All energies presented here are in atomic units (i.e. hartrees). The geometries are given in Angstroms.

The geometry optimizations were performed with the Gaussian 03 program package [1] using UB3LYP/6-31G(d)

(cartesian gaussians) with default convergence. The structures are essentially of D2h symmetry up to the convergence threshold of the geometry optimization. The DFT wavefunctions were checked for stability. Our DFT geometries and energies show no substantial difference to those reported by Bendikov et al. [2], we refer to their supporting material for further details.

The presented results do not contain zero-point energy corrections.

The DMRG results are converged to an accuracy of a few microhartree. We note that the frozen core for both singlet and triplet calculations is closed-shell and derived from the singlet Slater-determinant. No point group symmetry was used.

At the end of our study we became aware that for triplet octacene, and both decacene and dodecacene the underlying PSI3 [3]

RHF/STO-3G calculations were not completely converged. We recomputed the DMRG results for triplet octacene and decacene using reconverged RHF calculations and the corrected results showed no substantial change (as reported below). We hence omitted the recalculation of the 12acene DMRG energies.

1. Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman,

J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone,

B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda,

J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian,

J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli,

J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich,

* 1. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz,
  2. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi,
  3. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
  4. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

1. Bendikov, M.; Duong, H. M.; Starkey, K.; Houk, K. N.; Carter, E. A.; Wudl, F. J. Am. Chem. Soc. 2004, 126, 7416.
2. T. D. Crawford, C. D. Sherrill, E. F. Valeev, J. T. Fermann, R. A. King, M. L. Leininger, S. T. Brown, C. L. Janssen, E. T. Seidl, J. P. Kenny, and W. D. Allen, PSI 3.2, 2003.

############################################################################################################################ Relaxed singlet-triplet gap (i.e. based on optimized geometries for both singlet and triplet state):

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| [n]acene | B3LYP/6-31G(d) | BLYP/6-31G(d) | DMRG(1000)/STO-3G | DMRG(1500)/DZ |
| 2 | 0.09983555 | 0.09628987 | 0.098081 | 0.097212 |
| 3 | 0.06657758 | 0.06400386 | 0.073222 | 0.070118 |
| 4 | 0.04414963 | 0.04255671 | 0.055363 | 0.050846 |
| 5 | 0.02848859 | 0.02776432 | 0.042547 | 0.037242 |
| 6 | 0.01742608 | 0.01736319 | 0.033405 | 0.027908 |
| 8 | 0.00919419 | 0.00474040 | 0.022554 |  |
| 10 | 0.00888014 | 0.00267079 | 0.018422 |  |
| 12 | 0.01155370 | 0.00395812 |  |  |
| [8 triplet unconverged |  |  | 0.022536] |  |
| [10 unconverged |  |  | 0.018347] |  |
| [12 unconverged |  |  | 0.016987] |  |

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Number of unpaired electrons in the singlet ground state DMRG wavefunction:

[n]acene Takatsuka measure\* Head-Gordon1 measure\*\* Head-Gordon2 measure\*\*

STO-3G DZ STO-3G DZ STO-3G DZ

1. 2.13 1.64 1.14 0.86 0.52 0.30
2. 3.10 2.41 1.67 1.27 0.83 0.48
3. 4.15 3.25 2.26 1.73 1.20 0.72
4. 5.26 4.15 2.89 2.23 1.64 1.02
5. 6.48 3.61 2.21

8 9.06 5.24 3.59 10 11.47 6.75 4.78 12\*\*\* 13.86 8.23 5.92

\* Takatsuka, K.; Fueno, T.; Yamaguchi, K. Theor. Chim. Acta 1978, 48, 175. \*\* Head-Gordon, M. Chem. Phys. Lett. 2003, 372, 508. Corresponding to eqns. 7 and 18, respectively.

\*\*\* underlying HF not fully converged

############################################################################################################################ Detailed results:

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singlet 2acene (naphthalene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -378.68387984 (PSI3)

DMRG(1000)/STO-3G = -378.86217348 (core = -365.08259953; active space = -13.77957395) RHF/DZ total energy = -383.24982220 (PSI3)

DMRG(1500)/DZ = -383.39790201 (core = -369.63881187; active space = -13.75909014)

UB3LYP/6-31G(d) total energy = -385.89272908 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -385.71047407 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -2.433661 0.708302 0.000000
2. 6 0 -2.433661 -0.708302 0.000000
3. 1 0 -3.378045 -1.245972 0.000000
4. 1 0 -3.378045 1.245972 0.000000
5. 6 0 -1.244629 1.402481 0.000000
6. 6 0 -1.244629 -1.402481 0.000000
7. 6 0 -0.000077 0.717168 0.000000
8. 6 0 -0.000077 -0.717168 0.000000
9. 1 0 -1.242734 2.490258 0.000000
10. 1 0 -1.242734 -2.490258 0.000000
11. 6 0 1.244779 1.402533 0.000000
12. 6 0 1.244779 -1.402533 0.000000
13. 6 0 2.433606 0.708405 0.000000
14. 6 0 2.433606 -0.708405 0.000000
15. 1 0 1.242448 2.490302 0.000000
16. 1 0 1.242448 -2.490302 0.000000
17. 1 0 3.378224 1.245662 0.000000
18. 1 0 3.378224 -1.245662 0.000000

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triplet 2acene (naphthalene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -378.65409116 (PSI3; singlet state)

DMRG(1000)/STO-3G = -378.76409267 (core = -365.18200251; active space = -13.58209017) RHF/DZ total energy = -383.22837228 (PSI3; singlet state)

DMRG(1500)/DZ = -383.30069014 (core = -369.73048446; active space = -13.57020568)

UB3LYP/6-31G(d) total energy = -385.79289353 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -385.61418420 (G03 with stable=(opt))

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 2.488282 0.681831 0.000000
2. 6 0 2.488282 -0.681831 0.000000
3. 1 0 3.419575 -1.241120 0.000000
4. 1 0 3.419575 1.241120 0.000000
5. 6 0 1.238411 1.400670 0.000000
6. 6 0 1.238411 -1.400670 0.000000
7. 6 0 -0.000001 0.725296 0.000000
8. 6 0 -0.000001 -0.725296 0.000000
9. 1 0 1.247313 2.487396 0.000000
10. 1 0 1.247313 -2.487396 0.000000
11. 6 0 -1.238411 1.400665 0.000000
12. 6 0 -1.238411 -1.400665 0.000000
13. 6 0 -2.488281 0.681833 0.000000
14. 6 0 -2.488281 -0.681833 0.000000
15. 1 0 -1.247325 2.487390 0.000000
16. 1 0 -1.247325 -2.487390 0.000000
17. 1 0 -3.419563 1.241141 0.000000
18. 1 0 -3.419563 -1.241141 0.000000

