 30.63148732 -1.40098422 0.00000000

C 30.63148349 1.40099785 0.00000000

C 29.40522300 -0.72512662 0.00000000

C 29.40522123 0.72513731 0.00000000

C 28.17768877 -1.40261600 0.00000000

C 28.17768568 1.40262364 0.00000000

C 26.95696199 -0.72697559 0.00000000

C 26.95696062 0.72698079 0.00000000

C 25.72690382 -1.40270102 0.00000000

C 25.72690128 1.40270385 0.00000000

C 24.50628010 -0.72766313 0.00000000

C 24.50627893 0.72766372 0.00000000

C 23.27712266 -1.40238158 0.00000000

C 23.27712040 1.40238028 0.00000000

C 22.05475096 -0.72772435 0.00000000

C 22.05474982 0.72772098 0.00000000

C 20.82741129 -1.40204145 0.00000000

C 20.82740923 1.40203644 0.00000000

C 19.60324619 -0.72752584 0.00000000

C 19.60324516 0.72751904 0.00000000

C 18.37739263 -1.40183537 0.00000000

C 18.37739092 1.40182711 0.00000000

C 17.15210239 -0.72730695 0.00000000

C 17.15210158 0.72729733 0.00000000

C 15.92703904 -1.40176390 0.00000000

C 15.92703783 1.40175312 0.00000000

C 14.70131975 -0.72716537 0.00000000

C 14.70131924 0.72715372 0.00000000

C 13.47647216 -1.40177171 0.00000000

C 13.47647157 1.40175936 0.00000000

C 12.25076104 -0.72710930 0.00000000

C 12.25076090 0.72709664 0.00000000

C 11.02582335 -1.40180685 0.00000000

C 11.02582346 1.40179407 0.00000000

C 9.80028472 -0.72710820 0.00000000

C 9.80028494 0.72709571 0.00000000

C 8.57517734 -1.40183967 0.00000000

C 8.57517808 1.40182766 0.00000000

C 7.34980250 -0.72712978 0.00000000

C 7.34980306 0.72711848 0.00000000

C 6.12456701 -1.40185969 0.00000000

C 6.12456825 1.40184940 0.00000000

C 4.89928141 -0.72715180 0.00000000

C 4.89928215 0.72714247 0.00000000

C 3.67399236 -1.40186788 0.00000000

C 3.67399379 1.40185992 0.00000000

C 2.44872485 -0.72716421 0.00000000

C 2.44872562 0.72715719 0.00000000

C 1.22343849 -1.40186906 0.00000000

C 1.22343991 1.40186357 0.00000000

C -0.00184586 -0.72716376 0.00000000

C -0.00184517 0.72715920 0.00000000

C -1.22711380 -1.40186535 0.00000000

C -1.22711247 1.40186228 0.00000000

C -2.45240417 -0.72715009 0.00000000

C -2.45240353 0.72714799 0.00000000

C -3.67768423 -1.40185477 0.00000000

C -3.67768292 1.40185404 0.00000000

C -4.90292719 -0.72712570 0.00000000

C -4.90292653 0.72712608 0.00000000

C -6.12828925 -1.40183306 0.00000000

C -6.12828788 1.40183471 0.00000000

C -7.35340823 -0.72710009 0.00000000

C -7.35340750 0.72710296 0.00000000

C -8.57893188 -1.40179906 0.00000000

C -8.57893046 1.40180320 0.00000000

C -9.80387667 -0.72709509 0.00000000

C -9.80387592 0.72710040 0.00000000

C -11.02958222 -1.40176373 0.00000000

C -11.02958090 1.40177030 0.00000000

C -12.25441844 -0.72714543 0.00000000

C -12.25441779 0.72715298 0.00000000

C -13.48015709 -1.40175723 0.00000000

C -13.48015610 1.40176586 0.00000000

C -14.70517726 -0.72728392 0.00000000

C -14.70517684 0.72729309 0.00000000

C -15.93051955 -1.40182922 0.00000000

C -15.93051912 1.40183912 0.00000000

C -17.15630245 -0.72750931 0.00000000

C -17.15630239 0.72751909 0.00000000

C -18.38053754 -1.40203348 0.00000000

C -18.38053795 1.40204340 0.00000000

C -19.60781137 -0.72772907 0.00000000

C -19.60781181 0.72773801 0.00000000

C -20.83022728 -1.40237114 0.00000000

C -20.83022859 1.40237953 0.00000000

C -22.05937940 -0.72770295 0.00000000

C -22.05938035 0.72770968 0.00000000

C -23.27996648 -1.40268810 0.00000000

C -23.27996853 1.40269351 0.00000000

C -24.51010980 -0.72702999 0.00000000

C -24.51011104 0.72703345 0.00000000

C -25.73071341 -1.40258288 0.00000000

C -25.73071567 1.40258446 0.00000000

C -26.95835390 -0.72516793 0.00000000

C -26.95835506 0.72516767 0.00000000

C -28.18445598 -1.40110092 0.00000000

C -28.18445801 1.40109869 0.00000000

C -29.40197618 -0.72170726 0.00000000

C -29.40197714 0.72170349 0.00000000

C -30.64589221 -1.40198605 0.00000000

C -30.64589392 1.40198062 0.00000000

C -31.82898839 -0.70814186 0.00000000

C -31.82898923 0.70813509 0.00000000

H 35.23058172 -1.24938861 0.00000000

H 35.23057783 1.24941605 0.00000000

H 33.08438935 -2.50078866 0.00000000

H 33.08438185 2.50080935 0.00000000

H 30.63200761 -2.50119428 0.00000000

H 30.63200080 2.50120772 0.00000000

H 28.17773479 -2.50266916 0.00000000

H 28.17772910 2.50267663 0.00000000

H 25.72691924 -2.50278544 0.00000000

H 25.72691447 2.50278825 0.00000000

H 23.27712402 -2.50249980 0.00000000

H 23.27711991 2.50249860 0.00000000

H 20.82739025 -2.50218353 0.00000000

H 20.82738668 2.50217864 0.00000000

H 18.37737365 -2.50198901 0.00000000

H 18.37737074 2.50198082 0.00000000

H 15.92703307 -2.50191984 0.00000000

H 15.92703100 2.50190907 0.00000000

H 13.47647654 -2.50192548 0.00000000

H 13.47647555 2.50191308 0.00000000

H 11.02583187 -2.50195744 0.00000000

H 11.02583208 2.50194459 0.00000000

H 8.57518444 -2.50198779 0.00000000

H 8.57518570 2.50197570 0.00000000

H 6.12457126 -2.50200642 0.00000000

H 6.12457332 2.50199611 0.00000000

H 3.67399458 -2.50201406 0.00000000

H 3.67399699 2.50200617 0.00000000

H 1.22343896 -2.50201507 0.00000000

H 1.22344149 2.50200970 0.00000000

H -1.22711678 -2.50201137 0.00000000

H -1.22711426 2.50200843 0.00000000

H -3.67769385 -2.50200115 0.00000000

H -3.67769134 2.50200052 0.00000000

H -6.12830744 -2.50198053 0.00000000

H -6.12830493 2.50198229 0.00000000

H -8.57895416 -2.50194869 0.00000000

H -8.57895168 2.50195299 0.00000000

H -11.02959243 -2.50191618 0.00000000

H -11.02959017 2.50192302 0.00000000

H -13.48012760 -2.50191152 0.00000000

H -13.48012596 2.50192054 0.00000000

H -15.93042703 -2.50198120 0.00000000

H -15.93042641 2.50199159 0.00000000

H -18.38039235 -2.50217484 0.00000000

H -18.38039317 2.50218530 0.00000000

H -20.83011494 -2.50249093 0.00000000

H -20.83011718 2.50249983 0.00000000

H -23.28005107 -2.50277907 0.00000000

H -23.28005442 2.50278480 0.00000000

H -25.73120991 -2.50265688 0.00000000

H -25.73121370 2.50265853 0.00000000

H -28.18529639 -2.50129419 0.00000000

H -28.18529999 2.50129190 0.00000000

H -30.63785570 -2.50079688 0.00000000

H -30.63785879 2.50079139 0.00000000

H -32.78331703 -1.24950252 0.00000000

H -32.78331856 1.24949454 0.00000000

$end

$comment

27-acene triplet

$end

$molecule

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C 34.27721929 0.70817248 0.00000000

C 33.09418448 -1.40194328 0.00000000

C 33.09419348 1.40187433 0.00000000

C 31.85006171 -0.72172073 0.00000000

C 31.85006621 0.72165962 0.00000000

C 30.63243008 -1.40094546 0.00000000

C 30.63243905 1.40089199 0.00000000

C 29.40632814 -0.72511428 0.00000000

C 29.40633254 0.72506825 0.00000000

C 28.17859740 -1.40258031 0.00000000

C 28.17860607 1.40254175 0.00000000

C 26.95785437 -0.72697359 0.00000000

C 26.95785854 0.72694210 0.00000000

C 25.72780762 -1.40266618 0.00000000

C 25.72781556 1.40264186 0.00000000

C 24.50693450 -0.72763840 0.00000000

C 24.50693840 0.72762057 0.00000000

C 23.27799347 -1.40235062 0.00000000

C 23.27800037 1.40233951 0.00000000

C 22.05523848 -0.72765816 0.00000000

C 22.05524198 0.72765290 0.00000000

C 20.82818524 -1.40202099 0.00000000

C 20.82819094 1.40202175 0.00000000

C 19.60367187 -0.72742859 0.00000000

C 19.60367492 0.72743443 0.00000000

C 18.37802131 -1.40182858 0.00000000

C 18.37802588 1.40183966 0.00000000

C 17.15253241 -0.72720338 0.00000000

C 17.15253501 0.72721880 0.00000000

C 15.92751791 -1.40176712 0.00000000

C 15.92752145 1.40178689 0.00000000

C 14.70175814 -0.72707372 0.00000000

C 14.70176030 0.72709712 0.00000000

C 13.47682921 -1.40177670 0.00000000

C 13.47683191 1.40180375 0.00000000

C 12.25117241 -0.72703323 0.00000000

C 12.25117420 0.72706329 0.00000000

C 11.02609259 -1.40180566 0.00000000

C 11.02609456 1.40183870 0.00000000

C 9.80062846 -0.72704126 0.00000000

C 9.80062991 0.72707670 0.00000000

C 8.57538042 -1.40182814 0.00000000

C 8.57538174 1.40186600 0.00000000

C 7.35005354 -0.72706342 0.00000000

C 7.35005467 0.72710310 0.00000000

C 6.12470945 -1.40183803 0.00000000

C 6.12471009 1.40187960 0.00000000

C 4.89943271 -0.72708132 0.00000000

C 4.89943346 0.72712405 0.00000000

C 3.67406945 -1.40183954 0.00000000

C 3.67406943 1.40188362 0.00000000

C 2.44877873 -0.72709028 0.00000000

C 2.44877912 0.72713493 0.00000000

C 1.22344435 -1.40183896 0.00000000

C 1.22344366 1.40188438 0.00000000

C -0.00188781 -0.72709073 0.00000000

C -0.00188774 0.72713618 0.00000000

C -1.22718008 -1.40183872 0.00000000

C -1.22718138 1.40188445 0.00000000

C -2.45254528 -0.72708231 0.00000000

C -2.45254554 0.72712748 0.00000000

C -3.67781811 -1.40183636 0.00000000

C -3.67782007 1.40188127 0.00000000

C -4.90317132 -0.72706386 0.00000000

C -4.90317198 0.72710753 0.00000000

C -6.12848647 -1.40182604 0.00000000

C -6.12848932 1.40186877 0.00000000

C -7.35374938 -0.72703931 0.00000000

C -7.35375055 0.72707987 0.00000000

C -8.57919756 -1.40180344 0.00000000

C -8.57920147 1.40184228 0.00000000

C -9.80428996 -0.72702629 0.00000000

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C -11.02993741 -1.40177511 0.00000000

C -11.02994251 1.40180803 0.00000000

C -12.25486213 -0.72706130 0.00000000

C -12.25486454 0.72708997 0.00000000

C -13.48063548 -1.40176746 0.00000000

C -13.48064168 1.40179240 0.00000000

C -14.70561349 -0.72718711 0.00000000

C -14.70561647 0.72720690 0.00000000

C -15.93114939 -1.40182969 0.00000000

C -15.93115653 1.40184481 0.00000000

C -17.15673269 -0.72741736 0.00000000

C -17.15673618 0.72742652 0.00000000

C -18.38131495 -1.40201970 0.00000000

C -18.38132288 1.40202329 0.00000000

C -19.60830108 -0.72766656 0.00000000

C -19.60830508 0.72766337 0.00000000

C -20.83110387 -1.40234483 0.00000000

C -20.83111242 1.40233520 0.00000000

C -22.06003463 -0.72768024 0.00000000

C -22.06003910 0.72766295 0.00000000

C -23.28087698 -1.40265461 0.00000000

C -23.28088606 1.40263003 0.00000000

C -24.51100256 -0.72702786 0.00000000

C -24.51100753 0.72699472 0.00000000

C -25.73162894 -1.40254572 0.00000000

C -25.73163856 1.40250440 0.00000000

C -26.95945951 -0.72515194 0.00000000

C -26.95946480 0.72510148 0.00000000

C -28.18540593 -1.40105944 0.00000000

C -28.18541604 1.40100014 0.00000000

C -29.40318752 -0.72166109 0.00000000

C -29.40319296 0.72159251 0.00000000

C -30.64693037 -1.40194049 0.00000000

C -30.64694084 1.40186256 0.00000000

C -31.83020266 -0.70808865 0.00000000

C -31.83020799 0.70800170 0.00000000

H 35.23174563 -1.24942252 0.00000000

H 35.23175355 1.24933995 0.00000000

H 33.08540265 -2.50075108 0.00000000

H 33.08541864 2.50068221 0.00000000

H 30.63294772 -2.50115750 0.00000000

H 30.63296340 2.50110412 0.00000000

H 28.17864073 -2.50263447 0.00000000

H 28.17865579 2.50259613 0.00000000

H 25.72782691 -2.50275107 0.00000000

H 25.72784086 2.50272712 0.00000000

H 23.27800528 -2.50246825 0.00000000

H 23.27801776 2.50245760 0.00000000

H 20.82817728 -2.50216086 0.00000000

H 20.82818798 2.50216209 0.00000000

H 18.37801244 -2.50197838 0.00000000

H 18.37802136 2.50198991 0.00000000

H 15.92751531 -2.50191812 0.00000000

H 15.92752248 2.50193827 0.00000000

H 13.47683015 -2.50192511 0.00000000

H 13.47683587 2.50195248 0.00000000

H 11.02609378 -2.50195105 0.00000000

H 11.02609815 2.50198435 0.00000000

H 8.57537976 -2.50197146 0.00000000

H 8.57538291 2.50200959 0.00000000

H 6.12470801 -2.50198045 0.00000000

H 6.12470994 2.50202229 0.00000000

H 3.67406918 -2.50198180 0.00000000

H 3.67406992 2.50202616 0.00000000

H 1.22344585 -2.50198128 0.00000000

H 1.22344541 2.50202698 0.00000000

H -1.22717854 -2.50198106 0.00000000

H -1.22718009 2.50202709 0.00000000

H -3.67782013 -2.50197881 0.00000000

H -3.67782289 2.50202409 0.00000000

H -6.12849550 -2.50196915 0.00000000

H -6.12849987 2.50201231 0.00000000

H -8.57921239 -2.50194821 0.00000000

H -8.57921858 2.50198755 0.00000000

H -11.02994593 -2.50192241 0.00000000

H -11.02995425 2.50195584 0.00000000

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H -13.48062291 2.50194223 0.00000000

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H -15.93108202 2.50199322 0.00000000

H -18.38118332 -2.50215867 0.00000000

H -18.38119691 2.50216257 0.00000000

H -20.83099998 -2.50246390 0.00000000

H -20.83101495 2.50245453 0.00000000

H -23.28096376 -2.50274599 0.00000000

H -23.28097996 2.50272165 0.00000000

H -25.73212238 -2.50262058 0.00000000

H -25.73213969 2.50257947 0.00000000

H -28.18623850 -2.50125368 0.00000000

H -28.18625664 2.50119454 0.00000000

H -30.63887965 -2.50075212 0.00000000

H -30.63889833 2.50067434 0.00000000

H -32.78449047 -1.24951888 0.00000000

H -32.78449984 1.24942483 0.00000000

$end

$comment

28-acene singlet

$end

$molecule

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C 33.09468052 1.40200128 0.00000000

C 31.85079791 -0.72173010 0.00000000

C 31.85079961 0.72171254 0.00000000

C 30.63322604 -1.40113518 0.00000000

C 30.63322916 1.40112052 0.00000000

C 29.40715329 -0.72522320 0.00000000

C 29.40715481 0.72521102 0.00000000

C 28.17947358 -1.40261383 0.00000000

C 28.17947634 1.40260438 0.00000000

C 26.95886293 -0.72708223 0.00000000

C 26.95886423 0.72707495 0.00000000

C 25.72872902 -1.40273003 0.00000000

C 25.72873137 1.40272505 0.00000000

C 24.50809977 -0.72773383 0.00000000

C 24.50810087 0.72773071 0.00000000

C 23.27899701 -1.40242130 0.00000000

C 23.27899895 1.40242009 0.00000000

C 22.05652585 -0.72773862 0.00000000

C 22.05652675 0.72773886 0.00000000

C 20.82930622 -1.40208294 0.00000000

C 20.82930772 1.40208476 0.00000000

C 19.60503014 -0.72750956 0.00000000

C 19.60503081 0.72751242 0.00000000

C 18.37927693 -1.40187217 0.00000000

C 18.37927807 1.40187628 0.00000000

C 17.15392146 -0.72728509 0.00000000

C 17.15392194 0.72728998 0.00000000

C 15.92890071 -1.40179237 0.00000000

C 15.92890154 1.40179819 0.00000000

C 14.70317090 -0.72715196 0.00000000

C 14.70317123 0.72715837 0.00000000

C 13.47831550 -1.40179522 0.00000000

C 13.47831610 1.40180232 0.00000000

C 12.25262708 -0.72710696 0.00000000

C 12.25262730 0.72711455 0.00000000

C 11.02765907 -1.40182882 0.00000000

C 11.02765952 1.40183685 0.00000000

C 9.80215070 -0.72711202 0.00000000

C 9.80215089 0.72712047 0.00000000

C 8.57701271 -1.40186093 0.00000000

C 8.57701310 1.40186969 0.00000000

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C 7.35166281 0.72714383 0.00000000

C 6.12640332 -1.40188051 0.00000000

C 6.12640370 1.40188993 0.00000000

C 4.90113655 -0.72715533 0.00000000

C 4.90113677 0.72716507 0.00000000

C 3.67582816 -1.40188814 0.00000000

C 3.67582845 1.40189815 0.00000000

C 2.45057699 -0.72716766 0.00000000

C 2.45057713 0.72717781 0.00000000

C 1.22527373 -1.40188993 0.00000000

C 1.22527382 1.40190027 0.00000000

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C -0.00000019 0.72718186 0.00000000

C -1.22527407 -1.40188994 0.00000000

C -1.22527421 1.40190023 0.00000000

C -2.45057731 -0.72716771 0.00000000

C -2.45057748 0.72717773 0.00000000

C -3.67582840 -1.40188818 0.00000000

C -3.67582874 1.40189801 0.00000000

C -4.90113673 -0.72715540 0.00000000

C -4.90113698 0.72716494 0.00000000

C -6.12640341 -1.40188057 0.00000000

C -6.12640383 1.40188974 0.00000000

C -7.35166261 -0.72713477 0.00000000

C -7.35166284 0.72714365 0.00000000

C -8.57701264 -1.40186104 0.00000000

C -8.57701306 1.40186949 0.00000000

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C -12.25262697 -0.72710716 0.00000000

