

Spin contamination and diagnostic T1

| | | | | | | |
|--------------------------|----------------|----------------|----------------|----------------|----------------|----------------|
| | R ₁ | R ₂ | R ₃ | R ₄ | R ₅ | R ₆ |
| $\langle s^2 \rangle$ | 1.07 | 1.15 | 0.97 | 1.05 | 0.96 | 0.88 |
| T_{1diag} | 0.030 | 0.033 | 0.028 | 0.028 | 0.023 | 0.025 |

| | | | | | | |
|--------------------------|----------------|----------------|----------------|-----------------|---------------------|-----------------------|
| | R ₇ | R ₈ | R ₉ | R ₁₀ | TS _{R1-R2} | TS _{R1-M8+H} |
| $\langle s^2 \rangle$ | 0.87 | 0.78 | 0.86 | 0.77 | 1.26 | 1.37 |
| T_{1diag} | 0.021 | 0.019 | 0.024 | 0.017 | 0.052 | 0.039 |

| | | | | | | |
|--------------------------|-----------------------|---------------------------|---------------------|----------------------|----------------------|-----------------------|
| | TS _{R31-R16} | TS _{R16-C5H7+CO} | TS _{R6-R7} | TS _{R12-M2} | TS _{R12-M3} | TS _{R12-R15} |
| $\langle s^2 \rangle$ | 1.23 | 1.27 | 0.96 | 1.37 | 1.2 | 1.14 |
| T_{1diag} | 0.035 | 0.038 | 0.026 | 0.043 | 0.039 | 0.037 |

| | | |
|--------------------------|---------------------------|----------------------------|
| | TS _{R15-C5H7+CO} | TS _{R7-c-C5H7+CO} |
| $\langle s^2 \rangle$ | 1.23 | 0.96 |
| T_{1diag} | 0.035 | 0.026 |

| | | | | | | |
|--------------------------|---------------------|----------------------|---------------------|----------------------|---------------------|---------------------|
| | TS _{R2-R3} | TS _{R3-R31} | TS _{R3-R5} | TS _{R5-R12} | TS _{R5-R6} | TS _{R5-M9} |
| $\langle s^2 \rangle$ | 0.90 | 1.22 | 1.48 | 1.08 | 0.81 | 0.79 |
| T_{1diag} | 0.028 | 0.033 | 0.04 | 0.032 | 0.020 | 0.02 |

Geometries obtained at the B3LYP/CBSB7 level of theory

R1

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.04496 | 0.005233 | -7.6e-005 |
| 2 | C | -0.598785 | 1.30441 | -0.000208 |
| 3 | C | 0.808829 | 1.26277 | 0.000218 |
| 4 | C | 1.18203 | -0.095457 | -4.7e-005 |
| 5 | O | 0.01723 | -0.853711 | -0.000207 |
| 6 | H | -1.22714 | 2.18157 | -0.000295 |
| 7 | H | 1.49401 | 2.09535 | 0.000252 |
| 8 | C | -2.39637 | -0.605289 | 0.000176 |
| 9 | H | -2.54398 | -1.23804 | -0.881416 |
| 10 | H | -2.5442 | -1.23689 | 0.882578 |
| 11 | H | -3.16151 | 0.172185 | -0.000434 |
| 12 | C | 2.39616 | -0.734033 | 6.5e-005 |
| 13 | H | 3.30971 | -0.157425 | 0.000262 |
| 14 | H | 2.4539 | -1.81285 | -6.2e-005 |