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singlet 3acene (anthracene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -529.46737463 (PSI3)

DMRG(1000)/STO-3G = -529.72168204 (core = -507.27923918; active space = -22.44244286) RHF/DZ total energy = -535.85016009 (PSI3)

DMRG(1500)/DZ = -536.06224403 (core = -513.65296095; active space = -22.40928308)

UB3LYP/6-31G(d) total energy = -539.53052332 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -539.283724697 (G03 with stable=(opt))

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -3.660857 0.713070 0.000000
2. 6 0 -3.660857 -0.713070 0.000000
3. 1 0 -4.607652 -1.246404 0.000000
4. 1 0 -4.607652 1.246404 0.000000
5. 6 0 -2.479632 1.407088 0.000000
6. 6 0 -2.479632 -1.407088 0.000000
7. 6 0 -1.224085 0.722636 0.000000
8. 6 0 -1.224085 -0.722636 0.000000
9. 1 0 -2.477321 2.494657 0.000000
10. 1 0 -2.477321 -2.494657 0.000000
11. 6 0 0.000029 1.403284 0.000000
12. 6 0 0.000029 -1.403284 0.000000
13. 6 0 1.224035 0.722646 0.000000
14. 6 0 1.224035 -0.722646 0.000000
15. 1 0 -0.000033 2.491609 0.000000
16. 1 0 -0.000033 -2.491609 0.000000
17. 6 0 2.479679 1.407102 0.000000
18. 6 0 2.479679 -1.407102 0.000000
19. 6 0 3.660841 0.713104 0.000000
20. 6 0 3.660841 -0.713104 0.000000
21. 1 0 2.477242 2.494663 0.000000
22. 1 0 2.477242 -2.494663 0.000000
23. 1 0 4.607703 1.246313 0.000000
24. 1 0 4.607703 -1.246313 0.000000

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triplet 3acene (anthracene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -529.44069487 (PSI3; singlet state)

DMRG(1000)/STO-3G = -529.64846038 (core = -507.36721026; active space = -22.28125012)

RHF/DZ total energy = -535.83148294 (PSI3; singlet state)

DMRG(1500)/DZ = -535.99212651 (core = -513.73841841; active space = -22.25370810)

UB3LYP/6-31G(d) total energy = -539.46394574 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -539.21972084 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 3.706046 0.691777 0.000000
2. 6 0 3.706046 -0.691777 0.000000
3. 1 0 4.641764 -1.243830 0.000000
4. 1 0 4.641764 1.243830 0.000000
5. 6 0 2.480846 1.395697 0.000000
6. 6 0 2.480846 -1.395697 0.000000
7. 6 0 1.255174 0.720576 0.000000
8. 6 0 1.255174 -0.720576 0.000000
9. 1 0 2.484966 2.483134 0.000000
10. 1 0 2.484966 -2.483134 0.000000
11. 6 0 0.000000 1.406192 0.000000
12. 6 0 0.000000 -1.406192 0.000000
13. 6 0 -1.255173 0.720575 0.000000
14. 6 0 -1.255173 -0.720575 0.000000
15. 1 0 -0.000001 2.493700 0.000000
16. 1 0 -0.000001 -2.493700 0.000000
17. 6 0 -2.480846 1.395696 0.000000
18. 6 0 -2.480846 -1.395696 0.000000
19. 6 0 -3.706045 0.691777 0.000000
20. 6 0 -3.706045 -0.691777 0.000000
21. 1 0 -2.484968 2.483133 0.000000
22. 1 0 -2.484968 -2.483133 0.000000
23. 1 0 -4.641762 1.243835 0.000000
24. 1 0 -4.641762 -1.243835 0.000000

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singlet 4acene (tetracene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -680.24601667 (PSI3)

DMRG(1000)/STO-3G = -680.57867814 (core = -648.50842303; active space = -32.07025511) RHF/DZ total energy = -688.44639369 (PSI3)

DMRG(1500)/DZ = -688.72424542 (core = -656.69809546; active space = -32.02614996)

UB3LYP/6-31G(d) total energy = -693.16581183 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -692.85488037 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 4.889184 0.715267 0.000000
2. 6 0 4.889184 -0.715267 0.000000
3. 1 0 5.837094 -1.246479 0.000000
4. 1 0 5.837094 1.246479 0.000000
5. 6 0 3.711380 1.409387 0.000000
6. 6 0 3.711380 -1.409387 0.000000
7. 6 0 2.450840 0.725941 0.000000
8. 6 0 2.450840 -0.725941 0.000000
9. 1 0 3.709630 2.496931 0.000000
10. 1 0 3.709630 -2.496931 0.000000
11. 6 0 1.235427 1.406152 0.000000
12. 6 0 1.235427 -1.406152 0.000000
13. 6 0 0.000016 0.726124 0.000000
14. 6 0 0.000016 -0.726124 0.000000
15. 1 0 1.235305 2.494321 0.000000
16. 1 0 1.235305 -2.494321 0.000000
17. 6 0 -1.235526 1.406147 0.000000
18. 6 0 -1.235526 -1.406147 0.000000
19. 6 0 -2.450799 0.725948 0.000000
20. 6 0 -2.450799 -0.725948 0.000000
21. 1 0 -1.235335 2.494309 0.000000
22. 1 0 -1.235335 -2.494309 0.000000
23. 6 0 -3.711407 1.409399 0.000000
24. 6 0 -3.711407 -1.409399 0.000000
25. 6 0 -4.889136 0.715307 0.000000
26. 6 0 -4.889136 -0.715307 0.000000
27. 1 0 -3.709510 2.496929 0.000000
28. 1 0 -3.709510 -2.496929 0.000000
29. 1 0 -5.837057 1.246476 0.000000
30. 1 0 -5.837057 -1.246476 0.000000

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triplet 4acene (tetracene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -680.22185991 (PSI3; singlet state)

DMRG(1000)/STO-3G = -680.52331507 (core = -648.58376709; active space = -31.93954798) RHF/DZ total energy = -688.42956675 (PSI3; singlet state)

