Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# A theoretical study of new representatives of closed- and open-circle benzofuran and benzocyclopentadienone oligomers

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## Electronic Supplementary Information

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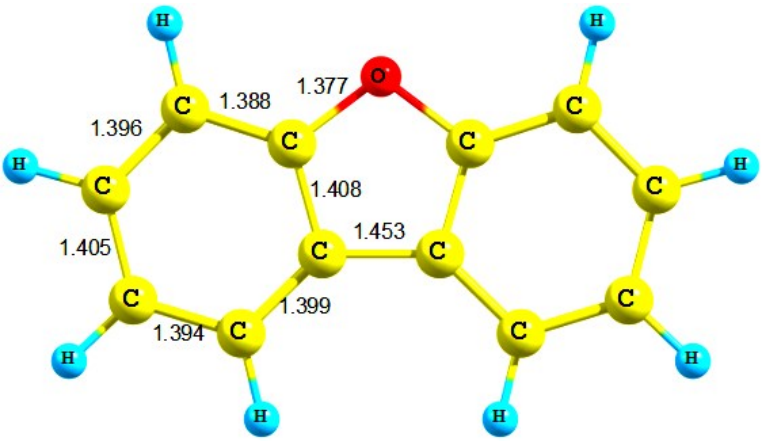


**Fig. S1.** Bond lengths in dibenzofuran calculated at the B3LYP/6-31(d) level of theory

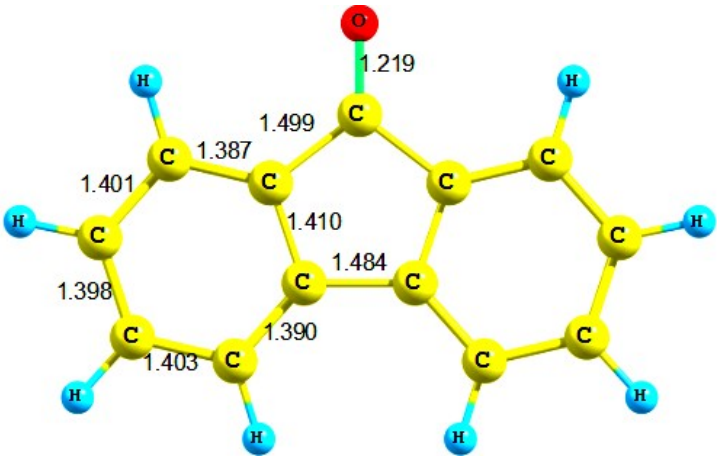


**Fig. S2.** Bond lengths in fluoren-9-on calculated at the B3LYP/6-31(d) level of theory

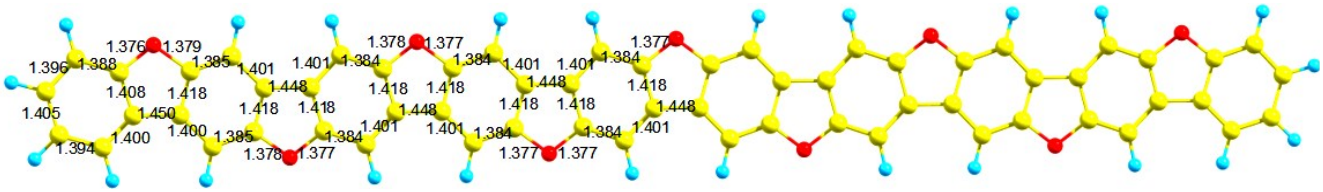


**Fig. S3.** Bond lengths in the linear benzofuran **A9** calculated at the B3LYP/6-31(d) level of theory

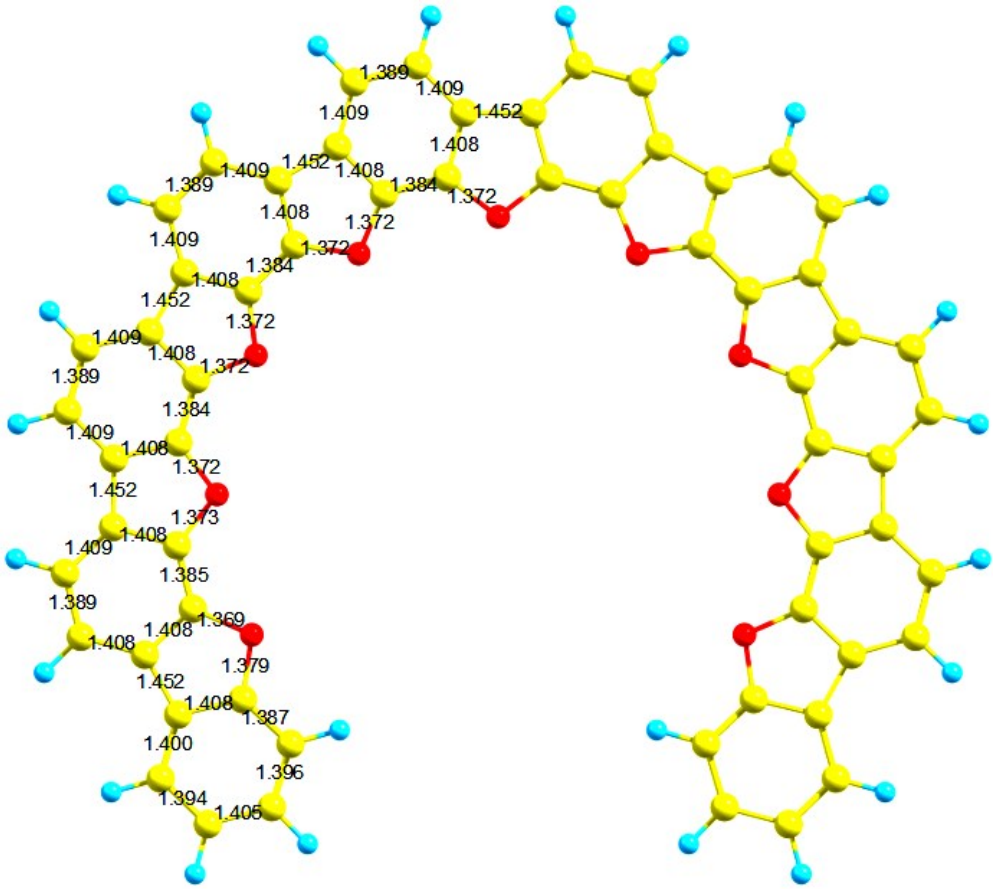


**Fig. S4.** Bond lengths in the fan-shaped benzofuran **B9** calculated at the B3LYP/6-31(d) level of theory

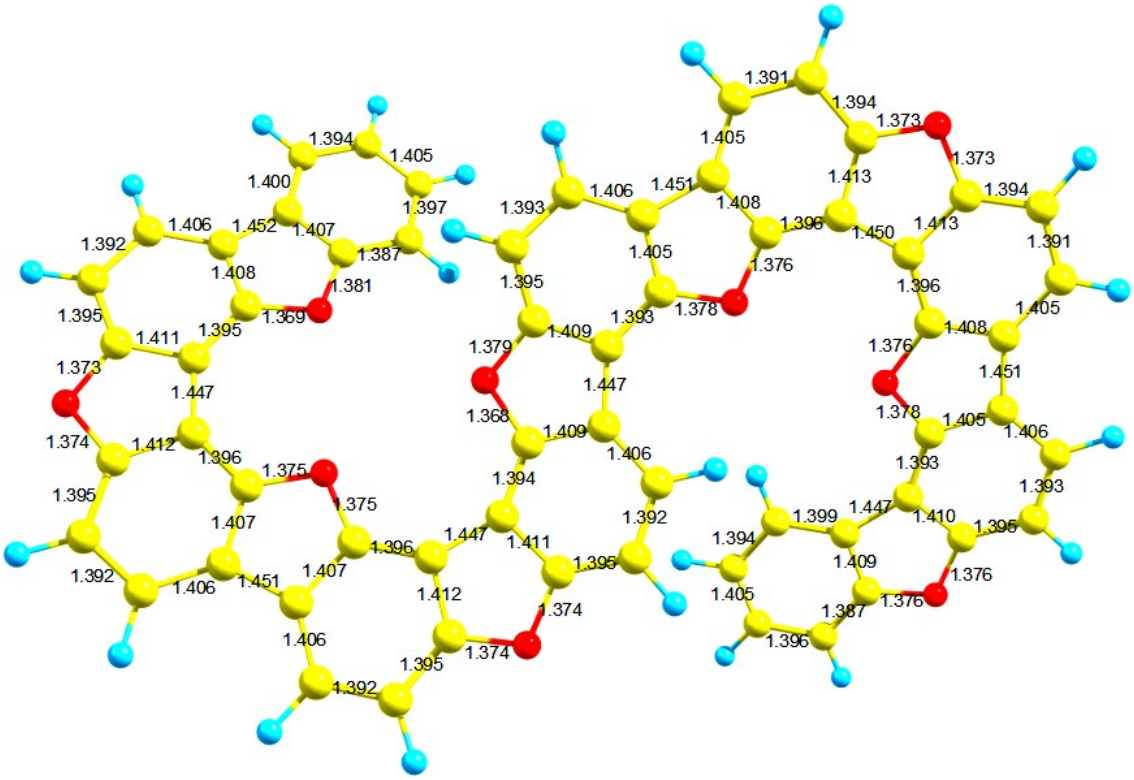


**Fig. S5.** Bond lengths in the S-shaped benzofuran **D9′** calculated at the B3LYP/6-31(d) level of theory

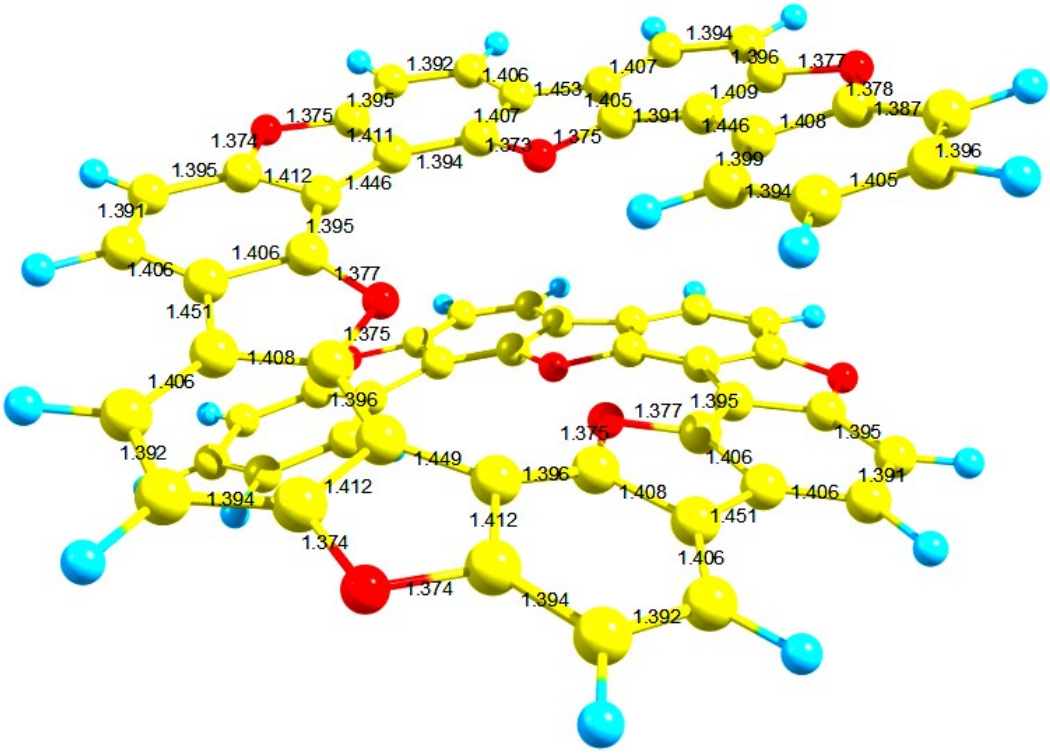


**Fig. S6.** Bond lengths in the helical benzofuran **D9** calculated at the B3LYP/6-31(d) level of theory

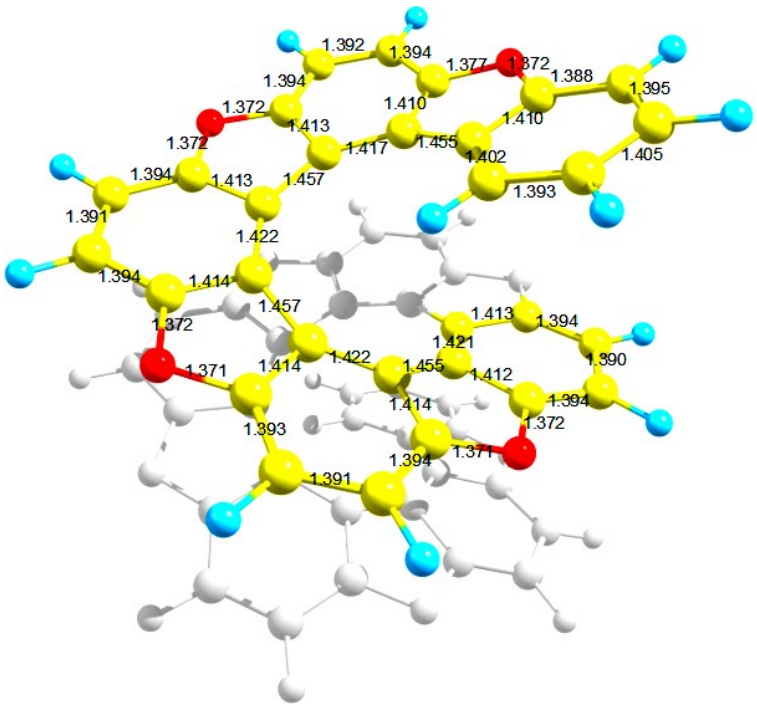


**Fig. S7.** Bond lengths in the helical benzofuran **C9** calculated at the B3LYP/6-31(d) level of theory

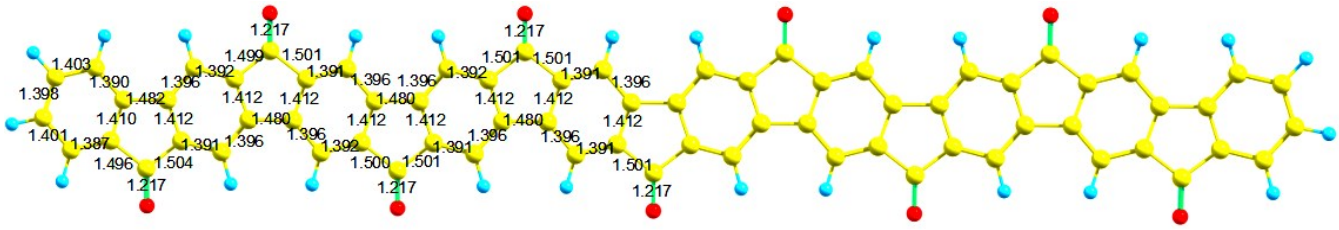


**Fig. S8.** Bond lengths in the linear benzocyclopentadienone **A9** calculated at the B3LYP/6-31(d) level of theory

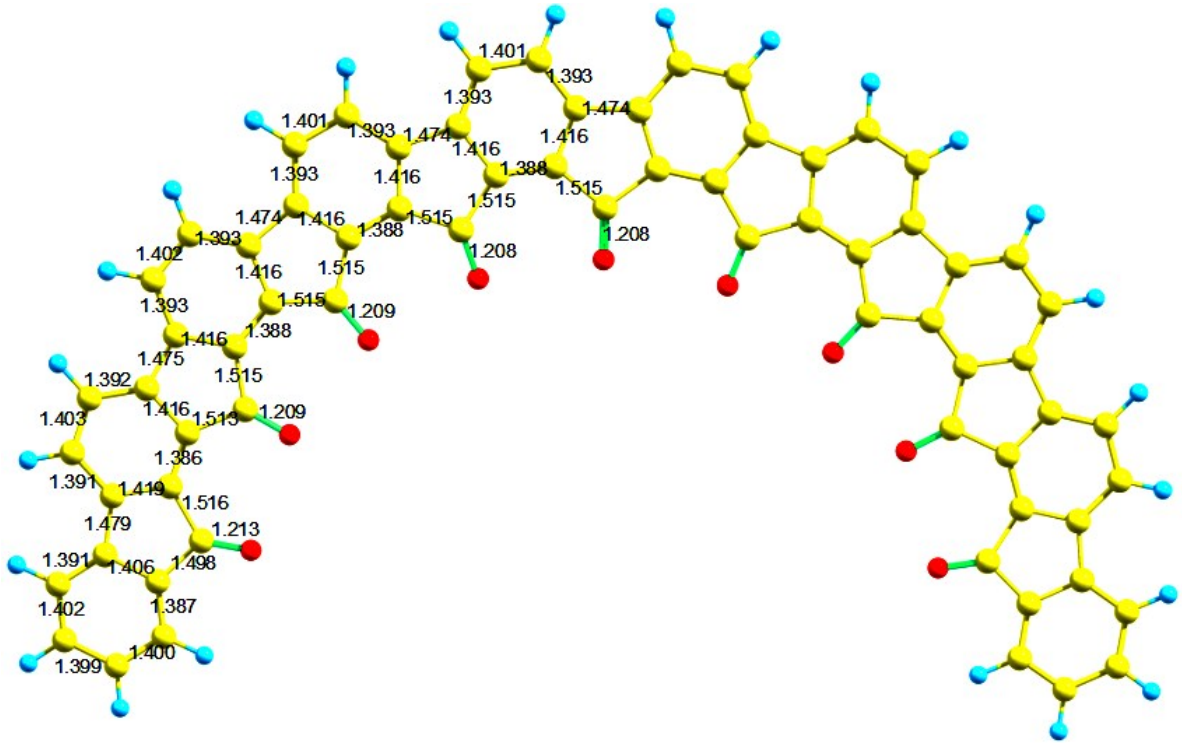


**Fig. S9.** Bond lengths in the fan-shaped benzocyclopentadienone **B9** calculated at the B3LYP/6-31(d) level of theory

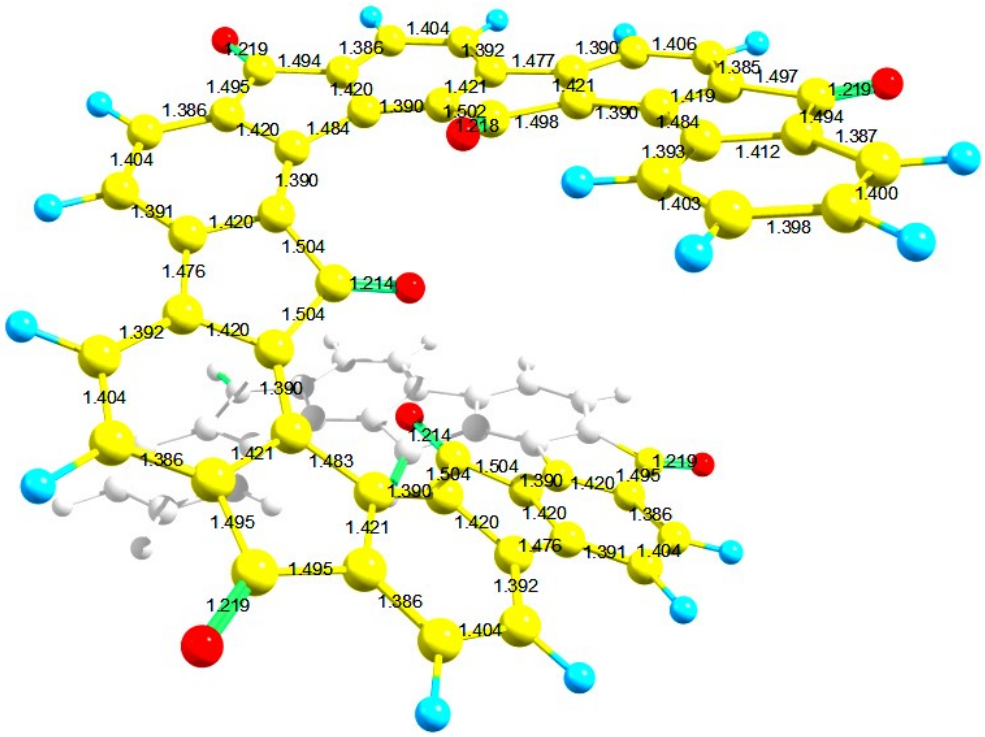


**Fig. S10.** Bond lengths in the helical benzocyclopentadienone **D9** calculated at the B3LYP/6-31(d) level of theory

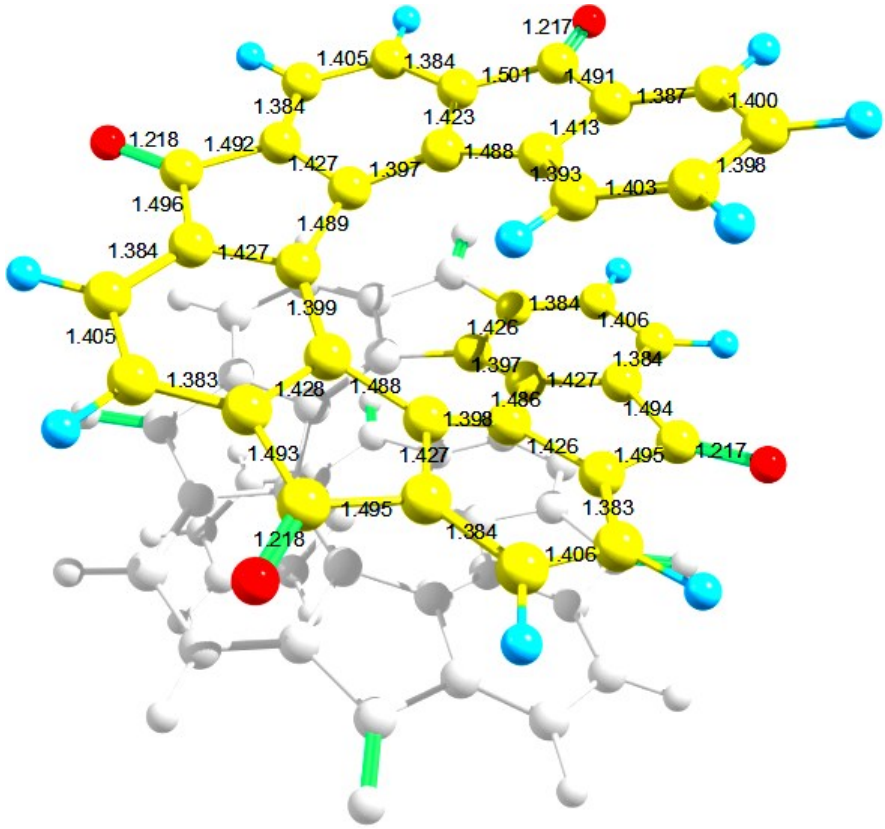


**Fig. S11.** Bond lengths in the helical benzocyclopentadienone **C9** calculated at the B3LYP/6-31(d) level of theory

**Table S1.** Total energies of the studied open-circle benzofuran and benzocyclopentadienone oligomers calculated at the B3LYP/6-31(d) level of theory

| | $E_{tot}$, *a.u.* | | $E_{tot}$, *a.u.* | | $E_{tot}$, *a.u.* | | $E_{tot}$, *a.u.* |
|---|---|---|---|---|---|---|---|
| [n]benzofuran systems | | | | | | | |
| **A1** | –537.4626 | | | | | | |
| **A2** | –842.4083 | **B2** | –842.4034 | **C2** | –842.6112 | **D2** | –842.6130 |
| **A3** | –1147.4875 | **B3** | –1147.4752 | **C3** | –1147.4737 | **D3** | –1147.4857 |
| **A4** | –1452.5668 | **B4** | –1452.5514 | **C4** | –1452.5429 | **D4** | –1452.5649 |
| **A5** | –1757.6460 | **B5** | –1757.6254 | **C5** | –1757.6096 | **D5** | –1757.6387 |
| **A6** | –2062.7252 | **B6** | –2062.6993 | **C6** | –2062.6771 | **D6** | –2062.7157 |
| **A7** | –2367.8044 | **B7** | –2367.7733 | **C7** | –2367.7440 | **D7** | –2367.7902 |
| **A8** | –2672.8836 | **B8** | –2672.8470 | **C8** | –2672.8105 | **D8** | –2672.8669 |
| **A9** | –2977.9628 | **B9** | –2977.9210 | **C9** | –2977.8770 | **D9** | –2978.6468 |
| [n]benzocyclopentadienone systems | | | | | | | |
| **A1** | –575.4370 | | | | | | |
| **A2** | –918.6249 | **B2** | –918.6164 | **C2** | –918.6180 | **D2** | –918.6274 |
| **A3** | –1261.8121 | **B3** | –1261.7948 | **C3** | –1261.7933 | **D3** | –1261.8166 |
| **A4** | –1605.3873 | **B4** | –1604.9730 | **C4** | –1604.9697 | **D4** | –1604.9886 |
| **A5** | –1948.1863 | **B5** | –1948.1509 | **C5** | –1948.1452 | **D5** | –1948.1783 |
| **A6** | –2291.3734 | **B6** | –2291.3290 | **C6** | –2291.3203 | **D6** | –2291.3476 |
| **A7** | –2634.5605 | **B7** | –2634.5068 | **C7** | –2634.4952 | **D7** | –2634.5371 |
| **A8** | –2977.7475 | **B8** | –2977.6847 | **C8** | –2977.6698 | **D8** | –2977.7063 |
| **A9** | –3320.9346 | **B9** | –3320.8625 | **C9** | –3320.8445 | **D9** | –3320.8960 |

