# Aromaticity in $P_8$ Allotropes and $(CH)_8$ Analogues: Significance of their 40 Valence Electrons?

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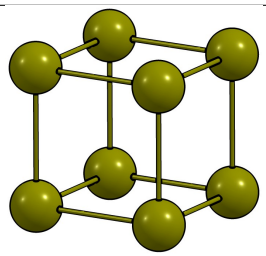
## Supporting Information

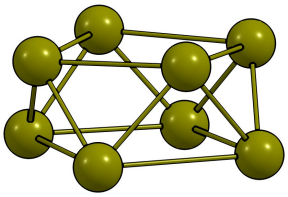
Complete Gaussian09 Reference.

Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

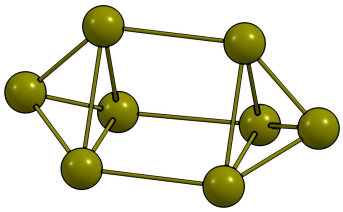
Table S1: Initial 8-vertex polyhedra upon which the starting structures are based.



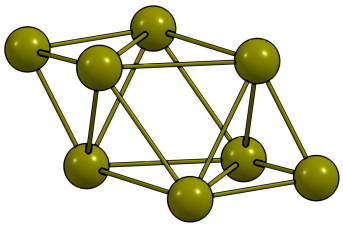
1. Cube



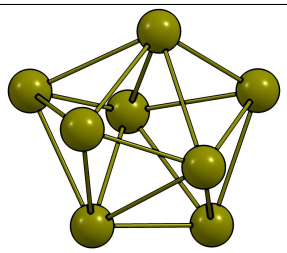
2. Antiprism



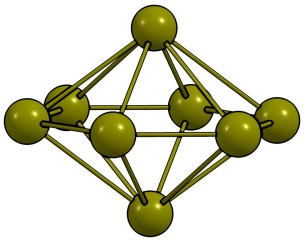
3. Trigonal Prism



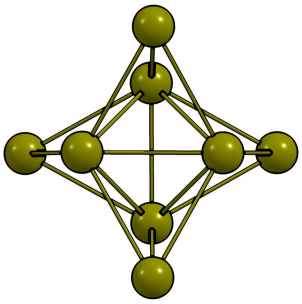
4. Trigonal Antiprism



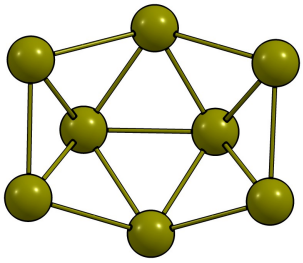
5. Bisdisphenoid



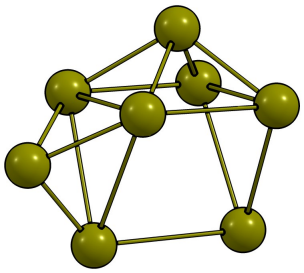
6. Hexagonal bipyramid



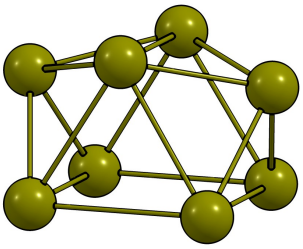
7. All-capped tetrahedron



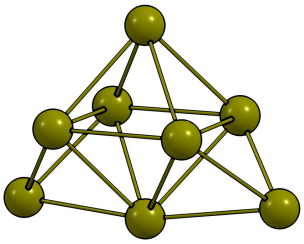
8. Nido structure



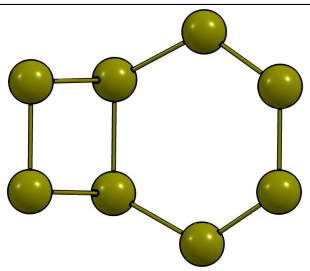
9. Dicapped trigonal prism ($C_s$)



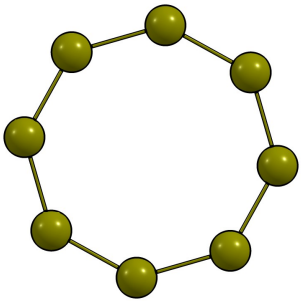
10. Dicapped trigonal prism ($C_{2v}$)



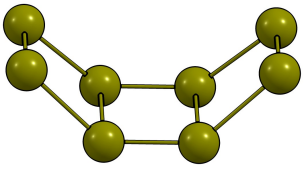
11. Dicapped octahedron



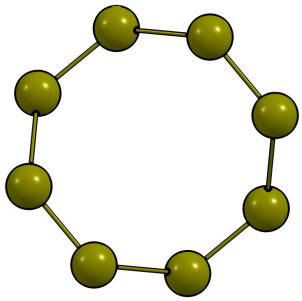
12. Bicyclooctatriene



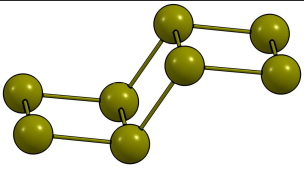
13. Cyclooctatetraene (planar)



14. *cis*-Tricyclooctadiene

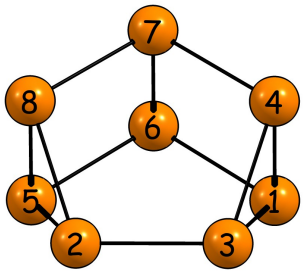


15. Cyclooctatetraene (non-planar)



16. *trans*-Tricyclooctadiene

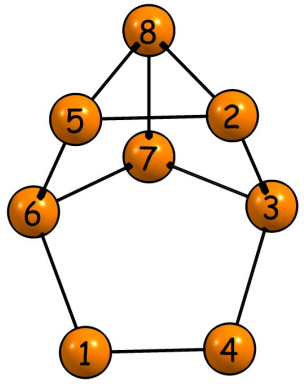
Table S2: Distance table for the lowest-lying $P_8$ optimized structures obtained at the M11/def2-TZVP level of theory. Included are the zero-point corrected absolute energy in (a.u.) at the DLPNO-CCSD(T)/def2-QZVP level of theory with zero-point energy obtained from the M11/def2-TZVP computations, relative energy in (kcal/mol) and symmetry.




1. -2727.491545 0.0 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 3.548864 | 0.000000 | | | |
| 3 | P | 2.180490 | 2.210211 | 0.000000 | | |
| 4 | P | 2.280445 | 3.548872 | 2.180495 | 0.000000 | |
| 5 | P | 3.547119 | 2.180494 | 3.548862 | 4.216929 | 0.000000 |
| 6 | P | 2.236614 | 3.466450 | 3.466445 | 3.164638 | 2.236612 |
| 7 | P | 3.164660 | 3.466451 | 3.466447 | 2.236611 | 3.164649 |
| 8 | P | 4.216933 | 2.180497 | 3.548865 | 3.547129 | 2.280440 |

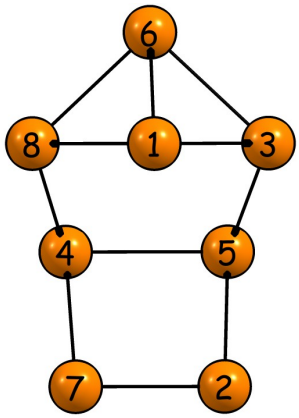
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 2.198067 | 0.000000 | |
| 8 | P | 3.164643 | 2.236608 | 0.000000 |