DMRG(1500)/DZ = -688.67339894 (core = -656.77361960; active space = -31.89977934)

UB3LYP/6-31G(d) total energy = -693.12166220 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -692.81232366 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -4.926099 0.698684 0.000000
2. 6 0 -4.926099 -0.698684 0.000000
3. 1 0 -5.865246 -1.244975 0.000000
4. 1 0 -5.865246 1.244975 0.000000
5. 6 0 -3.716632 1.397315 0.000000
6. 6 0 -3.716632 -1.397315 0.000000
7. 6 0 -2.486849 0.717519 0.000000
8. 6 0 -2.486849 -0.717519 0.000000
9. 1 0 -3.717388 2.484893 0.000000
10. 1 0 -3.717388 -2.484893 0.000000
11. 6 0 -1.231329 1.404734 0.000000
12. 6 0 -1.231329 -1.404734 0.000000
13. 6 0 0.000000 0.730940 0.000000
14. 6 0 0.000000 -0.730940 0.000000
15. 1 0 -1.236114 2.492628 0.000000
16. 1 0 -1.236114 -2.492628 0.000000
17. 6 0 1.231329 1.404734 0.000000
18. 6 0 1.231329 -1.404734 0.000000
19. 6 0 2.486848 0.717519 0.000000
20. 6 0 2.486848 -0.717519 0.000000
21. 1 0 1.236114 2.492628 0.000000
22. 1 0 1.236114 -2.492628 0.000000
23. 6 0 3.716633 1.397314 0.000000
24. 6 0 3.716633 -1.397314 0.000000
25. 6 0 4.926099 0.698684 0.000000
26. 6 0 4.926099 -0.698684 0.000000
27. 1 0 3.717391 2.484892 0.000000
28. 1 0 3.717391 -2.484892 0.000000
29. 1 0 5.865245 1.244978 0.000000
30. 1 0 5.865245 -1.244978 0.000000

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singlet 5acene (pentacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -831.02200266 (PSI3)

DMRG(1000)/STO-3G = -831.43462990 (core = -788.97948564; active space = -42.45514426) RHF/DZ total energy = -841.04035794 (PSI3)

DMRG(1500)/DZ = -841.38529937 (core = -798.98431887; active space = -42.40098050)

UB3LYP/6-31G(d) total energy = -846.79994340 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -846.42513205 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 6.117721 0.716456 0.000000
2. 6 0 6.117721 -0.716456 0.000000
3. 1 0 7.065952 -1.247064 0.000000
4. 1 0 7.065952 1.247064 0.000000
5. 6 0 4.941657 1.410527 0.000000
6. 6 0 4.941657 -1.410527 0.000000
7. 6 0 3.678746 0.727647 0.000000
8. 6 0 3.678746 -0.727647 0.000000
9. 1 0 4.939919 2.498020 0.000000
10. 1 0 4.939919 -2.498020 0.000000
11. 6 0 2.467582 1.407836 0.000000
12. 6 0 2.467582 -1.407836 0.000000
13. 6 0 1.226500 0.728534 0.000000
14. 6 0 1.226500 -0.728534 0.000000
15. 1 0 2.467624 2.495998 0.000000
16. 1 0 2.467624 -2.495998 0.000000
17. 6 0 -0.000028 1.408524 0.000000
18. 6 0 -0.000028 -1.408524 0.000000
19. 6 0 -1.226469 0.728539 0.000000
20. 6 0 -1.226469 -0.728539 0.000000
21. 1 0 -0.000017 2.496573 0.000000
22. 1 0 -0.000017 -2.496573 0.000000
23. 6 0 -2.467625 1.407846 0.000000
24. 6 0 -2.467625 -1.407846 0.000000
25. 6 0 -3.678713 0.727655 0.000000
26. 6 0 -3.678713 -0.727655 0.000000
27. 1 0 -2.467643 2.496006 0.000000
28. 1 0 -2.467643 -2.496006 0.000000
29. 6 0 -4.941671 1.410535 0.000000
30. 6 0 -4.941671 -1.410535 0.000000
31. 6 0 -6.117708 0.716482 0.000000
32. 6 0 -6.117708 -0.716482 0.000000
33. 1 0 -4.939849 2.498024 0.000000
34. 1 0 -4.939849 -2.498024 0.000000
35. 1 0 -7.065930 1.247100 0.000000
36. 1 0 -7.065930 -1.247100 0.000000

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triplet 5acene (pentacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -830.99997557 (PSI3; singlet state)

DMRG(1000)/STO-3G = -831.39208282 (core = -789.04458421; active space = -42.34749861) RHF/DZ total energy = -841.02488137 (PSI3; singlet state)

DMRG(1500)/DZ = -841.34805717 (core = -799.05111620; active space = -42.29694097)

UB3LYP/6-31G(d) total energy = -846.77145481 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -846.39736773 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -6.148662 0.703577 0.000000
2. 6 0 -6.148662 -0.703577 0.000000
3. 1 0 -7.090330 -1.245586 0.000000
4. 1 0 -7.090330 1.245586 0.000000
5. 6 0 -4.949456 1.399985 0.000000
6. 6 0 -4.949456 -1.399985 0.000000
7. 6 0 -3.712886 0.717632 0.000000
8. 6 0 -3.712886 -0.717632 0.000000
9. 1 0 -4.948444 2.487564 0.000000
10. 1 0 -4.948444 -2.487564 0.000000
11. 6 0 -2.464142 1.403071 0.000000
12. 6 0 -2.464142 -1.403071 0.000000
13. 6 0 -1.244230 0.729785 0.000000
14. 6 0 -1.244230 -0.729785 0.000000
15. 1 0 -2.468456 2.491214 0.000000
16. 1 0 -2.468456 -2.491214 0.000000
17. 6 0 0.000000 1.408308 0.000000
18. 6 0 0.000000 -1.408308 0.000000
19. 6 0 1.244230 0.729785 0.000000
20. 6 0 1.244230 -0.729785 0.000000
21. 1 0 0.000000 2.496125 0.000000
22. 1 0 0.000000 -2.496125 0.000000
23. 6 0 2.464142 1.403071 0.000000
24. 6 0 2.464142 -1.403071 0.000000
25. 6 0 3.712886 0.717632 0.000000
26. 6 0 3.712886 -0.717632 0.000000
27. 1 0 2.468456 2.491214 0.000000
28. 1 0 2.468456 -2.491214 0.000000
29. 6 0 4.949456 1.399985 0.000000
30. 6 0 4.949456 -1.399985 0.000000
31. 6 0 6.148662 0.703577 0.000000
32. 6 0 6.148662 -0.703577 0.000000
33. 1 0 4.948445 2.487564 0.000000
34. 1 0 4.948445 -2.487564 0.000000
35. 1 0 7.090329 1.245586 0.000000
36. 1 0 7.090329 -1.245586 0.000000