R2

| | | | | |
|----|---|----------|-----------|-----------|
| 1 | C | 1.19056 | -0.216631 | -2.1e-005 |
| 2 | C | 0.468081 | 1.05299 | 3.4e-005 |
| 3 | C | -0.93446 | 1.18353 | 2.6e-005 |
| 4 | C | -1.8541 | 0.206535 | -3.8e-005 |
| 5 | O | 0.612977 | -1.29543 | 6.3e-005 |
| 6 | H | 1.05057 | 1.96837 | 0.000104 |
| 7 | H | -1.32637 | 2.19973 | -8.5e-005 |
| 8 | C | 2.71015 | -0.132094 | -6.7e-005 |
| 9 | H | 3.12548 | -1.13877 | -0.000501 |
| 10 | H | 3.06847 | 0.409959 | -0.880999 |
| 11 | H | 3.0684 | 0.408989 | 0.881521 |
| 12 | C | -2.81956 | -0.657062 | -2.7e-005 |
| 13 | H | -3.22721 | -1.05413 | 0.92679 |
| 14 | H | -3.22717 | -1.05433 | -0.926772 |

R3

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.49093 | 0.020757 | -0.000217 |
| 2 | C | 0.437479 | -0.998001 | 0.265898 |
| 3 | C | -0.901663 | -0.875221 | 0.193526 |
| 4 | C | -1.68143 | 0.287771 | -0.199971 |
| 5 | O | 2.57591 | -0.348116 | -0.475651 |
| 6 | H | 0.855797 | -1.97697 | 0.478082 |
| 7 | H | -1.48937 | -1.76378 | 0.41541 |
| 8 | C | 1.30604 | 1.39848 | 0.363713 |
| 9 | H | 0.455091 | 1.74406 | 0.935825 |
| 10 | H | 2.10175 | 2.09239 | 0.122441 |
| 11 | C | -3.01944 | 0.313353 | -0.168794 |
| 12 | H | -3.57858 | 1.18671 | -0.481876 |
| 13 | H | -3.59475 | -0.542142 | 0.171026 |
| 14 | H | -1.14867 | 1.16181 | -0.560624 |

R4

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.10665 | 0.033577 | 0.005117 |
| 2 | C | -0.356509 | 1.28327 | 0.001409 |
| 3 | C | 1.04148 | 1.30174 | 0.074266 |
| 4 | C | 1.79273 | 0.149661 | -0.003953 |
| 5 | O | -2.31953 | -0.000205 | -0.150485 |
| 6 | H | -0.933663 | 2.19904 | -0.05062 |
| 7 | H | 1.54943 | 2.25785 | 0.158878 |
| 8 | C | -0.299743 | -1.23066 | 0.296036 |
| 9 | H | -0.281271 | -1.33202 | 1.38912 |
| 10 | H | -0.84921 | -2.08813 | -0.094986 |
| 11 | C | 1.14568 | -1.1831 | -0.228402 |
| 12 | H | 1.74158 | -1.98171 | 0.223357 |
| 13 | H | 1.15199 | -1.38768 | -1.31057 |
| 14 | H | 2.8755 | 0.207299 | 0.021857 |

R5

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.50229 | 0.329424 | -0.056995 |
| 2 | C | 0.630021 | -0.762665 | -0.53568 |
| 3 | C | -0.836132 | -0.743275 | -0.401598 |
| 4 | C | -1.57729 | 0.344358 | 0.049778 |
| 5 | O | 1.82556 | 1.47434 | -0.179269 |
| 6 | H | 1.01819 | -1.33665 | -1.37484 |
| 7 | H | -1.35953 | -1.66178 | -0.656462 |
| 8 | C | 1.59344 | -0.892148 | 0.747681 |
| 9 | H | 2.44746 | -1.5537 | 0.644862 |
| 10 | H | 1.11816 | -0.889815 | 1.7242 |
| 11 | C | -2.94337 | 0.341221 | 0.234358 |
| 12 | H | -3.46732 | 1.22454 | 0.575363 |
| 13 | H | -3.5355 | -0.545837 | 0.037137 |
| 14 | H | -1.03971 | 1.26705 | 0.258639 |