2. -2727.476942 +9.2 $C_s$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 4.005192 | 0.000000 | | | |
| 3 | P | 3.404191 | 2.241488 | 0.000000 | | |
| 4 | P | 2.015391 | 3.410715 | 2.206398 | 0.000000 | |
| 5 | P | 3.410707 | 2.187033 | 3.509487 | 4.004971 | 0.000000 |
| 6 | P | 2.206376 | 3.509589 | 3.334449 | 3.404146 | 2.241505 |
| 7 | P | 3.486326 | 3.218339 | 2.194622 | 3.486344 | 3.218334 |
| 8 | P | 4.607047 | 2.224056 | 3.009563 | 4.607019 | 2.224064 |

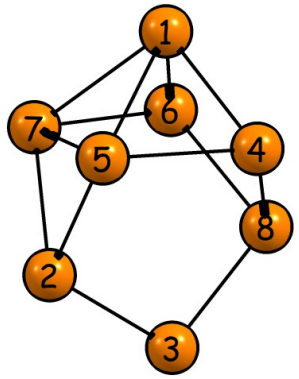
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 2.194625 | 0.000000 | |
| 8 | P | 3.009536 | 2.296244 | 0.000000 |




3. -2727.473942 +11.0 $C_s$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 3.879415 | 0.000000 | | | |
| 3 | P | 2.198256 | 3.361203 | 0.000000 | | |
| 4 | P | 3.556607 | 3.065659 | 3.446342 | 0.000000 | |
| 5 | P | 3.556607 | 2.220461 | 2.190181 | 2.207016 | 0.000000 |
| 6 | P | 2.209599 | 4.911601 | 2.203242 | 3.484419 | 3.484419 |
| 7 | P | 3.879415 | 2.024370 | 4.218070 | 2.220461 | 3.065659 |
| 8 | P | 2.198256 | 4.218070 | 3.208124 | 2.190181 | 3.446342 |

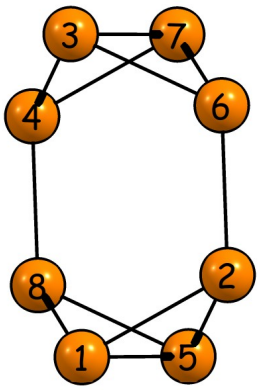
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 4.911601 | 0.000000 | |
| 8 | P | 2.203242 | 3.361203 | 0.000000 |




4. -2727.473615 +11.3 $C_s$

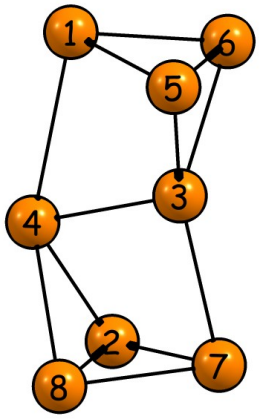
| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 3.682724 | 0.000000 | | | |
| 3 | P | 4.397099 | 2.128154 | 0.000000 | | |
| 4 | P | 2.225681 | 3.428232 | 3.434931 | 0.000000 | |
| 5 | P | 2.391854 | 2.225643 | 3.550229 | 2.160775 | 0.000000 |
| 6 | P | 2.225681 | 3.428232 | 3.434931 | 3.150228 | 3.547572 |
| 7 | P | 2.391854 | 2.225643 | 3.550229 | 3.547572 | 2.512934 |
| 8 | P | 3.176388 | 3.216579 | 2.103177 | 2.248391 | 3.450144 |

| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 2.160775 | 0.000000 | |
| 8 | P | 2.248391 | 3.450144 | 0.000000 |



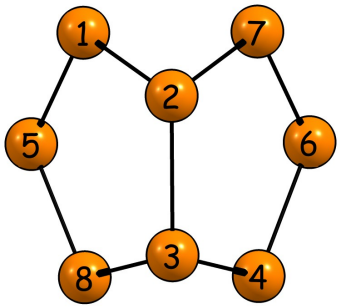

5. -2727.465219 +16.5 $D_{2h}$

| | | 1 | 2 | 3 | 4 | 5 | |
|---|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | | |
| 2 | P | 2.200516 | 0.000000 | | | | |
| 3 | P | 4.251534 | 3.785499 | 0.000000 | | | |
| 4 | P | 3.785499 | 3.928879 | 2.200516 | 0.000000 | | |
| 5 | P | 2.198896 | 2.200489 | 4.786511 | 3.785809 | 0.000000 | |
| 6 | P | 3.785809 | 2.231892 | 2.200489 | 3.233380 | 3.785499 | |
| 7 | P | 4.786511 | 3.785809 | 2.198896 | 2.200489 | 4.251534 | |
| 8 | P | 2.200489 | 3.233380 | 3.785809 | 2.231892 | 2.200516 | |
| | | 6 | 7 | 8 | | | |
| 6 | P | 0.000000 | | | | | |
| 7 | P | 2.200516 | 0.000000 | | | | |
| 8 | P | 3.928879 | 3.785499 | 0.000000 | | | |




6. -2727.458943 +20.5 $C_s$

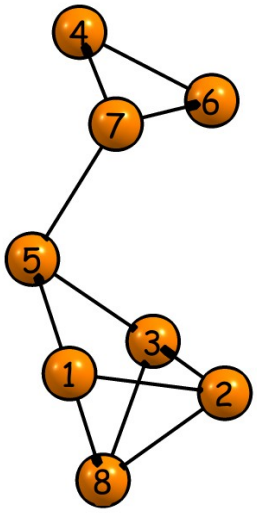
| | | 1 | 2 | 3 | 4 | 5 | |
|---|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | | |
| 2 | P | 4.758016 | 0.000000 | | | | |
| 3 | P | 2.634593 | 3.023641 | 0.000000 | | | |
| 4 | P | 2.769935 | 2.319466 | 2.165268 | 0.000000 | | |
| 5 | P | 2.159759 | 5.140850 | 2.192604 | 3.590039 | 0.000000 | |
| 6 | P | 2.159531 | 4.659117 | 2.192926 | 3.590381 | 2.213040 | |
| 7 | P | 4.923707 | 2.177781 | 2.383899 | 3.162833 | 4.338925 | |
| 8 | P | 4.755253 | 2.142426 | 3.022724 | 2.318868 | 4.654496 | |
| | | 6 | 7 | 8 | | | |
| 6 | P | 0.000000 | | | | | |
| 7 | P | 4.341093 | 0.000000 | | | | |
| 8 | P | 5.140612 | 2.178133 | 0.000000 | | | |




7. -2727.456872 +21.8 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 2.205481 | 0.000000 | | | |
| 3 | P | 3.528392 | 2.220962 | 0.000000 | | |
| 4 | P | 4.175671 | 3.528392 | 2.205481 | 0.000000 | |
| 5 | P | 2.082082 | 3.494396 | 3.494396 | 3.685401 | 0.000000 |
| 6 | P | 3.685401 | 3.494396 | 3.494396 | 2.082082 | 3.849128 |
| 7 | P | 2.402392 | 2.205481 | 3.528392 | 3.415368 | 3.685401 |
| 8 | P | 3.415368 | 3.528392 | 2.205481 | 2.402392 | 2.082082 |