C -12.25262721 0.72711438 0.00000000

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C -13.47831604 1.40180218 0.00000000

C -14.70317090 -0.72715216 0.00000000

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C -15.92890079 -1.40179258 0.00000000

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C -17.15392210 0.72728985 0.00000000

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C -18.37927830 1.40187615 0.00000000

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C -19.60503111 0.72751230 0.00000000

C -20.82930656 -1.40208306 0.00000000

C -20.82930804 1.40208462 0.00000000

C -22.05652618 -0.72773872 0.00000000

C -22.05652706 0.72773874 0.00000000

C -23.27899731 -1.40242135 0.00000000

C -23.27899919 1.40241997 0.00000000

C -24.50809997 -0.72773385 0.00000000

C -24.50810105 0.72773061 0.00000000

C -25.72872914 -1.40272999 0.00000000

C -25.72873140 1.40272495 0.00000000

C -26.95886290 -0.72708217 0.00000000

C -26.95886416 0.72707492 0.00000000

C -28.17947345 -1.40261369 0.00000000

C -28.17947611 1.40260433 0.00000000

C -29.40715302 -0.72522307 0.00000000

C -29.40715448 0.72521104 0.00000000

C -30.63322568 -1.40113499 0.00000000

C -30.63322870 1.40112055 0.00000000

C -31.85079743 -0.72172991 0.00000000

C -31.85079908 0.72171266 0.00000000

C -33.09467667 -1.40202147 0.00000000

C -33.09467988 1.40200142 0.00000000

C -34.27779984 -0.70812160 0.00000000

C -34.27780145 0.70809881 0.00000000

H 35.23206937 -1.24964997 0.00000000

H 35.23207232 1.24962445 0.00000000

H 33.08685975 -2.50084221 0.00000000

H 33.08686560 2.50082182 0.00000000

H 30.63423188 -2.50133640 0.00000000

H 30.63423733 2.50132188 0.00000000

H 28.17993126 -2.50269857 0.00000000

H 28.17993624 2.50268929 0.00000000

H 25.72862556 -2.50282987 0.00000000

H 25.72862979 2.50282508 0.00000000

H 23.27868649 -2.50254666 0.00000000

H 23.27868991 2.50254563 0.00000000

H 20.82904347 -2.50222802 0.00000000

H 20.82904615 2.50223002 0.00000000

H 18.37915618 -2.50202826 0.00000000

H 18.37915827 2.50203251 0.00000000

H 15.92889727 -2.50195220 0.00000000

H 15.92889885 2.50195814 0.00000000

H 13.47836268 -2.50195441 0.00000000

H 13.47836389 2.50196158 0.00000000

H 11.02770710 -2.50198588 0.00000000

H 11.02770802 2.50199393 0.00000000

H 8.57704054 -2.50201592 0.00000000

H 8.57704128 2.50202466 0.00000000

H 6.12641220 -2.50203404 0.00000000

H 6.12641278 2.50204346 0.00000000

H 3.67582786 -2.50204097 0.00000000

H 3.67582824 2.50205103 0.00000000

H 1.22527272 -2.50204249 0.00000000

H 1.22527280 2.50205292 0.00000000

H -1.22527293 -2.50204248 0.00000000

H -1.22527314 2.50205286 0.00000000

H -3.67582808 -2.50204096 0.00000000

H -3.67582854 2.50205085 0.00000000

H -6.12641228 -2.50203405 0.00000000

H -6.12641293 2.50204322 0.00000000

H -8.57704049 -2.50201599 0.00000000

H -8.57704125 2.50202442 0.00000000

H -11.02770698 -2.50198604 0.00000000

H -11.02770794 2.50199373 0.00000000

H -13.47836265 -2.50195465 0.00000000

H -13.47836384 2.50196144 0.00000000

H -15.92889737 -2.50195244 0.00000000

H -15.92889892 2.50195804 0.00000000

H -18.37915643 -2.50202846 0.00000000

H -18.37915847 2.50203240 0.00000000

H -20.82904380 -2.50222814 0.00000000

H -20.82904644 2.50222987 0.00000000

H -23.27868679 -2.50254668 0.00000000

H -23.27869012 2.50254547 0.00000000

H -25.72862571 -2.50282976 0.00000000

H -25.72862977 2.50282491 0.00000000

H -28.17993115 -2.50269836 0.00000000

H -28.17993600 2.50268916 0.00000000

H -30.63423156 -2.50133615 0.00000000

H -30.63423684 2.50132184 0.00000000

H -33.08685926 -2.50084189 0.00000000

H -33.08686492 2.50082192 0.00000000

H -35.23206883 -1.24964967 0.00000000

H -35.23207166 1.24962473 0.00000000

$end

$comment

28-acene triplet

$end

$molecule

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C 34.27893758 0.70801512 0.00000000

C 33.09564493 -1.40193612 0.00000000

C 33.09564557 1.40193307 0.00000000

C 31.85193697 -0.72164907 0.00000000

C 31.85193741 0.72164684 0.00000000

C 30.63411570 -1.40106399 0.00000000

C 30.63411630 1.40106254 0.00000000

C 29.40819337 -0.72518258 0.00000000

C 29.40819394 0.72518213 0.00000000

C 28.18033815 -1.40255440 0.00000000

C 28.18033874 1.40255482 0.00000000

C 26.95970257 -0.72706065 0.00000000

C 26.95970311 0.72706195 0.00000000

C 25.72959566 -1.40268329 0.00000000

C 25.72959629 1.40268538 0.00000000

C 24.50872035 -0.72769713 0.00000000

C 24.50872068 0.72769971 0.00000000

C 23.27983550 -1.40239015 0.00000000

C 23.27983618 1.40239317 0.00000000

C 22.05699822 -0.72767063 0.00000000

C 22.05699832 0.72767372 0.00000000

C 20.83005201 -1.40207023 0.00000000

C 20.83005272 1.40207338 0.00000000

C 19.60545321 -0.72742235 0.00000000

C 19.60545315 0.72742525 0.00000000

C 18.37988440 -1.40187840 0.00000000

C 18.37988516 1.40188110 0.00000000

C 17.15435378 -0.72720220 0.00000000

C 17.15435365 0.72720451 0.00000000

C 15.92936870 -1.40181373 0.00000000

C 15.92936947 1.40181563 0.00000000

C 14.70361148 -0.72708832 0.00000000

C 14.70361132 0.72708977 0.00000000

C 13.47867341 -1.40182360 0.00000000

C 13.47867421 1.40182454 0.00000000

C 12.25303961 -0.72706286 0.00000000

C 12.25303948 0.72706342 0.00000000

C 11.02794009 -1.40185612 0.00000000

C 11.02794099 1.40185618 0.00000000

C 9.80249685 -0.72707886 0.00000000

C 9.80249679 0.72707869 0.00000000

C 8.57723642 -1.40188200 0.00000000

C 8.57723750 1.40188146 0.00000000

C 7.35192040 -0.72710271 0.00000000

C 7.35192046 0.72710216 0.00000000

C 6.12657270 -1.40189427 0.00000000

C 6.12657397 1.40189352 0.00000000

C 4.90130220 -0.72711875 0.00000000

C 4.90130237 0.72711820 0.00000000

C 3.67593570 -1.40189621 0.00000000

C 3.67593707 1.40189562 0.00000000

C 2.45065660 -0.72712574 0.00000000

C 2.45065685 0.72712541 0.00000000

C 1.22531029 -1.40189499 0.00000000

C 1.22531172 1.40189476 0.00000000

C -0.00000042 -0.72712729 0.00000000

C -0.00000016 0.72712734 0.00000000

C -1.22531232 -1.40189478 0.00000000

C -1.22531089 1.40189502 0.00000000

C -2.45065739 -0.72712538 0.00000000

C -2.45065716 0.72712579 0.00000000

C -3.67593760 -1.40189569 0.00000000

C -3.67593622 1.40189625 0.00000000

C -4.90130282 -0.72711821 0.00000000

C -4.90130267 0.72711878 0.00000000

C -6.12657439 -1.40189362 0.00000000

C -6.12657310 1.40189429 0.00000000

C -7.35192083 -0.72710218 0.00000000

C -7.35192077 0.72710273 0.00000000

C -8.57723782 -1.40188152 0.00000000

C -8.57723668 1.40188200 0.00000000

C -9.80249708 -0.72707869 0.00000000

C -9.80249712 0.72707888 0.00000000

C -11.02794123 -1.40185620 0.00000000

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C -12.25303968 -0.72706339 0.00000000

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C -13.47867439 -1.40182450 0.00000000

C -13.47867355 1.40182353 0.00000000

C -14.70361147 -0.72708970 0.00000000

C -14.70361161 0.72708832 0.00000000

C -15.92936960 -1.40181553 0.00000000

C -15.92936881 1.40181368 0.00000000

C -17.15435371 -0.72720438 0.00000000

C -17.15435383 0.72720226 0.00000000

C -18.37988520 -1.40188097 0.00000000

C -18.37988447 1.40187839 0.00000000

C -19.60545315 -0.72742512 0.00000000

C -19.60545319 0.72742241 0.00000000

C -20.83005270 -1.40207325 0.00000000

C -20.83005200 1.40207025 0.00000000

C -22.05699823 -0.72767358 0.00000000

C -22.05699809 0.72767073 0.00000000

C -23.27983603 -1.40239306 0.00000000

C -23.27983538 1.40239024 0.00000000

C -24.50872049 -0.72769958 0.00000000

C -24.50872013 0.72769725 0.00000000

C -25.72959601 -1.40268528 0.00000000

C -25.72959537 1.40268342 0.00000000

C -26.95970279 -0.72706181 0.00000000

C -26.95970221 0.72706079 0.00000000

C -28.18033835 -1.40255470 0.00000000

C -28.18033767 1.40255459 0.00000000

C -29.40819351 -0.72518192 0.00000000

C -29.40819288 0.72518282 0.00000000

C -30.63411581 -1.40106233 0.00000000

C -30.63411511 1.40106430 0.00000000

C -31.85193686 -0.72164652 0.00000000

C -31.85193634 0.72164939 0.00000000

C -33.09564499 -1.40193272 0.00000000

C -33.09564422 1.40193651 0.00000000

C -34.27893695 -0.70801470 0.00000000

C -34.27893649 0.70801925 0.00000000

H 35.23315819 -1.24962786 0.00000000

H 35.23315887 1.24962362 0.00000000

H 33.08783716 -2.50075664 0.00000000

H 33.08783848 2.50075360 0.00000000

H 30.63513130 -2.50126571 0.00000000

H 30.63513270 2.50126425 0.00000000

H 28.18079140 -2.50263970 0.00000000

H 28.18079268 2.50264010 0.00000000

H 25.72948523 -2.50278297 0.00000000

H 25.72948637 2.50278503 0.00000000

H 23.27953335 -2.50251408 0.00000000

H 23.27953431 2.50251708 0.00000000

H 20.82981522 -2.50221251 0.00000000

H 20.82981602 2.50221563 0.00000000

H 18.37979249 -2.50203044 0.00000000

H 18.37979322 2.50203311 0.00000000

H 15.92938176 -2.50196857 0.00000000

H 15.92938245 2.50197043 0.00000000

H 13.47872069 -2.50197733 0.00000000

H 13.47872142 2.50197821 0.00000000

H 11.02797677 -2.50200770 0.00000000

H 11.02797766 2.50200767 0.00000000

H 8.57725032 -2.50203184 0.00000000

H 8.57725151 2.50203118 0.00000000

H 6.12657091 -2.50204315 0.00000000

H 6.12657239 2.50204230 0.00000000

H 3.67592953 -2.50204487 0.00000000

H 3.67593115 2.50204422 0.00000000

H 1.22530731 -2.50204368 0.00000000

H 1.22530902 2.50204341 0.00000000

H -1.22530967 -2.50204347 0.00000000

H -1.22530797 2.50204368 0.00000000

H -3.67593169 -2.50204434 0.00000000

H -3.67593008 2.50204491 0.00000000

H -6.12657278 -2.50204246 0.00000000

H -6.12657127 2.50204316 0.00000000

H -8.57725176 -2.50203129 0.00000000

H -8.57725052 2.50203182 0.00000000

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H -11.02797691 2.50200763 0.00000000

H -13.47872155 -2.50197816 0.00000000

H -13.47872078 2.50197720 0.00000000

H -15.92938260 -2.50197030 0.00000000

H -15.92938183 2.50196844 0.00000000

H -18.37979331 -2.50203295 0.00000000

H -18.37979261 2.50203035 0.00000000

H -20.82981605 -2.50221549 0.00000000

H -20.82981529 2.50221247 0.00000000

H -23.27953421 -2.50251698 0.00000000

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H -25.72948612 -2.50278497 0.00000000

H -25.72948499 2.50278310 0.00000000

H -28.18079231 -2.50264002 0.00000000

H -28.18079088 2.50263992 0.00000000

H -30.63513226 -2.50126408 0.00000000

H -30.63513068 2.50126604 0.00000000

H -33.08783792 -2.50075327 0.00000000

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H -35.23315828 -1.24962319 0.00000000

H -35.23315748 1.24962832 0.00000000

$end

$comment

29-acene singlet

$end

$molecule

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C 36.72608960 0.70826186 0.00000000

C 35.54322196 -1.40194672 0.00000000

C 35.54321592 1.40200519 0.00000000

C 34.29898822 -0.72178683 0.00000000

C 34.29898517 0.72183996 0.00000000

C 33.08162127 -1.40102794 0.00000000

C 33.08161543 1.40107595 0.00000000

C 31.85538304 -0.72510535 0.00000000

C 31.85538005 0.72514831 0.00000000

C 30.62784455 -1.40258618 0.00000000

C 30.62783878 1.40262406 0.00000000

C 29.40709992 -0.72695577 0.00000000

C 29.40709693 0.72698859 0.00000000

C 28.17705134 -1.40268967 0.00000000

C 28.17704548 1.40271750 0.00000000

C 26.95641927 -0.72764992 0.00000000

C 26.95641619 0.72767246 0.00000000

C 25.72726770 -1.40237398 0.00000000

C 25.72726168 1.40239146 0.00000000

C 24.50489187 -0.72771470 0.00000000

C 24.50488869 0.72772680 0.00000000

C 23.27755598 -1.40203744 0.00000000

C 23.27754990 1.40204429 0.00000000

C 22.05338894 -0.72752020 0.00000000

C 22.05338578 0.72752177 0.00000000

C 20.82753758 -1.40183522 0.00000000

C 20.82753175 1.40183161 0.00000000

C 19.60224561 -0.72730573 0.00000000

C 19.60224266 0.72729728 0.00000000

C 18.37718411 -1.40176799 0.00000000

C 18.37717887 1.40175466 0.00000000

C 17.15146285 -0.72716786 0.00000000

C 17.15146031 0.72715037 0.00000000

C 15.92661747 -1.40177896 0.00000000

C 15.92661310 1.40175719 0.00000000

C 14.70090423 -0.72711421 0.00000000

C 14.70090222 0.72708911 0.00000000

C 13.47596973 -1.40181700 0.00000000

C 13.47596633 1.40178845 0.00000000

C 12.25043099 -0.72711521 0.00000000

C 12.25042948 0.72708413 0.00000000

C 11.02532452 -1.40185150 0.00000000

C 11.02532197 1.40181781 0.00000000

C 9.79995606 -0.72713752 0.00000000

C 9.79995494 0.72710188 0.00000000

C 8.57471398 -1.40187220 0.00000000

C 8.57471207 1.40183466 0.00000000

C 7.34944602 -0.72716061 0.00000000

C 7.34944517 0.72712158 0.00000000

C 6.12413795 -1.40188051 0.00000000

C 6.12413652 1.40184008 0.00000000

C 4.89890040 -0.72717620 0.00000000

C 4.89889978 0.72713466 0.00000000

C 3.67358456 -1.40188213 0.00000000

C 3.67358358 1.40183959 0.00000000

C 2.44833195 -0.72718374 0.00000000

C 2.44833156 0.72714051 0.00000000

C 1.22304192 -1.40188222 0.00000000

C 1.22304141 1.40183837 0.00000000

C -0.00224412 -0.72718460 0.00000000

C -0.00224427 0.72714047 0.00000000

C -1.22749925 -1.40188269 0.00000000

C -1.22749930 1.40183833 0.00000000

C -2.45281305 -0.72717878 0.00000000

C -2.45281296 0.72713449 0.00000000

C -3.67804853 -1.40188176 0.00000000

C -3.67804812 1.40183768 0.00000000

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C -6.12861855 -1.40187446 0.00000000

C -6.12861763 1.40183149 0.00000000

C -7.35386977 -0.72714200 0.00000000

C -7.35386916 0.72710007 0.00000000

C -8.57922278 -1.40185481 0.00000000

C -8.57922113 1.40181402 0.00000000

C -9.80434171 -0.72711805 0.00000000

C -9.80434064 0.72707914 0.00000000

C -11.02986364 -1.40182135 0.00000000

C -11.02986097 1.40178426 0.00000000

C -12.25480512 -0.72711332 0.00000000

C -12.25480342 0.72707918 0.00000000

C -13.48051167 -1.40178464 0.00000000

C -13.48050772 1.40175331 0.00000000

C -14.70534394 -0.72716124 0.00000000

C -14.70534152 0.72713399 0.00000000

C -15.93108355 -1.40177466 0.00000000

C -15.93107828 1.40175137 0.00000000

C -17.15609971 -0.72729594 0.00000000

C -17.15609663 0.72727784 0.00000000

C -18.38144291 -1.40184205 0.00000000

C -18.38143644 1.40182905 0.00000000

C -19.60722018 -0.72751555 0.00000000

C -19.60721651 0.72750866 0.00000000

C -20.83145770 -1.40203974 0.00000000

C -20.83145023 1.40203895 0.00000000

C -22.05872455 -0.72772821 0.00000000

C -22.05872043 0.72773430 0.00000000

C -23.28114476 -1.40236988 0.00000000

C -23.28113644 1.40238285 0.00000000

C -24.51028960 -0.72769454 0.00000000

C -24.51028507 0.72771513 0.00000000

C -25.73088210 -1.40267767 0.00000000

C -25.73087292 1.40270584 0.00000000

C -26.96101974 -0.72701286 0.00000000

C -26.96101478 0.72704950 0.00000000

C -28.18162732 -1.40256167 0.00000000

C -28.18161721 1.40260663 0.00000000

C -29.40926553 -0.72514056 0.00000000

C -29.40926005 0.72519487 0.00000000

C -30.63536804 -1.40106831 0.00000000

C -30.63535704 1.40113186 0.00000000

C -31.85288889 -0.72166774 0.00000000

C -31.85288304 0.72174121 0.00000000

C -33.09680312 -1.40194231 0.00000000

C -33.09679157 1.40202585 0.00000000

C -34.27989822 -0.70808880 0.00000000

C -34.27989235 0.70818223 0.00000000

H 37.68049697 -1.24944384 0.00000000

H 37.68049160 1.24951159 0.00000000

H 35.53474935 -2.50075909 0.00000000

H 35.53473838 2.50081751 0.00000000

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H 33.08202058 2.50127245 0.00000000

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H 30.62786392 2.50267606 0.00000000