**Table S2.** Total energies of the studied oxa[n]circulenes and [n]circulene ketones calculated at the B3LYP/6-31(d) level of theory

| | $E_{tot}$, *a.u.* | n | $E_{tot}$, *a.u.* |
|---|---|---|---|
| oxa[n]circulenes | | [n]circulene ketones | |
| 4 | –609.7764 | 4 | –686.0339 |
| 6 | –915.0820 | 6 | –1029.4618 |
| 8 | –1220.3120 | 8 | –1372.7399 |
| 10 | –1525.3038 | 10 | –1715.8051 |
| 12 | –1830.2833 | 12 | –2058.9329 |
| 14 | –2135.3288 | 14 | –2402.1067 |
| 16 | –2440.4037 | 16 | –2745.2820 |
| 18 | –2745.4659 | 18 | –3088.3972 |
| 20 | –3050.4694 | 20 | –3431.4424 |
| 22 | –3355.4095 | 22 | –3774.5666 |
| 24 | –3660.3612 | 24 | –4117.7468 |
| 26 | –3965.4620 | 26 | –4460.9183 |
| 28 | –4270.5420 | 28 | –4804.0571 |
| 30 | –4575.5983 | 30 | –5147.1444 |

**Table S3.** HOMO-LUMO gap for [n]benzofurans and [n]benzocyclopentadienones calculated at the B3LYP/6-31(d) level of theory

| | HOMO-LUMO gap, eV | | HOMO-LUMO gap, eV | | HOMO-LUMO gap, eV | | HOMO-LUMO gap, eV |
|---|---|---|---|---|---|---|---|
| [n]benzofuran systems | | | | | | | |
| **A1** | 4.95 | | | | | | |
| **A2** | 4.32 | **B2** | 4.52 | **C2** | 4.37 | **D2** | 4.73 |
| **A3** | 3.91 | **B3** | 4.23 | **C3** | 4.08 | **D3** | 4.59 |
| **A4** | 3.67 | **B4** | 4.04 | **C4** | 3.87 | **D4** | 4.48 |
| **A5** | 3.50 | **B5** | 3.93 | **C5** | 3.73 | **D5** | 4.43 |
| **A6** | 3.39 | **B6** | 3.84 | **C6** | 3.62 | **D6** | 4.40 |
| **A7** | 3.31 | **B7** | 3.79 | **C7** | 3.56 | **D7** | 4.38 |
| **A8** | 3.25 | **B8** | 3.74 | **C8** | 3.51 | **D8** | 4.32 |
| **A9** | 3.21 | **B9** | 3.71 | **C9** | 3.47 | **D9** | 4.14 |
| [n]benzocyclopentadienone systems | | | | | | | |
| **A1** | 3.99 | | | | | | |
| **A2** | 3.17 | **B2** | 3.44 | **C2** | 3.45 | **D2** | 3.68 |
| **A3** | 2.79 | **B3** | 3.13 | **C3** | 3.23 | **D3** | 3.42 |
| **A4** | 2.51 | **B4** | 2.97 | **C4** | 3.14 | **D4** | 3.39 |
| **A5** | 2.46 | **B5** | 2.87 | **C5** | 3.09 | **D5** | 3.28 |
| **A6** | 2.38 | **B6** | 2.81 | **C6** | 3.06 | **D6** | 3.27 |
| **A7** | 2.33 | **B7** | 2.77 | **C7** | 3.06 | **D7** | 3.21 |
| **A8** | 2.29 | **B8** | 2.74 | **C8** | 3.05 | **D8** | 3.22 |
| **A9** | 2.26 | **B9** | 2.72 | **C9** | 3.02 | **D9** | 3.19 |

**Table S4.** The optimized Cartesian coordinates of the oxa[4]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.807697 | 1.204138 | -0.731835 |
| 2 | 6 | 0.807697 | 1.204138 | 0.731835 |
| 3 | 6 | -0.671432 | 1.285107 | -0.731835 |
| 4 | 6 | -0.671432 | 1.285107 | 0.731835 |
| 5 | 6 | 1.122738 | 0.042302 | 1.379954 |
| 6 | 6 | 1.122738 | 0.042302 | -1.379954 |
| 7 | 6 | 1.963377 | -0.921491 | -0.693797 |
| 8 | 6 | 1.963377 | -0.921491 | 0.693797 |
| 9 | 8 | -0.023788 | -0.434572 | 2.078264 |
| 10 | 6 | -1.111411 | 0.164601 | 1.379954 |
| 11 | 6 | -1.111411 | 0.164601 | -1.379954 |
| 12 | 6 | -2.052230 | -0.701673 | -0.693797 |
| 13 | 6 | -2.052230 | -0.701673 | 0.693797 |
| 14 | 8 | -0.023788 | -0.434572 | -2.078264 |
| 15 | 1 | 2.425333 | -1.755756 | -1.215229 |
| 16 | 1 | 2.425333 | -1.755756 | 1.215229 |
| 17 | 1 | -2.602489 | -1.480528 | -1.215229 |
| 18 | 1 | -2.602489 | -1.480528 | 1.215229 |

**Table S5.** The optimized Cartesian coordinates of the oxa[6]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.301785 | 0.550066 | -0.880875 |
| 2 | 6 | 0.191301 | 1.400229 | -0.880897 |
| 3 | 6 | 1.116983 | -0.865786 | -0.880897 |
| 4 | 6 | -0.174521 | -1.402412 | -0.880875 |
| 5 | 6 | -1.308285 | -0.534443 | -0.880897 |
| 6 | 6 | -1.127264 | 0.852346 | -0.880875 |
| 7 | 6 | 2.393946 | 0.817232 | -0.065232 |
| 8 | 6 | 0.164040 | 2.524167 | -0.065117 |
| 9 | 6 | 2.103972 | -1.404146 | -0.065117 |
| 10 | 6 | -0.489229 | -2.481834 | -0.065232 |
| 11 | 6 | -2.268012 | -1.120021 | -0.065117 |
| 12 | 6 | -1.904716 | 1.664602 | -0.065232 |
| 13 | 6 | -3.196090 | -0.297334 | 0.604655 |
| 14 | 6 | -3.012824 | 1.107520 | 0.604530 |
| 15 | 6 | 1.340546 | 2.916562 | 0.604655 |
| 16 | 6 | 2.465552 | 2.055422 | 0.604530 |
| 17 | 6 | 0.547272 | -3.162942 | 0.604530 |
| 18 | 6 | 1.855544 | -2.619228 | 0.604655 |
| 19 | 8 | 3.010527 | -0.392826 | 0.305640 |
| 20 | 8 | -1.165066 | 2.803606 | 0.305640 |
| 21 | 8 | -1.845461 | -2.410780 | 0.305640 |
| 22 | 1 | -3.953328 | -0.722708 | 1.255407 |
| 23 | 1 | -3.635693 | 1.712863 | 1.255214 |
| 24 | 1 | 1.350780 | 3.785037 | 1.255407 |
| 25 | 1 | 3.301229 | 2.292170 | 1.255214 |
| 26 | 1 | 0.334463 | -4.005034 | 1.255214 |
| 27 | 1 | 2.602548 | -3.062329 | 1.255407 |

**Table S6.** The optimized Cartesian coordinates of the oxa[8]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.701413 | 4.166565 | 0.000000 |
| 2 | 6 | -0.701413 | 4.166565 | 0.000000 |
| 3 | 6 | -1.372083 | 2.937192 | 0.000000 |
| 4 | 6 | -0.698099 | 1.710140 | 0.000000 |
| 5 | 6 | 0.698099 | 1.710140 | 0.000000 |
| 6 | 6 | 1.372083 | 2.937192 | 0.000000 |
| 7 | 8 | 2.743680 | 2.743680 | 0.000000 |
| 8 | 6 | 2.937192 | 1.372083 | 0.000000 |
| 9 | 6 | 1.710140 | 0.698099 | 0.000000 |
| 10 | 6 | 4.166565 | 0.701413 | 0.000000 |
| 11 | 6 | 4.166565 | -0.701413 | 0.000000 |
| 12 | 1 | 1.252684 | 5.100490 | 0.000000 |
| 13 | 1 | -1.252684 | 5.100490 | 0.000000 |
| 14 | 1 | 5.100490 | 1.252684 | 0.000000 |
| 15 | 1 | 5.100490 | -1.252684 | 0.000000 |
| 16 | 6 | 1.710140 | -0.698099 | 0.000000 |
| 17 | 6 | 2.937192 | -1.372083 | 0.000000 |
| 18 | 8 | 2.743680 | -2.743680 | 0.000000 |
| 19 | 6 | 1.372083 | -2.937192 | 0.000000 |
| 20 | 6 | 0.698099 | -1.710140 | 0.000000 |
| 21 | 6 | 0.701413 | -4.166565 | 0.000000 |
| 22 | 6 | -0.701413 | -4.166565 | 0.000000 |
| 23 | 1 | 1.252684 | -5.100490 | 0.000000 |
| 24 | 1 | -1.252684 | -5.100490 | 0.000000 |
| 25 | 6 | -0.698099 | -1.710140 | 0.000000 |
| 26 | 6 | -1.372083 | -2.937192 | 0.000000 |
| 27 | 8 | -2.743680 | -2.743680 | 0.000000 |
| 28 | 6 | -2.937192 | -1.372083 | 0.000000 |
| 29 | 6 | -1.710140 | -0.698099 | 0.000000 |
| 30 | 6 | -4.166565 | -0.701413 | 0.000000 |
| 31 | 6 | -4.166565 | 0.701413 | 0.000000 |
| 32 | 6 | -2.937192 | 1.372083 | 0.000000 |
| 33 | 6 | -1.710140 | 0.698099 | 0.000000 |
| 34 | 1 | -5.100490 | -1.252684 | 0.000000 |
| 35 | 1 | -5.100490 | 1.252684 | 0.000000 |
| 36 | 8 | -2.743680 | 2.743680 | 0.000000 |

**Table S7.** The optimized Cartesian coordinates of the oxa[10]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.725059 | -0.157754 | -2.206279 |
| 2 | 6 | 1.881594 | -0.193089 | -1.339108 |
| 3 | 6 | 2.312084 | 0.233475 | 0.013689 |
| 4 | 6 | 1.801994 | 0.593810 | 1.315692 |
| 5 | 6 | -0.725059 | 0.157754 | -2.206279 |
| 6 | 6 | -1.881594 | 0.193089 | -1.339108 |
| 7 | 6 | -0.644200 | -0.324569 | 2.197262 |
| 8 | 6 | -2.312084 | -0.233475 | 0.013689 |
| 9 | 6 | -1.801994 | -0.593810 | 1.315692 |
| 10 | 6 | 0.644200 | 0.324569 | 2.197262 |
| 11 | 6 | -2.769825 | -1.164436 | 2.186848 |

| | | | | |
|---|---|---|---|---|
| 12 | 8 | -2.307069 | -1.327458 | 3.453147 |
| 13 | 6 | -1.093888 | -0.720605 | 3.485175 |
| 14 | 6 | -0.555054 | -0.405132 | 4.730776 |
| 15 | 6 | 0.555054 | 0.405132 | 4.730776 |
| 16 | 6 | 1.093888 | 0.720605 | 3.485175 |
| 17 | 8 | 2.307069 | 1.327458 | 3.453147 |
| 18 | 6 | 2.769825 | 1.164436 | 2.186848 |
| 19 | 6 | 4.131396 | 1.364042 | 1.970969 |
| 20 | 6 | 4.643236 | 0.851822 | 0.803192 |
| 21 | 6 | 3.729505 | 0.282574 | -0.079661 |
| 22 | 6 | -3.729505 | -0.282574 | -0.079661 |
| 23 | 6 | -4.643236 | -0.851822 | 0.803192 |
| 24 | 6 | -4.131396 | -1.364042 | 1.970969 |
| 25 | 6 | -3.104428 | 0.478623 | -2.009303 |
| 26 | 8 | -4.196635 | 0.229263 | -1.243998 |
| 27 | 6 | -3.318533 | 0.816374 | -3.342047 |
| 28 | 6 | -2.232024 | 0.711602 | -4.176275 |
| 29 | 6 | -1.035222 | 0.319397 | -3.585729 |
| 30 | 8 | 0.000000 | 0.000000 | -4.399440 |
| 31 | 6 | 1.035222 | -0.319397 | -3.585729 |
| 32 | 6 | 2.232024 | -0.711602 | -4.176275 |
| 33 | 6 | 3.318533 | -0.816374 | -3.342047 |
| 34 | 6 | 3.104428 | -0.478623 | -2.009303 |
| 35 | 8 | 4.196635 | -0.229263 | -1.243998 |
| 36 | 1 | -1.049739 | -0.743289 | 5.633989 |
| 37 | 1 | 1.049739 | 0.743289 | 5.633989 |
| 38 | 1 | 4.742713 | 1.805258 | 2.749737 |
| 39 | 1 | 5.696966 | 0.873203 | 0.550089 |
| 40 | 1 | -5.696966 | -0.873203 | 0.550089 |
| 41 | 1 | -4.742713 | -1.805258 | 2.749737 |
| 42 | 1 | -4.321039 | 1.038533 | -3.689180 |
| 43 | 1 | -2.284195 | 0.853589 | -5.249581 |
| 44 | 1 | 2.284195 | -0.853589 | -5.249581 |
| 45 | 1 | 4.321039 | -1.038533 | -3.689180 |

**Table S8.** The optimized Cartesian coordinates of the oxa[12]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.246534 | -0.345688 | 0.933092 |
| 2 | 6 | 1.974873 | 1.064613 | 0.981162 |
| 3 | 6 | -2.044941 | 1.418528 | -0.044737 |
| 4 | 6 | -2.246294 | 0.345671 | 0.933297 |
| 5 | 6 | -1.974668 | -1.064628 | 0.981280 |
| 6 | 6 | 2.045089 | -1.418561 | -0.044925 |
| 7 | 6 | 1.075452 | -1.915613 | -0.978333 |
| 8 | 6 | -0.371659 | -2.188256 | -0.931177 |
| 9 | 6 | -1.408582 | -2.044705 | 0.049489 |
| 10 | 6 | -1.075393 | 1.915597 | -0.978224 |
| 11 | 6 | 0.371707 | 2.188339 | -0.931108 |
| 12 | 6 | 1.408720 | 2.044758 | 0.049455 |
| 13 | 6 | 2.857582 | 1.818860 | 1.791990 |
| 14 | 6 | 3.766966 | 1.322771 | 2.726554 |
| 15 | 6 | 4.038690 | -0.032834 | 2.668800 |
| 16 | 6 | 3.369282 | -0.764417 | 1.687883 |
| 17 | 8 | 3.934990 | -1.901674 | 1.178293 |
| 18 | 6 | 3.212808 | -2.206229 | 0.060444 |
| 19 | 6 | 2.200657 | 3.198379 | 0.237627 |
| 20 | 8 | 2.959726 | 3.117479 | 1.369854 |

| | | | | |
|---|---|---|---|---|
| 21 | 6 | 0.559796 | 3.238668 | -1.855520 |
| 22 | 6 | 1.552393 | 4.225041 | -1.799667 |
| 23 | 6 | 2.344840 | 4.253624 | -0.666766 |
| 24 | 6 | -1.572716 | 2.826262 | -1.936254 |
| 25 | 8 | -0.565564 | 3.477534 | -2.600805 |
| 26 | 6 | -2.861328 | 3.372582 | -1.973409 |
| 27 | 6 | -3.681620 | 3.115408 | -0.890153 |
| 28 | 6 | -3.212785 | 2.205997 | 0.060524 |
| 29 | 8 | -3.934885 | 1.901530 | 1.178444 |
| 30 | 6 | -3.369047 | 0.764365 | 1.688100 |
| 31 | 6 | -4.038409 | 0.032748 | 2.669023 |
| 32 | 6 | -3.766732 | -1.322866 | 2.726661 |
| 33 | 6 | -2.857419 | -1.818914 | 1.792013 |
| 34 | 6 | -2.200779 | -3.198187 | 0.237350 |
| 35 | 8 | -2.959776 | -3.117428 | 1.369616 |
| 36 | 6 | -2.345176 | -4.253178 | -0.667330 |
| 37 | 6 | -0.559961 | -3.238298 | -1.855873 |
| 38 | 6 | -1.552748 | -4.224465 | -1.800242 |
| 39 | 8 | 0.565393 | -3.477292 | -2.601079 |
| 40 | 6 | 1.572635 | -2.826445 | -1.936226 |
| 41 | 6 | 3.681461 | -3.115925 | -0.890034 |
| 42 | 6 | 2.861112 | -3.373147 | -1.973222 |
| 43 | 1 | 4.348150 | 2.002664 | 3.339524 |
| 44 | 1 | 4.845244 | -0.485185 | 3.235021 |
| 45 | 1 | 1.571772 | 5.015227 | -2.541845 |
| 46 | 1 | 3.060235 | 5.045252 | -0.474360 |
| 47 | 1 | -3.120023 | 4.096847 | -2.737738 |
| 48 | 1 | -4.646555 | 3.592901 | -0.762160 |
| 49 | 1 | -4.844969 | 0.485065 | 3.235259 |
| 50 | 1 | -4.347956 | -2.002790 | 3.339558 |
| 51 | 1 | -3.060709 | -5.044726 | -0.475117 |
| 52 | 1 | -1.572285 | -5.014484 | -2.542594 |
| 53 | 1 | 4.646317 | -3.593557 | -0.761953 |
| 54 | 1 | 3.119683 | -4.097535 | -2.737474 |