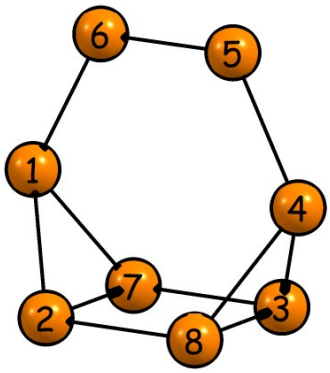
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 2.082082 | 0.000000 | |
| 8 | P | 3.685401 | 4.175671 | 0.000000 |




8. -2727.455876 +22.4 $C_1$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 2.220596 | 0.000000 | | | |
| 3 | P | 2.889997 | 2.216223 | 0.000000 | | |
| 4 | P | 5.271178 | 5.537284 | 4.267233 | 0.000000 | |
| 5 | P | 2.239687 | 3.235827 | 2.230152 | 3.286289 | 0.000000 |
| 6 | P | 4.889992 | 4.352020 | 3.327592 | 1.994409 | 3.382974 |
| 7 | P | 3.498908 | 3.884167 | 3.444955 | 2.204164 | 2.238566 |
| 8 | P | 2.211492 | 2.181740 | 2.221770 | 6.102996 | 3.112503 |

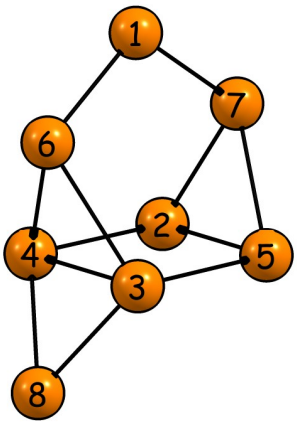
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 2.211167 | 0.000000 | |
| 8 | P | 5.393998 | 4.836024 | 0.000000 |




9. -2727.447434 +27.7 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 2.185881 | 0.000000 | | | |
| 3 | P | 3.724360 | 3.164984 | 0.000000 | | |
| 4 | P | 4.026170 | 3.724365 | 2.185877 | 0.000000 | |
| 5 | P | 3.588163 | 4.334971 | 3.776765 | 2.191425 | 0.000000 |
| 6 | P | 2.191425 | 3.776735 | 4.334995 | 3.588163 | 2.005025 |
| 7 | P | 2.185864 | 2.217269 | 2.258422 | 3.724350 | 4.334998 |
| 8 | P | 3.724352 | 2.258424 | 2.217268 | 2.185868 | 3.776749 |

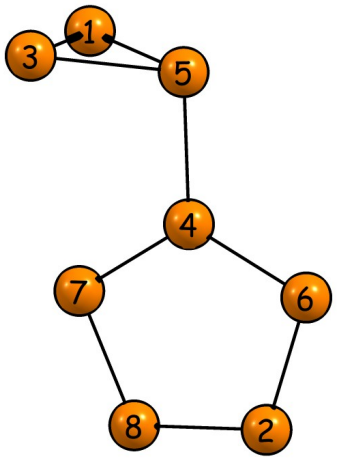
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 3.776778 | 0.000000 | |
| 8 | P | 4.334972 | 3.164867 | 0.000000 |




10. -2727.447249 +27.8 $C_s$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 3.619078 | 0.000000 | | | |
| 3 | P | 3.496746 | 3.213452 | 0.000000 | | |
| 4 | P | 3.496160 | 2.326141 | 2.250506 | 0.000000 | |
| 5 | P | 3.619002 | 2.181869 | 2.326554 | 3.212185 | 0.000000 |
| 6 | P | 2.022842 | 3.681649 | 2.304631 | 2.304026 | 3.681602 |
| 7 | P | 2.229378 | 2.184356 | 3.499077 | 3.498322 | 2.184247 |
| 8 | P | 5.080452 | 3.703070 | 2.115798 | 2.115637 | 3.702871 |

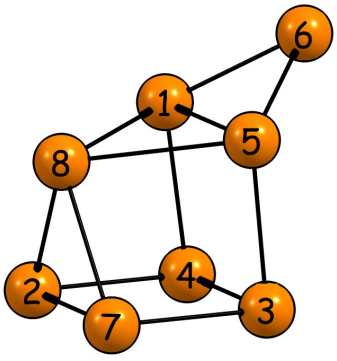
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 3.378472 | 0.000000 | |
| 8 | P | 3.500971 | 4.963782 | 0.000000 |




11. -2727.446015 +28.6 $C_s$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 6.348964 | 0.000000 | | | |
| 3 | P | 1.995078 | 6.348964 | 0.000000 | | |
| 4 | P | 3.345527 | 3.142409 | 3.345527 | 0.000000 | |
| 5 | P | 2.201620 | 5.269405 | 2.201620 | 2.212183 | 0.000000 |
| 6 | P | 5.236080 | 2.081585 | 5.236080 | 2.059808 | 3.668588 |
| 7 | P | 3.738711 | 3.447444 | 3.738711 | 2.067478 | 3.722253 |
| 8 | P | 5.692078 | 2.094317 | 5.692078 | 3.137982 | 5.285058 |

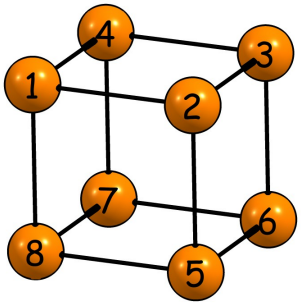
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 3.589843 | 0.000000 | |
| 8 | P | 3.437172 | 2.080749 | 0.000000 |




12. -2727.436978 +34.2 $C_s$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 2.983291 | 0.000000 | | | |
| 3 | P | 3.259089 | 3.144040 | 0.000000 | | |
| 4 | P | 2.294025 | 2.233655 | 2.217858 | 0.000000 | |
| 5 | P | 2.416815 | 3.773639 | 2.294276 | 3.259585 | 0.000000 |
| 6 | P | 2.095654 | 4.795097 | 3.638465 | 3.638371 | 2.095476 |
| 7 | P | 3.772507 | 2.207651 | 2.233539 | 3.144112 | 2.983483 |
| 8 | P | 2.456330 | 2.230730 | 3.284219 | 3.283900 | 2.457682 |

| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 4.794730 | 0.000000 | |
| 8 | P | 3.741928 | 2.230800 | 0.000000 |

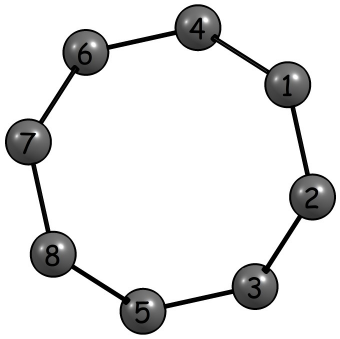



13. -2727.432774 +36.9
$T_{\mathrm{d}}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | P | 0.000000 | | | | |
| 2 | P | 2.264933 | 0.000000 | | | |
| 3 | P | 3.202774 | 2.264723 | 0.000000 | | |
| 4 | P | 2.264723 | 3.203127 | 2.264933 | 0.000000 | |
| 5 | P | 3.203536 | 2.264933 | 3.202774 | 3.922858 | 0.000000 |
| 6 | P | 3.922858 | 3.203127 | 2.264933 | 3.202662 | 2.264723 |
| 7 | P | 3.202774 | 3.922858 | 3.203536 | 2.264933 | 3.202774 |
| 8 | P | 2.264933 | 3.202662 | 3.922858 | 3.203127 | 2.264933 |