R6

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.12467 | 0.047057 | -0.001177 |
| 2 | C | -0.309065 | 1.27916 | 0.008066 |
| 3 | C | 1.02977 | 1.26386 | 0.031756 |
| 4 | C | 1.85656 | 0.009515 | 0.005096 |
| 5 | O | -2.33257 | 0.077607 | -0.12214 |
| 6 | H | -0.867957 | 2.20882 | -0.003359 |
| 7 | H | 1.57516 | 2.20377 | 0.063401 |
| 8 | C | -0.378031 | -1.27396 | 0.207698 |
| 9 | H | -0.478088 | -1.49097 | 1.28934 |
| 10 | H | -0.935486 | -2.06462 | -0.300288 |
| 11 | C | 1.05174 | -1.22749 | -0.205539 |
| 12 | H | 1.54818 | -2.13424 | -0.529034 |
| 13 | H | 2.62964 | 0.105769 | -0.769211 |
| 14 | H | 2.43124 | -0.038234 | 0.950868 |

R7

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.35076 | -1.27637 | -0.664419 |
| 2 | C | 0.417067 | -1.56604 | 0.250402 |
| 3 | C | -0.869565 | -0.990635 | 0.358745 |
| 4 | C | -1.39445 | 0.069172 | -0.557121 |
| 5 | O | 2.17709 | -1.04366 | -1.45216 |
| 6 | H | 0.734708 | -2.32853 | 0.956522 |
| 7 | H | -1.47611 | -1.30518 | 1.19796 |
| 8 | C | -0.708149 | 1.90386 | 1.06202 |
| 9 | H | -0.247232 | 1.20218 | 1.74899 |
| 10 | H | -0.676556 | 2.95316 | 1.33222 |
| 11 | C | -1.28412 | 1.50085 | -0.065448 |
| 12 | H | -1.73266 | 2.24134 | -0.726057 |
| 13 | H | -0.898015 | 0.00762 | -1.53658 |
| 14 | H | -2.45497 | -0.126584 | -0.769076 |

R8

| | | | | |
|----|---|----------|-----------|-----------|
| 1 | C | -1.40257 | -0.449627 | 0.244254 |
| 2 | C | 1.3533 | -1.50666 | 0.489698 |
| 3 | C | 1.67214 | -0.540497 | -0.374268 |
| 4 | C | 1.42337 | 0.89682 | -0.202666 |
| 5 | O | -2.15447 | -1.04502 | -0.444901 |
| 6 | H | 1.5857 | -2.54439 | 0.278815 |
| 7 | H | 2.2214 | -0.809017 | -1.27577 |
| 8 | C | -1.1311 | 1.049 | 0.221126 |
| 9 | H | -1.74982 | 1.48879 | -0.574466 |
| 10 | H | -1.53374 | 1.42097 | 1.17287 |
| 11 | C | 0.28532 | 1.54207 | 0.077609 |
| 12 | H | 0.347267 | 2.62476 | 0.158618 |
| 13 | H | 0.865833 | -1.2946 | 1.43279 |
| 14 | H | 2.29634 | 1.5271 | -0.368164 |

R9

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.64752 | -0.311716 | 0.013724 |
| 2 | C | -1.34882 | 0.971501 | -0.044732 |
| 3 | C | -0.020093 | 1.5675 | -0.205379 |
| 4 | C | 1.18397 | 1.03901 | 0.057233 |
| 5 | O | -1.94529 | -1.4343 | 0.050687 |
| 6 | H | -2.21667 | 1.6228 | -0.022158 |
| 7 | H | -0.052945 | 2.58273 | -0.588875 |
| 8 | C | 1.8518 | -1.3008 | -0.472821 |
| 9 | H | 1.08845 | -1.77007 | -1.08159 |
| 10 | H | 2.88008 | -1.37797 | -0.804403 |
| 11 | C | 1.46955 | -0.341421 | 0.612648 |
| 12 | H | 0.592933 | -0.709996 | 1.15694 |
| 13 | H | 2.28197 | -0.262738 | 1.34328 |
| 14 | H | 2.05516 | 1.64514 | -0.172726 |