**Table S9.** The optimized Cartesian coordinates of the oxa[14]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.499899 | 1.098400 | -1.544440 |
| 2 | 6 | 2.197097 | -0.091718 | -1.164407 |
| 3 | 6 | -0.501613 | -2.410168 | 0.614117 |
| 4 | 6 | -0.961984 | -2.214987 | -0.750130 |
| 5 | 6 | -1.448629 | -1.133178 | -1.546298 |
| 6 | 6 | 0.954077 | 2.191241 | -0.742023 |
| 7 | 6 | 0.499408 | 2.393427 | 0.592405 |
| 8 | 6 | -0.495496 | 1.837563 | 1.504968 |
| 9 | 6 | -2.150230 | 0.098573 | -1.176210 |
| 10 | 6 | 0.437825 | -1.817993 | 1.511395 |
| 11 | 6 | 1.724854 | -1.157531 | 1.275915 |
| 12 | 6 | 2.432676 | -0.767803 | 0.101782 |
| 13 | 6 | 3.311297 | -0.426344 | -1.963673 |
| 14 | 6 | 1.919079 | 1.706398 | -2.746695 |
| 15 | 8 | 1.681118 | 3.063012 | -2.741720 |
| 16 | 6 | 1.287537 | 3.355651 | -1.457816 |
| 17 | 6 | 3.771750 | -1.198401 | 0.034063 |
| 18 | 8 | 4.262586 | -1.109817 | -1.243766 |
| 19 | 6 | 2.513468 | -1.508605 | 2.387422 |
| 20 | 6 | 0.576011 | -2.438182 | 2.768501 |

| | | | | |
|---|---|---|---|---|
| 21 | 8 | 1.761401 | -2.095127 | 3.380295 |
| 22 | 6 | -0.909680 | -3.717886 | 0.947387 |
| 23 | 8 | -1.349347 | -4.403466 | -0.156901 |
| 24 | 6 | -1.331939 | -3.502131 | -1.192022 |
| 25 | 6 | -1.960165 | -1.473048 | -2.814570 |
| 26 | 6 | -3.075130 | 0.305878 | -2.216267 |
| 27 | 8 | -2.816131 | -0.507177 | -3.296118 |
| 28 | 6 | -0.423857 | 2.649916 | 2.656939 |
| 29 | 8 | 0.495507 | 3.664203 | 2.507832 |
| 30 | 6 | 0.896957 | 3.600876 | 1.195588 |
| 31 | 6 | -2.434598 | 0.757136 | 0.054856 |
| 32 | 6 | -3.779198 | 1.128908 | 0.244693 |
| 33 | 6 | -1.754452 | 1.201922 | 1.262531 |
| 34 | 6 | -2.793145 | 1.541987 | 2.156143 |
| 35 | 8 | -4.026241 | 1.466779 | 1.551166 |
| 36 | 6 | -4.323409 | 0.925584 | -2.067106 |
| 37 | 6 | -4.719341 | 1.271170 | -0.781024 |
| 38 | 6 | -2.625496 | 2.148929 | 3.402255 |
| 39 | 6 | -1.384127 | 2.711358 | 3.670873 |
| 40 | 6 | 1.387770 | 4.713775 | 0.502254 |
| 41 | 6 | 1.501101 | 4.613068 | -0.879318 |
| 42 | 6 | 3.564110 | 0.062805 | -3.246627 |
| 43 | 6 | 2.818966 | 1.157313 | -3.665931 |
| 44 | 6 | 3.906781 | -1.661433 | 2.367410 |
| 45 | 6 | 4.543236 | -1.582066 | 1.135317 |
| 46 | 6 | -0.828533 | -4.284046 | 2.221881 |
| 47 | 6 | -0.111690 | -3.586212 | 3.184714 |
| 48 | 6 | -2.005677 | -2.766649 | -3.350843 |
| 49 | 6 | -1.735453 | -3.822155 | -2.490198 |
| 50 | 1 | -5.001860 | 0.991719 | -2.910518 |
| 51 | 1 | -5.712497 | 1.651161 | -0.568841 |
| 52 | 1 | -3.475245 | 2.309793 | 4.056552 |
| 53 | 1 | -1.222359 | 3.336697 | 4.542055 |
| 54 | 1 | 1.594172 | 5.639081 | 1.028629 |
| 55 | 1 | 1.834328 | 5.445527 | -1.489120 |
| 56 | 1 | 4.404399 | -0.307475 | -3.823540 |
| 57 | 1 | 3.057353 | 1.687240 | -4.581655 |
| 58 | 1 | 4.430580 | -1.985548 | 3.259952 |
| 59 | 1 | 5.596364 | -1.811942 | 1.017683 |
| 60 | 1 | -1.250431 | -5.262995 | 2.420564 |
| 61 | 1 | 0.073240 | -4.003682 | 4.168433 |
| 62 | 1 | -2.425059 | -2.932156 | -4.337219 |
| 63 | 1 | -1.914477 | -4.852704 | -2.776136 |

**Table S10.** The optimized Cartesian coordinates of the oxa[16]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.010530 | -1.737294 | -1.604297 |
| 2 | 6 | -0.376089 | -2.050982 | -1.606467 |
| 3 | 6 | 1.840379 | 0.540766 | 1.509644 |
| 4 | 6 | 1.010545 | 1.737286 | 1.604292 |
| 5 | 6 | -0.376071 | 2.050984 | 1.606463 |
| 6 | 6 | 1.576826 | 0.842604 | -1.751062 |
| 7 | 6 | 0.376029 | 1.606496 | -2.050828 |
| 8 | 6 | -1.010607 | 1.604418 | -1.737230 |
| 9 | 6 | -1.576918 | 1.751301 | 0.842630 |
| 10 | 6 | 0.376023 | -1.606502 | 2.050829 |
| 11 | 6 | -1.010613 | -1.604416 | 1.737232 |

| | | | | |
|---|---|---|---|---|
| 12 | 6 | -1.840493 | -1.509864 | 0.540748 |
| 13 | 6 | -0.782064 | -3.014650 | -2.549392 |
| 14 | 6 | 1.865303 | -2.723871 | -2.130505 |
| 15 | 6 | -3.150225 | -1.790825 | 0.985504 |
| 16 | 6 | -1.865310 | -2.130731 | 2.723827 |
| 17 | 6 | 0.782101 | -2.549477 | 3.014415 |
| 18 | 6 | 3.150146 | 0.985489 | 1.790488 |
| 19 | 8 | 3.182489 | 2.334111 | 2.066300 |
| 20 | 6 | 1.865326 | 2.723858 | 2.130494 |
| 21 | 6 | -0.782036 | 3.014658 | 2.549387 |
| 22 | 6 | -2.627597 | 2.344372 | 1.575706 |
| 23 | 8 | -2.151818 | 3.080923 | 2.636449 |
| 24 | 6 | -1.865302 | 2.130747 | -2.723820 |
| 25 | 6 | 0.782114 | 2.549474 | -3.014410 |
| 26 | 8 | -3.182491 | -2.066662 | 2.334124 |
| 27 | 8 | 2.151904 | 2.636498 | -3.080530 |
| 28 | 6 | -3.150217 | 1.790842 | -0.985498 |
| 29 | 8 | -3.182484 | 2.066684 | -2.334117 |
| 30 | 6 | -1.840486 | 1.509871 | -0.540746 |
| 31 | 6 | 1.840372 | -0.540780 | -1.509645 |
| 32 | 8 | 3.182468 | -2.334132 | -2.066316 |
| 33 | 6 | 3.150136 | -0.985511 | -1.790496 |
| 34 | 6 | 1.576824 | -0.842616 | 1.751063 |
| 35 | 6 | 2.627565 | -1.575699 | 2.344010 |
| 36 | 8 | 2.151891 | -2.636513 | 3.080533 |
| 37 | 6 | -1.576931 | -1.751294 | -0.842628 |
| 38 | 6 | -2.627616 | -2.344357 | -1.575702 |
| 39 | 8 | -2.151846 | -3.080908 | -2.636449 |
| 40 | 6 | 3.959723 | -1.165476 | 2.412748 |
| 41 | 6 | 4.234072 | 0.162910 | 2.106684 |
| 42 | 6 | 1.439573 | 3.816951 | 2.894255 |
| 43 | 6 | -3.959736 | 2.413249 | 1.165450 |
| 44 | 6 | -4.234104 | 2.107162 | -0.162933 |
| 45 | 6 | -0.080834 | 3.181935 | -3.914793 |
| 46 | 6 | 4.234067 | -0.162938 | -2.106689 |
| 47 | 6 | 3.959727 | 1.165451 | -2.412746 |
| 48 | 6 | 0.080989 | -3.914982 | -3.181798 |
| 49 | 6 | -4.234117 | -2.107138 | 0.162943 |
| 50 | 6 | -3.959754 | -2.413228 | -1.165441 |
| 51 | 6 | -1.439426 | -2.894484 | 3.816871 |
| 52 | 6 | -0.080850 | -3.181929 | 3.914802 |
| 53 | 1 | 4.717587 | -1.820054 | 2.828925 |
| 54 | 1 | 5.215689 | 0.591578 | 2.276463 |
| 55 | 1 | -4.717569 | 2.829556 | 1.819982 |
| 56 | 1 | -5.215697 | 2.277061 | -0.591610 |
| 57 | 1 | 0.311119 | 3.834703 | -4.686881 |
| 58 | 1 | 5.215681 | -0.591612 | -2.276470 |
| 59 | 1 | 4.717596 | 1.820027 | -2.828919 |
| 60 | 1 | -5.215709 | -2.277030 | 0.591623 |
| 61 | 1 | -4.717593 | -2.829530 | -1.819970 |
| 62 | 1 | -2.164509 | -3.327725 | 4.496958 |
| 63 | 1 | 0.311099 | -3.834697 | 4.686891 |
| 64 | 6 | 1.439540 | -3.816956 | -2.894272 |
| 65 | 6 | -1.439412 | 2.894502 | -3.816861 |
| 66 | 1 | -2.164492 | 3.327751 | -4.496946 |
| 67 | 6 | 0.081024 | 3.914988 | 3.181785 |
| 68 | 1 | 2.164740 | 4.497011 | 3.327397 |
| 69 | 1 | -0.310836 | 4.687144 | 3.834526 |
| 70 | 1 | -0.310878 | -4.687132 | -3.834542 |
| 71 | 1 | 2.164700 | -4.497019 | -3.327421 |
| 72 | 6 | 2.627572 | 1.575681 | -2.344008 |

**Table S11.** The optimized Cartesian coordinates of the oxa[18]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.729474 | 0.012766 | 2.726912 |
| 2 | 6 | 0.729474 | -0.012766 | 2.726912 |
| 3 | 6 | -1.839644 | -0.395815 | -1.878882 |
| 4 | 6 | -0.715061 | -0.015096 | -2.738750 |
| 5 | 6 | 0.715061 | 0.015096 | -2.738750 |
| 6 | 6 | -2.080932 | 1.328221 | 0.780637 |
| 7 | 6 | -1.374437 | 2.389562 | 0.124125 |
| 8 | 6 | 0.000000 | 2.870193 | 0.000632 |
| 9 | 6 | 1.839644 | 0.395815 | -1.878882 |
| 10 | 6 | 0.000000 | -2.870193 | 0.000632 |
| 11 | 6 | 1.374437 | -2.389562 | 0.124125 |
| 12 | 6 | 2.080932 | -1.328221 | 0.780637 |
| 13 | 6 | 1.080035 | 0.165304 | 4.086035 |
| 14 | 6 | -1.080035 | -0.165304 | 4.086035 |
| 15 | 6 | -3.491902 | 1.418679 | 0.724776 |
| 16 | 6 | 3.491902 | -1.418679 | 0.724776 |
| 17 | 6 | 2.165724 | -3.515164 | -0.216580 |
| 18 | 6 | 0.124552 | -4.276313 | -0.056300 |
| 19 | 8 | 1.414656 | -4.657032 | -0.310165 |
| 20 | 6 | -2.985471 | -0.026405 | -2.627628 |
| 21 | 8 | -2.663346 | 0.409117 | -3.885110 |
| 22 | 6 | -1.307322 | 0.263366 | -3.990152 |
| 23 | 6 | 1.307322 | -0.263366 | -3.990152 |
| 24 | 6 | 2.985471 | 0.026405 | -2.627628 |
| 25 | 8 | 2.663346 | -0.409117 | -3.885110 |
| 26 | 6 | -0.124552 | 4.276313 | -0.056300 |
| 27 | 8 | -1.414656 | 4.657032 | -0.310165 |
| 28 | 6 | -2.165724 | 3.515164 | -0.216580 |
| 29 | 8 | 0.000000 | 0.000000 | 4.911762 |
| 30 | 6 | 2.334536 | 3.306368 | 0.287425 |
| 31 | 6 | -1.819624 | 0.364036 | 1.866642 |
| 32 | 6 | -3.100800 | 0.043277 | 2.369192 |
| 33 | 8 | -4.103763 | 0.547945 | 1.586263 |
| 34 | 6 | -1.341165 | -2.385307 | -0.110644 |
| 35 | 6 | -2.334536 | -3.306368 | 0.287425 |
| 36 | 6 | 1.819624 | -0.364036 | 1.866642 |
| 37 | 6 | 3.100800 | -0.043277 | 2.369192 |
| 38 | 8 | 4.103763 | -0.547945 | 1.586263 |
| 39 | 6 | -3.443941 | -1.642364 | -0.576196 |
| 40 | 8 | -3.592951 | -2.782874 | 0.165644 |
| 41 | 6 | -2.082588 | -1.319784 | -0.803033 |
| 42 | 6 | 3.443941 | 1.642364 | -0.576196 |
| 43 | 8 | 3.592951 | 2.782874 | 0.165644 |
| 44 | 6 | 2.082588 | 1.319784 | -0.803033 |
| 45 | 6 | 1.341165 | 2.385307 | -0.110644 |
| 46 | 6 | -4.554758 | -1.077412 | -1.200362 |
| 47 | 6 | -4.316595 | -0.245926 | -2.280775 |
| 48 | 6 | -0.668099 | 0.185544 | -5.230319 |
| 49 | 6 | 0.668099 | -0.185544 | -5.230319 |
| 50 | 6 | -0.890015 | -5.193311 | 0.222280 |
| 51 | 6 | -2.148126 | -4.676991 | 0.493310 |
| 52 | 6 | 4.240121 | -2.427498 | 0.117176 |
| 53 | 6 | 3.552765 | -3.544485 | -0.329739 |
| 54 | 6 | 2.353469 | 0.464593 | 4.567106 |
| 55 | 6 | 3.393515 | 0.430846 | 3.651443 |
| 56 | 6 | -3.393515 | -0.430846 | 3.651443 |
| 57 | 6 | -2.353469 | -0.464593 | 4.567106 |

| | | | | |
|---|---|---|---|---|
| 58 | 6 | -3.552765 | 3.544485 | -0.329739 |
| 59 | 6 | -4.240121 | 2.427498 | 0.117176 |
| 60 | 6 | 2.148126 | 4.676991 | 0.493310 |
| 61 | 6 | 0.890015 | 5.193311 | 0.222280 |
| 62 | 6 | 4.316595 | 0.245926 | -2.280775 |
| 63 | 6 | 4.554758 | 1.077412 | -1.200362 |
| 64 | 1 | -5.553182 | -1.393468 | -0.920111 |
| 65 | 1 | -5.114520 | 0.126409 | -2.913447 |
| 66 | 1 | -1.230051 | 0.335080 | -6.145393 |
| 67 | 1 | 1.230051 | -0.335080 | -6.145393 |
| 68 | 1 | -0.680346 | -6.256808 | 0.244877 |
| 69 | 1 | -2.995115 | -5.310073 | 0.732916 |
| 70 | 1 | 5.323212 | -2.387998 | 0.143336 |
| 71 | 1 | 4.059487 | -4.440443 | -0.670303 |
| 72 | 1 | 2.511592 | 0.676513 | 5.618574 |
| 73 | 1 | 4.423206 | 0.610745 | 3.939463 |
| 74 | 1 | -4.423206 | -0.610745 | 3.939463 |
| 75 | 1 | -2.511592 | -0.676513 | 5.618574 |
| 76 | 1 | -4.059487 | 4.440443 | -0.670303 |
| 77 | 1 | -5.323212 | 2.387998 | 0.143336 |
| 78 | 1 | 2.995115 | 5.310073 | 0.732916 |
| 79 | 1 | 0.680346 | 6.256808 | 0.244877 |
| 80 | 1 | 5.114520 | -0.126409 | -2.913447 |
| 81 | 1 | 5.553182 | 1.393468 | -0.920111 |

**Table S12.** The optimized Cartesian coordinates of the oxa[20]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.325320 | 2.835042 | -1.070872 |
| 2 | 6 | 0.404093 | 3.051739 | 0.388161 |
| 3 | 6 | -0.617839 | -1.847752 | -2.091666 |
| 4 | 6 | -0.325320 | -2.835042 | -1.070872 |
| 5 | 6 | -0.199328 | -2.401605 | 1.666856 |
| 6 | 6 | 1.458742 | 0.631352 | -2.335207 |
| 7 | 6 | 2.445246 | -0.218651 | -1.689278 |
| 8 | 6 | 3.090225 | -0.414406 | -0.374198 |
| 9 | 6 | 0.695359 | -1.411836 | 2.343721 |
| 10 | 6 | -2.869791 | 0.286402 | 1.047351 |
| 11 | 6 | -1.875552 | 0.588874 | 2.109835 |
| 12 | 6 | -0.695359 | 1.411836 | 2.343721 |
| 13 | 6 | 0.660911 | 4.443913 | 0.500228 |
| 14 | 6 | 0.130633 | 4.148925 | -1.583432 |
| 15 | 6 | 1.434235 | 0.489530 | -3.749360 |
| 16 | 6 | -0.383568 | 1.586053 | 3.721194 |
| 17 | 6 | -2.540000 | 0.161834 | 3.298208 |
| 18 | 6 | -4.049599 | -0.044277 | 1.757109 |
| 19 | 8 | -3.807446 | -0.278052 | 3.073300 |
| 20 | 6 | -0.247681 | -2.270368 | -3.396454 |
| 21 | 6 | -0.130633 | -4.148925 | -1.583432 |
| 22 | 6 | -0.822898 | -3.091861 | 2.737641 |
| 23 | 6 | 0.383568 | -1.586053 | 3.721194 |
| 24 | 8 | -0.585521 | -2.510183 | 3.941748 |
| 25 | 6 | 4.409201 | -0.818319 | -0.697967 |
| 26 | 8 | 4.513943 | -1.225396 | -1.991154 |
| 27 | 6 | 3.345282 | -0.861688 | -2.587530 |
| 28 | 8 | 0.389593 | 5.110200 | -0.654645 |
| 29 | 6 | 4.049599 | 0.044277 | 1.757109 |
| 30 | 6 | 0.617839 | 1.847752 | -2.091666 |

| | | | | |
|---|---|---|---|---|
| 31 | 6 | 0.247681 | 2.270368 | -3.396454 |
| 32 | 8 | 0.643294 | 1.404114 | -4.364382 |
| 33 | 6 | -3.090225 | 0.414406 | -0.374198 |
| 34 | 6 | -4.409201 | 0.818319 | -0.697967 |
| 35 | 6 | 0.199328 | 2.401605 | 1.666856 |
| 36 | 6 | 0.822898 | 3.091861 | 2.737641 |
| 37 | 8 | 0.585521 | 2.510183 | 3.941748 |
| 38 | 6 | -3.345282 | 0.861688 | -2.587530 |
| 39 | 8 | -4.513943 | 1.225396 | -1.991154 |
| 40 | 6 | -2.445246 | 0.218651 | -1.689278 |
| 41 | 6 | 2.540000 | -0.161834 | 3.298208 |
| 42 | 8 | 3.807446 | 0.278052 | 3.073300 |
| 43 | 6 | 1.875552 | -0.588874 | 2.109835 |
| 44 | 6 | 2.869791 | -0.286402 | 1.047351 |
| 45 | 6 | -5.371977 | 0.100192 | 1.328704 |
| 46 | 6 | -5.555200 | 0.660622 | 0.082428 |
| 47 | 6 | -1.022245 | 1.064987 | 4.842817 |
| 48 | 6 | -2.153525 | 0.318837 | 4.623926 |
| 49 | 6 | 1.201506 | 5.118707 | 1.591678 |
| 50 | 6 | 1.377277 | 4.374384 | 2.737501 |
| 51 | 6 | -0.247681 | 3.506780 | -3.808431 |
| 52 | 6 | -0.241031 | 4.516005 | -2.871077 |
| 53 | 6 | 3.226556 | -1.026579 | -3.962557 |
| 54 | 6 | 2.202181 | -0.337266 | -4.566217 |
| 55 | 6 | 5.371977 | -0.100192 | 1.328704 |
| 56 | 6 | 5.555200 | -0.660622 | 0.082428 |
| 57 | 6 | 1.022245 | -1.064987 | 4.842817 |
| 58 | 6 | 2.153525 | -0.318837 | 4.623926 |
| 59 | 1 | -6.187324 | -0.113767 | 2.010168 |
| 60 | 1 | -6.529183 | 0.914613 | -0.319873 |
| 61 | 1 | -0.659451 | 1.323614 | 5.830484 |
| 62 | 1 | -2.783995 | -0.062052 | 5.418883 |
| 63 | 1 | 1.459224 | 6.168853 | 1.515715 |
| 64 | 1 | 1.778516 | 4.785391 | 3.656765 |
| 65 | 1 | -0.474379 | 3.671334 | -4.855417 |
| 66 | 1 | -0.455956 | 5.551946 | -3.106971 |
| 67 | 1 | 3.968417 | -1.596341 | -4.510289 |
| 68 | 1 | 2.036376 | -0.331649 | -5.637046 |
| 69 | 1 | 6.187324 | 0.113767 | 2.010168 |
| 70 | 1 | 6.529183 | -0.914613 | -0.319873 |
| 71 | 1 | 0.659451 | -1.323614 | 5.830484 |
| 72 | 1 | 2.783995 | 0.062052 | 5.418883 |
| 73 | 6 | -0.404093 | -3.051739 | 0.388161 |
| 74 | 6 | -0.660911 | -4.443913 | 0.500228 |
| 75 | 8 | -0.389593 | -5.110200 | -0.654645 |
| 76 | 6 | -1.458742 | -0.631352 | -2.335207 |
| 77 | 6 | -1.434235 | -0.489530 | -3.749360 |
| 78 | 8 | -0.643294 | -1.404114 | -4.364382 |
| 79 | 6 | -2.202181 | 0.337266 | -4.566217 |
| 80 | 6 | -3.226556 | 1.026579 | -3.962557 |
| 81 | 1 | -2.036376 | 0.331649 | -5.637046 |
| 82 | 1 | -3.968417 | 1.596341 | -4.510289 |
| 83 | 6 | -1.377277 | -4.374384 | 2.737501 |
| 84 | 6 | -1.201506 | -5.118707 | 1.591678 |
| 85 | 6 | 0.241031 | -4.516005 | -2.871077 |
| 86 | 6 | 0.247681 | -3.506780 | -3.808431 |
| 87 | 1 | -1.778516 | -4.785391 | 3.656765 |
| 88 | 1 | -1.459224 | -6.168853 | 1.515715 |
| 89 | 1 | 0.455956 | -5.551946 | -3.106971 |
| 90 | 1 | 0.474379 | -3.671334 | -4.855417 |