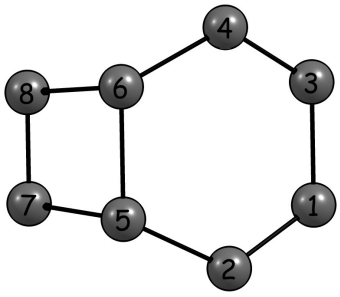
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | P | 0.000000 | | |
| 7 | P | 2.264933 | 0.000000 | |
| 8 | P | 3.203127 | 2.264723 | 0.000000 |

Table S3: Distance table for the lowest-lying $C_8H_8$ optimized structures obtained at the M11/def2-TZVP level of theory. Included are the zero-point corrected absolute energy in (a.u.) at the DLPNO-CCSD(T)/def2-QZVP level of theory with zero-point energy obtained from the M11/def2-TZVP computations, relative energy in (kcal/mol) and symmetry. H atoms are omitted for clarity



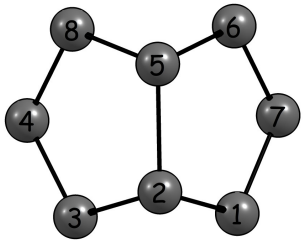

1. -308.955098 0.0 $D_{2d}$

| | | 1 | 2 | 3 | 4 | 5 | |
|---|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | | |
| 2 | C | 1.328183 | 0.000000 | | | | |
| 3 | C | 2.499143 | 1.473756 | 0.000000 | | | |
| 4 | C | 1.473756 | 2.499144 | 3.067169 | 0.000000 | | |
| 5 | C | 3.212394 | 2.499144 | 1.328182 | 3.342393 | 0.000000 | |
| 6 | C | 2.499143 | 3.212395 | 3.342393 | 1.328183 | 3.067168 | |
| 7 | C | 3.067169 | 3.342394 | 3.212394 | 2.499144 | 2.499143 | |
| 8 | C | 3.342393 | 3.067169 | 2.499143 | 3.212395 | 1.473756 | |
| | | 6 | 7 | 8 | | | |
| 6 | C | 0.000000 | | | | | |
| 7 | C | 1.473756 | 0.000000 | | | | |
| 8 | C | 2.499143 | 1.328182 | 0.000000 | | | |




2. -308.942539 +7.9 $C_s$

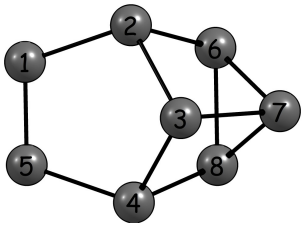
| | | 1 | 2 | 3 | 4 | 5 | |
|---|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | | |
| 2 | C | 1.329682 | 0.000000 | | | | |
| 3 | C | 1.467354 | 2.446565 | 0.000000 | | | |
| 4 | C | 2.446565 | 2.874307 | 1.329682 | 0.000000 | | |
| 5 | C | 2.479400 | 1.499065 | 2.908740 | 2.603584 | 0.000000 | |
| 6 | C | 2.908739 | 2.603584 | 2.479400 | 1.499065 | 1.576538 | |
| 7 | C | 3.386879 | 2.541760 | 3.663375 | 3.206093 | 1.520105 | |
| 8 | C | 3.663374 | 3.206093 | 3.386880 | 2.541761 | 2.098840 | |
| | | 6 | 7 | 8 | | | |
| 6 | C | 0.000000 | | | | | |
| 7 | C | 2.098841 | 0.000000 | | | | |
| 8 | C | 1.520105 | 1.328488 | 0.000000 | | | |




3. -308.939379 +9.9 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.497471 | 0.000000 | | | |
| 3 | C | 1.962270 | 1.497471 | 0.000000 | | |
| 4 | C | 2.810098 | 2.372350 | 1.384864 | 0.000000 | |
| 5 | C | 2.400566 | 1.547510 | 2.400566 | 2.372350 | 0.000000 |
| 6 | C | 2.274814 | 2.400566 | 3.004211 | 2.810098 | 1.497471 |
| 7 | C | 1.384864 | 2.372350 | 2.810098 | 3.046880 | 2.372350 |
| 8 | C | 3.004211 | 2.400566 | 2.274814 | 1.384864 | 1.497471 |

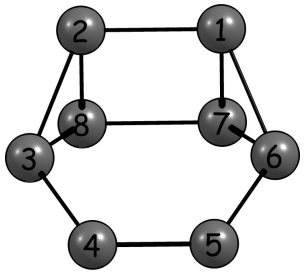
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.384864 | 0.000000 | |
| 8 | C | 1.962270 | 2.810098 | 0.000000 |




4. -308.908832 +29.0 $C_{s}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.505392 | 0.000000 | | | |
| 3 | C | 2.436422 | 1.555300 | 0.000000 | | |
| 4 | C | 2.305716 | 2.289696 | 1.555193 | 0.000000 | |
| 5 | C | 1.332107 | 2.305678 | 2.436310 | 1.505335 | 0.000000 |
| 6 | C | 2.559397 | 1.557199 | 2.090785 | 2.428799 | 2.927734 |
| 7 | C | 3.368174 | 2.224821 | 1.562722 | 2.224702 | 3.368079 |
| 8 | C | 2.927826 | 2.429045 | 2.090700 | 1.556826 | 2.559189 |

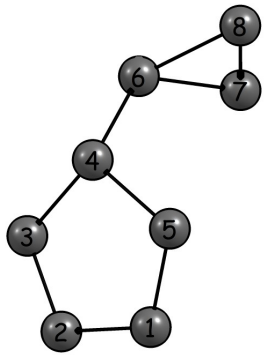
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.498437 | 0.000000 | |
| 8 | C | 1.517832 | 1.498531 | 0.000000 |




5. -308.905486 +31.1 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.535468 | 0.000000 | | | |
| 3 | C | 2.536605 | 1.521566 | 0.000000 | | |
| 4 | C | 2.971996 | 2.606321 | 1.466701 | 0.000000 | |
| 5 | C | 2.606975 | 2.972363 | 2.390485 | 1.328090 | 0.000000 |
| 6 | C | 1.522113 | 2.537034 | 2.682868 | 2.390482 | 1.466776 |
| 7 | C | 1.500599 | 2.147165 | 2.536846 | 2.972450 | 2.606712 |
| 8 | C | 2.147207 | 1.501231 | 1.521781 | 2.606590 | 2.971915 |

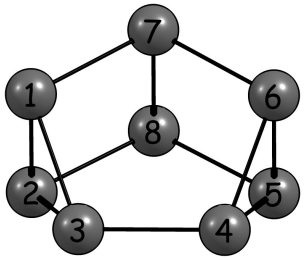
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.521905 | 0.000000 | |
| 8 | C | 2.536796 | 1.535467 | 0.000000 |




6. -308.898515 +35.5 $C_1$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.471868 | 0.000000 | | | |
| 3 | C | 2.286903 | 1.336482 | 0.000000 | | |
| 4 | C | 2.323720 | 2.327516 | 1.506661 | 0.000000 | |
| 5 | C | 1.336735 | 2.290224 | 2.344654 | 1.502090 | 0.000000 |
| 6 | C | 3.497870 | 3.483221 | 2.531959 | 1.531529 | 2.564065 |
| 7 | C | 3.826503 | 4.040168 | 3.450436 | 2.645334 | 3.034575 |
| 8 | C | 4.197218 | 4.600118 | 3.885357 | 2.657322 | 3.072970 |