H 28.17706539 -2.50277358 0.00000000

H 28.17705487 2.50280147 0.00000000

H 25.72727051 -2.50249182 0.00000000

H 25.72725983 2.50250935 0.00000000

H 23.27753767 -2.50217922 0.00000000

H 23.27752694 2.50218605 0.00000000

H 20.82752152 -2.50198861 0.00000000

H 20.82751129 2.50198483 0.00000000

H 18.37718073 -2.50192366 0.00000000

H 18.37717151 2.50191003 0.00000000

H 15.92662493 -2.50193227 0.00000000

H 15.92661717 2.50191011 0.00000000

H 13.47598016 -2.50196677 0.00000000

H 13.47597405 2.50193783 0.00000000

H 11.02533231 -2.50199844 0.00000000

H 11.02532766 2.50196442 0.00000000

H 8.57471724 -2.50201751 0.00000000

H 8.57471376 2.50197973 0.00000000

H 6.12413833 -2.50202520 0.00000000

H 6.12413576 2.50198459 0.00000000

H 3.67358469 -2.50202672 0.00000000

H 3.67358295 2.50198402 0.00000000

H 1.22304323 -2.50202675 0.00000000

H 1.22304233 2.50198274 0.00000000

H -1.22749746 -2.50202705 0.00000000

H -1.22749758 2.50198254 0.00000000

H -3.67804938 -2.50202603 0.00000000

H -3.67804864 2.50198177 0.00000000

H -6.12862648 -2.50201911 0.00000000

H -6.12862474 2.50197589 0.00000000

H -8.57924056 -2.50200079 0.00000000

H -8.57923747 2.50195965 0.00000000

H -11.02988695 -2.50196977 0.00000000

H -11.02988209 2.50193221 0.00000000

H -13.48052377 -2.50193603 0.00000000

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H -15.93105687 -2.50192790 0.00000000

H -15.93104753 2.50190412 0.00000000

H -18.38135224 -2.50199290 0.00000000

H -18.38134080 2.50197947 0.00000000

H -20.83131361 -2.50218000 0.00000000

H -20.83130034 2.50217886 0.00000000

H -23.28103218 -2.50248878 0.00000000

H -23.28101735 2.50250144 0.00000000

H -25.73096667 -2.50276796 0.00000000

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H -28.18212741 -2.50263510 0.00000000

H -28.18210936 2.50267971 0.00000000

H -30.63621774 -2.50126086 0.00000000

H -30.63619820 2.50132413 0.00000000

H -33.08877963 -2.50075221 0.00000000

H -33.08875910 2.50083553 0.00000000

H -35.23422621 -1.24944973 0.00000000

H -35.23421588 1.24955099 0.00000000

$end

$comment

29-acene triplet

$end

$molecule

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C 35.54415810 1.40191962 0.00000000

C 34.30007917 -0.72173279 0.00000000

C 34.30007658 0.72175949 0.00000000

C 33.08248925 -1.40097760 0.00000000

C 33.08248487 1.40100011 0.00000000

C 31.85638940 -0.72508128 0.00000000

C 31.85638675 0.72509972 0.00000000

C 30.62868812 -1.40254569 0.00000000

C 30.62868402 1.40255988 0.00000000

C 29.40793046 -0.72694785 0.00000000

C 29.40792803 0.72695832 0.00000000

C 28.17789732 -1.40265674 0.00000000

C 28.17789344 1.40266329 0.00000000

C 26.95705319 -0.72762881 0.00000000

C 26.95705121 0.72763220 0.00000000

C 25.72809234 -1.40235005 0.00000000

C 25.72808858 1.40235013 0.00000000

C 24.50538937 -0.72766305 0.00000000

C 24.50538783 0.72766060 0.00000000

C 23.27830369 -1.40202675 0.00000000

C 23.27829990 1.40202148 0.00000000

C 22.05383958 -0.72744551 0.00000000

C 22.05383831 0.72743802 0.00000000

C 20.82816619 -1.40183934 0.00000000

C 20.82816238 1.40182939 0.00000000

C 19.60270610 -0.72722827 0.00000000

C 19.60270499 0.72721633 0.00000000

C 18.37768924 -1.40178300 0.00000000

C 18.37768546 1.40176882 0.00000000

C 17.15193592 -0.72710289 0.00000000

C 17.15193492 0.72708692 0.00000000

C 15.92702259 -1.40179751 0.00000000

C 15.92701902 1.40177955 0.00000000

C 14.70135720 -0.72706478 0.00000000

C 14.70135638 0.72704543 0.00000000

C 13.47630312 -1.40183223 0.00000000

C 13.47629997 1.40181125 0.00000000

C 12.25082543 -0.72707541 0.00000000

C 12.25082482 0.72705347 0.00000000

C 11.02560349 -1.40185960 0.00000000

C 11.02560097 1.40183649 0.00000000

C 9.80026724 -0.72709880 0.00000000

C 9.80026694 0.72707531 0.00000000

C 8.57494132 -1.40187257 0.00000000

C 8.57493960 1.40184851 0.00000000

C 7.34966729 -0.72711673 0.00000000

C 7.34966732 0.72709289 0.00000000

C 6.12430648 -1.40187456 0.00000000

C 6.12430560 1.40185083 0.00000000

C 4.89903712 -0.72712506 0.00000000

C 4.89903749 0.72710211 0.00000000

C 3.67368415 -1.40187183 0.00000000

C 3.67368401 1.40184965 0.00000000

C 2.44839208 -0.72712700 0.00000000

C 2.44839270 0.72710603 0.00000000

C 1.22306531 -1.40186939 0.00000000

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C -0.00225763 -0.72712609 0.00000000

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H 3.67368337 2.50199260 0.00000000

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H -8.57947991 2.50199015 0.00000000

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H -25.73184180 2.50274842 0.00000000

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$comment

30-acene singlet

$end

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C 34.30130634 -0.72172797 0.00000000

C 34.30130741 0.72171497 0.00000000

C 33.08373392 -1.40113631 0.00000000

C 33.08373604 1.40112514 0.00000000

C 31.85766221 -0.72522151 0.00000000

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C 30.62998752 1.40260735 0.00000000

C 29.40937451 -0.72708138 0.00000000

C 29.40937556 0.72707552 0.00000000

C 28.17924478 -1.40273175 0.00000000

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C 26.95861500 0.72773001 0.00000000

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C 8.57695092 1.40189057 0.00000000

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C 7.35168976 0.72716076 0.00000000

C 6.12637553 -1.40188984 0.00000000

C 6.12637645 1.40189817 0.00000000

C 4.90114027 -0.72716372 0.00000000

C 4.90114065 0.72717265 0.00000000

C 3.67581934 -1.40188869 0.00000000

C 3.67581993 1.40189843 0.00000000

C 2.45057250 -0.72716765 0.00000000

C 2.45057266 0.72717775 0.00000000

C 1.22527064 -1.40188663 0.00000000

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H 20.82968360 2.50203295 0.00000000

H 18.37942627 -2.50195671 0.00000000

H 18.37942704 2.50195890 0.00000000

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H 15.92889930 2.50196090 0.00000000

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H 13.47824870 2.50199324 0.00000000

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$end

$comment

30-acene triplet

$end

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C 31.85862304 -0.72518946 0.00000000

C 31.85862311 0.72518398 0.00000000

C 30.63079435 -1.40256653 0.00000000

C 30.63079511 1.40256133 0.00000000

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C 28.18005619 -1.40269482 0.00000000

C 28.18005683 1.40269017 0.00000000

C 26.95921302 -0.72770438 0.00000000

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H 25.72999982 2.50252104 0.00000000

H 23.28029610 -2.50221968 0.00000000

H 23.28029696 2.50221751 0.00000000

H 20.83029567 -2.50203412 0.00000000

H 20.83029647 2.50203370 0.00000000

H 18.37990725 -2.50196964 0.00000000

H 18.37990783 2.50197106 0.00000000

H 15.92926954 -2.50197511 0.00000000

H 15.92926981 2.50197835 0.00000000

H 13.47854378 -2.50200443 0.00000000

H 13.47854373 2.50200931 0.00000000

H 11.02783060 -2.50202954 0.00000000

H 11.02783011 2.50203571 0.00000000

H 8.57716281 -2.50204133 0.00000000

H 8.57716183 2.50204807 0.00000000

H 6.12653152 -2.50204337 0.00000000

H 6.12653011 2.50205016 0.00000000

H 3.67591726 -2.50204096 0.00000000

H 3.67591536 2.50204731 0.00000000

H 1.22530628 -2.50203904 0.00000000

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$comment

31-acene singlet

$end

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C 24.50407260 -0.72751967 0.00000000

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C 9.80017450 0.72716106 0.00000000

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C 8.57486625 1.40188487 0.00000000

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C 6.12430892 1.40188512 0.00000000

C 4.89907203 -0.72713545 0.00000000

C 4.89907236 0.72718147 0.00000000

C 3.67375903 -1.40183647 0.00000000

C 3.67375953 1.40188296 0.00000000

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$end

$comment

31-acene triplet

$end

$molecule

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H -28.18210143 2.50275357 0.00000000

H -30.63325700 -2.50260433 0.00000000

H -30.63325485 2.50262355 0.00000000

H -33.08736293 -2.50122988 0.00000000

H -33.08736116 2.50125166 0.00000000

H -35.53998127 -2.50072220 0.00000000

H -35.53997983 2.50074581 0.00000000

H -37.68553759 -1.24946556 0.00000000

H -37.68553681 1.24949043 0.00000000

$end

$comment

32-acene singlet

$end

$molecule

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C 39.17880567 -0.70809239 0.00000000

C 39.17880419 0.70812461 0.00000000

C 37.99568346 -1.40200128 0.00000000

C 37.99568053 1.40203100 0.00000000

C 36.75181182 -0.72170726 0.00000000

C 36.75181033 0.72173444 0.00000000

C 35.53424038 -1.40111973 0.00000000

C 35.53423753 1.40114436 0.00000000

C 34.30817221 -0.72520548 0.00000000

C 34.30817078 0.72522772 0.00000000

C 33.08049784 -1.40260318 0.00000000

C 33.08049509 1.40262292 0.00000000

C 31.85988753 -0.72706902 0.00000000

C 31.85988616 0.72708641 0.00000000

C 30.62976369 -1.40272342 0.00000000

C 30.62976108 1.40273847 0.00000000

C 29.40913299 -0.72772479 0.00000000

C 29.40913166 0.72773759 0.00000000

C 28.18003981 -1.40242031 0.00000000

C 28.18003729 1.40243093 0.00000000

C 26.95756783 -0.72773289 0.00000000

C 26.95756652 0.72774132 0.00000000

C 25.73035591 -1.40208628 0.00000000

C 25.73035344 1.40209259 0.00000000

C 24.50608112 -0.72750715 0.00000000

C 24.50607982 0.72751133 0.00000000

C 23.28033304 -1.40187814 0.00000000

C 23.28033059 1.40188019 0.00000000

C 22.05498034 -0.72728672 0.00000000

C 22.05497908 0.72728666 0.00000000

C 20.82996271 -1.40180234 0.00000000

C 20.82996035 1.40180017 0.00000000

C 19.60423615 -0.72715749 0.00000000

C 19.60423496 0.72715335 0.00000000

C 18.37938396 -1.40180771 0.00000000

C 18.37938182 1.40180161 0.00000000

C 17.15369716 -0.72711393 0.00000000

C 17.15369610 0.72710613 0.00000000

C 15.92873474 -1.40184235 0.00000000

C 15.92873291 1.40183277 0.00000000

C 14.70322735 -0.72712075 0.00000000

C 14.70322649 0.72710979 0.00000000

C 13.47809639 -1.40187674 0.00000000

C 13.47809493 1.40186431 0.00000000

C 12.25274753 -0.72714512 0.00000000

C 12.25274692 0.72713158 0.00000000

C 11.02749418 -1.40189782 0.00000000

C 11.02749318 1.40188323 0.00000000

C 9.80223238 -0.72716462 0.00000000

C 9.80223198 0.72714930 0.00000000

C 8.57692378 -1.40190493 0.00000000

C 8.57692316 1.40188891 0.00000000

C 7.35168871 -0.72717510 0.00000000

C 7.35168846 0.72715862 0.00000000

C 6.12637030 -1.40190445 0.00000000

C 6.12636994 1.40188760 0.00000000

C 4.90112947 -0.72717822 0.00000000

C 4.90112931 0.72716107 0.00000000

C 3.67582221 -1.40190119 0.00000000

C 3.67582194 1.40188378 0.00000000

C 2.45056483 -0.72717815 0.00000000

C 2.45056469 0.72716048 0.00000000

C 1.22527405 -1.40189905 0.00000000

C 1.22527378 1.40188117 0.00000000

C -0.00000036 -0.72717794 0.00000000

C -0.00000052 0.72715981 0.00000000

C -1.22527463 -1.40189931 0.00000000

C -1.22527497 1.40188088 0.00000000

C -2.45056546 -0.72717867 0.00000000

C -2.45056561 0.72715991 0.00000000

C -3.67582259 -1.40190196 0.00000000

C -3.67582288 1.40188294 0.00000000

C -4.90112982 -0.72717924 0.00000000

C -4.90112992 0.72715997 0.00000000

C -6.12637038 -1.40190567 0.00000000

C -6.12637048 1.40188628 0.00000000

C -7.35168874 -0.72717654 0.00000000

C -7.35168869 0.72715710 0.00000000

C -8.57692353 -1.40190655 0.00000000

C -8.57692328 1.40188722 0.00000000

C -9.80223210 -0.72716642 0.00000000

C -9.80223187 0.72714744 0.00000000

C -11.02749371 -1.40189977 0.00000000

C -11.02749298 1.40188124 0.00000000

C -12.25274710 -0.72714719 0.00000000

C -12.25274659 0.72712949 0.00000000

C -13.47809587 -1.40187891 0.00000000

C -13.47809457 1.40186213 0.00000000

C -14.70322694 -0.72712300 0.00000000

C -14.70322613 0.72710756 0.00000000

C -15.92873441 -1.40184461 0.00000000

C -15.92873258 1.40183055 0.00000000

C -17.15369699 -0.72711621 0.00000000

C -17.15369588 0.72710390 0.00000000

C -18.37938398 -1.40180992 0.00000000

C -18.37938165 1.40179946 0.00000000

C -19.60423629 -0.72715961 0.00000000

C -19.60423496 0.72715129 0.00000000

C -20.82996311 -1.40180430 0.00000000

C -20.82996039 1.40179826 0.00000000

C -22.05498078 -0.72728850 0.00000000

C -22.05497929 0.72728491 0.00000000

C -23.28033375 -1.40187967 0.00000000

C -23.28033077 1.40187868 0.00000000

C -24.50608174 -0.72750843 0.00000000

C -24.50608015 0.72751006 0.00000000

C -25.73035674 -1.40208725 0.00000000

C -25.73035363 1.40209161 0.00000000

C -26.95756844 -0.72773355 0.00000000

C -26.95756679 0.72774063 0.00000000

C -28.18004054 -1.40242065 0.00000000

C -28.18003731 1.40243055 0.00000000

C -29.40913340 -0.72772478 0.00000000

C -29.40913169 0.72773753 0.00000000

C -30.62976415 -1.40272307 0.00000000

C -30.62976076 1.40273878 0.00000000

C -31.85988761 -0.72706830 0.00000000

C -31.85988583 0.72708704 0.00000000

C -33.08049794 -1.40260212 0.00000000

C -33.08049439 1.40262391 0.00000000

C -34.30817195 -0.72520407 0.00000000

C -34.30817009 0.72522904 0.00000000

C -35.53424016 -1.40111796 0.00000000

C -35.53423650 1.40114605 0.00000000

C -36.75181128 -0.72170515 0.00000000

C -36.75180937 0.72173648 0.00000000

C -37.99568303 -1.40199880 0.00000000

C -37.99567928 1.40203338 0.00000000

C -39.17880497 -0.70808957 0.00000000

C -39.17880307 0.70812736 0.00000000

H 40.13306904 -1.24961737 0.00000000

H 40.13306644 1.24965156 0.00000000

H 37.98787235 -2.50082067 0.00000000

H 37.98786716 2.50085035 0.00000000

H 35.53525038 -2.50132000 0.00000000

H 35.53524532 2.50134461 0.00000000

H 33.08095942 -2.50268708 0.00000000

H 33.08095444 2.50270679 0.00000000

H 30.62966174 -2.50282255 0.00000000

H 30.62965704 2.50283757 0.00000000

H 28.17972761 -2.50254484 0.00000000

H 28.17972315 2.50255545 0.00000000

H 25.73009326 -2.50223056 0.00000000

H 25.73008892 2.50223687 0.00000000

H 23.28021471 -2.50203362 0.00000000

H 23.28021035 2.50203565 0.00000000

H 20.82996113 -2.50196155 0.00000000

H 20.82995694 2.50195932 0.00000000

H 18.37943393 -2.50196627 0.00000000

H 18.37943018 2.50196008 0.00000000

H 15.92878693 -2.50199856 0.00000000

H 15.92878370 2.50198886 0.00000000

H 13.47812752 -2.50203066 0.00000000

H 13.47812487 2.50201809 0.00000000

H 11.02750317 -2.50205037 0.00000000

H 11.02750133 2.50203564 0.00000000

H 8.57691951 -2.50205683 0.00000000

H 8.57691834 2.50204072 0.00000000

H 6.12636226 -2.50205617 0.00000000

H 6.12636162 2.50203926 0.00000000

H 3.67581624 -2.50205303 0.00000000

H 3.67581578 2.50203563 0.00000000

H 1.22527201 -2.50205101 0.00000000

H 1.22527156 2.50203317 0.00000000

H -1.22527252 -2.50205126 0.00000000

H -1.22527322 2.50203287 0.00000000

H -3.67581650 -2.50205378 0.00000000

H -3.67581705 2.50203477 0.00000000

H -6.12636218 -2.50205736 0.00000000

H -6.12636238 2.50203792 0.00000000

H -8.57691903 -2.50205843 0.00000000

H -8.57691856 2.50203900 0.00000000

H -11.02750245 -2.50205229 0.00000000

H -11.02750110 2.50203364 0.00000000

H -13.47812677 -2.50203283 0.00000000

H -13.47812443 2.50201591 0.00000000

H -15.92878648 -2.50200084 0.00000000

H -15.92878326 2.50198665 0.00000000

H -18.37943398 -2.50196852 0.00000000

H -18.37942989 2.50195795 0.00000000

H -20.82996173 -2.50196352 0.00000000

H -20.82995689 2.50195744 0.00000000

H -23.28021576 -2.50203516 0.00000000

H -23.28021044 2.50203416 0.00000000

H -25.73009452 -2.50223153 0.00000000

H -25.73008899 2.50223589 0.00000000

H -28.17972875 -2.50254516 0.00000000

H -28.17972300 2.50255505 0.00000000

H -30.62966253 -2.50282216 0.00000000

H -30.62965642 2.50283784 0.00000000

H -33.08095977 -2.50268598 0.00000000

H -33.08095337 2.50270774 0.00000000

H -35.53525040 -2.50131820 0.00000000

H -35.53524389 2.50134626 0.00000000

H -37.98787220 -2.50081816 0.00000000

H -37.98786554 2.50085271 0.00000000

H -40.13306844 -1.24961428 0.00000000

H -40.13306510 1.24965460 0.00000000

$end

$comment

32-acene triplet

$end

$molecule

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C 39.17977174 0.70802774 0.00000000

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C 37.99652153 1.40194897 0.00000000