**Table S13.** The optimized Cartesian coordinates of the oxa[22]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.728595 | -3.272354 | 0.130759 |
| 2 | 6 | 0.724524 | -3.247905 | 0.433278 |
| 3 | 6 | -2.598719 | 1.365953 | -0.945801 |
| 4 | 6 | -0.712094 | 3.267001 | -0.120818 |
| 5 | 6 | 2.597935 | 1.512699 | 0.691565 |
| 6 | 6 | -2.616871 | -1.328332 | 0.918064 |
| 7 | 6 | -2.420233 | -0.258421 | 1.920209 |
| 8 | 6 | -1.416366 | 0.374207 | 2.857351 |
| 9 | 6 | 2.372813 | 0.589664 | 1.889612 |
| 10 | 6 | 1.421395 | -0.130385 | -2.878541 |
| 11 | 6 | 2.423127 | -0.590496 | -1.843719 |
| 12 | 6 | 2.616690 | -1.469869 | -0.670717 |
| 13 | 6 | 0.977778 | -4.587404 | 0.849300 |
| 14 | 6 | -0.983579 | -4.662639 | -0.053484 |
| 15 | 6 | -3.991467 | -1.518924 | 0.580663 |
| 16 | 6 | 3.990202 | -1.599967 | -0.301818 |
| 17 | 6 | 3.652758 | -0.096780 | -2.379259 |
| 18 | 6 | 2.224863 | 0.423428 | -3.908803 |
| 19 | 8 | 3.516051 | 0.578667 | -3.541043 |
| 20 | 6 | -4.014744 | 1.356479 | -0.784499 |
| 21 | 6 | -1.136520 | 4.565876 | 0.249991 |
| 22 | 6 | 4.013497 | 1.477239 | 0.530761 |
| 23 | 6 | 3.693725 | 0.167649 | 2.220178 |
| 24 | 8 | 4.639881 | 0.654029 | 1.393674 |
| 25 | 6 | -2.217566 | 1.101015 | 3.775734 |
| 26 | 8 | -3.508860 | 1.192335 | 3.387566 |
| 27 | 6 | -3.648148 | 0.323793 | 2.362320 |
| 28 | 8 | -0.003387 | -5.443139 | 0.467231 |
| 29 | 6 | 0.047136 | 0.301962 | 4.739442 |
| 30 | 6 | -1.948288 | -2.470622 | 0.172027 |
| 31 | 6 | -3.024987 | -3.137836 | -0.472463 |
| 32 | 8 | -4.209621 | -2.509623 | -0.310155 |
| 33 | 6 | 0.035083 | -0.295089 | -3.320851 |
| 34 | 6 | -0.040773 | -0.526716 | -4.720529 |
| 35 | 6 | 1.945331 | -2.466193 | 0.258995 |
| 36 | 6 | 3.019858 | -3.014438 | 1.010260 |
| 37 | 8 | 4.205383 | -2.423600 | 0.745926 |
| 38 | 6 | -2.008916 | -1.029244 | -3.993967 |
| 39 | 8 | -1.208366 | -1.103756 | -5.085554 |
| 40 | 6 | -1.396626 | -0.353564 | -2.891793 |
| 41 | 6 | 2.015310 | -0.317576 | 4.109677 |
| 42 | 8 | 1.215298 | -0.202492 | 5.198255 |
| 43 | 6 | 1.401410 | 0.155930 | 2.907575 |
| 44 | 6 | -0.029883 | 0.287000 | 3.320973 |
| 45 | 6 | 1.969770 | 0.527269 | -5.281273 |
| 46 | 6 | 0.829529 | -0.092869 | -5.720386 |
| 47 | 6 | 5.147875 | -1.108733 | -0.895848 |
| 48 | 6 | 4.970314 | -0.317087 | -1.990605 |
| 49 | 6 | 2.051569 | -5.074849 | 1.583959 |
| 50 | 6 | 3.095027 | -4.198683 | 1.747040 |
| 51 | 6 | -3.102380 | -4.429010 | -0.999218 |
| 52 | 6 | -2.058870 | -5.266053 | -0.693576 |
| 53 | 6 | -4.966865 | 0.039261 | 2.022438 |
| 54 | 6 | -5.147559 | -0.931720 | 1.083765 |
| 55 | 6 | -0.821740 | 0.904946 | 5.648996 |
| 56 | 6 | -1.960869 | 1.441809 | 5.109003 |
| 57 | 6 | 4.183823 | -0.557287 | 3.304861 |

| | | | | |
|---|---|---|---|---|
| 58 | 6 | 3.306152 | -0.778204 | 4.329594 |
| 59 | 1 | 2.734129 | 0.925855 | -5.938028 |
| 60 | 1 | 0.567610 | -0.220779 | -6.764251 |
| 61 | 1 | 6.112031 | -1.377580 | -0.481679 |
| 62 | 1 | 5.775517 | 0.108365 | -2.577417 |
| 63 | 1 | 2.051060 | -6.094643 | 1.951055 |
| 64 | 1 | 4.020054 | -4.452885 | 2.251239 |
| 65 | 1 | -4.028684 | -4.763125 | -1.451786 |
| 66 | 1 | -2.059570 | -6.333084 | -0.883767 |
| 67 | 1 | -5.770252 | 0.561644 | 2.527790 |
| 68 | 1 | -6.112929 | -1.267992 | 0.725411 |
| 69 | 1 | -0.559372 | 0.960199 | 6.699107 |
| 70 | 1 | -2.723850 | 1.950319 | 5.686707 |
| 71 | 1 | 5.237663 | -0.805819 | 3.341427 |
| 72 | 1 | 3.579761 | -1.198378 | 5.290399 |
| 73 | 6 | 0.706463 | 3.241395 | -0.441699 |
| 74 | 6 | 1.127970 | 4.459991 | -1.026514 |
| 75 | 6 | -2.369842 | 0.249019 | -1.965182 |
| 76 | 6 | -3.689309 | -0.227482 | -2.218372 |
| 77 | 8 | -4.637857 | 0.393639 | -1.491114 |
| 78 | 6 | -4.177106 | -1.131275 | -3.160389 |
| 79 | 6 | -3.298534 | -1.524185 | -4.131291 |
| 80 | 1 | -5.230440 | -1.384459 | -3.153184 |
| 81 | 1 | -3.570434 | -2.105146 | -5.004853 |
| 82 | 6 | 1.974520 | 2.484463 | -0.223801 |
| 83 | 6 | 2.909609 | 3.243030 | -1.000303 |
| 84 | 8 | 2.385703 | 4.382268 | -1.519070 |
| 85 | 6 | -1.978493 | 2.481335 | -0.208972 |
| 86 | 6 | -2.916424 | 3.358792 | 0.426127 |
| 87 | 8 | -2.395017 | 4.569984 | 0.746505 |
| 88 | 6 | 4.862649 | 2.179002 | -0.321280 |
| 89 | 6 | 4.284302 | 3.109232 | -1.136179 |
| 90 | 6 | 0.553543 | 5.728986 | -0.890500 |
| 91 | 6 | -0.563783 | 5.795090 | -0.096200 |
| 92 | 6 | -4.291722 | 3.249310 | 0.577512 |
| 93 | 6 | -4.867090 | 2.193239 | -0.068668 |
| 94 | 1 | 5.929198 | 1.999191 | -0.265922 |
| 95 | 1 | 4.833196 | 3.784054 | -1.782283 |
| 96 | 1 | 1.056162 | 6.596686 | -1.301728 |
| 97 | 1 | -1.067814 | 6.718650 | 0.163837 |
| 98 | 1 | -4.842901 | 4.023869 | 1.097497 |
| 99 | 1 | -5.933355 | 2.005363 | -0.095626 |

**Table S14.** The optimized Cartesian coordinates of the oxa[24]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 8 | 3.291043 | -3.319643 | 2.470491 |
| 2 | 6 | 1.551540 | -0.895127 | 4.563950 |
| 3 | 6 | -1.630149 | -2.975204 | -0.085447 |
| 4 | 6 | -1.439901 | -2.417129 | -1.382546 |
| 5 | 6 | -1.891957 | -1.187590 | -2.055831 |
| 6 | 6 | 5.907529 | 0.405094 | -0.941054 |
| 7 | 6 | 5.925486 | 0.244852 | 0.441370 |
| 8 | 6 | 3.466988 | 1.374326 | 2.581544 |
| 9 | 6 | 2.701576 | 1.353285 | 1.397926 |
| 10 | 8 | 4.614815 | 0.611874 | 2.465451 |
| 11 | 6 | 4.697725 | 0.307603 | 1.123800 |
| 12 | 6 | 3.461694 | 0.485581 | 0.488466 |

| | | | | |
|---|---|---|---|---|
| 13 | 6 | 3.444389 | 0.186974 | -0.904933 |
| 14 | 6 | 4.656869 | 0.396065 | -1.578531 |
| 15 | 1 | 6.822162 | 0.464089 | -1.520632 |
| 16 | 1 | 6.855941 | 0.205424 | 0.997130 |
| 17 | 6 | -2.559847 | 3.916643 | 1.331469 |
| 18 | 6 | -2.017283 | 2.730505 | 0.798302 |
| 19 | 6 | -2.935795 | 4.098962 | 2.667429 |
| 20 | 6 | -3.083667 | 2.958221 | 3.440569 |
| 21 | 6 | -2.995317 | 1.723845 | 2.770570 |
| 22 | 6 | -2.466563 | 1.539615 | 1.479780 |
| 23 | 1 | -3.214157 | 5.079176 | 3.038600 |
| 24 | 1 | -3.501466 | 3.005151 | 4.440404 |
| 25 | 8 | -3.947807 | 0.768573 | 3.079507 |
| 26 | 6 | -4.264121 | 0.196818 | 1.864383 |
| 27 | 6 | -3.265122 | 0.438776 | 0.910108 |
| 28 | 6 | -3.582636 | 0.056439 | -0.426398 |
| 29 | 6 | -4.953193 | 0.073495 | -0.738263 |
| 30 | 6 | -5.971201 | -0.084252 | 0.210075 |
| 31 | 6 | -5.595353 | -0.125893 | 1.549396 |
| 32 | 1 | -6.330411 | -0.222963 | 2.340901 |
| 33 | 1 | -7.008045 | -0.170983 | -0.095206 |
| 34 | 8 | -5.146854 | 0.163455 | -2.097679 |
| 35 | 6 | -3.905583 | -0.030401 | -2.664370 |
| 36 | 6 | -2.923208 | -0.262534 | -1.679543 |
| 37 | 6 | -1.797960 | -1.478733 | -3.430545 |
| 38 | 6 | -2.581258 | -0.895192 | -4.437403 |
| 39 | 6 | -3.711306 | -0.192511 | -4.038152 |
| 40 | 1 | -4.476086 | 0.102645 | -4.748113 |
| 41 | 1 | -2.433035 | -1.179291 | -5.473637 |
| 42 | 6 | -1.258920 | -3.342604 | -2.425198 |
| 43 | 8 | -1.245181 | -2.724127 | -3.655949 |
| 44 | 6 | -2.122199 | -4.295951 | -0.064013 |
| 45 | 6 | -1.981698 | -5.205708 | -1.114270 |
| 46 | 6 | -1.452198 | -4.725319 | -2.308659 |
| 47 | 1 | -1.338125 | -5.363486 | -3.177737 |
| 48 | 1 | -2.303634 | -6.235480 | -1.005857 |
| 49 | 8 | -2.769376 | -4.562817 | 1.121092 |
| 50 | 6 | -2.581376 | -3.450221 | 1.909741 |
| 51 | 6 | -1.717321 | -2.526093 | 1.288369 |
| 52 | 6 | -1.030600 | -1.639785 | 2.171993 |
| 53 | 6 | -1.641571 | -1.438024 | 3.423173 |
| 54 | 6 | -2.732707 | -2.170900 | 3.910802 |
| 55 | 6 | -3.161738 | -3.264877 | 3.166482 |
| 56 | 1 | -3.890122 | -3.969081 | 3.553020 |
| 57 | 1 | -3.109570 | -1.978805 | 4.909043 |
| 58 | 8 | -0.823749 | -0.741855 | 4.283887 |
| 59 | 6 | 0.432570 | -0.828712 | 3.722429 |
| 60 | 6 | 0.384682 | -1.289546 | 2.391102 |
| 61 | 6 | 2.621844 | -1.677680 | 4.147409 |
| 62 | 6 | 2.545830 | -2.231561 | 2.868541 |
| 63 | 6 | 1.596402 | -1.870122 | 1.889032 |
| 64 | 1 | 3.435489 | -1.933764 | 4.816741 |
| 65 | 1 | 1.485102 | -0.525579 | 5.581473 |
| 66 | 6 | 2.833161 | -3.645617 | 1.214000 |
| 67 | 6 | 1.968025 | -2.650603 | 0.723343 |
| 68 | 6 | 3.092981 | -4.849590 | 0.550973 |
| 69 | 6 | 2.527642 | -5.023581 | -0.711416 |
| 70 | 6 | 1.906433 | -3.916290 | -1.305809 |
| 71 | 6 | 1.762952 | -2.666278 | -0.682517 |
| 72 | 8 | 1.693335 | -3.823324 | -2.664082 |
| 73 | 6 | 1.760577 | -2.475876 | -2.948811 |
| 74 | 6 | 1.833295 | -1.695417 | -1.777088 |
| 75 | 6 | 2.125660 | -2.049921 | -4.231719 |

| | | | | |
|---|---|---|---|---|
| 76 | 6 | 2.918896 | -0.913865 | -4.317603 |
| 77 | 6 | 3.247995 | -0.277416 | -3.116404 |
| 78 | 6 | 2.593261 | -0.478386 | -1.883366 |
| 79 | 8 | 4.483762 | 0.313451 | -2.941785 |
| 80 | 1 | 1.971592 | -2.697057 | -5.088010 |
| 81 | 1 | 3.415713 | -0.641582 | -5.242483 |
| 82 | 1 | 2.675198 | -5.936632 | -1.277715 |
| 83 | 1 | 3.693884 | -5.622217 | 1.017590 |
| 84 | 6 | 1.623427 | 3.165448 | -0.216034 |
| 85 | 6 | 2.198908 | 4.445385 | -0.188776 |
| 86 | 6 | 2.009633 | 2.578686 | 1.066304 |
| 87 | 6 | 2.396030 | 3.684314 | 1.853698 |
| 88 | 6 | 2.927706 | 3.615813 | 3.145725 |
| 89 | 6 | 3.446922 | 2.393862 | 3.545634 |
| 90 | 8 | 2.507891 | 4.827427 | 1.092529 |
| 91 | 1 | 3.086629 | 4.516423 | 3.728797 |
| 92 | 1 | 4.036283 | 2.303024 | 4.451603 |
| 93 | 6 | -1.678185 | 3.073282 | -0.578673 |
| 94 | 6 | -2.416262 | 4.244969 | -0.828251 |
| 95 | 6 | -0.888066 | 3.369308 | -2.833721 |
| 96 | 6 | -1.964946 | 4.220842 | -3.159845 |
| 97 | 6 | -2.682248 | 4.758840 | -2.104707 |
| 98 | 1 | -3.380536 | 5.577056 | -2.241583 |
| 99 | 1 | -2.044702 | 4.625128 | -4.163127 |
| 100 | 6 | -0.649353 | 2.821345 | -1.562554 |
| 101 | 6 | 0.826400 | 2.916406 | -1.393177 |
| 102 | 6 | 2.188046 | 4.642286 | -2.561832 |
| 103 | 6 | 2.569209 | 5.165222 | -1.337315 |
| 104 | 1 | 2.407231 | 5.153850 | -3.492637 |
| 105 | 1 | 3.142187 | 6.082126 | -1.254825 |
| 106 | 6 | 1.255761 | 3.580714 | -2.550512 |
| 107 | 8 | -2.852240 | 4.821299 | 0.338684 |
| 108 | 8 | 0.286743 | 3.571559 | -3.535817 |

**Table S15.** The optimized Cartesian coordinates of the oxa[26]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.716459 | 1.036029 | 1.628727 |
| 2 | 6 | 3.473837 | 0.815676 | 0.405337 |
| 3 | 6 | -0.854060 | -2.996132 | 1.332908 |
| 4 | 6 | -0.930538 | -2.972731 | -1.368955 |
| 5 | 6 | -3.415419 | -0.714859 | -0.731305 |
| 6 | 6 | 1.092926 | 3.356725 | -0.282522 |
| 7 | 6 | -0.607355 | 2.267343 | -2.003594 |
| 8 | 6 | -1.937003 | 2.375449 | -1.384792 |
| 9 | 6 | -3.409978 | -0.752673 | 0.718134 |
| 10 | 6 | 2.376196 | -2.488765 | -0.724393 |
| 11 | 6 | 2.161360 | -1.530939 | -1.805178 |
| 12 | 6 | 2.506222 | -0.136866 | -1.916915 |
| 13 | 6 | 4.818672 | 0.906320 | 0.798521 |
| 14 | 6 | 3.664225 | 0.878455 | 2.662428 |
| 15 | 6 | 1.665966 | 4.600123 | -0.595993 |
| 16 | 6 | 2.902176 | 0.297023 | -3.200684 |
| 17 | 6 | 2.314879 | -2.292387 | -2.984130 |
| 18 | 6 | 2.936930 | -3.613091 | -1.351465 |
| 19 | 8 | 2.710965 | -3.584138 | -2.709825 |
| 20 | 6 | -1.579179 | -3.697222 | 2.310302 |
| 21 | 6 | -0.820177 | -4.144793 | -2.148284 |

| | | | | |
|---|---|---|---|---|
| 22 | 6 | -4.777429 | -0.805599 | -1.082434 |
| 23 | 6 | -4.682609 | -1.248221 | 1.065403 |
| 24 | 8 | -5.540008 | -1.210233 | -0.010473 |
| 25 | 6 | -2.797895 | 2.689206 | -2.448019 |
| 26 | 8 | -2.207244 | 2.426717 | -3.665724 |
| 27 | 6 | -0.856622 | 2.335407 | -3.389344 |
| 28 | 8 | 4.943045 | 0.747802 | 2.161212 |
| 29 | 6 | -2.656325 | 3.462307 | 2.029418 |
| 30 | 6 | 1.097139 | 3.025010 | 1.102740 |
| 31 | 6 | 1.027911 | 4.112170 | 1.985969 |
| 32 | 6 | 2.430878 | -2.492499 | 0.697073 |
| 33 | 6 | 3.521621 | -3.182790 | 1.251934 |
| 34 | 6 | 3.253066 | 0.721213 | -0.997109 |
| 35 | 6 | 4.215069 | 1.351135 | -1.800882 |
| 36 | 8 | 3.869316 | 1.280481 | -3.132556 |
| 37 | 6 | 2.428106 | -2.348202 | 2.957828 |
| 38 | 8 | 3.623790 | -2.934240 | 2.602369 |
| 39 | 6 | 1.593173 | -2.145501 | 1.837690 |
| 40 | 6 | -2.051598 | 1.269682 | 3.443223 |
| 41 | 6 | -2.066311 | 1.133492 | 2.041591 |
| 42 | 6 | -2.181120 | 2.353884 | 1.298875 |
| 43 | 6 | 3.859582 | -4.470083 | -0.734516 |
| 44 | 6 | 4.238133 | -4.178771 | 0.575186 |
| 45 | 6 | 2.719438 | -0.416841 | -4.389453 |
| 46 | 6 | 2.425352 | -1.769443 | -4.275416 |
| 47 | 6 | 5.844601 | 1.353415 | -0.045779 |
| 48 | 6 | 5.503946 | 1.684845 | -1.356118 |
| 49 | 1 | 4.331837 | -5.266590 | -1.298917 |
| 50 | 1 | 5.007342 | -4.748061 | 1.085249 |
| 51 | 1 | 3.007739 | 0.018014 | -5.340215 |
| 52 | 1 | 2.469177 | -2.429892 | -5.134271 |
| 53 | 1 | 6.848927 | 1.500926 | 0.335716 |
| 54 | 1 | 6.236717 | 2.081853 | -2.050012 |
| 55 | 6 | -1.381170 | -1.807793 | -2.076467 |
| 56 | 6 | -1.300255 | -1.876230 | -3.481993 |
| 57 | 6 | 0.181903 | -2.277690 | 2.085589 |
| 58 | 6 | -0.188342 | -2.441146 | 3.437982 |
| 59 | 8 | -1.331514 | -3.200477 | 3.570264 |
| 60 | 6 | 0.658854 | -2.281205 | 4.540848 |
| 61 | 6 | 2.024331 | -2.263243 | 4.292061 |
| 62 | 1 | 0.269392 | -2.386593 | 5.547460 |
| 63 | 1 | 2.747798 | -2.347897 | 5.095387 |
| 64 | 6 | -2.499838 | -0.881825 | -1.816310 |
| 65 | 6 | -3.010293 | -0.580819 | -3.092235 |
| 66 | 8 | -2.154278 | -0.982978 | -4.092610 |
| 67 | 6 | -1.025501 | -3.456925 | -0.003161 |
| 68 | 6 | -1.342805 | -4.822091 | -0.127577 |
| 69 | 8 | -1.083664 | -5.271844 | -1.401916 |
| 70 | 6 | -5.283057 | -0.533891 | -2.356310 |
| 71 | 6 | -4.360453 | -0.327983 | -3.376370 |
| 72 | 6 | -0.835201 | -2.975896 | -4.215938 |
| 73 | 6 | -0.647639 | -4.171132 | -3.532879 |
| 74 | 6 | -1.953527 | -5.577388 | 0.879401 |
| 75 | 6 | -2.166721 | -4.954543 | 2.106894 |
| 76 | 1 | -6.351547 | -0.524016 | -2.540925 |
| 77 | 1 | -4.673753 | -0.155543 | -4.400061 |
| 78 | 1 | -0.834381 | -2.939102 | -5.299899 |
| 79 | 1 | -0.480896 | -5.106768 | -4.054817 |
| 80 | 1 | -2.265850 | -6.599326 | 0.695368 |
| 81 | 1 | -2.643900 | -5.472670 | 2.931441 |
| 82 | 6 | -2.416973 | 2.704775 | -0.086607 |
| 83 | 6 | -3.328199 | 3.775995 | -0.037721 |
| 84 | 8 | -3.378362 | 4.318643 | 1.227069 |

| | | | | |
|---|---|---|---|---|
| 85 | 6 | -2.663505 | -0.194768 | 1.802201 |
| 86 | 6 | -3.012677 | -0.655983 | 3.083699 |
| 87 | 6 | -5.035729 | -1.689603 | 2.343366 |
| 88 | 6 | -4.126181 | -1.459756 | 3.369856 |
| 89 | 6 | -2.160075 | 2.483934 | 4.137976 |
| 90 | 6 | -2.543513 | 3.606366 | 3.413576 |
| 91 | 6 | -3.916004 | 3.529073 | -2.335896 |
| 92 | 6 | -4.127893 | 4.168194 | -1.115680 |
| 93 | 1 | -5.999729 | -2.151037 | 2.526738 |
| 94 | 1 | -4.347051 | -1.731329 | 4.396066 |
| 95 | 1 | -2.158530 | 2.487898 | 5.222552 |
| 96 | 1 | -2.838920 | 4.526639 | 3.905136 |
| 97 | 1 | -4.492215 | 3.787138 | -3.217657 |
| 98 | 1 | -4.883418 | 4.937127 | -0.998531 |
| 99 | 8 | -2.431141 | 0.103048 | 4.076442 |
| 100 | 6 | 0.643335 | 2.825717 | -1.560247 |
| 101 | 6 | 1.325547 | 3.601454 | -2.520111 |
| 102 | 8 | 1.963015 | 4.677353 | -1.938480 |
| 103 | 6 | 1.622516 | 1.924124 | 1.919895 |
| 104 | 6 | 1.556697 | 2.403276 | 3.244899 |
| 105 | 8 | 1.059380 | 3.691474 | 3.298836 |
| 106 | 6 | 3.431091 | 1.151397 | 4.012701 |
| 107 | 6 | 2.315113 | 1.920911 | 4.319058 |
| 108 | 6 | 1.312741 | 5.436889 | 1.614619 |
| 109 | 6 | 1.747965 | 5.665761 | 0.310630 |
| 110 | 6 | 1.169152 | 3.479892 | -3.903830 |
| 111 | 6 | 0.060037 | 2.776450 | -4.355693 |
| 112 | 1 | 4.183307 | 0.927060 | 4.761159 |
| 113 | 1 | 2.170165 | 2.325702 | 5.314879 |
| 114 | 1 | 1.330690 | 6.221276 | 2.363347 |
| 115 | 1 | 2.102047 | 6.639713 | -0.008608 |
| 116 | 1 | 1.803868 | 4.035289 | -4.585435 |
| 117 | 1 | -0.213054 | 2.772534 | -5.405408 |