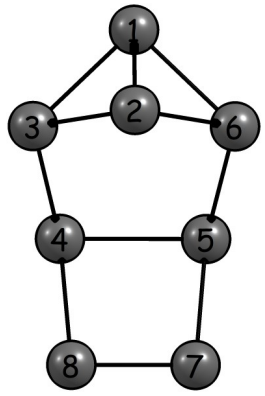
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.496470 | 0.000000 | |
| 8 | C | 1.497297 | 1.286624 | 0.000000 |




7. -308.898190 +35.7 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.515622 | 0.000000 | | | |
| 3 | C | 1.505088 | 1.505002 | 0.000000 | | |
| 4 | C | 2.471608 | 2.471326 | 1.521581 | 0.000000 | |
| 5 | C | 2.945996 | 2.526047 | 2.471761 | 1.504944 | 0.000000 |
| 6 | C | 2.526416 | 2.945913 | 2.471765 | 1.504954 | 1.515418 |
| 7 | C | 1.544660 | 2.180132 | 2.355688 | 2.355485 | 2.180048 |
| 8 | C | 2.180071 | 1.544384 | 2.355601 | 2.355379 | 1.544558 |

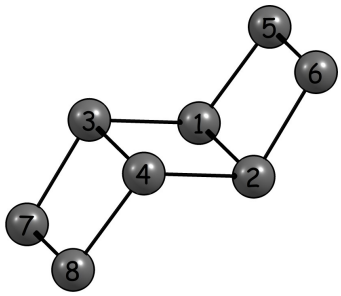
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.544698 | 0.000000 | |
| 8 | C | 2.180159 | 1.561930 | 0.000000 |




8. -308.895159 +37.6 $C_{\mathrm{s}}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.463958 | 0.000000 | | | |
| 3 | C | 1.505862 | 1.497951 | 0.000000 | | |
| 4 | C | 2.484965 | 2.477728 | 1.524467 | 0.000000 | |
| 5 | C | 2.484965 | 2.477728 | 2.388709 | 1.564816 | 0.000000 |
| 6 | C | 1.505862 | 1.497951 | 2.161232 | 2.388709 | 1.524467 |
| 7 | C | 3.661046 | 3.068842 | 3.107237 | 2.095286 | 1.520302 |
| 8 | C | 3.661046 | 3.068842 | 2.604546 | 1.520302 | 2.095286 |

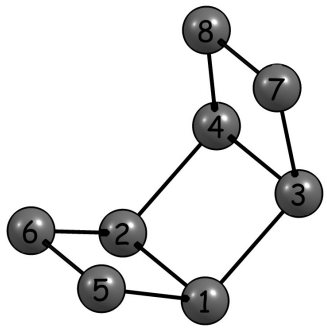
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 2.604546 | 0.000000 | |
| 8 | C | 3.107237 | 1.328530 | 0.000000 |




9. -308.888275 +41.9 $C_{2\mathrm{h}}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.571827 | 0.000000 | | | |
| 3 | C | 1.555475 | 2.211366 | 0.000000 | | |
| 4 | C | 2.211366 | 1.555475 | 1.571827 | 0.000000 | |
| 5 | C | 1.510588 | 2.091031 | 2.554884 | 2.935638 | 0.000000 |
| 6 | C | 2.091032 | 1.510588 | 2.935639 | 2.554885 | 1.330004 |
| 7 | C | 2.554886 | 2.935639 | 1.510589 | 2.091032 | 3.891099 |
| 8 | C | 2.935639 | 2.554885 | 2.091031 | 1.510588 | 4.112123 |

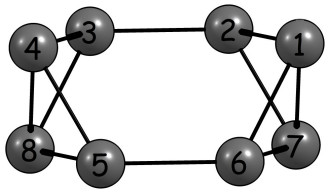
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 4.112124 | 0.000000 | |
| 8 | C | 3.891099 | 1.330004 | 0.000000 |




10. -308.878301 +48.2 $C_{2v}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.557021 | 0.000000 | | | |
| 3 | C | 1.582895 | 2.220331 | 0.000000 | | |
| 4 | C | 2.220332 | 1.582895 | 1.557021 | 0.000000 | |
| 5 | C | 1.507677 | 2.085317 | 2.637758 | 3.005531 | 0.000000 |
| 6 | C | 2.085317 | 1.507678 | 3.005532 | 2.637757 | 1.332966 |
| 7 | C | 2.637757 | 3.005531 | 1.507677 | 2.085317 | 2.959560 |
| 8 | C | 3.005532 | 2.637758 | 2.085317 | 1.507677 | 3.245889 |

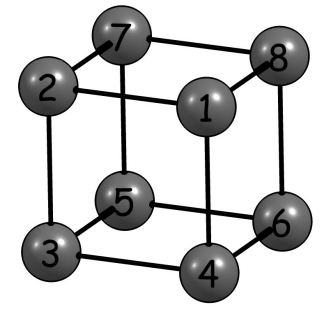
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 3.245888 | 0.000000 | |
| 8 | C | 2.959560 | 1.332966 | 0.000000 |




11. -308.865822 +56.0 $D_{2h}$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.498415 | 0.000000 | | | |
| 3 | C | 2.587619 | 1.524080 | 0.000000 | | |
| 4 | C | 2.920028 | 2.587419 | 1.498182 | 0.000000 | |
| 5 | C | 2.587419 | 2.682411 | 2.207376 | 1.498415 | 0.000000 |
| 6 | C | 1.498182 | 2.207376 | 2.682411 | 2.587619 | 1.524080 |
| 7 | C | 1.469154 | 1.498182 | 2.587419 | 3.268788 | 2.587619 |
| 8 | C | 3.268788 | 2.587619 | 1.498415 | 1.469154 | 1.498182 |

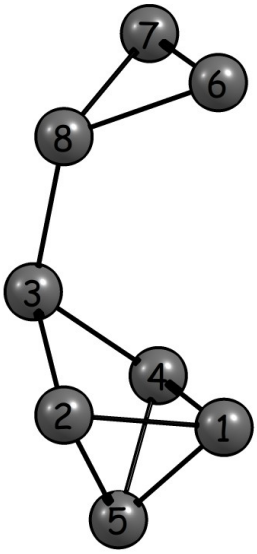
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.498415 | 0.000000 | |
| 8 | C | 2.587419 | 2.920028 | 0.000000 |




12. -308.837027 +74.1 $T_d$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.562403 | 0.000000 | | | |
| 3 | C | 2.209450 | 1.562229 | 0.000000 | | |
| 4 | C | 1.562229 | 2.209446 | 1.562403 | 0.000000 | |
| 5 | C | 2.705960 | 2.209328 | 1.562229 | 2.209446 | 0.000000 |
| 6 | C | 2.209322 | 2.705960 | 2.209450 | 1.562229 | 1.562403 |
| 7 | C | 2.209450 | 1.562229 | 2.209322 | 2.705960 | 1.562229 |
| 8 | C | 1.562229 | 2.209446 | 2.705960 | 2.209328 | 2.209446 |

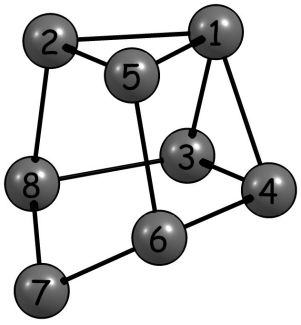
| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 2.209450 | 0.000000 | |
| 8 | C | 1.562229 | 1.562403 | 0.000000 |