C 36.75277846 -0.72167265 0.00000000

C 36.75278011 0.72165774 0.00000000

C 35.53501687 -1.40108908 0.00000000

C 35.53501985 1.40107668 0.00000000

C 34.30906487 -0.72519538 0.00000000

C 34.30906621 0.72518499 0.00000000

C 33.08125644 -1.40257579 0.00000000

C 33.08125874 1.40256733 0.00000000

C 31.86062961 -0.72706802 0.00000000

C 31.86063056 0.72706108 0.00000000

C 30.63052520 -1.40270090 0.00000000

C 30.63052688 1.40269531 0.00000000

C 29.40970995 -0.72770773 0.00000000

C 29.40971069 0.72770347 0.00000000

C 28.18078152 -1.40240523 0.00000000

C 28.18078288 1.40240208 0.00000000

C 26.95803286 -0.72768769 0.00000000

C 26.95803353 0.72768594 0.00000000

C 25.73102859 -1.40208083 0.00000000

C 25.73102984 1.40208023 0.00000000

C 24.50650894 -0.72744277 0.00000000

C 24.50650955 0.72744374 0.00000000

C 23.28090128 -1.40188266 0.00000000

C 23.28090254 1.40188489 0.00000000

C 22.05541574 -0.72722084 0.00000000

C 22.05541633 0.72722474 0.00000000

C 20.83042486 -1.40181374 0.00000000

C 20.83042617 1.40181898 0.00000000

C 19.60467880 -0.72710169 0.00000000

C 19.60467938 0.72710860 0.00000000

C 18.37976187 -1.40182010 0.00000000

C 18.37976312 1.40182837 0.00000000

C 17.15411926 -0.72706928 0.00000000

C 17.15411974 0.72707911 0.00000000

C 15.92905368 -1.40185029 0.00000000

C 15.92905464 1.40186138 0.00000000

C 14.70359853 -0.72708170 0.00000000

C 14.70359881 0.72709398 0.00000000

C 13.47837219 -1.40187720 0.00000000

C 13.47837263 1.40189040 0.00000000

C 12.25304934 -0.72710531 0.00000000

C 12.25304932 0.72711916 0.00000000

C 11.02773098 -1.40189140 0.00000000

C 11.02773081 1.40190575 0.00000000

C 9.80246084 -0.72712058 0.00000000

C 9.80246051 0.72713498 0.00000000

C 8.57711770 -1.40189424 0.00000000

C 8.57711689 1.40190855 0.00000000

C 7.35184930 -0.72712644 0.00000000

C 7.35184866 0.72714025 0.00000000

C 6.12651491 -1.40189253 0.00000000

C 6.12651348 1.40190571 0.00000000

C 4.90123087 -0.72712657 0.00000000

C 4.90122997 0.72713872 0.00000000

C 3.67591199 -1.40189017 0.00000000

C 3.67591003 1.40190116 0.00000000

C 2.45061433 -0.72712556 0.00000000

C 2.45061322 0.72713513 0.00000000

C 1.22530564 -1.40188971 0.00000000

C 1.22530335 1.40189777 0.00000000

C 0.00000100 -0.72712610 0.00000000

C -0.00000022 0.72713256 0.00000000

C -1.22530254 -1.40189141 0.00000000

C -1.22530491 1.40189617 0.00000000

C -2.45061252 -0.72712881 0.00000000

C -2.45061369 0.72713199 0.00000000

C -3.67590937 -1.40189504 0.00000000

C -3.67591155 1.40189656 0.00000000

C -4.90122951 -0.72713265 0.00000000

C -4.90123056 0.72713282 0.00000000

C -6.12651310 -1.40189989 0.00000000

C -6.12651490 1.40189869 0.00000000

C -7.35184855 -0.72713452 0.00000000

C -7.35184941 0.72713237 0.00000000

C -8.57711683 -1.40190312 0.00000000

C -8.57711818 1.40189999 0.00000000

C -9.80246072 -0.72712968 0.00000000

C -9.80246136 0.72712603 0.00000000

C -11.02773098 -1.40190075 0.00000000

C -11.02773183 1.40189657 0.00000000

C -12.25304970 -0.72711438 0.00000000

C -12.25305012 0.72711014 0.00000000

C -13.47837282 -1.40188595 0.00000000

C -13.47837323 1.40188162 0.00000000

C -14.70359911 -0.72708986 0.00000000

C -14.70359934 0.72708575 0.00000000

C -15.92905458 -1.40185767 0.00000000

C -15.92905469 1.40185378 0.00000000

C -17.15411976 -0.72707590 0.00000000

C -17.15411987 0.72707233 0.00000000

C -18.37976264 -1.40182566 0.00000000

C -18.37976265 1.40182249 0.00000000

C -19.60467899 -0.72710650 0.00000000

C -19.60467911 0.72710360 0.00000000

C -20.83042521 -1.40181742 0.00000000

C -20.83042530 1.40181497 0.00000000

C -22.05541549 -0.72722389 0.00000000

C -22.05541568 0.72722153 0.00000000

C -23.28090116 -1.40188472 0.00000000

C -23.28090145 1.40188260 0.00000000

C -24.50650841 -0.72744433 0.00000000

C -24.50650866 0.72744211 0.00000000

C -25.73102822 -1.40208161 0.00000000

C -25.73102869 1.40207940 0.00000000

C -26.95803233 -0.72768812 0.00000000

C -26.95803259 0.72768555 0.00000000

C -28.18078129 -1.40240516 0.00000000

C -28.18078182 1.40240229 0.00000000

C -29.40970974 -0.72770739 0.00000000

C -29.40970998 0.72770397 0.00000000

C -30.63052560 -1.40270016 0.00000000

C -30.63052591 1.40269633 0.00000000

C -31.86063000 -0.72706677 0.00000000

C -31.86063008 0.72706254 0.00000000

C -33.08125787 -1.40257398 0.00000000

C -33.08125761 1.40256948 0.00000000

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C -34.30906579 0.72518811 0.00000000

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C -35.53501847 1.40108096 0.00000000

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C -36.75277971 0.72166351 0.00000000

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C -37.99652013 1.40195649 0.00000000

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C -39.17977150 0.70803697 0.00000000

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H 40.13399834 1.24961443 0.00000000

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H 37.98871694 2.50076819 0.00000000

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H 28.18047625 2.50252506 0.00000000

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H 25.73078594 2.50222196 0.00000000

H 23.28080284 -2.50203486 0.00000000

H 23.28080500 2.50203699 0.00000000

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H 18.37980915 -2.50197466 0.00000000

H 18.37981115 2.50198291 0.00000000

H 15.92909530 -2.50200259 0.00000000

H 15.92909675 2.50201375 0.00000000

H 13.47839238 -2.50202745 0.00000000

H 13.47839293 2.50204080 0.00000000

H 11.02773287 -2.50204050 0.00000000

H 11.02773241 2.50205502 0.00000000

H 8.57711160 -2.50204284 0.00000000

H 8.57711006 2.50205734 0.00000000

H 6.12650882 -2.50204099 0.00000000

H 6.12650627 2.50205433 0.00000000

H 3.67590905 -2.50203876 0.00000000

H 3.67590561 2.50204987 0.00000000

H 1.22530549 -2.50203845 0.00000000

H 1.22530149 2.50204655 0.00000000

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H -3.67590480 -2.50204385 0.00000000

H -3.67590865 2.50204524 0.00000000

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H -6.12650892 2.50204726 0.00000000

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H -8.57711227 2.50204869 0.00000000

H -11.02773237 -2.50205008 0.00000000

H -11.02773401 2.50204573 0.00000000

H -13.47839285 -2.50203633 0.00000000

H -13.47839378 2.50203186 0.00000000

H -15.92909631 -2.50200996 0.00000000

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H -18.37981018 -2.50198008 0.00000000

H -18.37981045 2.50197694 0.00000000

H -20.83043412 -2.50197259 0.00000000

H -20.83043446 2.50197024 0.00000000

H -23.28080296 -2.50203673 0.00000000

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H -25.73078360 -2.50222333 0.00000000

H -25.73078449 2.50222120 0.00000000

H -28.18047387 -2.50252820 0.00000000

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H -33.08171478 -2.50265816 0.00000000

H -33.08171425 2.50265346 0.00000000

H -35.53603532 -2.50128572 0.00000000

H -35.53603384 2.50128133 0.00000000

H -37.98871592 -2.50077855 0.00000000

H -37.98871390 2.50077571 0.00000000

H -40.13399845 -1.24962631 0.00000000

H -40.13399740 1.24962521 0.00000000

$end

$comment

33-acene singlet

$end

$molecule

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C 40.44456433 1.40192784 0.00000000

C 39.20037402 -0.72185283 0.00000000

C 39.20037664 0.72180540 0.00000000

C 37.98293733 -1.40108004 0.00000000

C 37.98294229 1.40103701 0.00000000

C 36.75674194 -0.72514601 0.00000000

C 36.75674444 0.72510713 0.00000000

C 35.52919405 -1.40262507 0.00000000

C 35.52919871 1.40259042 0.00000000

C 34.30846767 -0.72699104 0.00000000

C 34.30847000 0.72696028 0.00000000

C 33.07842611 -1.40272191 0.00000000

C 33.07843052 1.40269515 0.00000000

C 31.85780224 -0.72767210 0.00000000

C 31.85780447 0.72764905 0.00000000

C 30.62866421 -1.40239309 0.00000000

C 30.62866838 1.40237377 0.00000000

C 29.40629085 -0.72772537 0.00000000

C 29.40629297 0.72770957 0.00000000

C 28.17896993 -1.40204800 0.00000000

C 28.17897390 1.40203579 0.00000000

C 26.95480670 -0.72752124 0.00000000

C 26.95480871 0.72751237 0.00000000

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C 25.72897088 1.40183237 0.00000000

C 24.50368235 -0.72729873 0.00000000

C 24.50368423 0.72729646 0.00000000

C 23.27862834 -1.40176286 0.00000000

C 23.27863187 1.40176380 0.00000000

C 22.05291635 -0.72715432 0.00000000

C 22.05291813 0.72715830 0.00000000

C 20.82807586 -1.40176756 0.00000000

C 20.82807913 1.40177448 0.00000000

C 19.60237146 -0.72709533 0.00000000

C 19.60237310 0.72710505 0.00000000

C 18.37744146 -1.40180047 0.00000000

C 18.37744444 1.40181290 0.00000000

C 17.15190880 -0.72709130 0.00000000

C 17.15191026 0.72710623 0.00000000

C 15.92680811 -1.40183097 0.00000000

C 15.92681073 1.40184832 0.00000000

C 14.70144256 -0.72710927 0.00000000

C 14.70144381 0.72712882 0.00000000

C 13.47620711 -1.40184836 0.00000000

C 13.47620939 1.40187002 0.00000000

C 12.25094106 -0.72712807 0.00000000

C 12.25094215 0.72715166 0.00000000

C 11.02563734 -1.40185327 0.00000000

C 11.02563933 1.40187865 0.00000000

C 9.80040592 -0.72713857 0.00000000

C 9.80040687 0.72716562 0.00000000

C 8.57508572 -1.40185100 0.00000000

C 8.57508749 1.40187965 0.00000000

C 7.34985109 -0.72714139 0.00000000

C 7.34985195 0.72717151 0.00000000

C 6.12453973 -1.40184638 0.00000000

C 6.12454126 1.40187787 0.00000000

C 4.89928898 -0.72714001 0.00000000

C 4.89928971 0.72717272 0.00000000

C 3.67399266 -1.40184235 0.00000000

C 3.67399391 1.40187625 0.00000000

C 2.44872585 -0.72713796 0.00000000

C 2.44872642 0.72717279 0.00000000

C 1.22344327 -1.40184045 0.00000000

C 1.22344417 1.40187622 0.00000000

C -0.00183718 -0.72713727 0.00000000

C -0.00183682 0.72717364 0.00000000

C -1.22710660 -1.40184103 0.00000000

C -1.22710613 1.40187799 0.00000000

C -2.45240126 -0.72713810 0.00000000

C -2.45240112 0.72717529 0.00000000

C -3.67765501 -1.40184383 0.00000000

C -3.67765497 1.40188127 0.00000000

C -4.90296572 -0.72713865 0.00000000

C -4.90296581 0.72717595 0.00000000

C -6.12820283 -1.40184760 0.00000000

C -6.12820325 1.40188473 0.00000000

C -7.35352478 -0.72713556 0.00000000

C -7.35352512 0.72717212 0.00000000

C -8.57875643 -1.40184924 0.00000000

C -8.57875738 1.40188522 0.00000000

C -9.80406643 -0.72712496 0.00000000

C -9.80406707 0.72715984 0.00000000

C -11.02932815 -1.40184405 0.00000000

C -11.02932974 1.40187783 0.00000000

C -12.25457613 -0.72710609 0.00000000

C -12.25457713 0.72713813 0.00000000

C -13.47993229 -1.40182693 0.00000000

C -13.47993462 1.40185729 0.00000000

C -14.70504927 -0.72708574 0.00000000

C -14.70505070 0.72711368 0.00000000

C -15.93057199 -1.40179705 0.00000000

C -15.93057511 1.40182262 0.00000000

C -17.15551375 -0.72708577 0.00000000

C -17.15551557 0.72710825 0.00000000

C -18.38121828 -1.40176575 0.00000000

C -18.38122213 1.40178519 0.00000000

C -19.60605258 -0.72714024 0.00000000

C -19.60605477 0.72715599 0.00000000

C -20.83178833 -1.40176308 0.00000000

C -20.83179286 1.40177515 0.00000000

C -22.05680677 -0.72728269 0.00000000

C -22.05680928 0.72729047 0.00000000

C -23.28214582 -1.40183952 0.00000000

C -23.28215098 1.40184309 0.00000000

C -24.50792390 -0.72751183 0.00000000

C -24.50792675 0.72751053 0.00000000

C -25.73215805 -1.40204815 0.00000000

C -25.73216387 1.40204211 0.00000000

C -26.95942320 -0.72773595 0.00000000

C -26.95942638 0.72772447 0.00000000

C -28.18184093 -1.40238997 0.00000000

C -28.18184734 1.40237323 0.00000000

C -29.41098247 -0.72771555 0.00000000

C -29.41098594 0.72769289 0.00000000

C -30.63157195 -1.40271048 0.00000000

C -30.63157894 1.40268205 0.00000000

C -31.86170728 -0.72704852 0.00000000

C -31.86171104 0.72701366 0.00000000

C -33.08230894 -1.40260900 0.00000000

C -33.08231651 1.40256786 0.00000000

C -34.30994871 -0.72519194 0.00000000

C -34.30995278 0.72514388 0.00000000

C -35.53604122 -1.40113167 0.00000000

C -35.53604929 1.40107678 0.00000000

C -36.75356789 -0.72173523 0.00000000

C -36.75357215 0.72167314 0.00000000

C -37.99747012 -1.40202326 0.00000000

C -37.99747846 1.40195382 0.00000000

C -39.18057010 -0.70817212 0.00000000

C -39.18057433 0.70809559 0.00000000

H 42.58182148 -1.24971414 0.00000000

H 42.58182603 1.24965429 0.00000000

H 40.43636374 -2.50079117 0.00000000

H 40.43637296 2.50073926 0.00000000

H 37.98332990 -2.50126938 0.00000000

H 37.98333868 2.50122645 0.00000000

H 35.52922286 -2.50267600 0.00000000

H 35.52923119 2.50264146 0.00000000

H 33.07842987 -2.50280241 0.00000000

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H 30.62865539 -2.50250704 0.00000000

H 30.62866281 2.50248779 0.00000000

H 28.17894151 -2.50218570 0.00000000

H 28.17894860 2.50217356 0.00000000

H 25.72894430 -2.50198725 0.00000000

H 25.72895102 2.50198186 0.00000000

H 23.27862115 -2.50191499 0.00000000

H 23.27862750 2.50191599 0.00000000

H 20.82808103 -2.50191785 0.00000000

H 20.82808686 2.50192486 0.00000000

H 18.37745056 -2.50194785 0.00000000

H 18.37745586 2.50196038 0.00000000

H 15.92681503 -2.50197617 0.00000000

H 15.92681974 2.50199363 0.00000000

H 13.47620914 -2.50199255 0.00000000

H 13.47621326 2.50201431 0.00000000

H 11.02563524 -2.50199743 0.00000000

H 11.02563880 2.50202288 0.00000000

H 8.57508165 -2.50199562 0.00000000

H 8.57508480 2.50202432 0.00000000

H 6.12453596 -2.50199160 0.00000000

H 6.12453863 2.50202316 0.00000000

H 3.67399046 -2.50198808 0.00000000

H 3.67399263 2.50202207 0.00000000

H 1.22344306 -2.50198646 0.00000000

H 1.22344464 2.50202234 0.00000000

H -1.22710472 -2.50198709 0.00000000

H -1.22710388 2.50202419 0.00000000

H -3.67765132 -2.50198974 0.00000000

H -3.67765123 2.50202732 0.00000000

H -6.12819875 -2.50199325 0.00000000

H -6.12819952 2.50203056 0.00000000

H -8.57875540 -2.50199477 0.00000000

H -8.57875714 2.50203096 0.00000000

H -11.02933480 -2.50198992 0.00000000

H -11.02933770 2.50202396 0.00000000

H -13.47994914 -2.50197398 0.00000000

H -13.47995333 2.50200463 0.00000000

H -15.93059413 -2.50194631 0.00000000

H -15.93059969 2.50197218 0.00000000

H -18.38122837 -2.50191773 0.00000000

H -18.38123523 2.50193745 0.00000000

H -20.83175842 -2.50191668 0.00000000

H -20.83176654 2.50192902 0.00000000

H -23.28205036 -2.50199050 0.00000000

H -23.28205962 2.50199433 0.00000000

H -25.73200664 -2.50218827 0.00000000

H -25.73201703 2.50218248 0.00000000

H -28.18171872 -2.50250858 0.00000000

H -28.18173015 2.50249208 0.00000000

H -30.63164692 -2.50280042 0.00000000

H -30.63165939 2.50277221 0.00000000

H -33.08280180 -2.50268192 0.00000000

H -33.08281529 2.50264100 0.00000000

H -35.53688708 -2.50132354 0.00000000

H -35.53690139 2.50126882 0.00000000

H -37.98944525 -2.50083241 0.00000000

H -37.98946009 2.50076311 0.00000000

H -40.13489275 -1.24954155 0.00000000

H -40.13490020 1.24945937 0.00000000

$end

$comment

33-acene triplet

$end

$molecule

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C 41.62851237 0.70811550 0.00000000