R10

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.69057 | 0.494054 | -0.034573 |
| 2 | C | 0.367247 | 0.357056 | 0.743153 |
| 3 | C | -0.67023 | 1.27483 | 0.125199 |
| 4 | C | -1.63561 | 0.586341 | -0.479211 |
| 5 | O | 2.25428 | -0.334542 | -0.657858 |
| 6 | H | 0.609453 | 0.648528 | 1.7709 |
| 7 | H | -0.579393 | 2.3533 | 0.153109 |
| 8 | C | -0.284375 | -1.0513 | 0.648063 |
| 9 | H | 0.443492 | -1.81024 | 0.360705 |
| 10 | H | -0.683886 | -1.32194 | 1.628 |
| 11 | C | -1.43948 | -0.906676 | -0.375461 |
| 12 | H | -1.17916 | -1.3281 | -1.35394 |
| 13 | H | -2.34611 | -1.42413 | -0.046975 |
| 14 | H | -2.46736 | 1.03309 | -1.01196 |

TSR1_R2

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.06682 | -0.108438 | 0.001175 |
| 2 | C | -0.556623 | 1.21589 | 0.05991 |
| 3 | C | 0.830635 | 1.25572 | -0.07823 |
| 4 | C | 1.51578 | 0.074142 | -0.076369 |
| 5 | O | -0.234061 | -1.04314 | -0.138126 |
| 6 | H | -1.18285 | 2.09461 | 0.116688 |
| 7 | H | 1.36123 | 2.17418 | -0.31028 |
| 8 | C | -2.53694 | -0.429372 | 0.075249 |
| 9 | H | -2.82959 | -1.00585 | -0.806096 |
| 10 | H | -2.73404 | -1.05353 | 0.951231 |
| 11 | H | -3.14871 | 0.471872 | 0.136064 |
| 12 | C | 2.55318 | -0.711941 | 0.115019 |
| 13 | H | 2.6334 | -1.67352 | -0.379461 |
| 14 | H | 3.33772 | -0.438707 | 0.816333 |

TSR1_M1+H

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.05151 | -0.034198 | -0.105763 |
| 2 | C | -0.581518 | 1.30796 | -0.013901 |
| 3 | C | 0.792915 | 1.25676 | 0.057744 |
| 4 | C | 1.16984 | -0.119729 | 0.011594 |
| 5 | O | 0.030525 | -0.867227 | -0.086555 |
| 6 | H | -1.20809 | 2.17654 | -0.004733 |
| 7 | H | 1.47832 | 2.07616 | 0.133806 |
| 8 | C | -2.31914 | -0.536019 | -0.185711 |
| 9 | H | -2.4876 | -1.58922 | -0.294413 |
| 10 | H | -3.07406 | -0.963724 | 2.0934 |
| 11 | H | -3.15727 | 0.130978 | -0.237939 |
| 12 | C | 2.39449 | -0.709667 | 0.048465 |
| 13 | H | 3.27871 | -0.107155 | 0.125256 |
| 14 | H | 2.4953 | -1.77639 | 0.002505 |

TSR2_R3

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.40153 | 0.06692 | 0.021471 |
| 2 | C | -0.55329 | -1.14617 | 0.12244 |
| 3 | C | 0.79362 | -1.11006 | 0.039556 |
| 4 | C | 1.52513 | 0.123512 | -0.093582 |
| 5 | O | -2.59746 | -0.019787 | -0.197693 |
| 6 | H | -1.09053 | -2.08615 | 0.176892 |
| 7 | H | 1.36075 | -2.04125 | 0.036896 |
| 8 | C | -0.704608 | 1.3916 | 0.152682 |
| 9 | H | -1.09453 | 2.1632 | -0.508491 |
| 10 | H | -0.61003 | 1.72914 | 1.18574 |
| 11 | H | 0.547165 | 1.08246 | -0.130478 |
| 12 | C | 2.82328 | 0.392137 | -0.081063 |
| 13 | H | 3.20675 | 1.39908 | -0.207563 |
| 14 | H | 3.56451 | -0.395837 | 0.059523 |