**Table S16.** The optimized Cartesian coordinates of the oxa[28]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.704266 | -2.970616 | -1.247803 |
| 2 | 6 | 2.014248 | -3.276184 | 0.140703 |
| 3 | 6 | 1.805261 | 2.762435 | -1.453562 |
| 4 | 6 | 1.703659 | 2.970860 | 1.247876 |
| 5 | 6 | -1.755284 | 3.195327 | 0.718838 |
| 6 | 6 | -1.754691 | -3.195540 | -0.718959 |
| 7 | 6 | -1.572102 | -2.370066 | 1.870704 |
| 8 | 6 | -1.965909 | -1.008026 | 2.304536 |
| 9 | 6 | -1.777087 | 3.223897 | -0.737378 |
| 10 | 6 | 3.609315 | 0.053580 | 0.710609 |
| 11 | 6 | 2.781812 | -0.320807 | 1.856172 |
| 12 | 6 | 1.955732 | -1.470373 | 2.146083 |
| 13 | 6 | 2.825758 | -4.426924 | 0.081515 |
| 14 | 6 | 2.662668 | -3.709544 | -1.980948 |
| 15 | 6 | -2.650650 | -4.223354 | -1.096168 |
| 16 | 6 | 1.831427 | -1.797724 | 3.515217 |
| 17 | 6 | 3.471646 | 0.218029 | 2.966203 |
| 18 | 6 | 4.837596 | 0.441707 | 1.272150 |
| 19 | 8 | 4.698599 | 0.728628 | 2.609799 |
| 20 | 6 | 1.857813 | 3.721438 | -2.480987 |
| 21 | 6 | 2.661986 | 3.709864 | 1.981082 |

| | | | | |
|---|---|---|---|---|
| 22 | 6 | -2.651484 | 4.222976 | 1.095903 |
| 23 | 6 | -2.316281 | 4.490578 | -1.050077 |
| 24 | 8 | -2.946859 | 5.044729 | 0.036220 |
| 25 | 6 | -1.703158 | -1.006363 | 3.695515 |
| 26 | 8 | -1.180683 | -2.198759 | 4.131986 |
| 27 | 6 | -1.322618 | -3.058090 | 3.073964 |
| 28 | 8 | 3.329641 | -4.607977 | -1.183386 |
| 29 | 6 | -0.915367 | -2.716551 | -1.783026 |
| 30 | 6 | -1.428468 | -2.923896 | -3.079796 |
| 31 | 6 | 3.609094 | -0.052588 | -0.711151 |
| 32 | 6 | 4.837157 | -0.440898 | -1.273073 |
| 33 | 6 | 1.806057 | -2.761714 | 1.453582 |
| 34 | 6 | 1.858659 | -3.720589 | 2.481122 |
| 35 | 8 | 1.649871 | -3.147938 | 3.712337 |
| 36 | 6 | 3.470641 | -0.217278 | -2.966674 |
| 37 | 8 | 4.697670 | -0.727937 | -2.610629 |
| 38 | 6 | 2.781181 | 0.321704 | -1.856465 |
| 39 | 6 | -1.703915 | 1.005451 | -3.695282 |
| 40 | 6 | -1.966434 | 1.007226 | -2.304258 |
| 41 | 6 | -3.839770 | -0.110714 | -0.704737 |
| 42 | 6 | 6.076977 | 0.281921 | 0.635845 |
| 43 | 6 | 6.076759 | -0.281184 | -0.637168 |
| 44 | 6 | 2.258875 | -1.013451 | 4.592333 |
| 45 | 6 | 3.142154 | 0.015692 | 4.308096 |
| 46 | 6 | 3.000164 | -5.327339 | 1.135478 |
| 47 | 6 | 2.404599 | -5.004141 | 2.350742 |
| 48 | 1 | 6.998153 | 0.506732 | 1.161910 |
| 49 | 1 | 6.997756 | -0.506058 | -1.163519 |
| 50 | 1 | 2.078796 | -1.343705 | 5.609419 |
| 51 | 1 | 3.681613 | 0.535950 | 5.091325 |
| 52 | 1 | 3.559450 | -6.245484 | 0.994663 |
| 53 | 1 | 2.481147 | -5.653302 | 3.215982 |
| 54 | 6 | 0.544829 | 2.559826 | 1.997061 |
| 55 | 6 | 0.698451 | 2.604398 | 3.399682 |
| 56 | 6 | 1.954975 | 1.471199 | -2.146228 |
| 57 | 6 | 1.830531 | 1.798683 | -3.515312 |
| 58 | 8 | 1.649002 | 3.148922 | -3.712263 |
| 59 | 6 | 2.257741 | 1.014445 | -4.592548 |
| 60 | 6 | 3.140945 | -0.014809 | -4.308508 |
| 61 | 1 | 2.077521 | 1.344773 | -5.609584 |
| 62 | 1 | 3.680181 | -0.535098 | -5.091872 |
| 63 | 6 | -0.915940 | 2.716571 | 1.782974 |
| 64 | 6 | -1.429114 | 2.923972 | 3.079701 |
| 65 | 8 | -0.508956 | 2.633096 | 4.054916 |
| 66 | 6 | 2.013564 | 3.276664 | -0.140604 |
| 67 | 6 | 2.824921 | 4.427502 | -0.081298 |
| 68 | 8 | 3.328829 | 4.608462 | 1.183598 |
| 69 | 6 | -3.132781 | 4.439382 | 2.385952 |
| 70 | 6 | -2.549570 | 3.698666 | 3.403735 |
| 71 | 6 | 1.834430 | 3.037898 | 4.094475 |
| 72 | 6 | 2.827723 | 3.672714 | 3.364552 |
| 73 | 6 | 2.999094 | 5.328130 | -1.135120 |
| 74 | 6 | 2.403580 | 5.005038 | -2.350428 |
| 75 | 1 | -3.886859 | 5.194023 | 2.579277 |
| 76 | 1 | -2.822222 | 3.840657 | 4.443368 |
| 77 | 1 | 1.823769 | 3.056690 | 5.178705 |
| 78 | 1 | 3.643577 | 4.204407 | 3.841222 |
| 79 | 1 | 3.558172 | 6.246378 | -0.994145 |
| 80 | 1 | 2.480009 | 5.654383 | -3.215543 |
| 81 | 6 | -3.839614 | 0.109806 | 0.705370 |
| 82 | 6 | -5.084621 | 0.511372 | 1.233860 |
| 83 | 6 | -1.572663 | 2.369382 | -1.870663 |
| 84 | 6 | -1.323445 | 3.057261 | -3.074063 |

| | | | | |
|---|---|---|---|---|
| 85 | 6 | -2.168949 | 5.138431 | -2.278613 |
| 86 | 6 | -1.553693 | 4.421791 | -3.295924 |
| 87 | 1 | -2.519220 | 6.155266 | -2.416348 |
| 88 | 1 | -1.394768 | 4.841561 | -4.282776 |
| 89 | 8 | -1.181570 | 2.197801 | -4.131985 |
| 90 | 6 | -1.776458 | -3.224362 | 0.737261 |
| 91 | 6 | -2.315474 | -4.491150 | 1.049792 |
| 92 | 8 | -2.945937 | -5.045265 | -0.036586 |
| 93 | 6 | 0.545424 | -2.559724 | -1.997055 |
| 94 | 6 | 0.699083 | -2.604263 | -3.399673 |
| 95 | 8 | -0.508302 | -2.632804 | -4.054948 |
| 96 | 6 | 2.828404 | -3.672479 | -3.364418 |
| 97 | 6 | 1.835065 | -3.037828 | -4.094413 |
| 98 | 6 | -2.548641 | -3.698934 | -3.403959 |
| 99 | 6 | -3.131739 | -4.439862 | -2.386276 |
| 100 | 6 | -2.168092 | -5.139166 | 2.278239 |
| 101 | 6 | -1.552810 | -4.422660 | 3.295638 |
| 102 | 1 | 3.644330 | -4.204111 | -3.841033 |
| 103 | 1 | 1.824416 | -3.056781 | -5.178641 |
| 104 | 1 | -2.821115 | -3.841035 | -4.443627 |
| 105 | 1 | -3.885578 | -5.194709 | -2.579715 |
| 106 | 1 | -2.518315 | -6.156035 | 2.415837 |
| 107 | 1 | -1.393856 | -4.842609 | 4.282411 |
| 108 | 6 | -2.980267 | -0.070870 | 1.876654 |
| 109 | 6 | -3.707138 | 0.545850 | 2.925077 |
| 110 | 8 | -4.963658 | 0.924642 | 2.533754 |
| 111 | 6 | -2.980616 | 0.069927 | -1.876161 |
| 112 | 6 | -3.707713 | -0.546775 | -2.924442 |
| 113 | 8 | -4.964217 | -0.925415 | -2.532904 |
| 114 | 6 | -2.251413 | 0.148733 | -4.654142 |
| 115 | 6 | -3.329601 | -0.622796 | -4.263096 |
| 116 | 6 | -6.325120 | -0.314056 | -0.618828 |
| 117 | 6 | -6.324959 | 0.313474 | 0.619933 |
| 118 | 6 | -3.328871 | 0.621739 | 4.263686 |
| 119 | 6 | -2.250637 | -0.149806 | 4.654539 |
| 120 | 1 | -1.963317 | 0.249895 | -5.694411 |
| 121 | 1 | -3.931897 | -1.178126 | -4.973016 |
| 122 | 1 | -7.241548 | -0.572841 | -1.137273 |
| 123 | 1 | -7.241258 | 0.572373 | 1.138552 |
| 124 | 1 | -3.931140 | 1.176950 | 4.973721 |
| 125 | 1 | -1.962429 | -0.251076 | 5.694768 |
| 126 | 6 | -5.084911 | -0.512136 | -1.232984 |

**Table S17.** The optimized Cartesian coordinates of the oxa[30]circulene in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.887537 | -1.752598 | 1.662249 |
| 2 | 6 | -0.097777 | 2.838221 | -4.569310 |
| 3 | 6 | -1.640067 | 1.946002 | -2.283349 |
| 4 | 6 | -0.497427 | 2.825561 | -2.076432 |
| 5 | 6 | -0.304176 | 5.393163 | 0.682445 |
| 6 | 6 | -0.077600 | 4.035802 | 0.360003 |
| 7 | 6 | 0.074026 | 3.376979 | 1.662249 |
| 8 | 6 | -0.459065 | 4.324531 | 2.575403 |
| 9 | 8 | -0.683006 | 5.539413 | 1.988544 |
| 10 | 6 | 0.905489 | 2.358458 | 2.278541 |
| 11 | 6 | 0.731292 | 2.233919 | 3.678358 |
| 12 | 6 | -0.060561 | 3.032556 | 4.509297 |

| | | | | |
|---|---|---|---|---|
| 13 | 6 | -0.620575 | 4.162396 | 3.948380 |
| 14 | 1 | -1.095542 | 4.936272 | 4.540496 |
| 15 | 1 | -0.058184 | 2.853525 | 5.578420 |
| 16 | 6 | 2.276571 | 1.809842 | 2.046012 |
| 17 | 6 | 2.750872 | 1.515921 | 3.342850 |
| 18 | 8 | 1.758168 | 1.556396 | 4.281727 |
| 19 | 6 | 3.323509 | 1.944256 | 1.064456 |
| 20 | 6 | 4.591407 | 2.289661 | 1.596453 |
| 21 | 6 | 5.026513 | 2.049188 | 2.896169 |
| 22 | 6 | 4.079170 | 1.564250 | 3.780219 |
| 23 | 1 | 4.300614 | 1.391603 | 4.826753 |
| 24 | 1 | 6.042082 | 2.281932 | 3.195740 |
| 25 | 6 | 3.482552 | 2.148267 | -0.369505 |
| 26 | 6 | 4.631274 | 2.966886 | -0.477955 |
| 27 | 8 | 5.358945 | 2.960558 | 0.681754 |
| 28 | 6 | 2.949908 | 1.703248 | -1.624200 |
| 29 | 6 | 3.217970 | 2.586951 | -2.691410 |
| 30 | 6 | 4.154033 | 3.627206 | -2.697219 |
| 31 | 6 | 4.962828 | 3.755040 | -1.579363 |
| 32 | 1 | 5.806539 | 4.434858 | -1.542159 |
| 33 | 1 | 4.318199 | 4.199398 | -3.603200 |
| 34 | 6 | 2.505320 | 0.447339 | -2.283349 |
| 35 | 6 | 2.354752 | 0.828899 | -3.640555 |
| 36 | 8 | 2.696814 | 2.133567 | -3.868038 |
| 37 | 6 | 2.695721 | -0.981997 | -2.076432 |
| 38 | 6 | 2.836244 | -1.730344 | -3.274872 |
| 39 | 6 | 2.506860 | -1.334433 | -4.569310 |
| 40 | 6 | 2.219823 | -0.000480 | -4.755194 |
| 41 | 1 | 2.083548 | 0.434791 | -5.738498 |
| 42 | 1 | 2.592116 | -2.037786 | -5.388995 |
| 43 | 6 | 3.279722 | -1.874503 | -1.051681 |
| 44 | 6 | 3.964805 | -2.859266 | -1.796193 |
| 45 | 8 | 3.554850 | -2.879572 | -3.099264 |
| 46 | 6 | 0.000000 | 6.485090 | -0.134059 |
| 47 | 6 | 0.525133 | 6.199806 | -1.384638 |
| 48 | 6 | 0.493795 | 4.863255 | -1.796193 |
| 49 | 6 | -0.016494 | 3.777574 | -1.051681 |
| 50 | 1 | 0.849238 | 6.973211 | -2.071823 |
| 51 | 1 | -0.112984 | 7.497812 | 0.236089 |
| 52 | 6 | 0.080400 | 3.321432 | -3.274872 |
| 53 | 8 | 0.716357 | 4.518376 | -3.099264 |
| 54 | 6 | -1.109496 | 1.922663 | -4.755194 |
| 55 | 6 | -1.895224 | 1.624825 | -3.640555 |
| 56 | 1 | 0.468717 | 3.263731 | -5.388995 |
| 57 | 1 | -1.418314 | 1.587010 | -5.738498 |
| 58 | 6 | -2.950010 | 1.703071 | -1.624200 |
| 59 | 6 | -3.849350 | 1.493368 | -2.691410 |
| 60 | 8 | -3.196130 | 1.268726 | -3.868038 |
| 61 | 6 | -3.601730 | 1.941845 | -0.369505 |
| 62 | 6 | -4.885036 | 2.527358 | -0.477955 |
| 63 | 6 | -5.733373 | 2.420415 | -1.579363 |
| 64 | 6 | -5.218269 | 1.783896 | -2.697219 |
| 65 | 8 | -5.243391 | 3.160703 | 0.681754 |
| 66 | 6 | -4.278608 | 2.831445 | 1.596453 |
| 67 | 6 | -3.345529 | 1.906115 | 1.064456 |
| 68 | 6 | -4.287906 | 3.328494 | 2.896169 |
| 69 | 6 | -3.394265 | 2.750540 | 3.780219 |
| 70 | 6 | -2.688262 | 1.624365 | 3.342850 |
| 71 | 6 | -2.705655 | 1.066648 | 2.046012 |
| 72 | 1 | -4.997252 | 4.091630 | 3.195740 |
| 73 | 1 | -3.355470 | 3.028639 | 4.826753 |
| 74 | 1 | -6.743969 | 2.811181 | -1.542159 |
| 75 | 1 | -5.795884 | 1.639971 | -3.603200 |

| | | | | |
|---|---|---|---|---|
| 76 | 6 | -2.495229 | -0.395053 | 2.278541 |
| 77 | 6 | -2.300277 | -0.483642 | 3.678358 |
| 78 | 8 | -2.226962 | 0.744420 | 4.281727 |
| 79 | 6 | -2.961563 | -1.624381 | 1.662249 |
| 80 | 6 | -3.515622 | -2.559828 | 2.575403 |
| 81 | 6 | -3.294453 | -2.618632 | 3.948380 |
| 82 | 6 | -2.595990 | -1.568726 | 4.509297 |
| 83 | 1 | -2.442133 | -1.477151 | 5.578420 |
| 84 | 1 | -3.727166 | -3.416903 | 4.540496 |
| 85 | 6 | -3.456307 | -2.085104 | 0.360003 |
| 86 | 6 | -4.518528 | -2.960005 | 0.682445 |
| 87 | 8 | -4.455770 | -3.361207 | 1.988544 |
| 88 | 6 | -3.263228 | -1.903071 | -1.051681 |
| 89 | 6 | -4.458600 | -2.003988 | -1.796193 |
| 90 | 6 | -5.631756 | -2.645125 | -1.384638 |
| 91 | 6 | -5.616253 | -3.242545 | -0.134059 |
| 92 | 1 | -6.436804 | -3.846753 | 0.236089 |
| 93 | 1 | -6.463597 | -2.751144 | -2.071823 |
| 94 | 6 | -2.198295 | -1.843565 | -2.076432 |
| 95 | 6 | -2.916644 | -1.591088 | -3.274872 |
| 96 | 8 | -4.271207 | -1.638805 | -3.099264 |
| 97 | 6 | -0.865253 | -2.393340 | -2.283349 |
| 98 | 6 | -0.459528 | -2.453725 | -3.640555 |
| 99 | 6 | -1.110327 | -1.922183 | -4.755194 |
| 100 | 6 | -2.409083 | -1.503788 | -4.569310 |
| 101 | 1 | -3.060832 | -1.225945 | -5.388995 |
| 102 | 1 | -0.665234 | -2.021801 | -5.738498 |
| 103 | 6 | 0.000102 | -3.406319 | -1.624200 |
| 104 | 6 | 0.631380 | -4.080319 | -2.691410 |
| 105 | 8 | 0.499316 | -3.402293 | -3.868038 |
| 106 | 6 | 1.064236 | -5.411101 | -2.697219 |
| 107 | 6 | 0.770546 | -6.175455 | -1.579363 |
| 108 | 6 | 0.253761 | -5.494244 | -0.477955 |
| 109 | 6 | 0.119178 | -4.090112 | -0.369505 |
| 110 | 1 | 0.937430 | -7.246039 | -1.542159 |
| 111 | 1 | 1.477686 | -5.839369 | -3.603200 |
| 112 | 6 | 0.022020 | -3.850371 | 1.064456 |
| 113 | 6 | -0.312799 | -5.121106 | 1.596453 |
| 114 | 8 | -0.115554 | -6.121261 | 0.681754 |
| 115 | 6 | -0.062610 | -3.140286 | 3.342850 |
| 116 | 6 | 0.429084 | -2.876490 | 2.046012 |
| 117 | 8 | 0.468795 | -2.300816 | 4.281727 |
| 118 | 6 | 1.568985 | -1.750277 | 3.678358 |
| 119 | 6 | 1.589740 | -1.963406 | 2.278541 |
| 120 | 6 | 2.656551 | -1.463830 | 4.509297 |
| 121 | 6 | 3.915028 | -1.543764 | 3.948380 |
| 122 | 6 | 3.974686 | -1.764704 | 2.575403 |
| 123 | 1 | 4.822707 | -1.519369 | 4.540496 |
| 124 | 1 | 2.500317 | -1.376373 | 5.578420 |
| 125 | 6 | 3.533907 | -1.950698 | 0.360003 |
| 126 | 6 | 4.822704 | -2.433157 | 0.682445 |
| 127 | 8 | 5.138776 | -2.178206 | 1.988544 |
| 128 | 6 | 5.106623 | -3.554681 | -1.384638 |
| 129 | 6 | 5.616253 | -3.242545 | -0.134059 |
| 130 | 1 | 5.614359 | -4.222067 | -2.071823 |
| 131 | 1 | 6.549788 | -3.651059 | 0.236089 |
| 132 | 6 | -0.684905 | -4.314790 | 3.780219 |
| 133 | 6 | -0.738608 | -5.377682 | 2.896169 |
| 134 | 1 | -0.945144 | -4.420242 | 4.826753 |
| 135 | 1 | -1.044829 | -6.373563 | 3.195740 |

**Table S18.** The optimized Cartesian coordinates of the [4]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.635285 | 0.825530 | 1.363271 |
| 2 | 6 | 0.780177 | 0.690208 | 1.363269 |
| 3 | 6 | -0.780177 | -0.690208 | 1.363269 |
| 4 | 6 | 0.635285 | -0.825530 | 1.363271 |
| 5 | 6 | 1.521239 | 1.085772 | 0.274714 |
| 6 | 6 | -1.287996 | 1.354362 | 0.274736 |
| 7 | 6 | -0.497853 | 2.177294 | -0.594171 |
| 8 | 6 | 0.901358 | 2.043512 | -0.594187 |
| 9 | 6 | 2.201519 | -0.210482 | -0.286245 |
| 10 | 6 | 1.287996 | -1.354362 | 0.274736 |
| 11 | 6 | -1.521239 | -1.085772 | 0.274714 |
| 12 | 6 | -0.901358 | -2.043512 | -0.594187 |
| 13 | 6 | 0.497853 | -2.177294 | -0.594171 |
| 14 | 6 | -2.201519 | 0.210482 | -0.286245 |
| 15 | 1 | -0.958182 | 2.707781 | -1.424376 |
| 16 | 1 | 1.453837 | 2.477152 | -1.424415 |
| 17 | 1 | -1.453837 | -2.477152 | -1.424415 |
| 18 | 1 | 0.958182 | -2.707781 | -1.424376 |
| 19 | 8 | 3.037645 | -0.290389 | -1.148212 |
| 20 | 8 | -3.037645 | 0.290389 | -1.148212 |