---------------------------------------------------------------------

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singlet 6acene (hexacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -981.79438703 (PSI3)

DMRG(1000)/STO-3G = -982.29006984 (core = -928.83956216; active space = -53.45050768) RHF/DZ total energy = -993.63184030 (PSI3)

DMRG(1500)/DZ = -994.04624673 (core = -940.65926366; active space = -53.38698307)

UB3LYP/6-31G(d) total energy = -1000.43368232 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -999.99516051 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -7.350517 0.715773 0.000000
2. 6 0 -7.350517 -0.715773 0.000000
3. 1 0 -8.298142 -1.247504 0.000000
4. 1 0 -8.298142 1.247504 0.000000
5. 6 0 -6.172862 1.409775 0.000000
6. 6 0 -6.172862 -1.409775 0.000000
7. 6 0 -4.911467 0.727133 0.000000
8. 6 0 -4.911467 -0.727133 0.000000
9. 1 0 -6.170427 2.497230 0.000000
10. 1 0 -6.170427 -2.497230 0.000000
11. 6 0 -3.698398 1.407935 0.000000
12. 6 0 -3.698398 -1.407935 0.000000
13. 6 0 -2.457546 0.729346 0.000000
14. 6 0 -2.457546 -0.729346 0.000000
15. 1 0 -3.698513 2.496086 0.000000
16. 1 0 -3.698513 -2.496086 0.000000
17. 6 0 -1.232079 1.409756 0.000000
18. 6 0 -1.232079 -1.409756 0.000000
19. 6 0 0.000001 0.730568 0.000000
20. 6 0 0.000001 -0.730568 0.000000
21. 1 0 -1.232324 2.497778 0.000000
22. 1 0 -1.232324 -2.497778 0.000000
23. 6 0 1.232076 1.409755 0.000000
24. 6 0 1.232076 -1.409755 0.000000
25. 6 0 2.457547 0.729345 0.000000
26. 6 0 2.457547 -0.729345 0.000000
27. 1 0 1.232315 2.497777 0.000000
28. 1 0 1.232315 -2.497777 0.000000
29. 6 0 3.698396 1.407933 0.000000
30. 6 0 3.698396 -1.407933 0.000000
31. 6 0 4.911470 0.727133 0.000000
32. 6 0 4.911470 -0.727133 0.000000
33. 1 0 3.698508 2.496084 0.000000
34. 1 0 3.698508 -2.496084 0.000000
35. 6 0 6.172863 1.409777 0.000000
36. 6 0 6.172863 -1.409777 0.000000
37. 6 0 7.350516 0.715771 0.000000
38. 6 0 7.350516 -0.715771 0.000000
39. 1 0 6.170439 2.497232 0.000000
40. 1 0 6.170439 -2.497232 0.000000
41. 1 0 8.298147 1.247490 0.000000
42. 1 0 8.298147 -1.247490 0.000000

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triplet 6acene (hexacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -981.77641132 (PSI3; singlet state)

DMRG(1000)/STO-3G = -982.25666437 (core = -928.88664107; active space = -53.37002331) RHF/DZ total energy = -993.61870455 (PSI3; singlet state)

DMRG(1500)/DZ = -994.01833852 (core = -940.70874258; active space = -53.30959594)

UB3LYP/6-31G(d) total energy = -1000.41625624 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -999.977797315 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -7.373375 0.707073 0.000000
2. 6 0 -7.373375 -0.707073 0.000000
3. 1 0 -8.316769 -1.246130 0.000000
4. 1 0 -8.316769 1.246130 0.000000
5. 6 0 -6.181007 1.402359 0.000000
6. 6 0 -6.181007 -1.402359 0.000000
7. 6 0 -4.938109 0.718996 0.000000
8. 6 0 -4.938109 -0.718996 0.000000
9. 1 0 -6.179284 2.489911 0.000000
10. 1 0 -6.179284 -2.489911 0.000000
11. 6 0 -3.697422 1.402780 0.000000
12. 6 0 -3.697422 -1.402780 0.000000
13. 6 0 -2.479315 0.727408 0.000000
14. 6 0 -2.479315 -0.727408 0.000000
15. 1 0 -3.700526 2.491010 0.000000
16. 1 0 -3.700526 -2.491010 0.000000
17. 6 0 -1.229341 1.408048 0.000000
18. 6 0 -1.229341 -1.408048 0.000000
19. 6 0 0.000000 0.733735 0.000000
20. 6 0 0.000000 -0.733735 0.000000
21. 1 0 -1.231922 2.495996 0.000000
22. 1 0 -1.231922 -2.495996 0.000000
23. 6 0 1.229341 1.408048 0.000000
24. 6 0 1.229341 -1.408048 0.000000
25. 6 0 2.479315 0.727408 0.000000
26. 6 0 2.479315 -0.727408 0.000000
27. 1 0 1.231923 2.495996 0.000000
28. 1 0 1.231923 -2.495996 0.000000
29. 6 0 3.697422 1.402780 0.000000
30. 6 0 3.697422 -1.402780 0.000000
31. 6 0 4.938108 0.718996 0.000000
32. 6 0 4.938108 -0.718996 0.000000
33. 1 0 3.700527 2.491010 0.000000
34. 1 0 3.700527 -2.491010 0.000000
35. 6 0 6.181007 1.402359 0.000000
36. 6 0 6.181007 -1.402359 0.000000
37. 6 0 7.373375 0.707073 0.000000
38. 6 0 7.373375 -0.707073 0.000000
39. 1 0 6.179284 2.489911 0.000000
40. 1 0 6.179284 -2.489911 0.000000
41. 1 0 8.316769 1.246130 0.000000
42. 1 0 8.316769 -1.246130 0.000000

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singlet 8acene (octacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -1283.33243811 (PSI3)

DMRG(1000)/STO-3G = -1284.00096366 (core = -1207.06363716; active space = -76.93732650)