TSR3_R4

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.13872 | 0.035663 | 0.089502 |
| 2 | C | -0.273548 | 1.25847 | 0.104372 |
| 3 | C | 1.07867 | 1.24065 | 0.083631 |
| 4 | C | 1.83481 | 0.009905 | 0.009855 |
| 5 | O | -2.23606 | 0.072654 | -0.451436 |
| 6 | H | -0.814974 | 2.19837 | 0.099825 |
| 7 | H | 1.62272 | 2.17834 | 0.164598 |
| 8 | C | -0.625804 | -1.19246 | 0.713393 |
| 9 | H | -0.06273 | -1.13628 | 1.63597 |
| 10 | H | -1.17568 | -2.10433 | 0.511565 |
| 11 | C | 1.3133 | -1.11245 | -0.581245 |
| 12 | H | 1.81256 | -2.07019 | -0.485103 |
| 13 | H | 0.60785 | -1.03138 | -1.39791 |
| 14 | H | 2.76649 | -0.054433 | 0.565491 |

TSR3_R5

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.49092 | 0.239945 | 0.013063 |
| 2 | C | 0.530682 | -0.635591 | -0.691962 |
| 3 | C | -0.874399 | -0.593541 | -0.608161 |
| 4 | C | -1.61155 | 0.377109 | 0.118239 |
| 5 | O | 2.22866 | 1.13694 | -0.298887 |
| 6 | H | 0.987547 | -1.2852 | -1.43264 |
| 7 | H | -1.43125 | -1.37305 | -1.12058 |
| 8 | C | 1.40879 | -0.776226 | 1.04161 |
| 9 | H | 2.26024 | -1.42113 | 1.23535 |
| 10 | H | 0.563503 | -0.822707 | 1.71177 |
| 11 | C | -2.9626 | 0.368923 | 0.259596 |
| 12 | H | -3.47841 | 1.1463 | 0.808666 |
| 13 | H | -3.57126 | -0.413037 | -0.182251 |
| 14 | H | -1.05074 | 1.18961 | 0.576502 |

TSR4_R6

| | | | | |
|----|---|----------|-----------|-----------|
| 1 | C | 1.10729 | 0.057319 | 8.7e-005 |
| 2 | C | 0.325923 | 1.28461 | -0.03921 |
| 3 | C | -1.04231 | 1.29529 | -0.056835 |
| 4 | C | -1.81107 | 0.089564 | 0.021204 |
| 5 | O | 2.32482 | 0.046834 | 0.095837 |
| 6 | H | 0.896253 | 2.20588 | -0.04005 |
| 7 | H | -1.57991 | 2.23649 | -0.087307 |
| 8 | C | 0.362506 | -1.28857 | -0.12097 |
| 9 | H | 0.614967 | -1.6874 | -1.11829 |
| 10 | H | 0.822926 | -1.98719 | 0.586054 |
| 11 | C | -1.12596 | -1.21581 | 0.024383 |
| 12 | H | -1.73492 | -2.10968 | -0.020898 |
| 13 | H | -1.6377 | -0.474634 | 1.10793 |
| 14 | H | -2.87853 | 0.107404 | -0.166086 |

TSR4_M2+H

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.11501 | -0.003204 | -0.004684 |
| 2 | C | 0.413889 | 1.28895 | 0.009262 |
| 3 | C | -0.935274 | 1.35783 | -0.014489 |
| 4 | C | -1.77689 | 0.175591 | -0.064034 |
| 5 | O | 2.32457 | -0.09122 | 0.101419 |
| 6 | H | 1.03586 | 2.17427 | 0.071906 |
| 7 | H | -1.42333 | 2.32715 | 0.017196 |
| 8 | C | 0.249917 | -1.25311 | -0.182839 |
| 9 | H | 0.501608 | -1.66417 | -1.17183 |
| 10 | H | 0.593325 | -2.01015 | 0.528903 |
| 11 | C | -1.2337 | -1.05678 | -0.108338 |
| 12 | H | -1.86518 | -1.93562 | -0.182026 |
| 13 | H | -1.58348 | -1.52085 | 2.16596 |
| 14 | H | -2.85305 | 0.303485 | -0.05073 |