**Table S19.** The optimized Cartesian coordinates of the [6]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.098074 | 1.407316 | -0.804786 |
| 2 | 6 | -1.149779 | 0.817380 | -0.804792 |
| 3 | 6 | 1.282762 | 0.587048 | -0.804792 |
| 4 | 6 | 1.169735 | -0.788593 | -0.804786 |
| 5 | 6 | -0.132983 | -1.404428 | -0.804792 |
| 6 | 6 | -1.267809 | -0.618724 | -0.804786 |
| 7 | 6 | 0.332310 | 2.630446 | -0.163113 |
| 8 | 6 | -2.243636 | 1.412698 | -0.163176 |
| 9 | 6 | 2.345251 | 1.236697 | -0.163176 |
| 10 | 6 | 2.111878 | -1.603012 | -0.163113 |
| 11 | 6 | -0.101614 | -2.649395 | -0.163176 |
| 12 | 6 | -2.444188 | -1.027434 | -0.163113 |
| 13 | 6 | -1.297823 | -3.131312 | 0.375914 |
| 14 | 6 | -2.474342 | -2.316706 | 0.376036 |
| 15 | 6 | -2.062885 | 2.689604 | 0.375914 |
| 16 | 6 | -0.769155 | 3.301196 | 0.376036 |
| 17 | 6 | 3.243497 | -0.984491 | 0.376036 |
| 18 | 6 | 3.360707 | 0.441709 | 0.375914 |
| 19 | 6 | 1.841635 | 2.659776 | 0.167746 |
| 20 | 6 | -3.224252 | 0.265015 | 0.167746 |
| 21 | 6 | 1.382616 | -2.924791 | 0.167746 |
| 22 | 1 | -1.314833 | -4.070368 | 0.922337 |
| 23 | 1 | -3.347233 | -2.662996 | 0.922682 |
| 24 | 1 | -2.867626 | 3.173862 | 0.922337 |
| 25 | 1 | -0.632606 | 4.230287 | 0.922682 |
| 26 | 1 | 3.979839 | -1.567290 | 0.922682 |
| 27 | 1 | 4.182458 | 0.896505 | 0.922337 |

| | | | | |
|---|---|---|---|---|
| 28 | 8 | 2.461861 | 3.555447 | 0.694060 |
| 29 | 8 | 1.848177 | -3.909758 | 0.694060 |
| 30 | 8 | -4.310038 | 0.354310 | 0.694060 |

**Table S20.** The optimized Cartesian coordinates of the [8]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.182375 | -3.089871 | 0.000000 |
| 2 | 6 | -0.748224 | -1.734205 | 0.000000 |
| 3 | 6 | -1.734205 | -0.748224 | 0.000000 |
| 4 | 6 | -1.734205 | 0.748224 | 0.000000 |
| 5 | 6 | -3.089871 | 1.182375 | 0.000000 |
| 6 | 6 | -3.089871 | -1.182375 | 0.000000 |
| 7 | 6 | -0.748224 | 1.734205 | 0.000000 |
| 8 | 6 | -3.993150 | 0.000000 | 0.000000 |
| 9 | 6 | -1.182375 | 3.089871 | 0.000000 |
| 10 | 6 | -3.495323 | -2.506201 | 0.000000 |
| 11 | 6 | -2.506201 | -3.495323 | 0.000000 |
| 12 | 6 | -2.506201 | 3.495323 | 0.000000 |
| 13 | 6 | -3.495323 | 2.506201 | 0.000000 |
| 14 | 1 | -4.554948 | -2.742680 | 0.000000 |
| 15 | 1 | -2.742680 | -4.554948 | 0.000000 |
| 16 | 1 | -2.742680 | 4.554948 | 0.000000 |
| 17 | 1 | -4.554948 | 2.742680 | 0.000000 |
| 18 | 6 | 0.748224 | -1.734205 | 0.000000 |
| 19 | 6 | 1.182375 | -3.089871 | 0.000000 |
| 20 | 6 | 1.734205 | -0.748224 | 0.000000 |
| 21 | 6 | 1.734205 | 0.748224 | 0.000000 |
| 22 | 6 | 0.748224 | 1.734205 | 0.000000 |
| 23 | 6 | 3.089871 | -1.182375 | 0.000000 |
| 24 | 6 | 3.089871 | 1.182375 | 0.000000 |
| 25 | 6 | 1.182375 | 3.089871 | 0.000000 |
| 26 | 6 | 3.495323 | -2.506201 | 0.000000 |
| 27 | 6 | 2.506201 | -3.495323 | 0.000000 |
| 28 | 6 | 2.506201 | 3.495323 | 0.000000 |
| 29 | 6 | 3.495323 | 2.506201 | 0.000000 |
| 30 | 1 | 4.554948 | -2.742680 | 0.000000 |
| 31 | 1 | 2.742680 | -4.554948 | 0.000000 |
| 32 | 1 | 2.742680 | 4.554948 | 0.000000 |
| 33 | 1 | 4.554948 | 2.742680 | 0.000000 |
| 34 | 6 | 3.993150 | 0.000000 | 0.000000 |
| 35 | 6 | 0.000000 | -3.993150 | 0.000000 |
| 36 | 6 | 0.000000 | 3.993150 | 0.000000 |
| 37 | 8 | 0.000000 | 5.212010 | 0.000000 |
| 38 | 8 | 5.212010 | 0.000000 | 0.000000 |
| 39 | 8 | 0.000000 | -5.212010 | 0.000000 |
| 40 | 8 | -5.212010 | 0.000000 | 0.000000 |

**Table S21.** The optimized Cartesian coordinates of the [10]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.755184 | -4.547133 | -0.623731 |

| | | | | |
|---|---|---|---|---|
| 2 | 6 | 1.490137 | 2.660502 | -1.875179 |
| 3 | 6 | 1.603196 | 4.010629 | -1.598742 |
| 4 | 6 | 0.745048 | 4.538724 | -0.630401 |
| 5 | 6 | -0.023823 | 3.646790 | 0.088431 |
| 6 | 6 | 0.037233 | 2.219016 | -0.009198 |
| 7 | 6 | 0.683969 | 1.721345 | -1.154820 |
| 8 | 6 | 0.409389 | 0.569927 | -2.087383 |
| 9 | 6 | -0.396106 | -0.583255 | -2.089350 |
| 10 | 6 | -0.680938 | -1.731394 | -1.156020 |
| 11 | 6 | -0.043017 | -2.228266 | -0.004982 |
| 12 | 6 | 0.666859 | -1.701203 | 1.215145 |
| 13 | 6 | 0.428048 | -0.620208 | 2.083210 |
| 14 | 6 | -0.436806 | 0.614376 | 2.080825 |
| 15 | 6 | -0.675743 | 1.692604 | 1.209437 |
| 16 | 6 | -1.110067 | 4.030982 | 1.023150 |
| 17 | 6 | -1.443313 | 2.779463 | 1.743907 |
| 18 | 6 | -2.054491 | 2.804605 | 2.983762 |
| 19 | 6 | -1.725662 | 1.786398 | 3.880973 |
| 20 | 6 | -0.869471 | 0.799178 | 3.435561 |
| 21 | 6 | -0.005077 | 0.001085 | 4.338010 |
| 22 | 6 | 0.858952 | -0.801167 | 3.438915 |
| 23 | 6 | 1.712323 | -1.788784 | 3.888709 |
| 24 | 6 | 2.039134 | -2.811263 | 2.995550 |
| 25 | 6 | 1.430001 | -2.788643 | 1.754548 |
| 26 | 1 | -2.615818 | 3.684637 | 3.282971 |
| 27 | 1 | -2.002788 | 1.821618 | 4.930194 |
| 28 | 1 | 1.988317 | -1.820852 | 4.938311 |
| 29 | 1 | 2.597400 | -3.691878 | 3.298742 |
| 30 | 6 | 1.094716 | -4.041009 | 1.036147 |
| 31 | 6 | 0.012767 | -3.655873 | 0.096724 |
| 32 | 6 | -1.605016 | -4.018782 | -1.599273 |
| 33 | 6 | -1.485053 | -2.669918 | -1.879479 |
| 34 | 6 | -1.828522 | -2.126718 | -3.215729 |
| 35 | 6 | -0.919862 | -0.963188 | -3.365950 |
| 36 | 6 | -0.508612 | -0.470959 | -4.588769 |
| 37 | 6 | 0.541454 | 0.452339 | -4.585621 |
| 38 | 6 | 0.943033 | 0.947285 | -3.360616 |
| 39 | 6 | 1.847509 | 2.113408 | -3.206169 |
| 40 | 1 | 2.232249 | 4.633216 | -2.227594 |
| 41 | 1 | 0.634032 | 5.604975 | -0.459309 |
| 42 | 1 | 0.997574 | 0.832585 | -5.494345 |
| 43 | 1 | -0.958247 | -0.852692 | -5.500083 |
| 44 | 1 | -2.232037 | -4.641143 | -2.230406 |
| 45 | 1 | -0.648995 | -5.613231 | -0.448761 |
| 46 | 8 | -1.570385 | 5.145939 | 1.195037 |
| 47 | 8 | 2.619394 | 2.570391 | -4.029693 |
| 48 | 8 | -2.593422 | -2.584741 | -4.045173 |
| 49 | 8 | 1.549809 | -5.157290 | 1.213342 |
| 50 | 8 | -0.004691 | 0.004231 | 5.556873 |

**Table S22.** The optimized Cartesian coordinates of the [12]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.370770 | 1.290247 | 1.246301 |
| 2 | 6 | -2.239668 | 0.367350 | 0.648700 |
| 3 | 6 | 0.374361 | -2.200919 | 0.591738 |
| 4 | 6 | 1.370772 | -1.290248 | 1.246299 |
| 5 | 6 | 2.239669 | -0.367351 | 0.648700 |

| | | | | |
|---|---|---|---|---|
| 6 | 6 | -0.374361 | 2.200919 | 0.591739 |
| 7 | 6 | 0.374753 | 2.200970 | -0.591451 |
| 8 | 6 | 1.370840 | 1.290182 | -1.246342 |
| 9 | 6 | 2.239620 | 0.366994 | -0.649022 |
| 10 | 6 | -0.374752 | -2.200970 | -0.591453 |
| 11 | 6 | -1.370839 | -1.290181 | -1.246343 |
| 12 | 6 | -2.239619 | -0.366994 | -0.649022 |
| 13 | 6 | -3.577494 | 0.338634 | 1.140601 |
| 14 | 6 | -3.968302 | 0.877240 | 2.354980 |
| 15 | 6 | -3.034299 | 1.649305 | 3.058511 |
| 16 | 6 | -1.820407 | 1.921974 | 2.441719 |
| 17 | 6 | -1.147774 | 3.248016 | 2.583481 |
| 18 | 6 | -0.491552 | 3.455843 | 1.254618 |
| 19 | 6 | -3.577337 | -0.337978 | -1.141205 |
| 20 | 6 | -4.484031 | 0.000468 | -0.000406 |
| 21 | 6 | -1.820432 | -1.922016 | -2.441720 |
| 22 | 6 | -3.034122 | -1.649101 | -3.058802 |
| 23 | 6 | -3.968040 | -0.876637 | -2.355594 |
| 24 | 6 | -0.492230 | -3.456021 | -1.254041 |
| 25 | 6 | -1.148200 | -3.248310 | -2.583048 |
| 26 | 6 | -0.197634 | -4.678100 | -0.672827 |
| 27 | 6 | 0.196626 | -4.677986 | 0.673705 |
| 28 | 6 | 0.491550 | -3.455843 | 1.254618 |
| 29 | 6 | 1.147775 | -3.248018 | 2.583480 |
| 30 | 6 | 1.820407 | -1.921975 | 2.441718 |
| 31 | 6 | 3.034298 | -1.649306 | 3.058511 |
| 32 | 6 | 3.968302 | -0.877241 | 2.354980 |
| 33 | 6 | 3.577495 | -0.338635 | 1.140601 |
| 34 | 6 | 3.577338 | 0.337977 | -1.141206 |
| 35 | 6 | 4.484032 | -0.000472 | -0.000407 |
| 36 | 6 | 3.968040 | 0.876638 | -2.355594 |
| 37 | 6 | 1.820433 | 1.922017 | -2.441719 |
| 38 | 6 | 3.034123 | 1.649102 | -3.058802 |
| 39 | 6 | 1.148202 | 3.248312 | -2.583046 |
| 40 | 6 | 0.492229 | 3.456022 | -1.254040 |
| 41 | 6 | -0.196631 | 4.677987 | 0.673704 |
| 42 | 6 | 0.197630 | 4.678100 | -0.672828 |
| 43 | 1 | -5.004304 | 0.804453 | 2.671833 |
| 44 | 1 | -3.306864 | 2.188840 | 3.960847 |
| 45 | 1 | -3.306677 | -2.188724 | -3.961089 |
| 46 | 1 | -5.003957 | -0.803611 | -2.672670 |
| 47 | 1 | -0.340965 | -5.594388 | -1.237140 |
| 48 | 1 | 0.339753 | -5.594174 | 1.238231 |
| 49 | 1 | 3.306864 | -2.188841 | 3.960847 |
| 50 | 1 | 5.004304 | -0.804454 | 2.671833 |
| 51 | 1 | 5.003957 | 0.803611 | -2.672671 |
| 52 | 1 | 3.306677 | 2.188724 | -3.961089 |
| 53 | 1 | -0.339759 | 5.594175 | 1.238230 |
| 54 | 1 | 0.340960 | 5.594388 | -1.237140 |
| 55 | 8 | -1.210972 | -4.038854 | -3.504365 |
| 56 | 8 | 1.210441 | -4.038353 | 3.504983 |
| 57 | 8 | -5.700735 | 0.000652 | -0.000539 |
| 58 | 8 | -1.210440 | 4.038352 | 3.504984 |
| 59 | 8 | 1.210970 | 4.038854 | -3.504365 |
| 60 | 8 | 5.700737 | -0.000649 | -0.000539 |

**Table S23.** The optimized Cartesian coordinates of the [14]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.814911 | 1.381394 | 0.454722 |
| 2 | 6 | 0.856590 | 2.285524 | -0.013870 |
| 3 | 6 | 0.571082 | -0.402218 | -2.316850 |
| 4 | 6 | 1.189106 | -1.386274 | -1.383654 |
| 5 | 6 | 0.559590 | -2.232603 | -0.459820 |
| 6 | 6 | 1.756149 | 0.258457 | 1.446994 |
| 7 | 6 | 0.734999 | -0.095185 | 2.334804 |
| 8 | 6 | -0.734999 | 0.095185 | 2.334804 |
| 9 | 6 | -0.856590 | -2.285524 | -0.013870 |
| 10 | 6 | -0.571082 | 0.402218 | -2.316850 |
| 11 | 6 | -1.189106 | 1.386274 | -1.383654 |
| 12 | 6 | -0.559590 | 2.232603 | -0.459820 |
| 13 | 6 | 1.246747 | 3.654140 | -0.056123 |
| 14 | 6 | 3.172629 | 1.799450 | 0.385796 |
| 15 | 6 | 4.046059 | 0.757255 | 1.016584 |
| 16 | 6 | 3.087867 | -0.052842 | 1.833274 |
| 17 | 6 | -1.120238 | 3.530029 | -0.279846 |
| 18 | 6 | 0.000000 | 4.488740 | -0.012028 |
| 19 | 6 | -2.410046 | 1.836108 | -1.960931 |
| 20 | 6 | -1.235178 | 0.557245 | -3.566420 |
| 21 | 6 | -2.551744 | 1.234313 | -3.325573 |
| 22 | 6 | 1.235178 | -0.557245 | -3.566420 |
| 23 | 6 | 2.551744 | -1.234313 | -3.325573 |
| 24 | 6 | 2.410046 | -1.836108 | -1.960931 |
| 25 | 6 | 1.120238 | -3.530029 | -0.279846 |
| 26 | 6 | -1.246747 | -3.654140 | -0.056123 |
| 27 | 6 | 0.000000 | -4.488740 | -0.012028 |
| 28 | 6 | -1.121578 | 0.410605 | 3.668029 |
| 29 | 6 | 0.000000 | 0.000000 | 4.576895 |
| 30 | 6 | 1.121578 | -0.410605 | 3.668029 |
| 31 | 6 | -1.814911 | -1.381394 | 0.454722 |
| 32 | 6 | -3.172629 | -1.799450 | 0.385796 |
| 33 | 6 | -1.756149 | -0.258457 | 1.446994 |
| 34 | 6 | -3.087867 | 0.052842 | 1.833274 |
| 35 | 6 | -4.046059 | -0.757255 | 1.016584 |
| 36 | 6 | -2.565304 | -4.075578 | -0.031330 |
| 37 | 6 | -3.566162 | -3.095795 | 0.086910 |
| 38 | 6 | -3.421437 | 0.629073 | 3.052736 |
| 39 | 6 | -2.418021 | 0.741178 | 4.028175 |
| 40 | 6 | 2.418021 | -0.741178 | 4.028175 |
| 41 | 6 | 3.421437 | -0.629073 | 3.052736 |
| 42 | 6 | 2.565304 | 4.075578 | -0.031330 |
| 43 | 6 | 3.566162 | 3.095795 | 0.086910 |
| 44 | 6 | -3.065011 | 2.995644 | -1.568281 |
| 45 | 6 | -2.384902 | 3.885981 | -0.722992 |
| 46 | 6 | 0.663582 | -0.233584 | -4.785550 |
| 47 | 6 | -0.663582 | 0.233584 | -4.785550 |
| 48 | 6 | 2.384902 | -3.885981 | -0.722992 |
| 49 | 6 | 3.065011 | -2.995644 | -1.568281 |
| 50 | 1 | -2.800501 | -5.134043 | -0.086122 |
| 51 | 1 | -4.621854 | -3.349678 | 0.081164 |
| 52 | 1 | -4.465318 | 0.815498 | 3.287366 |
| 53 | 1 | -2.651345 | 0.985120 | 5.060163 |
| 54 | 1 | 2.651345 | -0.985120 | 5.060163 |
| 55 | 1 | 4.465318 | -0.815498 | 3.287366 |
| 56 | 1 | 2.800501 | 5.134043 | -0.086122 |
| 57 | 1 | 4.621854 | 3.349678 | 0.081164 |

| | | | | |
|---|---|---|---|---|
| 58 | 1 | -3.991612 | 3.279326 | -2.058657 |
| 59 | 1 | -2.756372 | 4.890925 | -0.545474 |
| 60 | 1 | 1.215112 | -0.402217 | -5.705393 |
| 61 | 1 | -1.215112 | 0.402217 | -5.705393 |
| 62 | 1 | 2.756372 | -4.890925 | -0.545474 |
| 63 | 1 | 3.991612 | -3.279326 | -2.058657 |
| 64 | 8 | 0.067480 | -5.692266 | 0.148010 |
| 65 | 8 | -5.257824 | -0.678309 | 0.977566 |
| 66 | 8 | 0.000000 | 0.000000 | 5.792890 |
| 67 | 8 | 5.257824 | 0.678309 | 0.977566 |
| 68 | 8 | -0.067480 | 5.692266 | 0.148010 |
| 69 | 8 | -3.471670 | 1.352430 | -4.111054 |
| 70 | 8 | 3.471670 | -1.352430 | -4.111054 |

**Table S24.** The optimized Cartesian coordinates of the [16]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.231535 | 0.629902 | 1.065268 |
| 2 | 6 | 2.561316 | 0.508132 | -0.291157 |
| 3 | 6 | -1.044723 | -1.084800 | 1.866829 |
| 4 | 6 | -2.231535 | -0.629902 | 1.065268 |
| 5 | 6 | -2.561316 | -0.508132 | -0.291157 |
| 6 | 6 | -0.048165 | 1.915967 | 1.557861 |
| 7 | 6 | -0.508064 | 2.561208 | 0.291171 |
| 8 | 6 | -0.629795 | 2.231426 | -1.065266 |
| 9 | 6 | -1.916078 | -0.048170 | -1.557848 |
| 10 | 6 | 0.508064 | -2.561208 | 0.291171 |
| 11 | 6 | 0.629795 | -2.231426 | -1.065266 |
| 12 | 6 | 1.084852 | -1.044669 | -1.866817 |
| 13 | 6 | 3.896685 | 0.885516 | -0.635476 |
| 14 | 6 | 3.332493 | 0.559626 | 1.972924 |
| 15 | 6 | 0.979061 | -1.401486 | -3.246367 |
| 16 | 6 | 0.559434 | -3.332374 | -1.972913 |
| 17 | 6 | 0.885565 | -3.896548 | 0.635461 |
| 18 | 6 | -1.401498 | -0.979004 | 3.246382 |
| 19 | 6 | -2.811661 | -0.518552 | 3.369151 |
| 20 | 6 | -3.332493 | -0.559626 | 1.972924 |
| 21 | 6 | -3.896685 | -0.885516 | -0.635476 |
| 22 | 6 | -2.665713 | -0.610960 | -2.637494 |
| 23 | 6 | -3.934941 | -1.180959 | -2.098134 |
| 24 | 6 | -0.559434 | 3.332374 | -1.972913 |
| 25 | 6 | -0.885565 | 3.896548 | 0.635461 |
| 26 | 6 | 0.518227 | -2.811522 | -3.369116 |
| 27 | 6 | -1.181051 | 3.934757 | 2.098125 |
| 28 | 6 | -0.979061 | 1.401486 | -3.246367 |
| 29 | 6 | -0.518227 | 2.811522 | -3.369116 |
| 30 | 6 | -1.084852 | 1.044669 | -1.866817 |
| 31 | 6 | 1.044723 | 1.084800 | 1.866829 |
| 32 | 6 | 2.811661 | 0.518552 | 3.369151 |
| 33 | 6 | 1.401498 | 0.979004 | 3.246382 |
| 34 | 6 | 0.048165 | -1.915967 | 1.557861 |
| 35 | 6 | 0.611085 | -2.665506 | 2.637481 |
| 36 | 6 | 1.181051 | -3.934757 | 2.098125 |
| 37 | 6 | 1.916078 | 0.048170 | -1.557848 |
| 38 | 6 | 2.665713 | 0.610960 | -2.637494 |
| 39 | 6 | 3.934941 | 1.180959 | -2.098134 |
| 40 | 6 | 0.327867 | -2.453380 | 3.974975 |

| | | | | |
|---|---|---|---|---|
| 41 | 6 | -0.702393 | -1.558798 | 4.290323 |
| 42 | 6 | -4.661558 | -0.682102 | 1.609613 |
| 43 | 6 | -2.453764 | -0.327577 | -3.974979 |
| 44 | 6 | -1.559099 | 0.702610 | -4.290320 |
| 45 | 6 | -0.979061 | 4.939830 | -0.265881 |
| 46 | 6 | 0.702393 | 1.558798 | 4.290323 |
| 47 | 6 | -0.327867 | 2.453380 | 3.974975 |
| 48 | 6 | 4.939972 | 0.978984 | 0.265846 |
| 49 | 6 | 1.559099 | -0.702610 | -4.290320 |
| 50 | 6 | 2.453764 | 0.327577 | -3.974979 |
| 51 | 6 | 0.682020 | -4.661438 | -1.609608 |
| 52 | 6 | 0.979061 | -4.939830 | -0.265881 |
| 53 | 1 | 0.806657 | -3.069423 | 4.730019 |
| 54 | 1 | -1.056870 | -1.426596 | 5.308213 |
| 55 | 1 | -3.069943 | -0.806252 | -4.729985 |
| 56 | 1 | -1.426927 | 1.057157 | -5.308188 |
| 57 | 1 | -1.250058 | 5.933061 | 0.078348 |
| 58 | 1 | 1.056870 | 1.426596 | 5.308213 |
| 59 | 1 | -0.806657 | 3.069423 | 4.730019 |
| 60 | 1 | 1.426927 | -1.057157 | -5.308188 |
| 61 | 1 | 3.069943 | 0.806252 | -4.729985 |
| 62 | 1 | 0.640818 | -5.434452 | -2.370654 |
| 63 | 1 | 1.250058 | -5.933061 | 0.078348 |
| 64 | 6 | 4.661558 | 0.682102 | 1.609613 |
| 65 | 6 | -0.682020 | 4.661438 | -1.609608 |
| 66 | 1 | -0.640818 | 5.434452 | -2.370654 |
| 67 | 6 | -4.939972 | -0.978984 | 0.265846 |
| 68 | 1 | -5.434581 | -0.640977 | 2.370654 |
| 69 | 1 | -5.933216 | -1.249902 | -0.078407 |
| 70 | 1 | 5.933216 | 1.249902 | -0.078407 |
| 71 | 1 | 5.434581 | 0.640977 | 2.370654 |
| 72 | 6 | -0.611085 | 2.665506 | 2.637481 |
| 73 | 8 | 0.262026 | -3.433003 | -4.383848 |
| 74 | 8 | 1.711092 | -4.838766 | 2.716428 |
| 75 | 8 | -3.433004 | -0.261817 | 4.383828 |
| 76 | 8 | -4.838903 | -1.711098 | -2.716433 |
| 77 | 8 | -0.262026 | 3.433003 | -4.383848 |
| 78 | 8 | -1.711092 | 4.838766 | 2.716428 |
| 79 | 8 | 3.433004 | 0.261817 | 4.383828 |
| 80 | 8 | 4.838903 | 1.711098 | -2.716433 |