UB3LYP/6-31G(d) total energy = -1307.70623333 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -1307.13536368 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 9.822751 0.713143 0.000000
2. 6 0 9.822751 -0.713143 0.000000
3. 1 0 10.769689 -1.246217 0.000000
4. 1 0 10.769689 1.246217 0.000000
5. 6 0 8.640499 1.406976 0.000000
6. 6 0 8.640499 -1.406976 0.000000
7. 6 0 7.384570 0.724117 0.000000
8. 6 0 7.384570 -0.724117 0.000000
9. 1 0 8.636571 2.494304 0.000000
10. 1 0 8.636571 -2.494304 0.000000
11. 6 0 6.162609 1.405479 0.000000
12. 6 0 6.162609 -1.405479 0.000000
13. 6 0 4.929929 0.727469 0.000000
14. 6 0 4.929929 -0.727469 0.000000
15. 1 0 6.161034 2.493535 0.000000
16. 1 0 6.161034 -2.493535 0.000000
17. 6 0 3.694126 1.408421 0.000000
18. 6 0 3.694126 -1.408421 0.000000
19. 6 0 2.467559 0.730635 0.000000
20. 6 0 2.467559 -0.730635 0.000000
21. 1 0 3.692886 2.496398 0.000000
22. 1 0 3.692886 -2.496398 0.000000
23. 6 0 1.230750 1.409903 0.000000
24. 6 0 1.230750 -1.409903 0.000000
25. 6 0 -0.000016 0.731730 0.000000
26. 6 0 -0.000016 -0.731730 0.000000
27. 1 0 1.230172 2.497885 0.000000
28. 1 0 1.230172 -2.497885 0.000000
29. 6 0 -1.230777 1.409902 0.000000
30. 6 0 -1.230777 -1.409902 0.000000
31. 6 0 -2.467583 0.730633 0.000000
32. 6 0 -2.467583 -0.730633 0.000000
33. 1 0 -1.230207 2.497883 0.000000
34. 1 0 -1.230207 -2.497883 0.000000
35. 6 0 -3.694139 1.408418 0.000000
36. 6 0 -3.694139 -1.408418 0.000000
37. 6 0 -4.929935 0.727466 0.000000
38. 6 0 -4.929935 -0.727466 0.000000
39. 1 0 -3.692907 2.496394 0.000000
40. 1 0 -3.692907 -2.496394 0.000000
41. 6 0 -6.162601 1.405476 0.000000
42. 6 0 -6.162601 -1.405476 0.000000
43. 6 0 -7.384554 0.724113 0.000000
44. 6 0 -7.384554 -0.724113 0.000000
45. 1 0 -6.161031 2.493529 0.000000
46. 1 0 -6.161031 -2.493529 0.000000
47. 6 0 -8.640472 1.406970 0.000000
48. 6 0 -8.640472 -1.406970 0.000000
49. 6 0 -9.822720 0.713143 0.000000
50. 6 0 -9.822720 -0.713143 0.000000
51. 1 0 -8.636541 2.494295 0.000000
52. 1 0 -8.636541 -2.494295 0.000000
53. 1 0 -10.769647 1.246231 0.000000
54. 1 0 -10.769647 -1.246231 0.000000

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triplet 8acene (octacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -1283.22124680 (PSI3, SCF not converged to minimum; singlet state)

DMRG(1000)/STO-3G (\*) = -1283.97842776 (\*unconv. HF; core = -1207.06020314; active space = -76.91822462)

RHF/STO-3G total energy = -1283.32634910 (G03 with stable=(opt,rrhf); singlet state)

DMRG(1000)/STO-3G = -1283.97840925 (core = -1207.06264653; active space = -76.91576272)

UB3LYP/6-31G(d) total energy = -1307.69703914 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -1307.13062328 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -9.825968 0.711479 0.000000
2. 6 0 -9.825968 -0.711479 0.000000
3. 1 0 -10.771697 -1.246535 0.000000
4. 1 0 -10.771697 1.246535 0.000000
5. 6 0 -8.641569 1.405924 0.000000
6. 6 0 -8.641569 -1.405924 0.000000
7. 6 0 -7.389595 0.722226 0.000000
8. 6 0 -7.389595 -0.722226 0.000000
9. 1 0 -8.639224 2.493446 0.000000
10. 1 0 -8.639224 -2.493446 0.000000
11. 6 0 -6.161777 1.404097 0.000000
12. 6 0 -6.161777 -1.404097 0.000000
13. 6 0 -4.937510 0.725939 0.000000
14. 6 0 -4.937510 -0.725939 0.000000
15. 1 0 -6.162721 2.492328 0.000000
16. 1 0 -6.162721 -2.492328 0.000000
17. 6 0 -3.691044 1.406977 0.000000
18. 6 0 -3.691044 -1.406977 0.000000
19. 6 0 -2.474742 0.731640 0.000000
20. 6 0 -2.474742 -0.731640 0.000000
21. 1 0 -3.693001 2.495073 0.000000
22. 1 0 -3.693001 -2.495073 0.000000
23. 6 0 -1.228646 1.409601 0.000000
24. 6 0 -1.228646 -1.409601 0.000000
25. 6 0 -0.000001 0.734990 0.000000
26. 6 0 -0.000001 -0.734990 0.000000
27. 1 0 -1.229852 2.497614 0.000000
28. 1 0 -1.229852 -2.497614 0.000000
29. 6 0 1.228645 1.409602 0.000000
30. 6 0 1.228645 -1.409602 0.000000
31. 6 0 2.474741 0.731640 0.000000
32. 6 0 2.474741 -0.731640 0.000000
33. 1 0 1.229849 2.497614 0.000000
34. 1 0 1.229849 -2.497614 0.000000
35. 6 0 3.691044 1.406978 0.000000
36. 6 0 3.691044 -1.406978 0.000000
37. 6 0 4.937510 0.725939 0.000000
38. 6 0 4.937510 -0.725939 0.000000
39. 1 0 3.693002 2.495074 0.000000
40. 1 0 3.693002 -2.495074 0.000000
41. 6 0 6.161777 1.404098 0.000000
42. 6 0 6.161777 -1.404098 0.000000
43. 6 0 7.389596 0.722226 0.000000
44. 6 0 7.389596 -0.722226 0.000000
45. 1 0 6.162723 2.492328 0.000000
46. 1 0 6.162723 -2.492328 0.000000
47. 6 0 8.641569 1.405924 0.000000
48. 6 0 8.641569 -1.405924 0.000000
49. 6 0 9.825969 0.711479 0.000000
50. 6 0 9.825969 -0.711479 0.000000
51. 1 0 8.639228 2.493446 0.000000
52. 1 0 8.639228 -2.493446 0.000000
53. 1 0 10.771696 1.246538 0.000000
54. 1 0 10.771696 -1.246538 0.000000