C 40.44543031 -1.40190599 0.00000000

C 40.44543121 1.40189695 0.00000000

C 39.20135554 -0.72178319 0.00000000

C 39.20135598 0.72177498 0.00000000

C 37.98374895 -1.40101717 0.00000000

C 37.98374980 1.40100968 0.00000000

C 36.75765230 -0.72510397 0.00000000

C 36.75765275 0.72509722 0.00000000

C 35.52997826 -1.40257417 0.00000000

C 35.52997912 1.40256818 0.00000000

C 34.30923398 -0.72696583 0.00000000

C 34.30923441 0.72696059 0.00000000

C 33.07920042 -1.40268153 0.00000000

C 33.07920125 1.40267703 0.00000000

C 31.85840701 -0.72764151 0.00000000

C 31.85840745 0.72763773 0.00000000

C 30.62941000 -1.40236418 0.00000000

C 30.62941080 1.40236109 0.00000000

C 29.40677981 -0.72767618 0.00000000

C 29.40678021 0.72767380 0.00000000

C 28.17964595 -1.40203393 0.00000000

C 28.17964673 1.40203226 0.00000000

C 26.95524899 -0.72745929 0.00000000

C 26.95524938 0.72745830 0.00000000

C 25.72954146 -1.40183990 0.00000000

C 25.72954221 1.40183957 0.00000000

C 24.50412127 -0.72723942 0.00000000

C 24.50412164 0.72723975 0.00000000

C 23.27909665 -1.40177781 0.00000000

C 23.27909735 1.40177877 0.00000000

C 22.05335409 -0.72710879 0.00000000

C 22.05335444 0.72711035 0.00000000

C 20.82845587 -1.40178899 0.00000000

C 20.82845651 1.40179113 0.00000000

C 19.60278407 -0.72706531 0.00000000

C 19.60278438 0.72706800 0.00000000

C 18.37775600 -1.40182243 0.00000000

C 18.37775656 1.40182561 0.00000000

C 17.15226793 -0.72707202 0.00000000

C 17.15226821 0.72707569 0.00000000

C 15.92707204 -1.40185018 0.00000000

C 15.92707255 1.40185430 0.00000000

C 14.70172905 -0.72709425 0.00000000

C 14.70172929 0.72709883 0.00000000

C 13.47642417 -1.40186442 0.00000000

C 13.47642459 1.40186939 0.00000000

C 12.25114860 -0.72711255 0.00000000

C 12.25114879 0.72711791 0.00000000

C 11.02580409 -1.40186741 0.00000000

C 11.02580441 1.40187305 0.00000000

C 9.80053847 -0.72712044 0.00000000

C 9.80053862 0.72712635 0.00000000

C 8.57519745 -1.40186475 0.00000000

C 8.57519770 1.40187088 0.00000000

C 7.34991812 -0.72712068 0.00000000

C 7.34991823 0.72712701 0.00000000

C 6.12459424 -1.40186071 0.00000000

C 6.12459440 1.40186718 0.00000000

C 4.89930080 -0.72711765 0.00000000

C 4.89930086 0.72712425 0.00000000

C 3.67399069 -1.40185745 0.00000000

C 3.67399077 1.40186412 0.00000000

C 2.44869063 -0.72711501 0.00000000

C 2.44869066 0.72712173 0.00000000

C 1.22338717 -1.40185585 0.00000000

C 1.22338717 1.40186258 0.00000000

C -0.00191460 -0.72711448 0.00000000

C -0.00191462 0.72712122 0.00000000

C -1.22721395 -1.40185594 0.00000000

C -1.22721406 1.40186257 0.00000000

C -2.45251946 -0.72711620 0.00000000

C -2.45251953 0.72712274 0.00000000

C -3.67781002 -1.40185767 0.00000000

C -3.67781021 1.40186404 0.00000000

C -4.90312658 -0.72711860 0.00000000

C -4.90312670 0.72712481 0.00000000

C -6.12840027 -1.40186057 0.00000000

C -6.12840055 1.40186651 0.00000000

C -7.35373299 -0.72711843 0.00000000

C -7.35373315 0.72712412 0.00000000

C -8.57898924 -1.40186261 0.00000000

C -8.57898961 1.40186797 0.00000000

C -9.80432801 -0.72711107 0.00000000

C -9.80432821 0.72711609 0.00000000

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C -12.25489477 -0.72709360 0.00000000

C -12.25489500 0.72709785 0.00000000

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C -13.48021905 1.40185039 0.00000000

C -14.70542100 -0.72706988 0.00000000

C -14.70542128 0.72707317 0.00000000

C -15.93088958 -1.40182027 0.00000000

C -15.93089014 1.40182308 0.00000000

C -17.15592271 -0.72705951 0.00000000

C -17.15592302 0.72706182 0.00000000

C -18.38158523 -1.40178886 0.00000000

C -18.38158587 1.40179059 0.00000000

C -19.60647295 -0.72709805 0.00000000

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C -22.05721619 0.72722559 0.00000000

C -23.28268337 -1.40184296 0.00000000

C -23.28268412 1.40184222 0.00000000

C -24.50832465 -0.72745088 0.00000000

C -24.50832505 0.72744948 0.00000000

C -25.73278879 -1.40203469 0.00000000

C -25.73278959 1.40203260 0.00000000

C -26.95986052 -0.72768652 0.00000000

C -26.95986094 0.72768373 0.00000000

C -28.18253379 -1.40236014 0.00000000

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C -29.41152755 -0.72768353 0.00000000

C -29.41152798 0.72767929 0.00000000

C -30.63228610 -1.40266704 0.00000000

C -30.63228694 1.40266205 0.00000000

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C -33.08302802 1.40254672 0.00000000

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C -34.31078932 0.72513712 0.00000000

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C -36.75447679 -0.72165718 0.00000000

C -36.75447724 0.72164843 0.00000000

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C -39.18148057 -0.70807834 0.00000000

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H 42.58278112 1.24966343 0.00000000

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H 40.43723131 2.50071003 0.00000000

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H 37.98414082 2.50120154 0.00000000

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H 33.07921211 2.50276014 0.00000000

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H 30.62941438 2.50247698 0.00000000

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H 28.17963248 2.50217080 0.00000000

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H 25.72953093 2.50198880 0.00000000

H 23.27909504 -2.50192912 0.00000000

H 23.27909630 2.50193008 0.00000000

H 20.82846105 -2.50193835 0.00000000

H 20.82846220 2.50194048 0.00000000

H 18.37776172 -2.50196913 0.00000000

H 18.37776272 2.50197232 0.00000000

H 15.92707507 -2.50199516 0.00000000

H 15.92707599 2.50199929 0.00000000

H 13.47642393 -2.50200873 0.00000000

H 13.47642471 2.50201370 0.00000000

H 11.02580202 -2.50201158 0.00000000

H 11.02580259 2.50201722 0.00000000

H 8.57519515 -2.50200875 0.00000000

H 8.57519558 2.50201488 0.00000000

H 6.12459276 -2.50200427 0.00000000

H 6.12459304 2.50201074 0.00000000

H 3.67399027 -2.50200036 0.00000000

H 3.67399039 2.50200703 0.00000000

H 1.22338765 -2.50199801 0.00000000

H 1.22338767 2.50200475 0.00000000

H -1.22721238 -2.50199735 0.00000000

H -1.22721258 2.50200399 0.00000000

H -3.67780703 -2.50199834 0.00000000

H -3.67780737 2.50200472 0.00000000

H -6.12839633 -2.50200053 0.00000000

H -6.12839686 2.50200648 0.00000000

H -8.57898687 -2.50200211 0.00000000

H -8.57898755 2.50200747 0.00000000

H -11.02959275 -2.50199941 0.00000000

H -11.02959353 2.50200404 0.00000000

H -13.48023137 -2.50198739 0.00000000

H -13.48023234 2.50199116 0.00000000

H -15.93090920 -2.50196342 0.00000000

H -15.93091020 2.50196623 0.00000000

H -18.38159715 -2.50193517 0.00000000

H -18.38159832 2.50193690 0.00000000

H -20.83220851 -2.50192831 0.00000000

H -20.83220976 2.50192885 0.00000000

H -23.28260084 -2.50198997 0.00000000

H -23.28260219 2.50198924 0.00000000

H -25.73265117 -2.50217220 0.00000000

H -25.73265260 2.50217011 0.00000000

H -28.18242219 -2.50247762 0.00000000

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H -30.63236715 -2.50275697 0.00000000

H -30.63236867 2.50275198 0.00000000

H -33.08352213 -2.50262665 0.00000000

H -33.08352365 2.50262017 0.00000000

H -35.53762761 -2.50125467 0.00000000

H -35.53762916 2.50124668 0.00000000

H -37.99023979 -2.50074939 0.00000000

H -37.99024136 2.50073984 0.00000000

H -40.13577925 -1.24948799 0.00000000

H -40.13578004 1.24947712 0.00000000

$end

$comment

34-acene singlet

$end

$molecule

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C 39.20231352 -0.72169980 0.00000000

C 39.20231140 0.72174156 0.00000000

C 37.98474015 -1.40111516 0.00000000

C 37.98473609 1.40115339 0.00000000

C 36.75867497 -0.72519972 0.00000000

C 36.75867290 0.72523446 0.00000000

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C 35.53099654 1.40263092 0.00000000

C 34.31039065 -0.72706413 0.00000000

C 34.31038864 0.72709205 0.00000000

C 33.08026864 -1.40272153 0.00000000

C 33.08026479 1.40274609 0.00000000

C 31.85963590 -0.72771996 0.00000000

C 31.85963388 0.72774115 0.00000000

C 30.63054738 -1.40241864 0.00000000

C 30.63054351 1.40243649 0.00000000

C 29.40807375 -0.72772965 0.00000000

C 29.40807172 0.72774412 0.00000000

C 28.18086504 -1.40208583 0.00000000

C 28.18086115 1.40209694 0.00000000

C 26.95658945 -0.72750465 0.00000000

C 26.95658742 0.72751239 0.00000000

C 25.73084439 -1.40187992 0.00000000

C 25.73084058 1.40188433 0.00000000

C 24.50549291 -0.72728534 0.00000000

C 24.50549096 0.72728648 0.00000000

C 23.28047731 -1.40180427 0.00000000

C 23.28047369 1.40180226 0.00000000

C 22.05475282 -0.72715693 0.00000000

C 22.05475101 0.72715185 0.00000000

C 20.82990263 -1.40181068 0.00000000

C 20.82989935 1.40180268 0.00000000

C 19.60421891 -0.72711537 0.00000000

C 19.60421732 0.72710463 0.00000000

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C 18.37925502 1.40183388 0.00000000

C 17.15375223 -0.72712299 0.00000000

C 17.15375094 0.72710742 0.00000000

C 15.92862271 -1.40188119 0.00000000

C 15.92862050 1.40186354 0.00000000

C 14.70327549 -0.72714667 0.00000000

C 14.70327447 0.72712720 0.00000000

C 13.47802468 -1.40190250 0.00000000

C 13.47802295 1.40188141 0.00000000

C 12.25276466 -0.72716830 0.00000000

C 12.25276388 0.72714576 0.00000000

C 11.02745875 -1.40191124 0.00000000

C 11.02745741 1.40188745 0.00000000

C 9.80222390 -0.72717917 0.00000000

C 9.80222327 0.72715425 0.00000000

C 8.57691049 -1.40191139 0.00000000

C 8.57690944 1.40188554 0.00000000

C 7.35166879 -0.72718239 0.00000000

C 7.35166830 0.72715564 0.00000000

C 6.12636671 -1.40190893 0.00000000

C 6.12636592 1.40188148 0.00000000

C 4.90111018 -0.72718162 0.00000000

C 4.90110983 0.72715353 0.00000000

C 3.67582132 -1.40190624 0.00000000

C 3.67582082 1.40187770 0.00000000

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C 2.45055307 0.72715119 0.00000000

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C 1.22527307 1.40187578 0.00000000

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C -0.00000128 0.72715027 0.00000000

C -1.22527577 -1.40190482 0.00000000

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C -4.90111150 -0.72718146 0.00000000

C -4.90111115 0.72715346 0.00000000

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C -8.57690997 -1.40191123 0.00000000

C -8.57690892 1.40188546 0.00000000

C -9.80222284 -0.72717902 0.00000000

C -9.80222223 0.72715418 0.00000000

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C -17.15375071 -0.72712307 0.00000000

C -17.15374942 0.72710748 0.00000000

C -18.37925667 -1.40184726 0.00000000

C -18.37925391 1.40183395 0.00000000

C -19.60421833 -0.72711550 0.00000000

C -19.60421677 0.72710472 0.00000000

C -20.82990262 -1.40181081 0.00000000

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C -22.05475339 -0.72715707 0.00000000

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C -23.28047845 -1.40180438 0.00000000

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C -26.95659145 -0.72750466 0.00000000

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C -28.18086713 -1.40208581 0.00000000

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C -30.63054898 -1.40241856 0.00000000

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C -37.98473865 -1.40111508 0.00000000

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C -39.20230950 0.72174143 0.00000000

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H 37.98574559 2.50135361 0.00000000

H 35.53146208 -2.50268370 0.00000000

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H 33.08016017 2.50284524 0.00000000

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H 13.47803580 -2.50205423 0.00000000

H 13.47803272 2.50203307 0.00000000

H 11.02745634 -2.50206228 0.00000000

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H 6.12636052 -2.50205984 0.00000000

H 6.12635912 2.50203241 0.00000000

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H -11.02745214 2.50203836 0.00000000

H -13.47803340 -2.50205418 0.00000000

H -13.47803037 2.50203303 0.00000000

H -15.92865261 -2.50203462 0.00000000

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H -18.37930803 -2.50200299 0.00000000

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H -20.82995338 -2.50196890 0.00000000

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H -23.28047768 -2.50196315 0.00000000

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H -25.73072770 -2.50203495 0.00000000

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$end

$comment

34-acene triplet

$end

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C 39.20322479 -0.72167452 0.00000000

C 39.20322508 0.72166822 0.00000000

C 37.98548466 -1.40109356 0.00000000

C 37.98548525 1.40108779 0.00000000

C 36.75952233 -0.72519627 0.00000000

C 36.75952263 0.72519101 0.00000000

C 35.53173015 -1.40258078 0.00000000

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C 34.31110688 -0.72706832 0.00000000

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C 33.08100316 1.40270248 0.00000000

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C 31.86020924 0.72770601 0.00000000

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C 7.35179217 0.72714066 0.00000000

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C 4.90117820 0.72713770 0.00000000

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H 15.92894906 2.50203819 0.00000000

H 13.47829173 -2.50204940 0.00000000

H 13.47829232 2.50205274 0.00000000

H 11.02767038 -2.50205347 0.00000000

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$end

$comment

35-acene singlet

$end

$molecule

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C -37.98636033 -1.40110102 0.00000000

C -37.98635759 1.40110961 0.00000000

C -39.20387939 -0.72169901 0.00000000

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C -41.63087998 -0.70812802 0.00000000

C -41.63087843 0.70814444 0.00000000

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H 45.03261511 1.24941813 0.00000000

H 42.88670022 -2.50079724 0.00000000

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H 40.43413244 -2.50122697 0.00000000

H 40.43413240 2.50122988 0.00000000

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H 35.52915728 2.50278757 0.00000000

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H 33.07938341 2.50250043 0.00000000

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H 30.62967160 2.50218268 0.00000000

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H 23.27882005 2.50192402 0.00000000

H 20.82819326 -2.50195178 0.00000000

H 20.82819320 2.50195680 0.00000000

H 18.37756047 -2.50198303 0.00000000

H 18.37756054 2.50198793 0.00000000

H 15.92695785 -2.50200155 0.00000000

H 15.92695814 2.50200661 0.00000000

H 13.47638709 -2.50200846 0.00000000

H 13.47638741 2.50201392 0.00000000

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H 11.02583709 2.50201418 0.00000000

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H 8.57529393 2.50201195 0.00000000

H 6.12475054 -2.50200405 0.00000000

H 6.12474989 2.50200961 0.00000000

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H 3.67420191 2.50200794 0.00000000

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H -3.67745002 2.50200780 0.00000000

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H -6.12799615 2.50200950 0.00000000

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H -15.93028732 2.50198530 0.00000000

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H -20.83156354 -2.50193361 0.00000000

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H -23.28209199 -2.50192814 0.00000000

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H -25.73238260 -2.50199689 0.00000000

H -25.73238069 2.50198987 0.00000000

H -28.18233846 -2.50218857 0.00000000

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H -30.63205079 -2.50250248 0.00000000

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H -33.08197698 -2.50278718 0.00000000

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$comment

35-acene triplet

$end

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C 14.70187474 0.72722339 0.00000000

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H 15.92715095 2.50211103 0.00000000

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H -23.28248730 -2.50193862 0.00000000

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$comment

36-acene singlet

$end

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C 13.47800431 1.40191711 0.00000000

C 12.25276624 -0.72714930 0.00000000

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H 30.63110245 -2.50224376 0.00000000

H 30.63111216 2.50222289 0.00000000

H 28.18122463 -2.50204098 0.00000000

H 28.18123418 2.50202959 0.00000000

H 25.73098727 -2.50196219 0.00000000

H 25.73099659 2.50196001 0.00000000

H 23.28047328 -2.50195936 0.00000000

H 23.28048205 2.50196603 0.00000000

H 20.82983285 -2.50198785 0.00000000

H 20.82984095 2.50200280 0.00000000

H 18.37917930 -2.50201443 0.00000000

H 18.37918646 2.50203687 0.00000000

H 15.92856550 -2.50202749 0.00000000

H 15.92857151 2.50205635 0.00000000

H 13.47800652 -2.50203229 0.00000000

H 13.47801132 2.50206639 0.00000000

H 11.02744838 -2.50203193 0.00000000

H 11.02745218 2.50207019 0.00000000

H 8.57690431 -2.50202750 0.00000000

H 8.57690720 2.50206909 0.00000000

H 6.12636585 -2.50202423 0.00000000

H 6.12636799 2.50206838 0.00000000

H 3.67582299 -2.50202157 0.00000000

H 3.67582432 2.50206758 0.00000000

H 1.22527480 -2.50202036 0.00000000

H 1.22527520 2.50206732 0.00000000

H -1.22527586 -2.50202033 0.00000000

H -1.22527638 2.50206722 0.00000000

H -3.67582394 -2.50202146 0.00000000

H -3.67582534 2.50206733 0.00000000

H -6.12636657 -2.50202408 0.00000000

H -6.12636879 2.50206805 0.00000000

H -8.57690474 -2.50202739 0.00000000

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H -11.02744856 -2.50203193 0.00000000

H -11.02745244 2.50206980 0.00000000

H -13.47800652 -2.50203244 0.00000000

H -13.47801138 2.50206605 0.00000000

H -15.92856549 -2.50202774 0.00000000

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H -18.37917928 -2.50201474 0.00000000

H -18.37918637 2.50203678 0.00000000

H -20.82983286 -2.50198818 0.00000000

H -20.82984091 2.50200280 0.00000000

H -23.28047332 -2.50195968 0.00000000

H -23.28048208 2.50196604 0.00000000

H -25.73098741 -2.50196241 0.00000000

H -25.73099655 2.50196002 0.00000000

H -28.18122468 -2.50204104 0.00000000

H -28.18123416 2.50202957 0.00000000

H -30.63110240 -2.50224369 0.00000000

H -30.63111202 2.50222282 0.00000000

H -33.08071807 -2.50256597 0.00000000

H -33.08072779 2.50253553 0.00000000

H -35.53063353 -2.50285013 0.00000000

H -35.53064333 2.50281015 0.00000000

H -37.98191861 -2.50272134 0.00000000

H -37.98192853 2.50267183 0.00000000

H -40.43620490 -2.50136272 0.00000000

H -40.43621493 2.50130358 0.00000000

H -42.88877627 -2.50088087 0.00000000

H -42.88878633 2.50081193 0.00000000

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H -45.03403721 1.24955226 0.00000000

$end

$comment

36-acene triplet

$end

$molecule

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C 42.89736527 1.40201474 0.00000000

C 41.65360160 -0.72164892 0.00000000

C 41.65359578 0.72169821 0.00000000

C 40.43590153 -1.40107687 0.00000000

C 40.43589110 1.40111610 0.00000000

C 39.20991487 -0.72518035 0.00000000

C 39.20990955 0.72521057 0.00000000

C 37.98215611 -1.40257187 0.00000000

C 37.98214697 1.40259254 0.00000000

C 36.76152374 -0.72705860 0.00000000

C 36.76151918 0.72707139 0.00000000

C 35.53143659 -1.40270515 0.00000000

C 35.53142873 1.40270990 0.00000000

C 34.31065199 -0.72770853 0.00000000

C 34.31064813 0.72770703 0.00000000

C 33.08170858 -1.40241606 0.00000000

C 33.08170205 1.40240824 0.00000000

C 31.85901244 -0.72770005 0.00000000

C 31.85900952 0.72768803 0.00000000

C 30.63198109 -1.40209427 0.00000000

C 30.63197611 1.40207758 0.00000000

C 29.40750940 -0.72746422 0.00000000

C 29.40750753 0.72744520 0.00000000

C 28.18187888 -1.40189866 0.00000000

C 28.18187544 1.40187669 0.00000000

C 26.95642545 -0.72724512 0.00000000

C 26.95642438 0.72722206 0.00000000

C 25.73143288 -1.40183023 0.00000000

C 25.73143065 1.40180568 0.00000000

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C 23.28079354 1.40181092 0.00000000