**Table S25.** The optimized Cartesian coordinates of the [18]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.017939 | 0.758070 | 2.686482 |
| 2 | 6 | 0.017939 | -0.758070 | 2.686482 |
| 3 | 6 | -0.393698 | 1.872855 | -1.852841 |
| 4 | 6 | -0.021477 | 0.706112 | -2.757187 |
| 5 | 6 | 0.021477 | -0.706112 | -2.757187 |
| 6 | 6 | 1.432411 | 2.102419 | 0.756167 |
| 7 | 6 | 2.440648 | 1.389200 | 0.062530 |
| 8 | 6 | 2.933732 | -0.039369 | 0.015502 |
| 9 | 6 | 0.393698 | -1.872855 | -1.852841 |
| 10 | 6 | -2.933732 | 0.039369 | 0.015502 |
| 11 | 6 | -2.440648 | -1.389200 | 0.062530 |
| 12 | 6 | -1.432411 | -2.102419 | 0.756167 |
| 13 | 6 | 0.375067 | -1.116494 | 4.034721 |
| 14 | 6 | -0.375067 | 1.116494 | 4.034721 |

| | | | | |
|---|---|---|---|---|
| 15 | 6 | 1.511636 | 3.528996 | 0.624073 |
| 16 | 6 | -1.511636 | -3.528996 | 0.624073 |
| 17 | 6 | -3.512381 | -2.180719 | -0.478984 |
| 18 | 6 | -4.368677 | -0.054049 | 0.029086 |
| 19 | 6 | -4.756487 | -1.379015 | -0.502954 |
| 20 | 6 | 0.118280 | 3.047614 | -2.511313 |
| 21 | 6 | 0.624575 | 2.711352 | -3.857055 |
| 22 | 6 | 0.284727 | 1.287458 | -4.037181 |
| 23 | 6 | -0.284727 | -1.287458 | -4.037181 |
| 24 | 6 | -0.118280 | -3.047614 | -2.511313 |
| 25 | 6 | -0.624575 | -2.711352 | -3.857055 |
| 26 | 6 | 4.368677 | 0.054049 | 0.029086 |
| 27 | 6 | 4.756487 | 1.379015 | -0.502954 |
| 28 | 6 | 3.512381 | 2.180719 | -0.478984 |
| 29 | 6 | 0.000000 | 0.000000 | 4.932373 |
| 30 | 6 | 3.343247 | -2.347689 | 0.423538 |
| 31 | 6 | 0.411070 | 1.836843 | 1.879601 |
| 32 | 6 | 0.000000 | 3.127046 | 2.358811 |
| 33 | 6 | 0.567787 | 4.206163 | 1.532444 |
| 34 | 6 | -2.440797 | 1.355809 | -0.090061 |
| 35 | 6 | -3.343247 | 2.347689 | 0.423538 |
| 36 | 6 | -0.411070 | -1.836843 | 1.879601 |
| 37 | 6 | 0.000000 | -3.127046 | 2.358811 |
| 38 | 6 | -0.567787 | -4.206163 | 1.532444 |
| 39 | 6 | -1.537312 | 3.502417 | -0.486807 |
| 40 | 6 | -2.705684 | 3.674801 | 0.400300 |
| 41 | 6 | -1.322337 | 2.116388 | -0.804967 |
| 42 | 6 | 1.537312 | -3.502417 | -0.486807 |
| 43 | 6 | 2.705684 | -3.674801 | 0.400300 |
| 44 | 6 | 1.322337 | -2.116388 | -0.804967 |
| 45 | 6 | 2.440797 | -1.355809 | -0.090061 |
| 46 | 6 | -0.941702 | 4.597889 | -1.075323 |
| 47 | 6 | -0.087704 | 4.360227 | -2.148176 |
| 48 | 6 | 0.224037 | 0.661419 | -5.263956 |
| 49 | 6 | -0.224037 | -0.661419 | -5.263956 |
| 50 | 6 | -5.247498 | 0.948227 | 0.377027 |
| 51 | 6 | -4.682000 | 2.178462 | 0.718068 |
| 52 | 6 | -2.455729 | -4.251387 | -0.078981 |
| 53 | 6 | -3.527549 | -3.551846 | -0.623810 |
| 54 | 6 | 0.738577 | -2.370481 | 4.475458 |
| 55 | 6 | 0.635024 | -3.410794 | 3.553658 |
| 56 | 6 | -0.635024 | 3.410794 | 3.553658 |
| 57 | 6 | -0.738577 | 2.370481 | 4.475458 |
| 58 | 6 | 3.527549 | 3.551846 | -0.623810 |
| 59 | 6 | 2.455729 | 4.251387 | -0.078981 |
| 60 | 6 | 4.682000 | -2.178462 | 0.718068 |
| 61 | 6 | 5.247498 | -0.948227 | 0.377027 |
| 62 | 6 | 0.087704 | -4.360227 | -2.148176 |
| 63 | 6 | 0.941702 | -4.597889 | -1.075323 |
| 64 | 1 | -1.208674 | 5.591848 | -0.732389 |
| 65 | 1 | 0.343614 | 5.152346 | -2.752287 |
| 66 | 1 | 0.458939 | 1.218187 | -6.165365 |
| 67 | 1 | -0.458939 | -1.218187 | -6.165365 |
| 68 | 1 | -6.316247 | 0.759521 | 0.372332 |
| 69 | 1 | -5.258276 | 3.022620 | 1.083058 |
| 70 | 1 | -2.393004 | -5.335150 | -0.080424 |
| 71 | 1 | -4.400005 | -4.037381 | -1.049652 |
| 72 | 1 | 1.011671 | -2.521000 | 5.515156 |
| 73 | 1 | 0.889948 | -4.440494 | 3.782954 |
| 74 | 1 | -0.889948 | 4.440494 | 3.782954 |
| 75 | 1 | -1.011671 | 2.521000 | 5.515156 |
| 76 | 1 | 4.400005 | 4.037381 | -1.049652 |
| 77 | 1 | 2.393004 | 5.335150 | -0.080424 |

| | | | | |
|---|---|---|---|---|
| 78 | 1 | 5.258276 | -3.022620 | 1.083058 |
| 79 | 1 | 6.316247 | -0.759521 | 0.372332 |
| 80 | 1 | -0.343614 | -5.152346 | -2.752287 |
| 81 | 1 | 1.208674 | -5.591848 | -0.732389 |
| 82 | 8 | 0.000000 | 0.000000 | 6.150945 |
| 83 | 8 | 0.383403 | 5.406862 | 1.649455 |
| 84 | 8 | 5.871523 | 1.738160 | -0.838569 |
| 85 | 8 | 3.104604 | -4.702540 | 0.920278 |
| 86 | 8 | -0.383403 | -5.406862 | 1.649455 |
| 87 | 8 | -1.141200 | -3.457220 | -4.671354 |
| 88 | 8 | 1.141200 | 3.457220 | -4.671354 |
| 89 | 8 | -3.104604 | 4.702540 | 0.920278 |
| 90 | 8 | -5.871523 | -1.738160 | -0.838569 |

**Table S26.** The optimized Cartesian coordinates of the [20]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.424040 | -0.759454 | -3.824586 |
| 2 | 6 | 2.475215 | 0.215299 | -4.124784 |
| 3 | 6 | 2.985141 | 0.145667 | -0.495195 |
| 4 | 6 | 4.386786 | 0.499904 | -0.593919 |
| 5 | 6 | 5.111745 | -0.197072 | 0.480547 |
| 6 | 6 | 4.067027 | -0.667257 | 1.406064 |
| 7 | 6 | 2.798568 | -0.100425 | 1.004792 |
| 8 | 6 | 5.015132 | 1.113021 | -1.650270 |
| 9 | 6 | 4.258209 | 1.241291 | -2.807275 |
| 10 | 6 | 3.059674 | 0.556196 | -2.834053 |
| 11 | 6 | 2.360690 | -0.086091 | -1.745983 |
| 12 | 1 | 4.624902 | 1.696539 | -3.723302 |
| 13 | 1 | 6.068569 | 1.372476 | -1.586379 |
| 14 | 6 | 4.386786 | -1.217026 | 2.625856 |
| 15 | 6 | 3.459749 | -1.021688 | 3.636204 |
| 16 | 6 | 2.390292 | -0.196322 | 3.352569 |
| 17 | 6 | 1.972525 | 0.332607 | 2.078177 |
| 18 | 1 | 5.371227 | -1.648262 | 2.787163 |
| 19 | 1 | 3.614542 | -1.344503 | 4.662437 |
| 20 | 6 | 1.250421 | -0.972980 | -2.409302 |
| 21 | 6 | 1.653965 | 0.401334 | 4.460750 |
| 22 | 6 | 0.745759 | 1.369493 | 3.844472 |
| 23 | 6 | 0.844821 | 1.375909 | 2.406487 |
| 24 | 6 | -0.026251 | 2.160870 | 4.667897 |
| 25 | 6 | -0.800382 | 3.135967 | 4.063689 |
| 26 | 6 | -0.720367 | 3.215674 | 2.692948 |
| 27 | 6 | 0.017019 | 2.361607 | 1.790039 |
| 28 | 1 | 0.035111 | 2.013388 | 5.742454 |
| 29 | 1 | -1.386499 | 3.869375 | 4.611421 |
| 30 | 6 | -1.097863 | 4.480723 | 2.041489 |
| 31 | 6 | -0.366369 | 4.453517 | 0.767084 |
| 32 | 6 | -0.063583 | 3.078502 | 0.445063 |
| 33 | 6 | -0.002576 | 5.575654 | 0.060937 |
| 34 | 6 | 0.754919 | 5.340911 | -1.086737 |
| 35 | 6 | 0.754014 | 4.042574 | -1.545599 |
| 36 | 6 | 0.139627 | 2.887804 | -0.938932 |
| 37 | 1 | -0.271547 | 6.564108 | 0.422402 |
| 38 | 1 | 1.246283 | 6.119873 | -1.662860 |
| 39 | 6 | 1.241059 | 3.687540 | -2.880837 |
| 40 | 6 | 0.437681 | 2.508512 | -3.239072 |
| 41 | 6 | -0.254920 | 1.955674 | -2.099155 |

| | | | | |
|---|---|---|---|---|
| 42 | 6 | 0.234433 | 2.252770 | -4.576169 |
| 43 | 6 | -0.765967 | 1.348689 | -4.880894 |
| 44 | 6 | -1.424040 | 0.759454 | -3.824586 |
| 45 | 6 | -1.250421 | 0.972980 | -2.409302 |
| 46 | 1 | 0.826661 | 2.779539 | -5.319062 |
| 47 | 1 | -1.053848 | 1.078390 | -5.893416 |
| 48 | 6 | -2.360690 | 0.086091 | -1.745983 |
| 49 | 6 | -3.059674 | -0.556196 | -2.834053 |
| 50 | 6 | -2.475215 | -0.215299 | -4.124784 |
| 51 | 6 | -4.258209 | -1.241291 | -2.807275 |
| 52 | 6 | -5.015132 | -1.113021 | -1.650270 |
| 53 | 6 | -4.386786 | -0.499904 | -0.593919 |
| 54 | 6 | -2.985141 | -0.145667 | -0.495195 |
| 55 | 1 | -4.624902 | -1.696539 | -3.723302 |
| 56 | 1 | -6.068569 | -1.372476 | -1.586379 |
| 57 | 6 | -5.111745 | 0.197072 | 0.480547 |
| 58 | 6 | -4.067027 | 0.667257 | 1.406064 |
| 59 | 6 | -2.798568 | 0.100425 | 1.004792 |
| 60 | 6 | -4.386786 | 1.217026 | 2.625856 |
| 61 | 6 | -3.459749 | 1.021688 | 3.636204 |
| 62 | 6 | -2.390292 | 0.196322 | 3.352569 |
| 63 | 6 | -1.972525 | -0.332607 | 2.078177 |
| 64 | 1 | -5.371227 | 1.648262 | 2.787163 |
| 65 | 1 | -3.614542 | 1.344503 | 4.662437 |
| 66 | 6 | 0.254920 | -1.955674 | -2.099155 |
| 67 | 6 | -0.437681 | -2.508512 | -3.239072 |
| 68 | 6 | -0.234433 | -2.252770 | -4.576169 |
| 69 | 6 | 0.765967 | -1.348689 | -4.880894 |
| 70 | 1 | 1.053848 | -1.078390 | -5.893416 |
| 71 | 1 | -0.826661 | -2.779539 | -5.319062 |
| 72 | 6 | -1.241059 | -3.687540 | -2.880837 |
| 73 | 6 | -0.754014 | -4.042574 | -1.545599 |
| 74 | 6 | -0.139627 | -2.887804 | -0.938932 |
| 75 | 6 | -0.754919 | -5.340911 | -1.086737 |
| 76 | 6 | 0.002576 | -5.575654 | 0.060937 |
| 77 | 6 | 0.366369 | -4.453517 | 0.767084 |
| 78 | 6 | 0.063583 | -3.078502 | 0.445063 |
| 79 | 6 | 1.097863 | -4.480723 | 2.041489 |
| 80 | 6 | 0.720367 | -3.215674 | 2.692948 |
| 81 | 6 | -0.017019 | -2.361607 | 1.790039 |
| 82 | 1 | 0.271547 | -6.564108 | 0.422402 |
| 83 | 1 | -1.246283 | -6.119873 | -1.662860 |
| 84 | 6 | 0.800382 | -3.135967 | 4.063689 |
| 85 | 6 | 0.026251 | -2.160870 | 4.667897 |
| 86 | 6 | -0.745759 | -1.369493 | 3.844472 |
| 87 | 6 | -0.844821 | -1.375909 | 2.406487 |
| 88 | 6 | -1.653965 | -0.401334 | 4.460750 |
| 89 | 1 | -0.035111 | -2.013388 | 5.742454 |
| 90 | 1 | 1.386499 | -3.869375 | 4.611421 |
| 91 | 8 | 6.318086 | -0.335949 | 0.586682 |
| 92 | 8 | 1.813953 | 0.197912 | 5.655786 |
| 93 | 8 | 2.827463 | 0.599090 | -5.231040 |
| 94 | 8 | -2.063562 | -4.277392 | -3.559808 |
| 95 | 8 | 1.799686 | -5.377750 | 2.474046 |
| 96 | 8 | -6.318086 | 0.335949 | 0.586682 |
| 97 | 8 | -1.813953 | -0.197912 | 5.655786 |
| 98 | 8 | -1.799686 | 5.377750 | 2.474046 |
| 99 | 8 | 2.063562 | 4.277392 | -3.559808 |
| 100 | 8 | -2.827463 | -0.599090 | -5.231040 |

**Table S27.** The optimized Cartesian coordinates of the [22]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.069071 | 4.066665 | -2.082551 |
| 2 | 6 | -0.447449 | 4.554095 | -0.953159 |
| 3 | 6 | 0.085250 | 3.624354 | -0.079409 |
| 4 | 6 | 0.001520 | 2.187695 | -0.098290 |
| 5 | 6 | -0.846912 | 1.694649 | -1.189740 |
| 6 | 6 | -1.188773 | 2.696269 | -2.168847 |
| 7 | 1 | -1.406324 | 4.680495 | -2.911569 |
| 8 | 1 | -0.292459 | 5.607254 | -0.743216 |
| 9 | 6 | 0.807551 | 4.152983 | 1.082599 |
| 10 | 6 | 1.136280 | 2.998162 | 1.908282 |
| 11 | 6 | 0.884401 | 1.763207 | 1.222918 |
| 12 | 6 | -1.398206 | 0.376154 | -1.887439 |
| 13 | 6 | -1.399940 | 0.653220 | -3.298424 |
| 14 | 6 | -1.482291 | 2.103577 | -3.487060 |
| 15 | 6 | 1.550378 | 3.205838 | 3.213350 |
| 16 | 6 | 1.629431 | 2.093265 | 4.036948 |
| 17 | 6 | 1.531863 | 0.875575 | 3.399541 |
| 18 | 6 | 1.407509 | 0.652203 | 1.982662 |
| 19 | 1 | 1.692349 | 4.226015 | 3.554204 |
| 20 | 1 | 1.771959 | 2.135828 | 5.111896 |
| 21 | 6 | 1.523015 | -0.422272 | 4.134473 |
| 22 | 6 | 1.754069 | -1.451976 | 3.101714 |
| 23 | 6 | 1.964307 | -0.771378 | 1.861293 |
| 24 | 6 | 2.195382 | -2.734500 | 3.395364 |
| 25 | 6 | 3.094588 | -3.352664 | 2.518314 |
| 26 | 6 | 3.566294 | -2.581629 | 1.468171 |
| 27 | 6 | 3.005119 | -1.325197 | 1.098438 |
| 28 | 6 | 4.974044 | -2.670835 | 0.948894 |
| 29 | 6 | 5.257870 | -1.297690 | 0.420165 |
| 30 | 6 | 4.020969 | -0.618308 | 0.302226 |
| 31 | 1 | 3.565750 | -4.302076 | 2.754025 |
| 32 | 1 | 1.970967 | -3.157577 | 4.370139 |
| 33 | 6 | 6.476322 | -0.683086 | 0.171618 |
| 34 | 6 | 6.476141 | 0.683139 | -0.174668 |
| 35 | 6 | 5.257490 | 1.297567 | -0.422685 |
| 36 | 6 | 4.020732 | 0.618025 | -0.304153 |
| 37 | 1 | 7.401236 | -1.238316 | 0.294492 |
| 38 | 1 | 7.400921 | 1.238483 | -0.298026 |
| 39 | 6 | 4.973305 | 2.670581 | -0.951531 |
| 40 | 6 | 3.565223 | 2.581264 | -1.469926 |
| 41 | 6 | 3.004352 | 1.324809 | -1.099828 |
| 42 | 6 | 3.092894 | 3.352256 | -2.519819 |
| 43 | 6 | 2.193279 | 2.733991 | -3.396366 |
| 44 | 6 | 1.752170 | 1.451470 | -3.102368 |
| 45 | 6 | 1.963026 | 0.770992 | -1.861993 |
| 46 | 6 | 1.405848 | -0.652509 | -1.982977 |
| 47 | 6 | 1.529288 | -0.876073 | -3.399824 |
| 48 | 6 | 1.520556 | 0.421708 | -4.134915 |
| 49 | 1 | 3.563927 | 4.301655 | -2.755830 |
| 50 | 1 | 1.968306 | 3.156969 | -4.371055 |
| 51 | 6 | -2.016092 | -0.888390 | -1.650133 |
| 52 | 6 | -1.914724 | -1.868861 | -2.688980 |
| 53 | 6 | -1.601146 | -1.603100 | -4.008077 |
| 54 | 6 | -1.495268 | -0.252167 | -4.338618 |
| 55 | 1 | -1.470335 | 0.113031 | -5.359602 |
| 56 | 1 | -1.596422 | -2.402212 | -4.741987 |
| 57 | 6 | -2.540122 | -3.165767 | -2.261166 |

| | | | | |
|---|---|---|---|---|
| 58 | 6 | -3.130106 | -1.424093 | -0.794778 |
| 59 | 6 | -3.465329 | -2.750479 | -1.174358 |
| 60 | 6 | 0.883045 | -1.763365 | -1.222699 |
| 61 | 6 | 1.134303 | -2.998434 | -1.908059 |
| 62 | 6 | 1.547382 | -3.206331 | -3.213442 |
| 63 | 6 | 1.626041 | -2.093892 | -4.037203 |
| 64 | 1 | 1.767831 | -2.136542 | -5.112246 |
| 65 | 1 | 1.688860 | -4.226590 | -3.554256 |
| 66 | 6 | 0.806038 | -4.153095 | -1.081913 |
| 67 | 6 | 0.084635 | -3.624179 | 0.080551 |
| 68 | 6 | 0.000959 | -2.187535 | 0.098964 |
| 69 | 6 | -0.846706 | -1.694068 | 1.190738 |
| 70 | 6 | -1.187738 | -2.695128 | 2.170649 |
| 71 | 6 | -1.068069 | -4.065561 | 2.084865 |
| 72 | 6 | -0.447431 | -4.553513 | 0.955113 |
| 73 | 1 | -0.292655 | -5.606780 | 0.745547 |
| 74 | 1 | -1.404575 | -4.679047 | 2.914444 |
| 75 | 6 | -1.480032 | -2.101582 | 3.488774 |
| 76 | 6 | -1.397501 | -0.375184 | 1.887900 |
| 77 | 6 | -1.397810 | -0.651307 | 3.299146 |
| 78 | 6 | -1.492298 | 0.254789 | 4.338769 |
| 79 | 6 | -1.599290 | 1.605474 | 4.007421 |
| 80 | 6 | -1.914356 | 1.870193 | 2.688506 |
| 81 | 6 | -2.015993 | 0.888952 | 1.650353 |
| 82 | 1 | -1.594206 | 2.405066 | 4.740811 |
| 83 | 1 | -1.466217 | -0.109683 | 5.359986 |
| 84 | 6 | -2.540999 | 3.166390 | 2.260415 |
| 85 | 6 | -3.466684 | 2.749857 | 1.174480 |
| 86 | 6 | -3.130765 | 1.423540 | 0.795302 |
| 87 | 6 | -4.716733 | 3.315615 | 0.947434 |
| 88 | 6 | -5.763698 | 2.504826 | 0.465093 |
| 89 | 6 | -5.466378 | 1.188326 | 0.155823 |
| 90 | 6 | -4.139161 | 0.695839 | 0.192789 |
| 91 | 6 | -4.138717 | -0.697305 | -0.191518 |
| 92 | 6 | -5.465542 | -1.190807 | -0.154019 |
| 93 | 6 | -5.762115 | -2.507397 | -0.463639 |
| 94 | 6 | -4.714843 | -3.317244 | -0.946855 |
| 95 | 6 | -6.382459 | -0.001628 | 0.001279 |
| 96 | 1 | -6.785944 | 2.868266 | 0.424671 |
| 97 | 1 | -4.908774 | 4.327703 | 1.291838 |
| 98 | 1 | -6.784099 | -2.871522 | -0.422762 |
| 99 | 1 | -4.906319 | -4.329321 | -1.291608 |
| 100 | 8 | 5.740528 | 3.609578 | -1.033247 |
| 101 | 8 | 5.741515 | -3.609652 | 1.030386 |
| 102 | 8 | -2.401935 | -4.250039 | -2.792047 |
| 103 | 8 | 1.451256 | -0.560701 | 5.342650 |
| 104 | 8 | 1.060470 | 5.324304 | 1.315663 |
| 105 | 8 | -1.733221 | 2.701901 | -4.520061 |
| 106 | 8 | 1.448421 | 0.559989 | -5.343086 |
| 107 | 8 | 1.058925 | -5.324463 | -1.314776 |
| 108 | 8 | -7.597263 | -0.002063 | 0.001384 |
| 109 | 8 | -2.403460 | 4.251004 | 2.790780 |
| 110 | 8 | -1.729802 | -2.699236 | 4.522439 |