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singlet 10acene (decacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -1584.78243939 (PSI3, SCF not converged to minimum)

DMRG(1000)/STO-3G (\*) = -1585.71323214 (\*unconv. HF; core = -1483.64454568; active space = -102.06868647)

RHF/STO-3G total energy = -1584.87473124 (G03 with stable=(opt,rrhf))

DMRG(1000)/STO-3G = -1585.71331102 (core = -1483.64649853; active space = -102.06681249)

UB3LYP/6-31G(d) total energy = -1614.98013084 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -1614.28024991 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1. 6 0 -12.286459 0.713204 0.000000
2. 6 0 -12.286459 -0.713204 0.000000
3. 1 0 -13.232858 -1.247136 0.000000
4. 1 0 -13.232858 1.247136 0.000000
5. 6 0 -11.104552 1.407441 0.000000
6. 6 0 -11.104552 -1.407441 0.000000
7. 6 0 -9.848699 0.724254 0.000000
8. 6 0 -9.848699 -0.724254 0.000000
9. 1 0 -11.102098 2.494931 0.000000
10. 1 0 -11.102098 -2.494931 0.000000
11. 6 0 -8.626957 1.405881 0.000000
12. 6 0 -8.626957 -1.405881 0.000000
13. 6 0 -7.395009 0.727344 0.000000
14. 6 0 -7.395009 -0.727344 0.000000
15. 1 0 -8.627386 2.494068 0.000000
16. 1 0 -8.627386 -2.494068 0.000000
17. 6 0 -6.158121 1.408266 0.000000
18. 6 0 -6.158121 -1.408266 0.000000
19. 6 0 -4.934211 0.730243 0.000000
20. 6 0 -4.934211 -0.730243 0.000000
21. 1 0 -6.158802 2.496330 0.000000
22. 1 0 -6.158802 -2.496330 0.000000
23. 6 0 -3.693580 1.409318 0.000000
24. 6 0 -3.693580 -1.409318 0.000000
25. 6 0 -2.468192 0.731552 0.000000
26. 6 0 -2.468192 -0.731552 0.000000
27. 1 0 -3.693840 2.497387 0.000000
28. 1 0 -3.693840 -2.497387 0.000000
29. 6 0 -1.231033 1.409431 0.000000
30. 6 0 -1.231033 -1.409431 0.000000
31. 6 0 -0.000005 0.731841 0.000000
32. 6 0 -0.000005 -0.731841 0.000000
33. 1 0 -1.231077 2.497521 0.000000
34. 1 0 -1.231077 -2.497521 0.000000
35. 6 0 1.231025 1.409431 0.000000
36. 6 0 1.231025 -1.409431 0.000000
37. 6 0 2.468184 0.731552 0.000000
38. 6 0 2.468184 -0.731552 0.000000
39. 1 0 1.231052 2.497521 0.000000
40. 1 0 1.231052 -2.497521 0.000000
41. 6 0 3.693573 1.409317 0.000000
42. 6 0 3.693573 -1.409317 0.000000
43. 6 0 4.934206 0.730244 0.000000
44. 6 0 4.934206 -0.730244 0.000000
45. 1 0 3.693823 2.497385 0.000000
46. 1 0 3.693823 -2.497385 0.000000
47. 6 0 6.158118 1.408263 0.000000
48. 6 0 6.158118 -1.408263 0.000000
49. 6 0 7.395010 0.727345 0.000000
50. 6 0 7.395010 -0.727345 0.000000
51. 1 0 6.158798 2.496327 0.000000
52. 1 0 6.158798 -2.496327 0.000000
53. 6 0 8.626961 1.405879 0.000000
54. 6 0 8.626961 -1.405879 0.000000
55. 6 0 9.848706 0.724254 0.000000
56. 6 0 9.848706 -0.724254 0.000000
57. 1 0 8.627398 2.494066 0.000000
58. 1 0 8.627398 -2.494066 0.000000
59. 6 0 11.104563 1.407439 0.000000
60. 6 0 11.104563 -1.407439 0.000000
61. 6 0 12.286471 0.713205 0.000000
62. 6 0 12.286471 -0.713205 0.000000
63. 1 0 11.102124 2.494928 0.000000
64. 1 0 11.102124 -2.494928 0.000000
65. 1 0 13.232869 1.247141 0.000000
66. 1 0 13.232869 -1.247141 0.000000

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triplet 10acene (decacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -1584.78934989 (PSI3, SCF not converged to minimum; singlet state)

DMRG(1000)/STO-3G (\*) = -1585.69488530 (\*unconv. HF; core = -1483.61667360; active space = -102.07821171)

RHF/STO-3G total energy = -1584.87423340 (G03 with stable=(opt,rrhf); singlet state)

DMRG(1000)/STO-3G = -1585.69488864 (core = -1483.61896067; active space = -102.07592797)