13. -308.803246 +95.3 $C_1$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.515549 | 0.000000 | | | |
| 3 | C | 2.225978 | 1.542419 | 0.000000 | | |
| 4 | C | 1.514684 | 1.940045 | 1.537978 | 0.000000 | |
| 5 | C | 1.443656 | 1.510522 | 2.227461 | 1.512783 | 0.000000 |
| 6 | C | 3.153517 | 3.375878 | 2.620689 | 3.022761 | 4.151640 |
| 7 | C | 3.817459 | 3.860117 | 2.629118 | 3.146001 | 4.479172 |
| 8 | C | 3.039370 | 2.611378 | 1.510608 | 2.604613 | 3.572877 |

| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.286072 | 0.000000 | |
| 8 | C | 1.500823 | 1.501961 | 0.000000 |




14. -308.773692 +113.8 $C_s$

| | | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 1 | C | 0.000000 | | | | |
| 2 | C | 1.613817 | 0.000000 | | | |
| 3 | C | 1.613817 | 2.130296 | 0.000000 | | |
| 4 | C | 1.614446 | 2.560414 | 1.420878 | 0.000000 | |
| 5 | C | 1.614446 | 1.420878 | 2.560414 | 2.129668 | 0.000000 |
| 6 | C | 2.377787 | 2.387293 | 2.387293 | 1.595754 | 1.595754 |
| 7 | C | 3.045744 | 2.427714 | 2.427714 | 2.427560 | 2.427560 |
| 8 | C | 2.376915 | 1.595985 | 1.595985 | 2.387116 | 2.387116 |

| | | 6 | 7 | 8 |
|---|---|---|---|---|
| 6 | C | 0.000000 | | |
| 7 | C | 1.455867 | 0.000000 | |
| 8 | C | 2.218309 | 1.455802 | 0.000000 |

Table S4: HOMO-LUMO gaps for the lowest-lying structures at the M11/def2-TZVP level of theory.

| Structure | HOMO (a.u.) | LUMO (a.u.) | H/L gap (a.u.) | H/L gap (eV) |
|---|---|---|---|---|
| C8H8-1 | -0.315898 | 0.030773 | 0.346671 | 9.43 |
| C8H8-2 | -0.309530 | 0.044760 | 0.354290 | 9.64 |
| C8H8-3 | -0.293892 | 0.079567 | 0.373459 | 10.16 |
| C8H8-4 | -0.338868 | 0.081737 | 0.420605 | 11.45 |
| C8H8-5 | -0.315435 | 0.093390 | 0.408825 | 11.12 |
| C8H8-6 | -0.316555 | 0.056530 | 0.373085 | 10.15 |
| C8H8-7 | -0.344320 | 0.110697 | 0.455017 | 12.38 |
| C8H8-8 | -0.333994 | 0.090825 | 0.424819 | 11.56 |
| C8H8-9 | -0.335069 | 0.077562 | 0.412631 | 11.23 |
| C8H8-10 | -0.341370 | 0.075014 | 0.416384 | 11.33 |
| C8H8-11 | -0.319572 | 0.110094 | 0.429666 | 11.69 |
| C8H8-12 | -0.354960 | 0.116205 | 0.471165 | 12.82 |
| C8H8-13 | -0.329993 | 0.084032 | 0.414025 | 11.27 |
| C8H8-14 | -0.201368 | 0.082285 | 0.283653 | 7.72 |
| P8-1 | -0.307112 | -0.034318 | 0.272794 | 7.42 |
| P8-2 | -0.329071 | -0.070062 | 0.259009 | 7.05 |
| P8-3 | -0.325684 | -0.058883 | 0.266801 | 7.26 |
| P8-4 | -0.298353 | -0.033674 | 0.264679 | 7.20 |
| P8-5 | -0.311281 | -0.028855 | 0.282426 | 7.69 |
| P8-6 | -0.290550 | -0.004223 | 0.286327 | 7.79 |
| P8-7 | -0.317724 | -0.091970 | 0.225754 | 6.14 |
| P8-8 | -0.307449 | -0.054637 | 0.252812 | 6.88 |
| P8-9 | -0.325472 | -0.067391 | 0.258081 | 7.02 |
| P8-10 | -0.306154 | -0.064388 | 0.241766 | 6.58 |
| P8-11 | -0.324445 | -0.071090 | 0.253355 | 6.89 |
| P8-12 | -0.301829 | -0.052821 | 0.249008 | 6.78 |
| P8-13 | -0.297076 | -0.052037 | 0.245039 | 6.67 |

Table S5: QTAIM analysis for the lowest-lying $P_8$ structures.