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C 22.05514895 0.72706855 0.00000000

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C 19.60464740 -0.72710610 0.00000000

C 19.60464738 0.72708137 0.00000000

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C 15.92881839 -1.40191031 0.00000000

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C 14.70355556 -0.72714425 0.00000000

C 14.70355520 0.72711981 0.00000000

C 13.47823061 -1.40191506 0.00000000

C 13.47822959 1.40189077 0.00000000

C 12.25297154 -0.72715338 0.00000000

C 12.25297092 0.72712856 0.00000000

C 11.02764607 -1.40191666 0.00000000

C 11.02764494 1.40189168 0.00000000

C 9.80237268 -0.72715370 0.00000000

C 9.80237216 0.72712875 0.00000000

C 8.57706284 -1.40191398 0.00000000

C 8.57706228 1.40188887 0.00000000

C 7.35177441 -0.72715061 0.00000000

C 7.35177447 0.72712673 0.00000000

C 6.12647718 -1.40191192 0.00000000

C 6.12647780 1.40188858 0.00000000

C 4.90118089 -0.72714705 0.00000000

C 4.90118185 0.72712633 0.00000000

C 3.67588842 -1.40190872 0.00000000

C 3.67589038 1.40188978 0.00000000

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C 2.45059269 0.72712795 0.00000000

C 1.22529790 -1.40190517 0.00000000

C 1.22530078 1.40189293 0.00000000

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C 0.00000486 0.72713127 0.00000000

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C -3.67588243 1.40190105 0.00000000

C -4.90117739 -0.72713502 0.00000000

C -4.90117626 0.72713941 0.00000000

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C -6.12647397 1.40190476 0.00000000

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C -23.28079291 1.40183358 0.00000000

C -24.50569337 -0.72710156 0.00000000

C -24.50569307 0.72712441 0.00000000

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C -25.73142772 1.40182921 0.00000000

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C -26.95641956 0.72724534 0.00000000

C -28.18187026 -1.40187498 0.00000000

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H 35.53130400 2.50280503 0.00000000

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H 18.37946394 -2.50204561 0.00000000

H 18.37946301 2.50202124 0.00000000

H 15.92882240 -2.50205709 0.00000000

H 15.92882126 2.50203323 0.00000000

H 13.47823449 -2.50206151 0.00000000

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H 11.02764195 -2.50206257 0.00000000

H 11.02764066 2.50203749 0.00000000

H 8.57705775 -2.50206020 0.00000000

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H 6.12647595 -2.50205819 0.00000000

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H 3.67588915 -2.50205506 0.00000000

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H 1.22529778 -2.50205154 0.00000000

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H -3.67588731 -2.50204517 0.00000000

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H -15.92882711 2.50205147 0.00000000

H -18.37946866 -2.50202459 0.00000000

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H -20.83015539 -2.50199646 0.00000000

H -20.83015405 2.50201544 0.00000000

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H -28.18176367 -2.50202399 0.00000000

H -28.18176610 2.50204923 0.00000000

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H -30.63172610 2.50223699 0.00000000

H -33.08138173 -2.50252392 0.00000000

H -33.08138877 2.50254270 0.00000000

H -35.53130493 -2.50279949 0.00000000

H -35.53131437 2.50281004 0.00000000

H -37.98259034 -2.50266524 0.00000000

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$end

$comment

37-acene singlet

$end

$molecule

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C 44.10253629 0.72184905 0.00000000

C 42.88509655 -1.40087818 0.00000000

C 42.88507570 1.40107240 0.00000000

C 41.65884256 -0.72503813 0.00000000

C 41.65883191 0.72521455 0.00000000

C 40.43135108 -1.40257284 0.00000000

C 40.43133094 1.40273140 0.00000000

C 39.21064123 -0.72691555 0.00000000

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C 37.98061432 -1.40265818 0.00000000

C 37.98059497 1.40278243 0.00000000

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C 35.53086979 -1.40234312 0.00000000

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C 34.30849416 -0.72767941 0.00000000

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C 31.85701110 0.72753820 0.00000000

C 30.63119330 -1.40182515 0.00000000

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C 29.40590573 -0.72728884 0.00000000

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C 28.18086204 -1.40176765 0.00000000

C 28.18084642 1.40176924 0.00000000

C 26.95514974 -0.72716136 0.00000000

C 26.95514192 0.72714947 0.00000000

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C 25.73030245 1.40176400 0.00000000

C 24.50461390 -0.72711836 0.00000000

C 24.50460667 0.72708119 0.00000000

C 23.27968958 -1.40183623 0.00000000

C 23.27967637 1.40178736 0.00000000

C 22.05415881 -0.72712907 0.00000000

C 22.05415227 0.72706898 0.00000000

C 20.82906309 -1.40188054 0.00000000

C 20.82905140 1.40180994 0.00000000

C 19.60369939 -0.72715998 0.00000000

C 19.60369370 0.72707964 0.00000000

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C 17.15320425 -0.72718945 0.00000000

C 17.15319950 0.72709172 0.00000000

C 15.92790625 -1.40192476 0.00000000

C 15.92789800 1.40181935 0.00000000

C 14.70267433 -0.72720921 0.00000000

C 14.70267050 0.72709701 0.00000000

C 13.47736195 -1.40193126 0.00000000

C 13.47735532 1.40181289 0.00000000

C 12.25212504 -0.72721975 0.00000000

C 12.25212201 0.72709585 0.00000000

C 11.02682243 -1.40193374 0.00000000

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C 9.80156630 0.72709069 0.00000000

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H 28.18083277 2.50192032 0.00000000

H 25.73032994 -2.50193837 0.00000000

H 25.73030411 2.50191354 0.00000000

H 23.27970693 -2.50198342 0.00000000

H 23.27968350 2.50193435 0.00000000

H 20.82907651 -2.50202580 0.00000000

H 20.82905584 2.50195492 0.00000000

H 18.37847609 -2.50205435 0.00000000

H 18.37845834 2.50196453 0.00000000

H 15.92790888 -2.50206935 0.00000000

H 15.92789413 2.50196366 0.00000000

H 13.47736237 -2.50207642 0.00000000

H 13.47735044 2.50195785 0.00000000

H 11.02682192 -2.50207948 0.00000000

H 11.02681255 2.50195070 0.00000000

H 8.57628062 -2.50208149 0.00000000

H 8.57627359 2.50194486 0.00000000

H 6.12573627 -2.50208346 0.00000000

H 6.12573159 2.50194119 0.00000000

H 3.67518807 -2.50208477 0.00000000

H 3.67518585 2.50193913 0.00000000

H 1.22463721 -2.50208532 0.00000000

H 1.22463757 2.50193879 0.00000000

H -1.22591425 -2.50208488 0.00000000

H -1.22591132 2.50194000 0.00000000

H -3.67646377 -2.50208369 0.00000000

H -3.67645837 2.50194291 0.00000000

H -6.12700979 -2.50208227 0.00000000

H -6.12700204 2.50194786 0.00000000

H -8.57755283 -2.50208048 0.00000000

H -8.57754265 2.50195469 0.00000000

H -11.02809734 -2.50207788 0.00000000

H -11.02808464 2.50196308 0.00000000

H -13.47865123 -2.50207160 0.00000000

H -13.47863578 2.50197042 0.00000000

H -15.92922661 -2.50205664 0.00000000

H -15.92920829 2.50197197 0.00000000

H -18.37983685 -2.50202881 0.00000000

H -18.37981565 2.50196360 0.00000000

H -20.83047793 -2.50198678 0.00000000

H -20.83045414 2.50194381 0.00000000

H -23.28110730 -2.50194189 0.00000000

H -23.28108128 2.50192343 0.00000000

H -25.73162934 -2.50192366 0.00000000

H -25.73160144 2.50193158 0.00000000

H -28.18191120 -2.50197872 0.00000000

H -28.18188169 2.50201463 0.00000000

H -30.63185694 -2.50215655 0.00000000

H -30.63182590 2.50222201 0.00000000

H -33.08155572 -2.50245626 0.00000000

H -33.08152319 2.50255279 0.00000000

H -35.53146912 -2.50272618 0.00000000

H -35.53143511 2.50285515 0.00000000

H -37.98261068 -2.50258469 0.00000000

H -37.98257512 2.50274752 0.00000000

H -40.43668710 -2.50120200 0.00000000

H -40.43665014 2.50140035 0.00000000

H -42.88922540 -2.50068884 0.00000000

H -42.88918766 2.50092402 0.00000000

H -45.03467672 -1.24934884 0.00000000

H -45.03465775 1.24961657 0.00000000

$end

$comment

37-acene triplet

$end

$molecule

0 3

C 46.53054972 -0.70826588 0.00000000

C 46.53054911 0.70825626 0.00000000

C 45.34757753 -1.40203044 0.00000000

C 45.34757625 1.40201974 0.00000000

C 44.10342512 -0.72171011 0.00000000

C 44.10342449 0.72169853 0.00000000

C 42.88583326 -1.40094715 0.00000000

C 42.88583230 1.40093488 0.00000000

C 41.65966046 -0.72511300 0.00000000

C 41.65966009 0.72510069 0.00000000

C 40.43206199 -1.40263122 0.00000000

C 40.43206150 1.40261860 0.00000000

C 39.21134142 -0.72698377 0.00000000

C 39.21134134 0.72697144 0.00000000

C 37.98131248 -1.40270560 0.00000000

C 37.98131246 1.40269337 0.00000000

C 36.76056128 -0.72765240 0.00000000

C 36.76056141 0.72764051 0.00000000

C 35.53153912 -1.40238086 0.00000000

C 35.53153947 1.40236925 0.00000000

C 34.30896225 -0.72769098 0.00000000

C 34.30896256 0.72767970 0.00000000

C 33.08179463 -1.40204851 0.00000000

C 33.08179529 1.40203754 0.00000000

C 31.85744399 -0.72747709 0.00000000

C 31.85744450 0.72746648 0.00000000

C 30.63171416 -1.40185117 0.00000000

C 30.63171511 1.40184099 0.00000000

C 29.40632089 -0.72725682 0.00000000

C 29.40632156 0.72724720 0.00000000

C 28.18129411 -1.40178662 0.00000000

C 28.18129530 1.40177753 0.00000000

C 26.95555985 -0.72712348 0.00000000

C 26.95556068 0.72711517 0.00000000

C 25.73067604 -1.40179637 0.00000000

C 25.73067746 1.40178880 0.00000000

C 24.50500193 -0.72707703 0.00000000

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C 23.27999546 -1.40182893 0.00000000

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C 22.05450390 -0.72708176 0.00000000

C 22.05450490 0.72707720 0.00000000

C 20.82932914 -1.40185694 0.00000000

C 20.82933077 1.40185337 0.00000000

C 19.60398793 -0.72710305 0.00000000

C 19.60398889 0.72710055 0.00000000

C 18.37869963 -1.40187123 0.00000000

C 18.37870118 1.40186974 0.00000000

C 17.15343268 -0.72712085 0.00000000

C 17.15343354 0.72712030 0.00000000

C 15.92810002 -1.40187407 0.00000000

C 15.92810142 1.40187450 0.00000000

C 14.70284649 -0.72712923 0.00000000

C 14.70284723 0.72713045 0.00000000

C 13.47751518 -1.40187177 0.00000000

C 13.47751641 1.40187380 0.00000000

C 12.25224766 -0.72713045 0.00000000

C 12.25224832 0.72713313 0.00000000

C 11.02693258 -1.40186822 0.00000000

C 11.02693370 1.40187155 0.00000000

C 9.80164777 -0.72712778 0.00000000

C 9.80164842 0.72713168 0.00000000

C 8.57634779 -1.40186560 0.00000000

C 8.57634894 1.40187007 0.00000000

C 7.35105226 -0.72712467 0.00000000

C 7.35105298 0.72712975 0.00000000

C 6.12576034 -1.40186433 0.00000000

C 6.12576159 1.40186999 0.00000000

C 4.90046212 -0.72712232 0.00000000

C 4.90046293 0.72712867 0.00000000

C 3.67517172 -1.40186334 0.00000000

C 3.67517306 1.40187028 0.00000000

C 2.44987580 -0.72712082 0.00000000

C 2.44987666 0.72712844 0.00000000

C 1.22458338 -1.40186246 0.00000000

C 1.22458471 1.40187074 0.00000000

C -0.00070830 -0.72711998 0.00000000

C -0.00070749 0.72712889 0.00000000

C -1.22600377 -1.40186153 0.00000000

C -1.22600261 1.40187098 0.00000000

C -2.45129206 -0.72711990 0.00000000

C -2.45129138 0.72712978 0.00000000

C -3.67658907 -1.40186090 0.00000000

C -3.67658816 1.40187118 0.00000000

C -4.90187755 -0.72712091 0.00000000

C -4.90187705 0.72713142 0.00000000

C -6.12717153 -1.40186123 0.00000000

C -6.12717089 1.40187195 0.00000000

C -7.35246674 -0.72712301 0.00000000

C -7.35246641 0.72713382 0.00000000

C -8.57775021 -1.40186270 0.00000000

C -8.57774978 1.40187351 0.00000000

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C -9.80305990 0.72713593 0.00000000

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C -20.83076744 -1.40181992 0.00000000

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C -22.05577790 0.72707251 0.00000000

C -23.28144193 -1.40178723 0.00000000

C -23.28144225 1.40179531 0.00000000

C -24.50631337 -0.72710463 0.00000000

C -24.50631358 0.72711181 0.00000000

C -25.73205835 -1.40177929 0.00000000

C -25.73205905 1.40178550 0.00000000

C -26.95704401 -0.72723489 0.00000000

C -26.95704445 0.72723991 0.00000000

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C -35.53200398 1.40267278 0.00000000

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C -36.76211443 0.72701524 0.00000000

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C -42.89793162 1.40194385 0.00000000

C -44.08110427 -0.70810364 0.00000000

C -44.08110632 0.70807750 0.00000000

H 47.48518922 -1.24944240 0.00000000

H 47.48518824 1.24943344 0.00000000

H 45.33911740 -2.50082193 0.00000000

H 45.33911487 2.50081115 0.00000000

H 42.88630208 -2.50115212 0.00000000

H 42.88630050 2.50113970 0.00000000

H 40.43209587 -2.50268951 0.00000000

H 40.43209493 2.50267673 0.00000000

H 37.98130974 -2.50278950 0.00000000

H 37.98130959 2.50277715 0.00000000

H 35.53152891 -2.50249738 0.00000000

H 35.53152953 2.50248567 0.00000000

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H 33.08177018 2.50217687 0.00000000

H 30.63169608 -2.50200149 0.00000000

H 30.63169804 2.50199124 0.00000000

H 28.18129023 -2.50193889 0.00000000

H 28.18129269 2.50192975 0.00000000

H 25.73068241 -2.50194640 0.00000000

H 25.73068528 2.50193878 0.00000000

H 23.28000406 -2.50197600 0.00000000

H 23.28000709 2.50197030 0.00000000

H 20.82933411 -2.50200180 0.00000000

H 20.82933712 2.50199824 0.00000000

H 18.37870025 -2.50201513 0.00000000

H 18.37870305 2.50201369 0.00000000

H 15.92809841 -2.50201772 0.00000000

H 15.92810096 2.50201823 0.00000000

H 13.47751325 -2.50201558 0.00000000

H 13.47751551 2.50201768 0.00000000

H 11.02693080 -2.50201210 0.00000000

H 11.02693292 2.50201545 0.00000000

H 8.57634636 -2.50200947 0.00000000

H 8.57634858 2.50201393 0.00000000

H 6.12575985 -2.50200801 0.00000000

H 6.12576230 2.50201364 0.00000000

H 3.67517163 -2.50200677 0.00000000

H 3.67517423 2.50201369 0.00000000

H 1.22458291 -2.50200560 0.00000000

H 1.22458553 2.50201389 0.00000000

H -1.22600481 -2.50200438 0.00000000

H -1.22600254 2.50201390 0.00000000

H -3.67658985 -2.50200352 0.00000000

H -3.67658805 2.50201388 0.00000000

H -6.12717089 -2.50200362 0.00000000

H -6.12716961 2.50201441 0.00000000

H -8.57774761 -2.50200488 0.00000000

H -8.57774676 2.50201572 0.00000000

H -11.02832274 -2.50200733 0.00000000

H -11.02832209 2.50201804 0.00000000

H -13.47890204 -2.50200874 0.00000000

H -13.47890148 2.50201930 0.00000000

H -15.92949715 -2.50200461 0.00000000

H -15.92949670 2.50201498 0.00000000

H -18.38012470 -2.50199054 0.00000000

H -18.38012437 2.50200056 0.00000000

H -20.83078834 -2.50196386 0.00000000

H -20.83078828 2.50197321 0.00000000

H -23.28145531 -2.50193362 0.00000000

H -23.28145572 2.50194179 0.00000000

H -25.73203599 -2.50192734 0.00000000

H -25.73203707 2.50193365 0.00000000

H -28.18239214 -2.50199126 0.00000000

H -28.18239401 2.50199506 0.00000000

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H -30.63241124 2.50217749 0.00000000

H -33.08215113 -2.50248570 0.00000000

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H -35.53207527 -2.50276782 0.00000000

H -35.53208013 2.50276129 0.00000000

H -37.98321411 -2.50264050 0.00000000

H -37.98321996 2.50262959 0.00000000

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H -40.43731041 2.50125612 0.00000000

H -42.88988242 -2.50077503 0.00000000

H -42.88988948 2.50075232 0.00000000

H -45.03541912 -1.24948249 0.00000000

H -45.03542266 1.24945371 0.00000000

$end

$comment

38-acene singlet

$end

$molecule

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C 44.10335479 -0.72168043 0.00000000

C 44.10335112 0.72176484 0.00000000

C 42.88577133 -1.40109524 0.00000000

C 42.88576428 1.40117350 0.00000000

C 41.65972402 -0.72518253 0.00000000

C 41.65972041 0.72525468 0.00000000

C 40.43204105 -1.40258411 0.00000000

C 40.43203415 1.40265026 0.00000000

C 39.21144731 -0.72705127 0.00000000

C 39.21144376 0.72711137 0.00000000

C 37.98131963 -1.40270981 0.00000000

C 37.98131283 1.40276410 0.00000000

C 36.76069997 -0.72770958 0.00000000

C 36.76069640 0.72775778 0.00000000

C 35.53160998 -1.40240970 0.00000000

C 35.53160315 1.40245213 0.00000000

C 34.30914332 -0.72772060 0.00000000

C 34.30913970 0.72775694 0.00000000

C 33.08193880 -1.40207907 0.00000000

C 33.08193191 1.40210952 0.00000000

C 31.85766523 -0.72749794 0.00000000

C 31.85766162 0.72752233 0.00000000

C 30.63192667 -1.40187537 0.00000000

C 30.63191981 1.40189388 0.00000000

C 29.40657418 -0.72728086 0.00000000

C 29.40657062 0.72729333 0.00000000

C 28.18156568 -1.40180313 0.00000000

C 28.18155890 1.40180979 0.00000000

C 26.95583967 -0.72715510 0.00000000

C 26.95583619 0.72715575 0.00000000

C 25.73099536 -1.40181238 0.00000000

C 25.73098872 1.40180738 0.00000000

C 24.50531040 -0.72711631 0.00000000

C 24.50530705 0.72710543 0.00000000

C 23.28035367 -1.40185214 0.00000000

C 23.28034739 1.40183588 0.00000000

C 22.05484799 -0.72712778 0.00000000

C 22.05484486 0.72710602 0.00000000

C 20.82972142 -1.40189032 0.00000000

C 20.82971570 1.40186358 0.00000000

C 19.60437415 -0.72715517 0.00000000

C 19.60437139 0.72712346 0.00000000

C 18.37912504 -1.40191460 0.00000000

C 18.37912014 1.40187858 0.00000000

C 17.15386466 -0.72717879 0.00000000

C 17.15386235 0.72713852 0.00000000

C 15.92855999 -1.40192537 0.00000000

C 15.92855598 1.40188158 0.00000000

C 14.70332503 -0.72719263 0.00000000

C 14.70332318 0.72714531 0.00000000

C 13.47801200 -1.40192795 0.00000000

C 13.47800881 1.40187788 0.00000000

C 12.25276958 -0.72719823 0.00000000

C 12.25276811 0.72714524 0.00000000

C 11.02746898 -1.40192745 0.00000000

C 11.02746648 1.40187240 0.00000000

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C 9.80220896 0.72714187 0.00000000