UB3LYP/6-31G(d) total energy = -1614.97125070 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -1614.27757912 (G03 with stable=(opt)) ---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 12.281767 0.713987 0.000000
2. 6 0 12.281767 -0.713987 0.000000
3. 1 0 13.228666 -1.246982 0.000000
4. 1 0 13.228666 1.246982 0.000000
5. 6 0 11.101565 1.408067 0.000000
6. 6 0 11.101565 -1.408067 0.000000
7. 6 0 9.844182 0.724718 0.000000
8. 6 0 9.844182 -0.724718 0.000000
9. 1 0 11.099350 2.495532 0.000000
10. 1 0 11.099350 -2.495532 0.000000
11. 6 0 8.624568 1.405643 0.000000
12. 6 0 8.624568 -1.405643 0.000000
13. 6 0 7.392839 0.726775 0.000000
14. 6 0 7.392839 -0.726775 0.000000
15. 1 0 8.624897 2.493833 0.000000
16. 1 0 8.624897 -2.493833 0.000000
17. 6 0 6.154767 1.407314 0.000000
18. 6 0 6.154767 -1.407314 0.000000
19. 6 0 4.936509 0.729877 0.000000
20. 6 0 4.936509 -0.729877 0.000000
21. 1 0 6.155625 2.495428 0.000000
22. 1 0 6.155625 -2.495428 0.000000
23. 6 0 3.689067 1.408951 0.000000
24. 6 0 3.689067 -1.408951 0.000000
25. 6 0 2.472220 0.733608 0.000000
26. 6 0 2.472220 -0.733608 0.000000
27. 1 0 3.690207 2.497067 0.000000
28. 1 0 3.690207 -2.497067 0.000000
29. 6 0 1.228635 1.410381 0.000000
30. 6 0 1.228635 -1.410381 0.000000
31. 6 0 -0.000004 0.735671 0.000000
32. 6 0 -0.000004 -0.735671 0.000000
33. 1 0 1.229314 2.498465 0.000000
34. 1 0 1.229314 -2.498465 0.000000
35. 6 0 -1.228642 1.410381 0.000000
36. 6 0 -1.228642 -1.410381 0.000000
37. 6 0 -2.472226 0.733608 0.000000
38. 6 0 -2.472226 -0.733608 0.000000
39. 1 0 -1.229323 2.498465 0.000000
40. 1 0 -1.229323 -2.498465 0.000000
41. 6 0 -3.689072 1.408951 0.000000
42. 6 0 -3.689072 -1.408951 0.000000
43. 6 0 -4.936512 0.729876 0.000000
44. 6 0 -4.936512 -0.729876 0.000000
45. 1 0 -3.690218 2.497067 0.000000
46. 1 0 -3.690218 -2.497067 0.000000
47. 6 0 -6.154769 1.407314 0.000000
48. 6 0 -6.154769 -1.407314 0.000000
49. 6 0 -7.392838 0.726774 0.000000
50. 6 0 -7.392838 -0.726774 0.000000
51. 1 0 -6.155634 2.495428 0.000000
52. 1 0 -6.155634 -2.495428 0.000000
53. 6 0 -8.624564 1.405643 0.000000
54. 6 0 -8.624564 -1.405643 0.000000
55. 6 0 -9.844175 0.724717 0.000000
56. 6 0 -9.844175 -0.724717 0.000000
57. 1 0 -8.624897 2.493833 0.000000
58. 1 0 -8.624897 -2.493833 0.000000
59. 6 0 -11.101557 1.408065 0.000000
60. 6 0 -11.101557 -1.408065 0.000000
61. 6 0 -12.281759 0.713988 0.000000
62. 6 0 -12.281759 -0.713988 0.000000
63. 1 0 -11.099341 2.495529 0.000000
64. 1 0 -11.099341 -2.495529 0.000000
65. 1 0 -13.228652 1.246991 0.000000
66. 1 0 -13.228652 -1.246991 0.000000

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singlet 12acene (dodecacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -1886.33790492 (PSI3, SCF not converged to minimum)

DMRG(1000)/STO-3G (\*) = -1887.42557476 (\*unconv. HF; core = -1758.90571049; active space = -128.51986427)

RHF/STO-3G total energy = -1886.41819716 (G03 with stable=(opt,rrhf))

DMRG(1000)/STO-3G = (core = -1758.90708587; active space = )

UB3LYP/6-31G(d) total energy = -1922.25353497 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -1921.42532899 (G03 with stable=(opt))

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 0.000000 0.713394 -14.748836
2. 6 0 0.000000 -0.713394 -14.748836
3. 1 0 0.000000 -1.247003 -15.695358
4. 1 0 0.000000 1.247003 -15.695358
5. 6 0 0.000000 1.407812 -13.567476
6. 6 0 0.000000 -1.407812 -13.567476
7. 6 0 0.000000 0.724478 -12.311353
8. 6 0 0.000000 -0.724478 -12.311353
9. 1 0 0.000000 2.495327 -13.565332
10. 1 0 0.000000 -2.495327 -13.565332
11. 6 0 0.000000 1.406129 -11.090439
12. 6 0 0.000000 -1.406129 -11.090439
13. 6 0 0.000000 0.727443 -9.858013
14. 6 0 0.000000 -0.727443 -9.858013
15. 1 0 0.000000 2.494335 -11.091319
16. 1 0 0.000000 -2.494335 -11.091319
17. 6 0 0.000000 1.408422 -8.622060
18. 6 0 0.000000 -1.408422 -8.622060
19. 6 0 0.000000 0.730154 -7.397949
20. 6 0 0.000000 -0.730154 -7.397949
21. 1 0 0.000000 2.496493 -8.623496
22. 1 0 0.000000 -2.496493 -8.623496
23. 6 0 0.000000 1.409295 -6.157676
24. 6 0 0.000000 -1.409295 -6.157676
25. 6 0 0.000000 0.731224 -4.933174
26. 6 0 0.000000 -0.731224 -4.933174
27. 1 0 0.000000 2.497354 -6.159031
28. 1 0 0.000000 -2.497354 -6.159031
29. 6 0 0.000000 1.409130 -3.694724
30. 6 0 0.000000 -1.409130 -3.694724
31. 6 0 0.000000 0.731313 -2.466697
32. 6 0 0.000000 -0.731313 -2.466697
33. 1 0 0.000000 2.497221 -3.695817
34. 1 0 0.000000 -2.497221 -3.695817
35. 6 0 0.000000 1.408825 -1.231658
36. 6 0 0.000000 -1.408825 -1.231658
37. 6 0 0.000000 0.731245 0.000000
38. 6 0 0.000000 -0.731245 0.000000
39. 1 0 0.000000 2.496953 -1.232101
40. 1 0 0.000000 -2.496953 -1.232101
41. 6 0 0.000000 1.408825 1.231656
42. 6 0 0.000000 -1.408825 1.231656
43. 6 0 0.000000 0.731313 2.466696
44. 6 0 0.000000 -0.731313 2.466696
45. 1 0 0.000000 2.496953 1.232094
46. 1 0 0.000000 -2.496953 1.232094
47. 6 0 0.000000 1.409130 3.694722
48. 6 0 0.000000 -1.409130 3.694722
49. 6 0 0.000000 0.731224 4.933172
50. 6 0 0.000000 -0.731224 4.933172
51. 1 0 0.000000 2.497220 3.695808
52. 1 0 0.000000 -2.497220 3.695808
53. 6 0 0.000000 1.409294 6.157673
54. 6 0 0.000000 -1.409294 6.157673
55. 6 0 0.000000 0.730154 7.397947
56. 6 0 0.000000 -0.730154 7.397947
57. 1 0 0.000000 2.497353 6.159021
58. 1 0 0.000000 -2.497353 6.159021
59. 6 0 0.000000 1.408421 8.622058
60. 6 0 0.000000 -1.408421 8.622058
61. 6 0 0.000000 0.727443 9.858013
62. 6 0 0.000000 -0.727443 9.858013
63. 1 0 0.000000 2.496492 8.623487
64. 1 0 0.000000 -2.496492 8.623487
65. 6 0 0.000000 1.406129 11.090441
66. 6 0 0.000000 -1.406129 11.090441
67. 6 0 0.000000 0.724478 12.311358
68. 6 0 0.000000 -0.724478 12.311358
69. 1 0 0.000000 2.494334 11.091314
70. 1 0 0.000000 -2.494334 11.091314
71. 6 0 0.000000 1.407813 13.567482
72. 6 0 0.000000 -1.407813 13.567482
73. 6 0 0.000000 0.713394 14.748844
74. 6 0 0.000000 -0.713394 14.748844
75. 1 0 0.000000 2.495328 13.565332
76. 1 0 0.000000 -2.495328 13.565332
77. 1 0 0.000000 1.246998 15.695371
78. 1 0 0.000000 -1.246998 15.695371