| Structure | N° P-Atom | N° P'-Atom | Distance (Å) | Nalewajski-Mrozek BO | BCP Rho | BCP-Laplacian |
|---|---|---|---|---|---|---|
| P–P ($P_2H_4$) | 1 | 2 | 2.264 | 1.05 | 0.1037 | -0.1119 |
| P=P ($P_2H_2$) | 1 | 2 | 2.046 | 2.05 | 0.1427 | -0.2041 |
| P8-1 | 1 | 3 | 2.180 | 0.99 | 0.1107 | -0.0923 |
| | 1 | 4 | 2.280 | 0.96 | 0.0956 | -0.0517 |
| | 1 | 6 | 2.237 | 0.97 | 0.1071 | -0.1061 |
| | 2 | 3 | 2.210 | 0.99 | 0.1082 | -0.1081 |
| | 2 | 5 | 2.180 | 0.99 | 0.1107 | -0.0923 |
| | 2 | 8 | 2.180 | 0.99 | 0.1107 | -0.0923 |
| | 3 | 4 | 2.180 | 0.99 | 0.1107 | -0.0923 |
| | 4 | 7 | 2.237 | 0.97 | 0.1071 | -0.1061 |
| | 5 | 6 | 2.237 | 0.97 | 0.1071 | -0.1061 |
| | 5 | 8 | 2.280 | 0.96 | 0.0956 | -0.0517 |
| | 6 | 7 | 2.198 | 1.02 | 0.1162 | -0.1364 |
| | 7 | 8 | 2.237 | 0.97 | 0.1071 | -0.1061 |
| P8-2 | 1 | 4 | 2.015 | 1.84 | 0.1470 | -0.2107 |
| | 1 | 6 | 2.206 | 1.02 | 0.1114 | -0.1152 |
| | 2 | 3 | 2.241 | 0.92 | 0.1028 | -0.0893 |
| | 2 | 5 | 2.187 | 1.00 | 0.1103 | -0.0868 |
| | 2 | 8 | 2.224 | 0.98 | 0.1052 | -0.0784 |
| | 3 | 4 | 2.206 | 1.02 | 0.1114 | -0.1152 |
| | 3 | 7 | 2.195 | 0.99 | 0.1145 | -0.1248 |
| | 5 | 6 | 2.242 | 0.92 | 0.1028 | -0.0893 |
| | 5 | 8 | 2.224 | 0.98 | 0.1052 | -0.0783 |
| | 6 | 7 | 2.195 | 0.99 | 0.1145 | -0.1248 |
| | 7 | 8 | 2.296 | 0.92 | 0.0979 | -0.0828 |
| P8-3 | 1 | 3 | 2.198 | 0.96 | 0.1084 | -0.0833 |
| | 1 | 6 | 2.210 | 0.95 | 0.1030 | -0.0461 |
| | 1 | 8 | 2.198 | 0.96 | 0.1084 | -0.0833 |
| | 2 | 5 | 2.220 | 1.01 | 0.1100 | -0.1149 |
| | 2 | 7 | 2.024 | 1.82 | 0.1477 | -0.2162 |
| | 3 | 5 | 2.190 | 1.00 | 0.1129 | -0.1184 |
| | 3 | 6 | 2.203 | 0.98 | 0.1078 | -0.0837 |
| | 4 | 5 | 2.207 | 0.96 | 0.1120 | -0.1222 |
| | 4 | 7 | 2.220 | 1.01 | 0.1100 | -0.1149 |
| | 4 | 8 | 2.190 | 1.00 | 0.1129 | -0.1184 |
| | 6 | 8 | 2.203 | 0.98 | 0.1078 | -0.0837 |
| P8-4 | 1 | 4 | 2.226 | 0.90 | 0.1046 | -0.0770 |
| | 1 | 5 | 2.392 | 0.53 | 0.0760 | 0.0220 |
| | 1 | 6 | 2.226 | 0.90 | 0.1046 | -0.0770 |
| | 1 | 7 | 2.392 | 0.53 | 0.0760 | 0.0220 |
| | 2 | 3 | 2.128 | 1.22 | 0.1221 | -0.1371 |
| | 2 | 5 | 2.226 | 0.87 | 0.1036 | -0.0781 |
| | 2 | 7 | 2.226 | 0.87 | 0.1036 | -0.0781 |
| | 3 | 8 | 2.103 | 1.24 | 0.1273 | -0.1537 |
| | 4 | 5 | 2.161 | 1.02 | 0.1154 | -0.1053 |
| | 4 | 8 | 2.248 | 0.88 | 0.1039 | -0.0935 |
| | 6 | 7 | 2.161 | 1.02 | 0.1154 | -0.1053 |
| | 6 | 8 | 2.248 | 0.88 | 0.1039 | -0.0935 |
| P8-5 | 1 | 2 | 2.201 | 0.98 | 0.1076 | -0.0807 |
| | 1 | 5 | 2.199 | 0.95 | 0.1052 | -0.0541 |
| | 1 | 8 | 2.200 | 0.98 | 0.1076 | -0.0807 |
| | 2 | 5 | 2.200 | 0.98 | 0.1076 | -0.0807 |
| | 2 | 6 | 2.232 | 0.98 | 0.1059 | -0.0977 |
| | 3 | 4 | 2.201 | 0.98 | 0.1076 | -0.0807 |
| | 3 | 6 | 2.200 | 0.98 | 0.1076 | -0.0807 |
| | 3 | 7 | 2.199 | 0.95 | 0.1052 | -0.0541 |
| | 4 | 7 | 2.200 | 0.98 | 0.1076 | -0.0807 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 4 | 8 | 2.232 | 0.98 | 0.1059 | -0.0977 |
| | 5 | 8 | 2.201 | 0.98 | 0.1076 | -0.0807 |
| | 6 | 7 | 2.201 | 0.98 | 0.1076 | -0.0807 |
| P8-6 | 1 | 4 | 2.770 | 0.34 | 0.0433 | 0.0371 |
| | 1 | 5 | 2.160 | 1.05 | 0.1130 | -0.0856 |
| | 1 | 6 | 2.160 | 1.05 | 0.1130 | -0.0857 |
| | 2 | 4 | 2.319 | 0.81 | 0.0885 | -0.0284 |
| | 2 | 7 | 2.178 | 1.04 | 0.1112 | -0.0824 |
| | 2 | 8 | 2.142 | 1.02 | 0.1153 | -0.0839 |
| | 3 | 4 | 2.165 | 0.94 | 0.1220 | -0.1515 |
| | 3 | 5 | 2.193 | 0.88 | 0.1083 | -0.0776 |
| | 3 | 6 | 2.193 | 0.88 | 0.1082 | -0.0773 |
| | 3 | 7 | 2.384 | 0.60 | 0.0821 | -0.0298 |
| | 4 | 8 | 2.319 | 0.81 | 0.0886 | -0.0287 |
| | 5 | 6 | 2.213 | 0.98 | 0.1037 | -0.0503 |
| | 7 | 8 | 2.178 | 1.04 | 0.1112 | -0.0822 |
| P8-7 | 1 | 2 | 2.205 | 0.96 | 0.1079 | -0.0931 |
| | 1 | 5 | 2.082 | 1.37 | 0.1327 | -0.1723 |
| | 1 | 7 | 2.402 | 0.61 | 0.0716 | 0.0176 |
| | 2 | 3 | 2.221 | 0.97 | 0.1078 | -0.1060 |
| | 2 | 7 | 2.205 | 0.96 | 0.1079 | -0.0931 |
| | 3 | 4 | 2.205 | 0.96 | 0.1079 | -0.0931 |
| | 3 | 8 | 2.205 | 0.96 | 0.1079 | -0.0931 |
| | 4 | 6 | 2.082 | 1.37 | 0.1327 | -0.1723 |
| | 4 | 8 | 2.402 | 0.61 | 0.0716 | 0.0176 |
| | 5 | 8 | 2.082 | 1.37 | 0.1327 | -0.1723 |
| | 6 | 7 | 2.082 | 1.37 | 0.1327 | -0.1723 |
| P8-8 | 1 | 2 | 2.221 | 0.99 | 0.1065 | -0.0825 |
| | 1 | 5 | 2.240 | 0.97 | 0.1078 | -0.1116 |
| | 1 | 8 | 2.211 | 0.99 | 0.1072 | -0.0827 |
| | 2 | 3 | 2.216 | 0.98 | 0.1079 | -0.0875 |
| | 2 | 8 | 2.182 | 1.00 | 0.1071 | -0.0598 |
| | 3 | 5 | 2.230 | 0.99 | 0.1100 | -0.1180 |
| | 3 | 8 | 2.222 | 0.95 | 0.1047 | -0.0757 |
| | 4 | 6 | 1.994 | 1.86 | 0.1491 | -0.1943 |
| | 4 | 7 | 2.204 | 1.01 | 0.1069 | -0.0695 |
| | 5 | 7 | 2.239 | 0.95 | 0.1090 | -0.1112 |
| | 6 | 7 | 2.211 | 1.01 | 0.1052 | -0.0625 |
| P8-9 | 1 | 2 | 2.186 | 0.95 | 0.1067 | -0.0730 |
| | 1 | 6 | 2.191 | 1.06 | 0.1104 | -0.1067 |
| | 1 | 7 | 2.186 | 0.95 | 0.1067 | -0.0730 |
| | 2 | 7 | 2.217 | 1.00 | 0.1073 | -0.0842 |
| | 2 | 8 | 2.258 | 0.95 | 0.1016 | -0.0867 |
| | 3 | 4 | 2.186 | 0.95 | 0.1067 | -0.0730 |
| | 3 | 7 | 2.258 | 0.95 | 0.1016 | -0.0867 |
| | 3 | 8 | 2.217 | 1.00 | 0.1073 | -0.0842 |
| | 4 | 5 | 2.191 | 1.06 | 0.1104 | -0.1067 |
| | 4 | 8 | 2.186 | 0.95 | 0.1067 | -0.0730 |
| | 5 | 6 | 2.005 | 1.78 | 0.1484 | -0.2158 |
| P8-10 | 1 | 6 | 2.023 | 1.55 | 0.1436 | -0.1971 |
| | 1 | 7 | 2.229 | 0.96 | 0.1024 | -0.0843 |
| | 2 | 4 | 2.326 | 0.74 | 0.0908 | -0.0573 |
| | 2 | 5 | 2.182 | 1.04 | 0.1119 | -0.0924 |
| | 2 | 7 | 2.184 | 1.01 | 0.1100 | -0.0844 |
| | 3 | 4 | 2.251 | 0.78 | 0.0963 | -0.0224 |
| | 3 | 5 | 2.327 | 0.74 | 0.0907 | -0.0572 |
| | 3 | 6 | 2.305 | 0.65 | 0.0887 | -0.0308 |
| | 3 | 8 | 2.116 | 1.10 | 0.1176 | -0.0874 |
| | 4 | 6 | 2.304 | 0.65 | 0.0888 | -0.0310 |
| | 4 | 8 | 2.116 | 1.10 | 0.1176 | -0.0875 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | 5 | 7 | 2.184 | 1.01 | 0.1100 | -0.0846 |
| P8-11 | 1 | 3 | 1.995 | 1.86 | 0.1492 | -0.1936 |
| | 1 | 5 | 2.202 | 1.01 | 0.1072 | -0.0671 |
| | 2 | 6 | 2.082 | 1.43 | 0.1319 | -0.1674 |
| | 2 | 8 | 2.094 | 1.42 | 0.1295 | -0.1605 |
| | 3 | 5 | 2.202 | 1.01 | 0.1072 | -0.0671 |
| | 4 | 5 | 2.212 | 0.92 | 0.1105 | -0.1159 |
| | 4 | 6 | 2.060 | 1.30 | 0.1343 | -0.1765 |
| | 4 | 7 | 2.067 | 1.25 | 0.1323 | -0.1691 |
| | 7 | 8 | 2.081 | 1.43 | 0.1318 | -0.1666 |
| P8-12 | 1 | 4 | 2.294 | 0.80 | 0.0976 | -0.0749 |
| | 1 | 6 | 2.096 | 1.18 | 0.1249 | -0.1220 |
| | 1 | 8 | 2.456 | 0.51 | 0.0706 | -0.0025 |
| | 2 | 4 | 2.234 | 0.97 | 0.1085 | -0.1087 |
| | 2 | 7 | 2.208 | 1.00 | 0.1078 | -0.0889 |
| | 2 | 8 | 2.231 | 0.87 | 0.1048 | -0.0743 |
| | 3 | 4 | 2.218 | 1.01 | 0.1117 | -0.1173 |
| | 3 | 5 | 2.294 | 0.80 | 0.0976 | -0.0748 |
| | 3 | 7 | 2.234 | 0.97 | 0.1085 | -0.1087 |
| | 5 | 6 | 2.095 | 1.18 | 0.1250 | -0.1223 |
| | 5 | 8 | 2.458 | 0.51 | 0.0705 | -0.0022 |
| | 7 | 8 | 2.231 | 0.87 | 0.1048 | -0.0743 |
| P8-13 | 1 | 2 | 2.265 | 1.00 | 0.1053 | -0.1083 |
| | 1 | 4 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 1 | 8 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 2 | 3 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 2 | 5 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 3 | 4 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 3 | 6 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 4 | 7 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 5 | 6 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 5 | 8 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 6 | 7 | 2.265 | 1.00 | 0.1053 | -0.1084 |
| | 7 | 8 | 2.265 | 1.00 | 0.1053 | -0.1084 |