C 8.57692461 -1.40192675 0.00000000

C 8.57692266 1.40186783 0.00000000

C 7.35165285 -0.72719874 0.00000000

C 7.35165192 0.72713800 0.00000000

C 6.12637718 -1.40192684 0.00000000

C 6.12637568 1.40186490 0.00000000

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C 4.90109868 0.72713494 0.00000000

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C 3.67582625 1.40186335 0.00000000

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H 33.08166020 2.50225306 0.00000000

H 30.63180541 -2.50202983 0.00000000

H 30.63179321 2.50204850 0.00000000

H 28.18156315 -2.50196144 0.00000000

H 28.18155103 2.50196824 0.00000000

H 25.73104570 -2.50197024 0.00000000

H 25.73103384 2.50196535 0.00000000

H 23.28040534 -2.50200795 0.00000000

H 23.28039413 2.50199172 0.00000000

H 20.82975233 -2.50204413 0.00000000

H 20.82974210 2.50201734 0.00000000

H 18.37913494 -2.50206714 0.00000000

H 18.37912616 2.50203102 0.00000000

H 15.92855766 -2.50207738 0.00000000

H 15.92855046 2.50203349 0.00000000

H 13.47800607 -2.50207989 0.00000000

H 13.47800035 2.50202978 0.00000000

H 11.02746431 -2.50207951 0.00000000

H 11.02745989 2.50202451 0.00000000

H 8.57692257 -2.50207895 0.00000000

H 8.57691919 2.50202012 0.00000000

H 6.12637720 -2.50207911 0.00000000

H 6.12637457 2.50201728 0.00000000

H 3.67582787 -2.50207978 0.00000000

H 3.67582623 2.50201574 0.00000000

H 1.22527624 -2.50208031 0.00000000

H 1.22527568 2.50201512 0.00000000

H -1.22527616 -2.50208036 0.00000000

H -1.22527565 2.50201514 0.00000000

H -3.67582792 -2.50207989 0.00000000

H -3.67582636 2.50201578 0.00000000

H -6.12637753 -2.50207926 0.00000000

H -6.12637487 2.50201732 0.00000000

H -8.57692311 -2.50207909 0.00000000

H -8.57691972 2.50202018 0.00000000

H -11.02746497 -2.50207962 0.00000000

H -11.02746054 2.50202455 0.00000000

H -13.47800664 -2.50207999 0.00000000

H -13.47800102 2.50202976 0.00000000

H -15.92855811 -2.50207743 0.00000000

H -15.92855090 2.50203339 0.00000000

H -18.37913515 -2.50206712 0.00000000

H -18.37912633 2.50203090 0.00000000

H -20.82975222 -2.50204409 0.00000000

H -20.82974199 2.50201721 0.00000000

H -23.28040504 -2.50200790 0.00000000

H -23.28039377 2.50199160 0.00000000

H -25.73104523 -2.50197018 0.00000000

H -25.73103337 2.50196524 0.00000000

H -28.18156265 -2.50196140 0.00000000

H -28.18155051 2.50196818 0.00000000

H -30.63180492 -2.50202983 0.00000000

H -30.63179273 2.50204848 0.00000000

H -33.08167189 -2.50222247 0.00000000

H -33.08165973 2.50225309 0.00000000

H -35.53129457 -2.50253341 0.00000000

H -35.53128247 2.50257597 0.00000000

H -37.98121911 -2.50280831 0.00000000

H -37.98120695 2.50286270 0.00000000

H -40.43252025 -2.50266793 0.00000000

H -40.43250785 2.50273415 0.00000000

H -42.88681043 -2.50129509 0.00000000

H -42.88679786 2.50137340 0.00000000

H -45.33945905 -2.50078512 0.00000000

H -45.33944627 2.50087581 0.00000000

H -47.48457487 -1.24963060 0.00000000

H -47.48456841 1.24973236 0.00000000

$end

$comment

38-acene triplet

$end

$molecule

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C 46.53112336 -0.70805494 0.00000000

C 46.53112392 0.70803614 0.00000000

C 45.34789449 -1.40198023 0.00000000

C 45.34789559 1.40196245 0.00000000

C 44.10413660 -0.72169246 0.00000000

C 44.10413717 0.72167596 0.00000000

C 42.88641843 -1.40110828 0.00000000

C 42.88641963 1.40109305 0.00000000

C 41.66045290 -0.72520741 0.00000000

C 41.66045360 0.72519377 0.00000000

C 40.43267352 -1.40259525 0.00000000

C 40.43267485 1.40258308 0.00000000

C 39.21206790 -0.72707813 0.00000000

C 39.21206868 0.72706756 0.00000000

C 37.98195043 -1.40271996 0.00000000

C 37.98195174 1.40271085 0.00000000

C 36.76120042 -0.72772076 0.00000000

C 36.76120112 0.72771286 0.00000000

C 35.53222252 -1.40242068 0.00000000

C 35.53222359 1.40241387 0.00000000

C 34.30955999 -0.72770774 0.00000000

C 34.30956050 0.72770162 0.00000000

C 33.08249836 -1.40209279 0.00000000

C 33.08249912 1.40208713 0.00000000

C 31.85805017 -0.72746772 0.00000000

C 31.85805057 0.72746229 0.00000000

C 30.63240767 -1.40189257 0.00000000

C 30.63240816 1.40188718 0.00000000

C 29.40695867 -0.72724609 0.00000000

C 29.40695898 0.72724060 0.00000000

C 28.18196623 -1.40182185 0.00000000

C 28.18196661 1.40181617 0.00000000

C 26.95622405 -0.72712394 0.00000000

C 26.95622433 0.72711818 0.00000000

C 25.73133144 -1.40182822 0.00000000

C 25.73133195 1.40182227 0.00000000

C 24.50567691 -0.72708916 0.00000000

C 24.50567731 0.72708348 0.00000000

C 23.28064519 -1.40186055 0.00000000

C 23.28064614 1.40185489 0.00000000

C 22.05517772 -0.72710022 0.00000000

C 22.05517841 0.72709549 0.00000000

C 20.82998219 -1.40188863 0.00000000

C 20.82998370 1.40188430 0.00000000

C 19.60465664 -0.72712229 0.00000000

C 19.60465764 0.72711944 0.00000000

C 18.37936032 -1.40190268 0.00000000

C 18.37936227 1.40190071 0.00000000

C 17.15409895 -0.72713787 0.00000000

C 17.15410016 0.72713762 0.00000000

C 15.92876887 -1.40190492 0.00000000

C 15.92877099 1.40190600 0.00000000

C 14.70351615 -0.72714349 0.00000000

C 14.70351734 0.72714621 0.00000000

C 13.47819136 -1.40190141 0.00000000

C 13.47819327 1.40190560 0.00000000

C 12.25292400 -0.72714251 0.00000000

C 12.25292499 0.72714798 0.00000000

C 11.02761617 -1.40189710 0.00000000

C 11.02761767 1.40190387 0.00000000

C 9.80233267 -0.72713925 0.00000000

C 9.80233339 0.72714687 0.00000000

C 8.57703847 -1.40189433 0.00000000

C 8.57703948 1.40190278 0.00000000

C 7.35174559 -0.72713651 0.00000000

C 7.35174607 0.72714534 0.00000000

C 6.12645776 -1.40189343 0.00000000

C 6.12645837 1.40190258 0.00000000

C 4.90116221 -0.72713516 0.00000000

C 4.90116252 0.72714434 0.00000000

C 3.67587521 -1.40189366 0.00000000

C 3.67587557 1.40190281 0.00000000

C 2.45058084 -0.72713486 0.00000000

C 2.45058107 0.72714383 0.00000000

C 1.22529196 -1.40189423 0.00000000

C 1.22529212 1.40190284 0.00000000

C 0.00000019 -0.72713517 0.00000000

C 0.00000035 0.72714336 0.00000000

C -1.22529153 -1.40189464 0.00000000

C -1.22529146 1.40190238 0.00000000

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C -2.45058044 0.72714297 0.00000000

C -3.67587505 -1.40189474 0.00000000

C -3.67587498 1.40190157 0.00000000

C -4.90116220 -0.72713647 0.00000000

C -4.90116207 0.72714297 0.00000000

C -6.12645806 -1.40189480 0.00000000

C -6.12645789 1.40190097 0.00000000

C -7.35174599 -0.72713784 0.00000000

C -7.35174579 0.72714394 0.00000000

C -8.57703938 -1.40189545 0.00000000

C -8.57703899 1.40190140 0.00000000

C -9.80233352 -0.72713991 0.00000000

C -9.80233317 0.72714611 0.00000000

C -11.02761769 -1.40189718 0.00000000

C -11.02761697 1.40190356 0.00000000

C -12.25292521 -0.72714173 0.00000000

C -12.25292467 0.72714868 0.00000000

C -13.47819324 -1.40189972 0.00000000

C -13.47819229 1.40190715 0.00000000

C -14.70351745 -0.72714081 0.00000000

C -14.70351680 0.72714883 0.00000000

C -15.92877075 -1.40190109 0.00000000

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C -17.15410003 -0.72713323 0.00000000

C -17.15409946 0.72714223 0.00000000

C -18.37936169 -1.40189693 0.00000000

C -18.37936107 1.40190653 0.00000000

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C -19.60465696 0.72712551 0.00000000

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C -20.82998280 1.40189125 0.00000000

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C -25.73133194 1.40182765 0.00000000

C -26.95622322 -0.72711981 0.00000000

C -26.95622408 0.72712239 0.00000000

C -28.18196491 -1.40181887 0.00000000

C -28.18196686 1.40181931 0.00000000

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C -29.40695881 0.72724247 0.00000000

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C -30.63240849 1.40188786 0.00000000

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C -35.53222185 -1.40242338 0.00000000

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C -36.76120094 0.72770987 0.00000000

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C -37.98195173 1.40270767 0.00000000

C -39.21206757 -0.72708114 0.00000000

C -39.21206844 0.72706449 0.00000000

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C -44.10413711 0.72167314 0.00000000

C -45.34789359 -1.40198319 0.00000000

C -45.34789580 1.40195942 0.00000000

C -46.53112275 -0.70805826 0.00000000

C -46.53112387 0.70803276 0.00000000

H 47.48532890 -1.24968689 0.00000000

H 47.48533000 1.24966722 0.00000000

H 45.34015146 -2.50079901 0.00000000

H 45.34015345 2.50078120 0.00000000

H 42.88746066 -2.50130888 0.00000000

H 42.88746282 2.50129359 0.00000000

H 40.43314759 -2.50268003 0.00000000

H 40.43314986 2.50266784 0.00000000

H 37.98184335 -2.50281924 0.00000000

H 37.98184562 2.50281019 0.00000000

H 35.53190882 -2.50254467 0.00000000

H 35.53191084 2.50253796 0.00000000

H 33.08224268 -2.50223591 0.00000000

H 33.08224415 2.50223036 0.00000000

H 30.63229875 -2.50204624 0.00000000

H 30.63229976 2.50204090 0.00000000

H 28.18196925 -2.50197888 0.00000000

H 28.18197016 2.50197316 0.00000000

H 25.73137812 -2.50198436 0.00000000

H 25.73137940 2.50197823 0.00000000

H 23.28068725 -2.50201422 0.00000000

H 23.28068930 2.50200827 0.00000000

H 20.83000267 -2.50203989 0.00000000

H 20.83000548 2.50203525 0.00000000

H 18.37936266 -2.50205226 0.00000000

H 18.37936602 2.50205007 0.00000000

H 15.92876283 -2.50205359 0.00000000

H 15.92876640 2.50205459 0.00000000

H 13.47818459 -2.50204967 0.00000000

H 13.47818788 2.50205393 0.00000000

H 11.02761192 -2.50204523 0.00000000

H 11.02761464 2.50205215 0.00000000

H 8.57703688 -2.50204245 0.00000000

H 8.57703882 2.50205106 0.00000000

H 6.12645769 -2.50204158 0.00000000

H 6.12645897 2.50205085 0.00000000

H 3.67587555 -2.50204183 0.00000000

H 3.67587647 2.50205106 0.00000000

H 1.22529213 -2.50204241 0.00000000

H 1.22529258 2.50205106 0.00000000

H -1.22529179 -2.50204283 0.00000000

H -1.22529150 2.50205055 0.00000000

H -3.67587568 -2.50204292 0.00000000

H -3.67587536 2.50204971 0.00000000

H -6.12645847 -2.50204299 0.00000000

H -6.12645796 2.50204905 0.00000000

H -8.57703853 -2.50204364 0.00000000

H -8.57703772 2.50204945 0.00000000

H -11.02761448 -2.50204537 0.00000000

H -11.02761317 2.50205162 0.00000000

H -13.47818762 -2.50204799 0.00000000

H -13.47818606 2.50205537 0.00000000

H -15.92876582 -2.50204965 0.00000000

H -15.92876430 2.50205845 0.00000000

H -18.37936497 -2.50204629 0.00000000

H -18.37936400 2.50205615 0.00000000

H -20.83000386 -2.50203283 0.00000000

H -20.83000388 2.50204257 0.00000000

H -23.28068718 -2.50200741 0.00000000

H -23.28068840 2.50201544 0.00000000

H -25.73137694 -2.50197908 0.00000000

H -25.73137933 2.50198388 0.00000000

H -28.18196747 -2.50197590 0.00000000

H -28.18197073 2.50197642 0.00000000

H -30.63229698 -2.50204572 0.00000000

H -30.63230054 2.50204159 0.00000000

H -33.08224136 -2.50223743 0.00000000

H -33.08224478 2.50222886 0.00000000

H -35.53190796 -2.50254744 0.00000000

H -35.53191122 2.50253507 0.00000000

H -37.98184260 -2.50282229 0.00000000

H -37.98184591 2.50280691 0.00000000

H -40.43314671 -2.50268271 0.00000000

H -40.43315020 2.50266491 0.00000000

H -42.88745953 -2.50131132 0.00000000

H -42.88746325 2.50129093 0.00000000

H -45.34015019 -2.50080189 0.00000000

H -45.34015409 2.50077818 0.00000000

H -47.48532801 -1.24969042 0.00000000

H -47.48532994 1.24966357 0.00000000

$end

$comment

39-acene singlet

$end

$molecule

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C 48.97926182 0.70812823 0.00000000

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C 47.79638898 1.40189393 0.00000000

C 46.55216452 -0.72188990 0.00000000

C 46.55217270 0.72172594 0.00000000

C 45.33478940 -1.40113716 0.00000000

C 45.33480514 1.40098699 0.00000000

C 44.10857001 -0.72519310 0.00000000

C 44.10857803 0.72505648 0.00000000

C 42.88102648 -1.40267308 0.00000000

C 42.88104170 1.40254999 0.00000000

C 41.66029728 -0.72702634 0.00000000

C 41.66030500 0.72691621 0.00000000

C 40.43024731 -1.40276024 0.00000000

C 40.43026185 1.40266310 0.00000000

C 39.20962814 -0.72770343 0.00000000

C 39.20963548 0.72761869 0.00000000

C 37.98047769 -1.40242709 0.00000000

C 37.98049144 1.40235467 0.00000000

C 36.75811181 -0.72775069 0.00000000

C 36.75811876 0.72768996 0.00000000

C 35.53077875 -1.40207419 0.00000000

C 35.53079170 1.40202507 0.00000000

C 34.30661998 -0.72753946 0.00000000

C 34.30662650 0.72750130 0.00000000

C 33.08077151 -1.40185633 0.00000000

C 33.08078356 1.40182902 0.00000000

C 31.85548713 -0.72730947 0.00000000

C 31.85549315 0.72729226 0.00000000

C 30.63042781 -1.40177449 0.00000000

C 30.63043881 1.40176728 0.00000000

C 29.40471366 -0.72715795 0.00000000

C 29.40471912 0.72715984 0.00000000

C 28.17986999 -1.40177280 0.00000000

C 28.17987990 1.40178382 0.00000000

C 26.95416269 -0.72709249 0.00000000

C 26.95416753 0.72711168 0.00000000

C 25.72923011 -1.40180002 0.00000000

C 25.72923887 1.40182734 0.00000000

C 24.50369499 -0.72708321 0.00000000

C 24.50369923 0.72711772 0.00000000

C 23.27859158 -1.40182574 0.00000000

C 23.27859923 1.40186737 0.00000000

C 22.05322432 -0.72709676 0.00000000

C 22.05322800 0.72714470 0.00000000

C 20.82798611 -1.40183885 0.00000000

C 20.82799276 1.40189297 0.00000000

C 19.60271889 -0.72711149 0.00000000

C 19.60272207 0.72717113 0.00000000

C 18.37741317 -1.40184013 0.00000000

C 18.37741888 1.40190502 0.00000000

C 17.15218059 -0.72711892 0.00000000

C 17.15218331 0.72718857 0.00000000

C 15.92686012 -1.40183475 0.00000000

C 15.92686494 1.40190881 0.00000000

C 14.70162361 -0.72711899 0.00000000

C 14.70162589 0.72719706 0.00000000

C 13.47631479 -1.40182758 0.00000000

C 13.47631874 1.40190928 0.00000000

C 12.25106133 -0.72711491 0.00000000

C 12.25106316 0.72719987 0.00000000

C 11.02577004 -1.40182147 0.00000000

C 11.02577309 1.40190928 0.00000000

C 9.80050155 -0.72710990 0.00000000

C 9.80050290 0.72720014 0.00000000

C 8.57522346 -1.40181741 0.00000000

C 8.57522555 1.40190973 0.00000000

C 7.34994693 -0.72710584 0.00000000

C 7.34994776 0.72719971 0.00000000

C 6.12467534 -1.40181525 0.00000000

C 6.12467642 1.40191039 0.00000000

C 4.89939709 -0.72710342 0.00000000

C 4.89939737 0.72719917 0.00000000

C 3.67412679 -1.40181449 0.00000000

C 3.67412679 1.40191058 0.00000000

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C 2.44885039 0.72719836 0.00000000

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C 1.22357776 1.40190985 0.00000000

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C -45.34870240 1.40191252 0.00000000