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triplet 12acene (dodecacene), UB3LYP/6-31G(d) geometry optimized, stationary point found

RHF/STO-3G total energy = -1886.34743932 (PSI3, SCF not converged to minimum; singlet state)

DMRG(1000)/STO-3G (\*) = -1887.40858761 (\*unconv. HF; core = -1758.85023318; active space = -128.55835443)

RHF/STO-3G total energy = -1886.42095876 (G03 with stable=(opt,rrhf); singlet state)

DMRG(1000)/STO-3G = (core = -1758.85210927; active space = )

UB3LYP/6-31G(d) total energy = -1922.24198127 (G03 with stable=(opt))

UBLYP/6-31G(d) total energy = -1921.42137087 (G03 with stable=(opt))

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1. 6 0 -14.737067 0.715485 0.000000
2. 6 0 -14.737067 -0.715485 0.000000
3. 1 0 -15.684601 -1.247349 0.000000
4. 1 0 -15.684601 1.247349 0.000000
5. 6 0 -13.559281 1.409578 0.000000
6. 6 0 -13.559281 -1.409578 0.000000
7. 6 0 -12.298661 0.726478 0.000000
8. 6 0 -12.298661 -0.726478 0.000000
9. 1 0 -13.557107 2.497071 0.000000
10. 1 0 -13.557107 -2.497071 0.000000
11. 6 0 -11.084094 1.407093 0.000000
12. 6 0 -11.084094 -1.407093 0.000000
13. 6 0 -9.846932 0.728015 0.000000
14. 6 0 -9.846932 -0.728015 0.000000
15. 1 0 -11.084300 2.495282 0.000000
16. 1 0 -11.084300 -2.495282 0.000000
17. 6 0 -8.615912 1.408278 0.000000
18. 6 0 -8.615912 -1.408278 0.000000
19. 6 0 -7.392454 0.729809 0.000000
20. 6 0 -7.392454 -0.729809 0.000000
21. 1 0 -8.616550 2.496358 0.000000
22. 1 0 -8.616550 -2.496358 0.000000
23. 6 0 -6.150319 1.409102 0.000000
24. 6 0 -6.150319 -1.409102 0.000000
25. 6 0 -4.934078 0.731907 0.000000
26. 6 0 -4.934078 -0.731907 0.000000
27. 1 0 -6.151146 2.497176 0.000000
28. 1 0 -6.151146 -2.497176 0.000000
29. 6 0 -3.687417 1.410020 0.000000
30. 6 0 -3.687417 -1.410020 0.000000
31. 6 0 -2.469847 0.734484 0.000000
32. 6 0 -2.469847 -0.734484 0.000000
33. 1 0 -3.688400 2.498088 0.000000
34. 1 0 -3.688400 -2.498088 0.000000
35. 6 0 -1.228397 1.410874 0.000000
36. 6 0 -1.228397 -1.410874 0.000000
37. 6 0 -0.000001 0.735873 0.000000
38. 6 0 -0.000001 -0.735873 0.000000
39. 1 0 -1.228915 2.498927 0.000000
40. 1 0 -1.228915 -2.498927 0.000000
41. 6 0 1.228395 1.410874 0.000000
42. 6 0 1.228395 -1.410874 0.000000
43. 6 0 2.469846 0.734484 0.000000
44. 6 0 2.469846 -0.734484 0.000000
45. 1 0 1.228913 2.498927 0.000000
46. 1 0 1.228913 -2.498927 0.000000
47. 6 0 3.687415 1.410020 0.000000
48. 6 0 3.687415 -1.410020 0.000000
49. 6 0 4.934077 0.731907 0.000000
50. 6 0 4.934077 -0.731907 0.000000
51. 1 0 3.688398 2.498088 0.000000
52. 1 0 3.688398 -2.498088 0.000000
53. 6 0 6.150318 1.409102 0.000000
54. 6 0 6.150318 -1.409102 0.000000
55. 6 0 7.392453 0.729810 0.000000
56. 6 0 7.392453 -0.729810 0.000000
57. 1 0 6.151145 2.497175 0.000000
58. 1 0 6.151145 -2.497175 0.000000
59. 6 0 8.615913 1.408277 0.000000
60. 6 0 8.615913 -1.408277 0.000000
61. 6 0 9.846932 0.728015 0.000000
62. 6 0 9.846932 -0.728015 0.000000
63. 1 0 8.616550 2.496357 0.000000
64. 1 0 8.616550 -2.496357 0.000000
65. 6 0 11.084096 1.407092 0.000000
66. 6 0 11.084096 -1.407092 0.000000
67. 6 0 12.298662 0.726478 0.000000
68. 6 0 12.298662 -0.726478 0.000000
69. 1 0 11.084300 2.495282 0.000000
70. 1 0 11.084300 -2.495282 0.000000
71. 6 0 13.559284 1.409579 0.000000
72. 6 0 13.559284 -1.409579 0.000000
73. 6 0 14.737070 0.715486 0.000000
74. 6 0 14.737070 -0.715486 0.000000
75. 1 0 13.557109 2.497072 0.000000
76. 1 0 13.557109 -2.497072 0.000000
77. 1 0 15.684604 1.247349 0.000000
78. 1 0 15.684604 -1.247349 0.000000

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