Table S6: Calculated molar magnetic susceptibility in cgs ppm units ($10^{-6}$ $cm^3$ $mol^{-1}$) at the (M11/def2-TZVP) level of theory, where for benzene ($C_6H_6$) the experimental value is found to be -54.4 ($10^{-6}$ $cm^3$ $mol^{-1}$)[a]

| Structure | Calculated $\chi$M ($10^{-6}$ $cm^3$ $mol^{-1}$) |
|---|---|
| C6H6 | -52.4448 |
| P8-1 | -119.9984 |
| P8-2 | -121.0013 |
| P8-3 | -107.6571 |
| P8-4 | -189.8174 |
| P8-5 | -136.2405 |
| P8-6 | -182.8385 |
| P8-7 | -111.5833 |
| P8-8 | -109.6991 |
| P8-9 | -152.4464 |
| P8-10 | -156.8422 |
| P8-11 | -112.8774 |
| P8-12 | -118.7701 |
| P8-13 | -2.0460 |
| C8H8-1 | -38.8016 |
| C8H8-2 | -51.6034 |
| C8H8-3 | -84.0608 |
| C8H8-4 | -68.5624 |
| C8H8-5 | -76.2359 |
| C8H8-6 | -60.5651 |
| C8H8-7 | -77.2472 |
| C8H8-8 | -74.5895 |
| C8H8-9 | -55.8549 |
| C8H8-10 | -57.9932 |
| C8H8-11 | -80.2488 |
| C8H8-12 | -46.6025 |
| C8H8-13 | -71.7029 |
| C8H8-14 | -88.0765 |

[a]J. Dauben, J. D. Wilson and J. L. Laity, Diamagnetic Susceptibility Exaltation in Hydrocarbons. *J. Am. Chem. Soc.* 1969, 91, 8, 1991–1998.

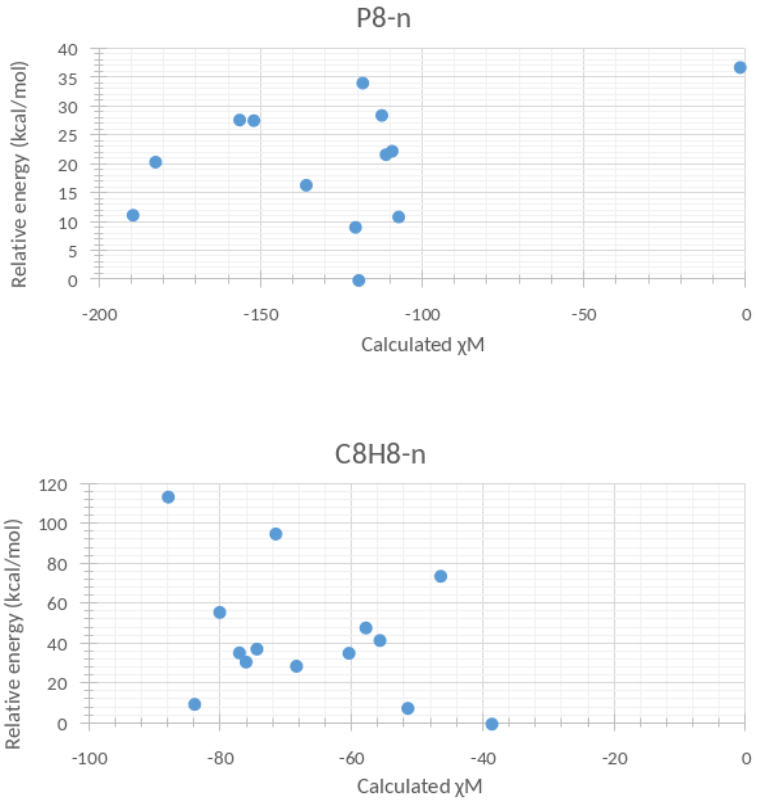



Figure S1. Correlation between the calculated $\chi$M and relative energy (kcal/mol) for the $P_8$ and $C_8H_8$ structures.