TSR4_R9

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.36745 | 0.228221 | -0.042549 |
| 2 | C | -0.550635 | 1.29083 | -0.066867 |
| 3 | C | 0.88716 | 1.35627 | 0.114892 |
| 4 | C | 1.77416 | 0.351985 | 0.042408 |
| 5 | O | -2.39593 | -0.348947 | -0.057987 |
| 6 | H | -1.0846 | 2.21262 | -0.287525 |
| 7 | H | 1.26704 | 2.35753 | 0.294231 |
| 8 | C | 0.079826 | -1.46356 | 0.305926 |
| 9 | H | -0.045718 | -1.35601 | 1.37893 |
| 10 | H | -0.52847 | -2.22181 | -0.172061 |
| 11 | C | 1.3798 | -1.06411 | -0.29236 |
| 12 | H | 2.15687 | -1.75467 | 0.076767 |
| 13 | H | 1.35802 | -1.20786 | -1.38184 |
| 14 | H | 2.82716 | 0.563974 | 0.186701 |

TSR6_R7

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.25418 | -0.233653 | 0.068838 |
| 2 | C | 0.340931 | -1.32028 | 0.166103 |
| 3 | C | -1.01715 | -1.26115 | 0.126552 |
| 4 | C | -1.77919 | -0.022354 | -0.272455 |
| 5 | O | 2.30126 | 0.062645 | -0.400942 |
| 6 | H | 0.836076 | -2.25468 | 0.41941 |
| 7 | H | -1.58977 | -2.14368 | 0.39068 |
| 8 | C | -0.008351 | 1.47462 | 0.644929 |
| 9 | H | -0.138104 | 1.06379 | 1.63999 |
| 10 | H | 0.677952 | 2.30797 | 0.553779 |
| 11 | C | -0.877754 | 1.17402 | -0.355077 |
| 12 | H | -0.805532 | 1.70261 | -1.30023 |
| 13 | H | -2.28633 | -0.191657 | -1.22996 |
| 14 | H | -2.5803 | 0.147301 | 0.460524 |

TSR6_M2+H

| | | | | |
|----|---|-----------|----------|-----------|
| 1 | C | -1.13082 | 0.034887 | 0.011924 |
| 2 | C | -0.346961 | 1.2795 | -0.003321 |
| 3 | C | 0.998667 | 1.26415 | -0.067922 |
| 4 | C | 1.7692 | 0.021542 | -0.122834 |
| 5 | O | -2.34745 | 0.028912 | -0.001048 |
| 6 | H | -0.912478 | 2.20395 | 0.009485 |
| 7 | H | 1.54944 | 2.19903 | -0.093305 |
| 8 | C | -0.342148 | -1.27669 | 0.062776 |
| 9 | H | -0.545792 | -1.71859 | 1.05084 |
| 10 | H | -0.794437 | -1.97584 | -0.648986 |
| 11 | C | 1.13538 | -1.17525 | -0.133333 |
| 12 | H | 1.70078 | -2.09504 | -0.240364 |
| 13 | H | 2.82998 | 0.082711 | -0.333215 |
| 14 | H | 2.4522 | 0.183638 | 1.78019 |

TSR6_M3+H

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | -1.10464 | 0.054851 | -0.033677 |
| 2 | C | -0.29501 | 1.28943 | 0.048285 |
| 3 | C | 1.04282 | 1.26463 | 0.047786 |
| 4 | C | 1.83377 | -0.002859 | -0.034384 |
| 5 | O | -2.32021 | 0.078666 | -0.116974 |
| 6 | H | -0.852982 | 2.21807 | 0.093208 |
| 7 | H | 1.60658 | 2.1916 | 0.103943 |
| 8 | C | -0.341805 | -1.22528 | -0.031855 |
| 9 | H | -0.666721 | -1.53121 | 1.94044 |
| 10 | H | -0.932584 | -2.12498 | -0.160274 |
| 11 | C | 1.00614 | -1.24244 | -0.124053 |
| 12 | H | 1.53406 | -2.18621 | -0.223324 |
| 13 | H | 2.52383 | 0.046765 | -0.889982 |
| 14 | H | 2.50181 | -0.073316 | 0.839169 |