C -46.53179326 -0.70820707 0.00000000

C -46.53179940 0.70804816 0.00000000

H 49.93364508 -1.24958615 0.00000000

H 49.93365929 1.24938387 0.00000000

H 47.78792767 -2.50088171 0.00000000

H 47.78795598 2.50070386 0.00000000

H 45.33520043 -2.50133078 0.00000000

H 45.33522848 2.50118074 0.00000000

H 42.88105940 -2.50272429 0.00000000

H 42.88108652 2.50260140 0.00000000

H 40.43026016 -2.50284329 0.00000000

H 40.43028609 2.50274638 0.00000000

H 37.98047279 -2.50254405 0.00000000

H 37.98049731 2.50247187 0.00000000

H 35.53074970 -2.50221515 0.00000000

H 35.53077273 2.50216630 0.00000000

H 33.08074491 -2.50200910 0.00000000

H 33.08076630 2.50198209 0.00000000

H 30.63041566 -2.50192988 0.00000000

H 30.63043519 2.50192299 0.00000000

H 28.17987048 -2.50192623 0.00000000

H 28.17988813 2.50193759 0.00000000

H 25.72923556 -2.50195040 0.00000000

H 25.72925123 2.50197804 0.00000000

H 23.27859549 -2.50197373 0.00000000

H 23.27860923 2.50201565 0.00000000

H 20.82798605 -2.50198556 0.00000000

H 20.82799802 2.50203991 0.00000000

H 18.37740999 -2.50198639 0.00000000

H 18.37742024 2.50205148 0.00000000

H 15.92685586 -2.50198095 0.00000000

H 15.92686450 2.50205519 0.00000000

H 13.47631114 -2.50197376 0.00000000

H 13.47631819 2.50205564 0.00000000

H 11.02576778 -2.50196748 0.00000000

H 11.02577318 2.50205550 0.00000000

H 8.57522251 -2.50196311 0.00000000

H 8.57522620 2.50205566 0.00000000

H 6.12467529 -2.50196053 0.00000000

H 6.12467718 2.50205591 0.00000000

H 3.67412716 -2.50195930 0.00000000

H 3.67412713 2.50205566 0.00000000

H 1.22357936 -2.50195901 0.00000000

H 1.22357753 2.50205448 0.00000000

H -1.22696717 -2.50195944 0.00000000

H -1.22697082 2.50205223 0.00000000

H -3.67751146 -2.50196078 0.00000000

H -3.67751680 2.50204911 0.00000000

H -6.12805235 -2.50196338 0.00000000

H -6.12805917 2.50204566 0.00000000

H -8.57858883 -2.50196766 0.00000000

H -8.57859689 2.50204260 0.00000000

H -11.02912116 -2.50197376 0.00000000

H -11.02913026 2.50204027 0.00000000

H -13.47965304 -2.50198072 0.00000000

H -13.47966302 2.50203792 0.00000000

H -15.93019341 -2.50198586 0.00000000

H -15.93020421 2.50203300 0.00000000

H -18.38075597 -2.50198461 0.00000000

H -18.38076763 2.50202090 0.00000000

H -20.83135283 -2.50197216 0.00000000

H -20.83136539 2.50199675 0.00000000

H -23.28197973 -2.50194796 0.00000000

H -23.28199330 2.50195987 0.00000000

H -25.73259523 -2.50192277 0.00000000

H -25.73260990 2.50192087 0.00000000

H -28.18310514 -2.50192536 0.00000000

H -28.18312093 2.50190849 0.00000000

H -30.63337637 -2.50200294 0.00000000

H -30.63339326 2.50196993 0.00000000

H -33.08331237 -2.50220446 0.00000000

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H -35.53300529 -2.50252887 0.00000000

H -35.53302407 2.50246081 0.00000000

H -37.98291608 -2.50282498 0.00000000

H -37.98293578 2.50273805 0.00000000

H -40.43405723 -2.50271053 0.00000000

H -40.43407780 2.50260385 0.00000000

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$end

$comment

39-acene triplet

$end

$molecule

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C 46.55293090 -0.72170286 0.00000000

C 46.55291901 0.72184283 0.00000000

C 45.33544272 -1.40097035 0.00000000

C 45.33542107 1.40109014 0.00000000

C 44.10928578 -0.72505615 0.00000000

C 44.10927408 0.72515669 0.00000000

C 42.88165863 -1.40254544 0.00000000

C 42.88163849 1.40262622 0.00000000

C 41.66090958 -0.72693107 0.00000000

C 41.66089881 0.72699431 0.00000000

C 40.43086978 -1.40266884 0.00000000

C 40.43085142 1.40271385 0.00000000

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C 39.21011286 0.72766194 0.00000000

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C 36.75851716 -0.72769030 0.00000000

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C 34.30698534 -0.72749023 0.00000000

C 34.30697928 0.72746970 0.00000000

C 33.08123640 -1.40186194 0.00000000

C 33.08122379 1.40183087 0.00000000

C 31.85584689 -0.72727865 0.00000000

C 31.85584225 0.72724049 0.00000000

C 30.63081575 -1.40180409 0.00000000

C 30.63080525 1.40175770 0.00000000

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C 29.40507093 0.72709898 0.00000000

C 28.18019769 -1.40181903 0.00000000

C 28.18018927 1.40176123 0.00000000

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C 24.50401482 0.72704610 0.00000000

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C 15.92705334 1.40182570 0.00000000

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C 14.70179279 0.72708840 0.00000000

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C 6.12475107 1.40182336 0.00000000

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C 4.89945844 0.72709049 0.00000000

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C -13.47984055 -1.40185778 0.00000000

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C -14.70516456 0.72713978 0.00000000

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H 35.53128603 2.50218080 0.00000000

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H 28.18019128 2.50191158 0.00000000

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H 23.27885995 -2.50203196 0.00000000

H 23.27885164 2.50195916 0.00000000

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H 18.37762862 2.50197140 0.00000000

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H 15.92705029 2.50196738 0.00000000

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H 13.47647706 2.50196250 0.00000000

H 11.02590310 -2.50205135 0.00000000

H 11.02590346 2.50195943 0.00000000

H 8.57532426 -2.50204748 0.00000000

H 8.57532882 2.50195950 0.00000000

H 6.12474516 -2.50204160 0.00000000

H 6.12475430 2.50196311 0.00000000

H 3.67416753 -2.50203369 0.00000000

H 3.67418031 2.50196986 0.00000000

H 1.22359180 -2.50202452 0.00000000

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H -42.88878525 -2.50126238 0.00000000

H -42.88879959 2.50126380 0.00000000

H -45.34138571 -2.50076492 0.00000000

H -45.34140096 2.50075031 0.00000000

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$end

$comment

40-acene singlet

$end

$molecule

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C 46.55384509 0.72177616 0.00000000

C 45.33626992 -1.40107598 0.00000000

C 45.33625669 1.40120425 0.00000000

C 44.11023843 -0.72516037 0.00000000

C 44.11023165 0.72527726 0.00000000

C 42.88254949 -1.40255616 0.00000000

C 42.88253662 1.40266158 0.00000000

C 41.66195794 -0.72703381 0.00000000

C 41.66195140 0.72712820 0.00000000

C 40.43182894 -1.40269276 0.00000000

C 40.43181659 1.40277615 0.00000000

C 39.21120798 -0.72769691 0.00000000

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C 37.98212263 -1.40240062 0.00000000

C 37.98211076 1.40246289 0.00000000

C 36.75965297 -0.72771191 0.00000000

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C -48.98081575 0.70817978 0.00000000

H 49.93509761 -1.24950551 0.00000000

H 49.93508559 1.24967781 0.00000000

H 47.78989265 -2.50077144 0.00000000

H 47.78986876 2.50092304 0.00000000

H 45.33736064 -2.50127288 0.00000000

H 45.33733713 2.50140103 0.00000000

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H 15.92853190 2.50201973 0.00000000

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H 13.47799445 2.50201308 0.00000000

H 11.02746255 -2.50209199 0.00000000

H 11.02745684 2.50200750 0.00000000

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H 8.57691545 2.50200384 0.00000000

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$end

$comment

40-acene triplet

$end

$molecule

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C 46.55458471 -0.72169164 0.00000000

C 46.55458885 0.72165061 0.00000000

C 45.33687682 -1.40112648 0.00000000

C 45.33688421 1.40109282 0.00000000

C 44.11092213 -0.72521628 0.00000000

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C 42.88314894 1.40257322 0.00000000

C 41.66254368 -0.72708017 0.00000000

C 41.66254696 0.72706603 0.00000000

C 40.43242143 -1.40271842 0.00000000

C 40.43242704 1.40271027 0.00000000

C 39.21168611 -0.72771941 0.00000000

C 39.21168894 0.72771599 0.00000000

C 37.98269980 -1.40241805 0.00000000

C 37.98270462 1.40241937 0.00000000

C 36.76005632 -0.72770462 0.00000000

C 36.76005854 0.72770911 0.00000000

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$end

$comment

41-acene singlet

$end

$molecule

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C -7.35255798 0.72713073 0.00000000

C -8.57782932 -1.40188411 0.00000000

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C -9.80309684 0.72713392 0.00000000

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C -15.92941630 -1.40188469 0.00000000

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C -17.15472574 -0.72716341 0.00000000

C -17.15472397 0.72714054 0.00000000

C -18.37994945 -1.40188245 0.00000000

C -18.37994588 1.40186270 0.00000000

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C -19.60524624 0.72713192 0.00000000

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C -35.53321660 -1.40204085 0.00000000

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C -41.66272261 -0.72701546 0.00000000

C -41.66272074 0.72704933 0.00000000

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C -42.88331019 1.40261153 0.00000000

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H 52.38493130 1.24956076 0.00000000

H 50.23933217 -2.50079743 0.00000000

H 50.23932603 2.50082414 0.00000000

H 47.78635739 -2.50121059 0.00000000

H 47.78635253 2.50123226 0.00000000

H 45.33221375 -2.50268792 0.00000000

H 45.33220866 2.50270478 0.00000000

H 42.88140360 -2.50279915 0.00000000

H 42.88139881 2.50281120 0.00000000

H 40.43162350 -2.50250733 0.00000000

H 40.43161911 2.50251489 0.00000000

H 37.98190898 -2.50219115 0.00000000

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H 35.53191016 2.50199734 0.00000000

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H 33.08159010 2.50192629 0.00000000

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H 30.63105261 2.50192978 0.00000000

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H 28.18042468 2.50195975 0.00000000

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H 25.72979165 2.50198756 0.00000000

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H 20.82862193 2.50200599 0.00000000

H 18.37808131 -2.50203620 0.00000000

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H 15.92754087 2.50199710 0.00000000

H 13.47700940 -2.50203354 0.00000000

H 13.47700668 2.50199245 0.00000000

H 11.02647232 -2.50203276 0.00000000

H 11.02647064 2.50198954 0.00000000

H 8.57593342 -2.50203260 0.00000000

H 8.57593262 2.50198817 0.00000000

H 6.12539372 -2.50203264 0.00000000

H 6.12539360 2.50198775 0.00000000

H 3.67485426 -2.50203248 0.00000000

H 3.67485455 2.50198769 0.00000000

H 1.22431550 -2.50203195 0.00000000

H 1.22431614 2.50198763 0.00000000

H -1.22622250 -2.50203097 0.00000000

H -1.22622155 2.50198743 0.00000000

H -3.67675960 -2.50202962 0.00000000

H -3.67675828 2.50198723 0.00000000

H -6.12729547 -2.50202816 0.00000000

H -6.12729352 2.50198738 0.00000000

H -8.57782910 -2.50202695 0.00000000

H -8.57782631 2.50198850 0.00000000

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H -11.02835564 2.50199120 0.00000000

H -13.47888661 -2.50202670 0.00000000

H -13.47888176 2.50199573 0.00000000

H -15.92941404 -2.50202692 0.00000000

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H -18.37995046 -2.50202452 0.00000000

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H -20.83050953 -2.50201510 0.00000000

H -20.83050295 2.50200180 0.00000000

H -23.28110340 -2.50199402 0.00000000

H -23.28109703 2.50198717 0.00000000

H -25.73172821 -2.50196085 0.00000000

H -25.73172227 2.50196010 0.00000000

H -28.18234284 -2.50192642 0.00000000

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H -30.63285346 -2.50191952 0.00000000

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$end

$comment

41-acene triplet

$end

$molecule

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C 49.00409557 -0.72169017 0.00000000

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C 47.78652038 -1.40095439 0.00000000

C 47.78650247 1.40103869 0.00000000

C 46.56034853 -0.72507392 0.00000000

C 46.56033892 0.72514166 0.00000000

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C 45.33271667 1.40264238 0.00000000

C 44.11201825 -0.72696104 0.00000000

C 44.11200913 0.72699640 0.00000000

C 42.88197444 -1.40269242 0.00000000

C 42.88195858 1.40271200 0.00000000

C 41.66124911 -0.72764967 0.00000000

C 41.66124105 0.72765598 0.00000000

C 40.43220242 -1.40238453 0.00000000

C 40.43218844 1.40237719 0.00000000

C 39.20966026 -0.72770247 0.00000000

C 39.20965359 0.72768478 0.00000000

C 37.98246665 -1.40206117 0.00000000

C 37.98245479 1.40203257 0.00000000

C 36.75814421 -0.72749930 0.00000000

C 36.75813892 0.72746301 0.00000000

C 35.53239986 -1.40187020 0.00000000

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C 29.40571324 -0.72711323 0.00000000

C 29.40570965 0.72704205 0.00000000

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C 4.90018770 0.72709751 0.00000000

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$end

$comment

42-acene singlet

$end

$molecule

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C 49.00432687 -0.72167659 0.00000000

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C 45.33301376 1.40264404 0.00000000

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C 44.11243182 0.72709957 0.00000000

C 42.88231405 -1.40271112 0.00000000

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42-acene triplet

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H -35.53331370 2.50202615 0.00000000

H -37.98323900 -2.50224101 0.00000000

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H -40.43289625 -2.50254682 0.00000000

H -40.43289119 2.50252663 0.00000000

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$end

$comment

43-acene singlet

$end

$molecule

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C 51.45335709 -0.72196097 0.00000000

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C 50.23599050 -1.40119681 0.00000000

C 50.23601612 1.40092334 0.00000000

C 49.00976672 -0.72524831 0.00000000

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C 47.78222941 -1.40273132 0.00000000

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C 46.56150288 -0.72707204 0.00000000

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C 45.33145188 -1.40280840 0.00000000

C 45.33147562 1.40262140 0.00000000

C 44.11083927 -0.72774341 0.00000000

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C 41.65932493 -0.72778459 0.00000000

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C 40.43198625 -1.40210621 0.00000000

C 40.43200783 1.40199842 0.00000000

C 39.20783431 -0.72756618 0.00000000

C 39.20784523 0.72747679 0.00000000

C 37.98198138 -1.40188089 0.00000000

C 37.98200177 1.40180975 0.00000000

C 36.75670144 -0.72732890 0.00000000

C 36.75671172 0.72727499 0.00000000

C 35.53163943 -1.40179191 0.00000000

C 35.53165842 1.40175517 0.00000000

C 34.30592750 -0.72717013 0.00000000

C 34.30593698 0.72714924 0.00000000

C 33.08108251 -1.40178369 0.00000000

C 33.08109980 1.40177866 0.00000000

C 31.85537610 -0.72709812 0.00000000

C 31.85538463 0.72710726 0.00000000

C 30.63044274 -1.40180500 0.00000000

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H 54.83487360 1.24928394 0.00000000

H 52.68908964 -2.50095916 0.00000000

H 52.68913588 2.50064050 0.00000000

H 50.23638474 -2.50139206 0.00000000

H 50.23643031 2.50111881 0.00000000

H 47.78225244 -2.50278179 0.00000000

H 47.78229663 2.50255274 0.00000000

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H 6.12479624 2.50208986 0.00000000

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H -13.47950970 2.50206610 0.00000000

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H -20.83109702 2.50204880 0.00000000

H -23.28163327 -2.50197146 0.00000000

H -23.28165404 2.50203272 0.00000000

H -25.73222220 -2.50196395 0.00000000

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H -28.18284154 -2.50194568 0.00000000

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H -35.53421917 -2.50202346 0.00000000

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$end

$comment

43-acene triplet

$end

$molecule

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C 26.95480606 -0.72710587 0.00000000

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C 22.05370759 0.72713770 0.00000000

C 20.82838057 -1.40186837 0.00000000

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C 19.60312475 -0.72713311 0.00000000

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$comment

44-acene singlet

$end

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$end

$comment

44-acene triplet

$end

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$comment

45-acene singlet

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$comment

45-acene triplet

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46-acene singlet

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$comment

46-acene triplet

$end

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$comment

47-acene singlet

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47-acene triplet

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H -6.12742630 -2.50193110 0.00000000

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H -23.28131268 -2.50197697 0.00000000

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H -37.98488290 -2.50196326 0.00000000

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$end

$comment

48-acene singlet

$end

$molecule

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$end

$comment

48-acene triplet

$end

$molecule

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49-acene singlet

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H -40.43266343 -2.50189902 0.00000000

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H -45.33289625 -2.50211752 0.00000000

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$end

$comment

49-acene triplet

$end

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$end

$comment

50-acene singlet

$end

$molecule

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50-acene triplet

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$end

$comment

51-acene singlet

$end

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$comment

51-acene triplet

$end

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52-acene singlet

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H -11.02751228 -2.50186465 0.00000000

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H -23.28020839 -2.50192101 0.00000000

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H -47.78552017 -2.50212270 0.00000000

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$comment

52-acene triplet

$end

$molecule

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$end

$comment

53-acene singlet

$end

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$comment

53-acene triplet

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$comment

54-acene singlet

$end

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$comment

54-acene triplet

$end

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55-acene triplet

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H 3.67778409 2.50184762 0.00000000

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$comment

56-acene singlet

$end

$molecule

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$end

$comment

56-acene triplet

$end

$molecule

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57-acene singlet

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57-acene triplet

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$comment

58-acene singlet

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$comment

58-acene triplet

$end

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59-acene singlet

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59-acene triplet

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$comment

60-acene triplet

$end

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$comment

61-acene singlet

$end

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61-acene triplet

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62-acene singlet

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62-acene triplet

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63-acene singlet

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H -64.93561254 -2.50288376 0.00000000

H -64.93569557 2.50217988 0.00000000

H -67.38551317 -2.50321061 0.00000000

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H -69.83664984 -2.50312489 0.00000000

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$comment

63-acene triplet

$end

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C 45.33711374 -1.40189173 0.00000000

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C 30.63384138 1.40202292 0.00000000

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$comment

64-acene singlet

$end

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64-acene triplet

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65-acene singlet

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65-acene triplet

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66-acene singlet

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66-acene triplet

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67-acene singlet

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67-acene triplet

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68-acene triplet

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69-acene singlet

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69-acene triplet

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70-acene singlet

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70-acene triplet

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71-acene singlet

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71-acene triplet

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72-acene singlet

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72-acene triplet

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73-acene singlet

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73-acene triplet

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74-acene singlet

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74-acene triplet

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75-acene singlet

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75-acene triplet

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76-acene singlet

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76-acene triplet

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77-acene singlet

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77-acene triplet

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78-acene singlet

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$comment

78-acene triplet

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79-acene singlet

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79-acene triplet

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80-acene singlet

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80-acene triplet

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81-acene singlet

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81-acene triplet

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82-acene singlet

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82-acene triplet

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83-acene singlet

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83-acene triplet

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84-acene singlet

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84-acene triplet

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85-acene singlet

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85-acene triplet

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86-acene triplet

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87-acene singlet

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87-acene triplet

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88-acene singlet

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$comment

88-acene triplet

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89-acene singlet

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89-acene triplet

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90-acene triplet

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91-acene singlet

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91-acene triplet

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92-acene singlet

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92-acene triplet

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93-acene singlet

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$comment

93-acene triplet

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94-acene triplet

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95-acene singlet

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$comment

95-acene triplet

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96-acene singlet

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96-acene triplet

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97-acene singlet

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97-acene triplet

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98-acene singlet

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98-acene triplet

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99-acene singlet

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99-acene triplet

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100-acene triplet

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