TSR7_C5H7+CO

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 2.62777 | -0.166998 | -0.477337 |
| 2 | C | 0.922727 | 1.44811 | -0.149275 |
| 3 | C | -0.24841 | 1.17692 | 0.372198 |
| 4 | C | -0.734049 | -0.141852 | 0.918824 |
| 5 | O | 2.42035 | -1.19863 | -0.047518 |
| 6 | H | 1.39612 | 2.3262 | -0.560407 |
| 7 | H | -0.975744 | 1.99676 | 0.429632 |
| 8 | C | -2.4677 | -0.286361 | -0.92752 |
| 9 | H | -2.03962 | 0.540751 | -1.48359 |
| 10 | H | -3.34009 | -0.76528 | -1.35698 |
| 11 | C | -1.94755 | -0.708775 | 0.220388 |
| 12 | H | -2.40952 | -1.55217 | 0.729915 |
| 13 | H | 0.072816 | -0.879966 | 0.897997 |
| 14 | H | -0.983453 | -0.003483 | 1.9799 |

TSR5_R8

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.67975 | 0.306445 | -0.142089 |
| 2 | C | 0.529189 | -1.04895 | -0.386221 |
| 3 | C | -0.809629 | -0.691039 | -0.539586 |
| 4 | C | -1.5613 | 0.163485 | 0.317768 |
| 5 | O | 1.85643 | 1.45879 | -0.361744 |
| 6 | H | 0.943998 | -1.81838 | -1.02464 |
| 7 | H | -1.31041 | -1.05124 | -1.43425 |
| 8 | C | 1.39784 | -0.697854 | 0.851227 |
| 9 | H | 2.18194 | -1.43962 | 0.990225 |
| 10 | H | 0.922351 | -0.409954 | 1.79328 |
| 11 | C | -2.85743 | 0.501279 | 0.117048 |
| 12 | H | -3.38702 | 1.14692 | 0.805919 |
| 13 | H | -3.41063 | 0.133263 | -0.740707 |
| 14 | H | -1.06223 | 0.568526 | 1.19524 |

TSR8_C5H7+CO

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.85931 | 0.788061 | 0.01028 |
| 2 | C | -1.7863 | 1.39758 | 0.07054 |
| 3 | C | -2.13144 | 0.128523 | -0.204581 |
| 4 | C | -1.25523 | -1.01045 | -0.415917 |
| 5 | O | 2.69792 | 0.364429 | -0.65666 |
| 6 | H | -2.54712 | 2.15902 | 0.197279 |
| 7 | H | -3.19113 | -0.086625 | -0.329738 |
| 8 | C | 0.723031 | -0.418137 | 1.00897 |
| 9 | H | 1.53227 | -0.901931 | 1.54943 |
| 10 | H | 0.161331 | 0.293562 | 1.60241 |
| 11 | C | -0.00871 | -1.24427 | 0.092261 |
| 12 | H | 0.490109 | -2.15102 | -0.238633 |
| 13 | H | -0.755904 | 1.72458 | 0.134702 |
| 14 | H | -1.67683 | -1.8009 | -1.03148 |

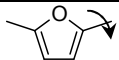
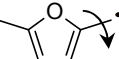

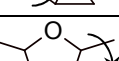
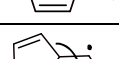
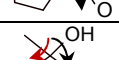

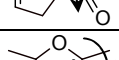
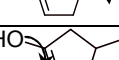


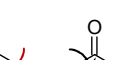
TSR9_R10

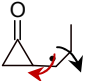

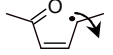

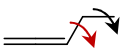
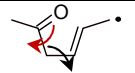
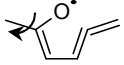
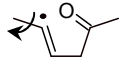
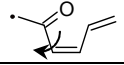
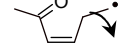
| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.79053 | 0.09065 | 0.053807 |
| 2 | C | 0.601934 | 0.221197 | 0.686729 |
| 3 | C | -0.352089 | 1.28261 | 0.213605 |
| 4 | C | -1.5262 | 0.926122 | -0.299571 |
| 5 | O | 2.69943 | -0.298301 | -0.569628 |
| 6 | H | 0.703289 | 0.071353 | 1.76122 |
| 7 | H | -0.064003 | 2.32474 | 0.304659 |
| 8 | C | -0.898964 | -1.38669 | 0.333425 |
| 9 | H | -0.342682 | -2.14132 | -0.209915 |
| 10 | H | -1.13257 | -1.64921 | 1.35986 |
| 11 | C | -1.893 | -0.535833 | -0.410129 |
| 12 | H | -1.94739 | -0.810738 | -1.47138 |
| 13 | H | -2.90994 | -0.674117 | -0.017318 |
| 14 | H | -2.2354 | 1.67735 | -0.637295 |

TSR10_C5H7+CO

| | | | | |
|----|---|-----------|-----------|-----------|
| 1 | C | 1.75347 | -0.472237 | -0.465798 |
| 2 | C | 0.225098 | -0.237771 | 0.751714 |
| 3 | C | -0.275938 | 1.10344 | 0.512119 |
| 4 | C | -1.39688 | 1.075 | -0.240577 |
| 5 | O | 2.67642 | 0.204459 | -0.319822 |
| 6 | H | 0.797767 | -0.456007 | 1.64921 |
| 7 | H | 0.227833 | 2.00002 | 0.851398 |
| 8 | C | -0.863471 | -1.2003 | 0.308916 |
| 9 | H | -0.462748 | -2.0736 | -0.209319 |
| 10 | H | -1.40774 | -1.56075 | 1.18877 |
| 11 | C | -1.79848 | -0.338527 | -0.581679 |
| 12 | H | -1.63252 | -0.536491 | -1.64842 |
| 13 | H | -2.85905 | -0.533565 | -0.393799 |
| 14 | H | -1.93777 | 1.94708 | -0.587427 |

Internal rotation database for DMF schemes established with relaxed scans at the B3LYP/6-31+G(d,p) level of theory.

| Species | Rotation characteristics | | |
|---|--------------------------|-------------|----------|
| | V (kcal/mol) | # minima | symmetry |
|  | 1.25 | 3 | 3 |
|  | 19 | 2 | 2 |
|  | 2.96 | 1 | 1 |
|  | 0.96 | 2 | 2 |
|  | 1.41 | 2 | 1 |
|  | 4.42 | 3 | 3 |
| | 3.1 | 1 | 1 |
|  | 3.05 | 2 | 1 |
|  | 1.4 | 3 | 3 |
|  | 3.93 | 2 | 1 |
|  | 6.3 | 1 | 1 |
| | 0.73 | 3 | 3 |
| | 1.2 | 3 | 3 |
|  | 7.04 | 1 | 1 |
| | 1.5 | 3 | 3 |
| | 0.71 | 3 | 3 |
|  | 2.77 | 1 | 1 |
| | 2.32 | 2 | 1 |

| | | | |
|---|------|---|---|
|  | 3.16 | 1 | 1 |
| | 3.17 | 2 | 1 |
|  | 10 | 1 | 1 |
|  | 0.36 | 3 | 3 |
|  | 2.42 | 3 | 3 |
| | 8.77 | 1 | 1 |
|  | 3.09 | 3 | 3 |
| | 1.66 | 3 | 1 |
|  | 5.09 | 1 | 1 |
| | 2.17 | 1 | 1 |
|  | 0.2 | 3 | 3 |
|  | 0.27 | 3 | 3 |
|  | 6.18 | 1 | 1 |
|  | 0.47 | 2 | 2 |

Full potential energy diagram of the decomposition of R₄ computed at the CBS-QB3 level of theory at 0K.
Potential energies are relative to the first reactant R₁.