**Table S28.** The optimized Cartesian coordinates of the [24]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 3.735070 | -3.135275 | 0.303513 |
| 2 | 6 | -0.102307 | -2.836896 | -1.456447 |
| 3 | 6 | -0.513476 | -3.416072 | -0.249860 |
| 4 | 6 | -0.546714 | -3.036497 | 1.182278 |
| 5 | 6 | -0.252563 | -4.212734 | 1.933787 |
| 6 | 6 | -0.493861 | -5.389219 | 1.032076 |
| 7 | 6 | -0.846491 | -4.801647 | -0.306452 |
| 8 | 6 | 3.774481 | 1.886941 | 1.937478 |
| 9 | 6 | 4.915071 | 2.265990 | 1.037030 |
| 10 | 6 | 4.583307 | 1.667828 | -0.302148 |
| 11 | 6 | 3.216710 | 1.263797 | -0.247057 |
| 12 | 6 | 2.903453 | 1.044586 | 1.184697 |
| 13 | 6 | 3.756183 | 1.955846 | 3.321043 |
| 14 | 6 | 2.970737 | 1.023543 | 4.016519 |
| 15 | 6 | 2.399359 | -0.016214 | 3.289152 |
| 16 | 6 | 2.359893 | -0.058546 | 1.866957 |
| 17 | 1 | 2.974235 | 0.977335 | 5.100907 |
| 18 | 1 | 4.430932 | 2.627056 | 3.843705 |
| 19 | 6 | 5.330681 | 1.659593 | -1.467456 |
| 20 | 6 | 4.677742 | 1.287717 | -2.656416 |
| 21 | 6 | 2.510727 | 1.330925 | -1.454228 |
| 22 | 6 | 3.292169 | 1.202657 | -2.635155 |
| 23 | 1 | 5.205114 | 1.219326 | -3.603089 |
| 24 | 1 | 6.373773 | 1.959887 | -1.454345 |
| 25 | 6 | 1.230886 | 2.015379 | -1.865240 |
| 26 | 6 | 1.214524 | 2.072743 | -3.287456 |
| 27 | 6 | 2.405529 | 1.348852 | -3.835522 |
| 28 | 6 | 0.600105 | 3.088503 | -4.013634 |
| 29 | 6 | 0.184610 | 4.233700 | -3.316660 |
| 30 | 6 | 0.252964 | 4.213143 | -1.933165 |
| 31 | 6 | 0.547021 | 3.036762 | -1.181863 |
| 32 | 6 | 0.494157 | 5.389402 | -1.031213 |
| 33 | 6 | 0.846582 | 4.801541 | 0.307207 |
| 34 | 6 | 0.513572 | 3.415938 | 0.250370 |
| 35 | 1 | -0.059197 | 5.154378 | -3.838066 |
| 36 | 1 | 0.642686 | 3.070143 | -5.098020 |
| 37 | 6 | 1.226839 | 5.443331 | 1.473444 |
| 38 | 6 | 1.222375 | 4.690455 | 2.661520 |
| 39 | 6 | 0.603777 | 3.447798 | 2.638523 |
| 40 | 6 | 0.102058 | 2.836655 | 1.456783 |
| 41 | 6 | 0.034046 | 2.751129 | 3.837921 |
| 42 | 6 | -1.188713 | 2.082953 | 3.289048 |
| 43 | 6 | -1.130880 | 2.070391 | 1.866878 |
| 44 | 1 | 1.544938 | 5.111923 | 3.608774 |
| 45 | 1 | 1.487853 | 6.496969 | 1.461843 |
| 46 | 6 | -2.375651 | 2.058591 | 4.015196 |
| 47 | 6 | -3.574940 | 2.273389 | 3.318528 |
| 48 | 6 | -2.357446 | 1.990463 | 1.183408 |
| 49 | 6 | -3.523077 | 2.323790 | 1.935055 |
| 50 | 1 | -2.338503 | 2.084523 | 5.099627 |
| 51 | 1 | -4.493969 | 2.522591 | 3.840298 |
| 52 | 6 | -4.420401 | 3.122818 | 1.034091 |
| 53 | 6 | -3.735077 | 3.135235 | -0.304296 |
| 54 | 6 | -2.702283 | 2.153336 | -0.248591 |
| 55 | 6 | -4.100217 | 3.787140 | -1.469748 |
| 56 | 6 | -3.450844 | 3.407675 | -2.658292 |
| 57 | 6 | -2.684496 | 2.250168 | -2.636606 |
| 58 | 6 | -2.406550 | 1.508726 | -1.455641 |
| 59 | 1 | -3.654645 | 3.898721 | -3.605049 |
| 60 | 1 | -4.881859 | 4.540318 | -1.457230 |
| 61 | 6 | -2.359618 | 0.058334 | -1.867106 |
| 62 | 6 | -2.398924 | 0.015845 | -3.289291 |
| 63 | 6 | -2.366340 | 1.409422 | -3.836788 |
| 64 | 6 | -2.970452 | -1.023906 | -4.016570 |

| | | | | |
|---|---|---|---|---|
| 65 | 6 | -2.903300 | -1.044667 | -1.184768 |
| 66 | 6 | -3.774255 | -1.887121 | -1.937481 |
| 67 | 6 | -3.755980 | -1.956121 | -3.321036 |
| 68 | 1 | -2.973902 | -0.977789 | -5.100963 |
| 69 | 1 | -4.430753 | -2.627345 | -3.843640 |
| 70 | 6 | -3.216512 | -1.263759 | 0.247040 |
| 71 | 6 | -4.583091 | -1.667960 | 0.302106 |
| 72 | 6 | -4.914812 | -2.266216 | -1.037046 |
| 73 | 6 | -2.510559 | -1.330730 | 1.454269 |
| 74 | 6 | -3.292113 | -1.202440 | 2.635131 |
| 75 | 6 | -4.677677 | -1.287675 | 2.656325 |
| 76 | 6 | -5.330529 | -1.659662 | 1.467364 |
| 77 | 1 | -5.205121 | -1.219241 | 3.602955 |
| 78 | 1 | -6.373608 | -1.960003 | 1.454237 |
| 79 | 6 | -2.405530 | -1.348427 | 3.835584 |
| 80 | 6 | -1.230666 | -2.015008 | 1.865452 |
| 81 | 6 | -1.214391 | -2.072164 | 3.287687 |
| 82 | 6 | -0.599842 | -3.087718 | 4.014044 |
| 83 | 6 | -0.184169 | -4.232980 | 3.317282 |
| 84 | 1 | 0.059746 | -5.153532 | 3.838870 |
| 85 | 1 | -0.642470 | -3.069195 | 5.098427 |
| 86 | 6 | -0.604280 | -3.448130 | -2.638023 |
| 87 | 6 | -1.222805 | -4.690827 | -2.660729 |
| 88 | 6 | -1.226928 | -5.443590 | -1.472562 |
| 89 | 1 | -1.487911 | -6.497232 | -1.460841 |
| 90 | 1 | -1.545572 | -5.112426 | -3.607854 |
| 91 | 6 | 1.130399 | -2.070494 | -1.866854 |
| 92 | 6 | 1.187801 | -2.082914 | -3.289048 |
| 93 | 6 | -0.034908 | -2.751434 | -3.837578 |
| 94 | 6 | 2.357083 | -1.990447 | -1.183705 |
| 95 | 6 | 3.522569 | -2.323479 | -1.935705 |
| 96 | 6 | 3.574079 | -2.272870 | -3.319172 |
| 97 | 6 | 2.374533 | -2.058240 | -4.015513 |
| 98 | 1 | 2.337074 | -2.084133 | -5.099933 |
| 99 | 1 | 4.492989 | -2.521957 | -3.841208 |
| 100 | 6 | 4.420149 | -3.122670 | -1.035063 |
| 101 | 6 | 2.702259 | -2.153420 | 0.248170 |
| 102 | 6 | 4.100470 | -3.787283 | 1.468831 |
| 103 | 6 | 3.451261 | -3.408027 | 2.657521 |
| 104 | 6 | 2.684988 | -2.250476 | 2.636158 |
| 105 | 6 | 2.406773 | -1.508892 | 1.455346 |
| 106 | 1 | 3.655265 | -3.899219 | 3.604156 |
| 107 | 1 | 4.882086 | -4.540484 | 1.456080 |
| 108 | 6 | 2.367098 | -1.409854 | 3.836517 |
| 109 | 8 | 2.266486 | -1.774445 | 4.990908 |
| 110 | 8 | 0.453334 | 6.568543 | -1.323488 |
| 111 | 8 | -2.265575 | 1.773859 | -4.991154 |
| 112 | 8 | -5.915532 | -2.890405 | -1.330762 |
| 113 | 8 | -0.453020 | -6.568250 | 1.324532 |
| 114 | 8 | -2.671537 | -1.080730 | 4.990258 |
| 115 | 8 | -5.461369 | 3.677805 | 1.327077 |
| 116 | 8 | 0.399271 | 2.845329 | 4.992617 |
| 117 | 8 | 5.461073 | -3.677474 | -1.328352 |
| 118 | 8 | -0.400488 | -2.845620 | -4.992208 |
| 119 | 8 | 5.915846 | 2.890097 | 1.330764 |
| 120 | 8 | 2.671298 | 1.080968 | -4.990257 |

**Table S29.** The optimized Cartesian coordinates of the [26]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -4.244898 | -1.691343 | 3.380972 |
| 2 | 6 | -4.144452 | -1.843485 | 2.013215 |
| 3 | 6 | -2.931003 | -1.693075 | 1.261915 |
| 4 | 6 | -1.734137 | -1.802722 | 1.997140 |
| 5 | 6 | -1.862510 | -1.623397 | 3.408966 |

| | | | | |
|---|---|---|---|---|
| 6 | 6 | -3.057851 | -1.486909 | 4.094921 |
| 7 | 1 | -3.044523 | -1.387677 | 5.175493 |
| 8 | 1 | -5.202579 | -1.817283 | 3.875716 |
| 9 | 6 | -5.135320 | -2.555336 | 1.153761 |
| 10 | 6 | -4.468111 | -2.713197 | -0.171678 |
| 11 | 6 | -3.304261 | -1.879143 | -0.170655 |
| 12 | 6 | -4.944609 | -3.389189 | -1.278260 |
| 13 | 6 | -4.252320 | -3.207188 | -2.483121 |
| 14 | 6 | -3.318755 | -2.184957 | -2.533872 |
| 15 | 6 | -2.926179 | -1.376420 | -1.425344 |
| 16 | 1 | -4.511196 | -3.739153 | -3.393358 |
| 17 | 1 | -5.827945 | -4.014992 | -1.198662 |
| 18 | 6 | -2.544044 | -0.024635 | -2.006094 |
| 19 | 6 | -2.453158 | -0.195215 | -3.423203 |
| 20 | 6 | -2.796563 | -1.597177 | -3.797466 |
| 21 | 6 | -2.820367 | 1.287978 | -1.556078 |
| 22 | 6 | -3.246530 | 2.222163 | -2.555229 |
| 23 | 6 | -3.070882 | 2.055101 | -3.916304 |
| 24 | 6 | -2.595279 | 0.817857 | -4.360654 |
| 25 | 1 | -2.534555 | 0.568169 | -5.415784 |
| 26 | 1 | -3.417906 | 2.822772 | -4.601253 |
| 27 | 6 | -4.279747 | 3.119492 | -1.957060 |
| 28 | 6 | -3.285411 | 1.836869 | -0.242819 |
| 29 | 6 | -4.416294 | 2.662854 | -0.542429 |
| 30 | 6 | -5.399617 | 3.003163 | 0.365712 |
| 31 | 6 | -5.269190 | 2.494481 | 1.668121 |
| 32 | 6 | -4.049102 | 1.939791 | 2.010750 |
| 33 | 6 | -2.947062 | 1.771310 | 1.115301 |
| 34 | 1 | -6.239793 | 3.617112 | 0.057062 |
| 35 | 1 | -6.040419 | 2.610208 | 2.423144 |
| 36 | 6 | -1.704083 | 1.837550 | 1.973358 |
| 37 | 6 | -2.125222 | 1.600407 | 3.320173 |
| 38 | 6 | -3.613611 | 1.569021 | 3.384363 |
| 39 | 6 | -1.378418 | 1.888295 | 4.450875 |
| 40 | 6 | -0.240193 | 2.682534 | 4.292049 |
| 41 | 6 | -0.241186 | 5.929180 | -0.660425 |
| 42 | 6 | 0.239388 | 5.929067 | 0.662104 |
| 43 | 6 | 0.306714 | 4.707444 | 1.307312 |
| 44 | 6 | -0.031020 | 3.457624 | 0.699392 |
| 45 | 6 | 0.029926 | 3.457825 | -0.698393 |
| 46 | 6 | -0.308182 | 4.707712 | -1.305958 |
| 47 | 1 | -0.487051 | 6.842672 | -1.192564 |
| 48 | 1 | 0.484971 | 6.842489 | 1.194495 |
| 49 | 6 | 0.682238 | 4.426430 | 2.725926 |
| 50 | 6 | 0.090597 | 3.084651 | 3.010681 |
| 51 | 6 | -0.505197 | 2.572472 | 1.814331 |
| 52 | 1 | 0.266020 | 3.129304 | 5.142188 |
| 53 | 1 | -1.792575 | 1.673685 | 5.431265 |
| 54 | 6 | 0.504309 | 2.573109 | -1.813595 |
| 55 | 6 | -0.091686 | 3.085439 | -3.009779 |
| 56 | 6 | -0.683692 | 4.426980 | -2.724632 |
| 57 | 6 | 1.703383 | 1.838558 | -1.972881 |
| 58 | 6 | 2.124482 | 1.601850 | -3.319792 |
| 59 | 6 | 1.377527 | 1.889813 | -4.450376 |
| 60 | 6 | 0.239111 | 2.683729 | -4.291270 |
| 61 | 1 | -0.267278 | 3.130603 | -5.141251 |
| 62 | 1 | 1.791673 | 1.675520 | -5.430839 |
| 63 | 6 | 2.946445 | 1.772385 | -1.114944 |
| 64 | 6 | 4.048363 | 1.941410 | -2.010451 |
| 65 | 6 | 3.612864 | 1.570871 | -3.384112 |
| 66 | 6 | 5.268305 | 2.496399 | -1.667815 |
| 67 | 6 | 5.398723 | 3.004768 | -0.365276 |
| 68 | 6 | 4.415602 | 2.663916 | 0.542873 |

| | | | | |
|---|---|---|---|---|
| 69 | 6 | 3.284914 | 1.837679 | 0.243152 |
| 70 | 1 | 6.238745 | 3.618891 | -0.056554 |
| 71 | 1 | 6.039425 | 2.612536 | -2.422886 |
| 72 | 6 | 2.820068 | 1.288444 | 1.556334 |
| 73 | 6 | 3.245989 | 2.222573 | 2.555640 |
| 74 | 6 | 4.278997 | 3.120238 | 1.957602 |
| 75 | 6 | 3.070394 | 2.055224 | 3.916690 |
| 76 | 6 | 2.595070 | 0.817788 | 4.360819 |
| 77 | 6 | 2.453185 | -0.195163 | 3.423198 |
| 78 | 6 | 2.544101 | -0.024320 | 2.006131 |
| 79 | 1 | 3.417207 | 2.822862 | 4.601780 |
| 80 | 1 | 2.534412 | 0.567909 | 5.415907 |
| 81 | 6 | 2.926607 | -1.375902 | 1.425157 |
| 82 | 6 | 3.319301 | -2.184552 | 2.533555 |
| 83 | 6 | 2.796938 | -1.597110 | 3.797243 |
| 84 | 6 | 3.304896 | -1.878285 | 0.170401 |
| 85 | 6 | 4.468914 | -2.712101 | 0.171315 |
| 86 | 6 | 4.945503 | -3.388185 | 1.277803 |
| 87 | 6 | 4.253109 | -3.206556 | 2.482663 |
| 88 | 1 | 4.512053 | -3.738634 | 3.392815 |
| 89 | 1 | 5.828969 | -4.013795 | 1.198136 |
| 90 | 6 | 5.136117 | -2.553917 | -1.154091 |
| 91 | 6 | 4.145227 | -1.841917 | -2.013398 |
| 92 | 6 | 2.931702 | -1.691915 | -1.262130 |
| 93 | 6 | 4.245734 | -1.689281 | -3.381086 |
| 94 | 6 | 3.058699 | -1.484716 | -4.095040 |
| 95 | 6 | 1.863335 | -1.621585 | -3.409212 |
| 96 | 6 | 1.734912 | -1.801493 | -1.997456 |
| 97 | 1 | 3.045444 | -1.385020 | -5.175568 |
| 98 | 1 | 5.203454 | -1.814954 | -3.875823 |
| 99 | 6 | 0.637910 | -2.090326 | -4.109972 |
| 100 | 6 | -0.023491 | -2.948105 | -3.084263 |
| 101 | 6 | 0.459588 | -2.609961 | -1.784231 |
| 102 | 6 | -0.026398 | -3.422782 | -0.743944 |
| 103 | 6 | -0.396665 | -4.751625 | -1.126671 |
| 104 | 6 | -0.766883 | -5.111519 | -2.408887 |
| 105 | 6 | -0.693194 | -4.122032 | -3.400184 |
| 106 | 1 | -1.003911 | -4.297516 | -4.425004 |
| 107 | 1 | -1.046280 | -6.136456 | -2.632537 |
| 108 | 6 | 0.027491 | -3.423118 | 0.742846 |
| 109 | 6 | 0.398123 | -4.752054 | 1.124944 |
| 110 | 6 | 0.000889 | -5.657453 | -0.001091 |
| 111 | 6 | -0.637067 | -2.092403 | 4.109508 |
| 112 | 6 | 0.024457 | -2.949580 | 3.083391 |
| 113 | 6 | -0.458708 | -2.610924 | 1.783512 |
| 114 | 6 | 0.694467 | -4.123469 | 3.398753 |
| 115 | 6 | 0.768432 | -5.112464 | 2.406984 |
| 116 | 1 | 1.048124 | -6.137429 | 2.630138 |
| 117 | 1 | 1.005206 | -4.299359 | 4.423498 |
| 118 | 8 | -6.239987 | -2.955808 | 1.471100 |
| 119 | 8 | -2.808887 | -2.102263 | -4.903707 |
| 120 | 8 | 0.332822 | -1.927015 | -5.274994 |
| 121 | 8 | 6.240964 | -2.953922 | -1.471403 |
| 122 | 8 | 2.809130 | -2.102463 | 4.903359 |
| 123 | 8 | 4.926951 | 3.986531 | 2.512698 |
| 124 | 8 | 1.259793 | 5.169436 | 3.496251 |
| 125 | 8 | -4.927900 | 3.985714 | -2.512032 |
| 126 | 8 | -1.261416 | 5.170065 | -3.494753 |
| 127 | 8 | 4.320717 | 1.409069 | -4.361689 |
| 128 | 8 | 0.000985 | -6.873507 | -0.001358 |
| 129 | 8 | -0.332005 | -1.929657 | 5.274618 |
| 130 | 8 | -4.321505 | 1.406580 | 4.361796 |

**Table S30.** The optimized Cartesian coordinates of the [28]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -3.488041 | 0.760099 | -4.175299 |
| 2 | 6 | -2.625131 | -0.099444 | -3.519509 |
| 3 | 6 | -2.690453 | -0.491063 | -2.142313 |
| 4 | 6 | -3.650891 | 0.217755 | -1.377908 |
| 5 | 6 | -4.662728 | 0.909435 | -2.133626 |
| 6 | 6 | -4.601574 | 1.220421 | -3.473152 |
| 7 | 1 | -3.359112 | 0.916877 | -5.241688 |
| 8 | 1 | -5.435060 | 1.727652 | -3.949021 |
| 9 | 6 | -5.932963 | 0.901121 | -1.363172 |
| 10 | 6 | -5.605598 | 0.234138 | -0.081359 |
| 11 | 6 | -4.174616 | 0.154132 | 0.028899 |
| 12 | 6 | -3.691146 | 0.102065 | 1.348029 |
| 13 | 6 | -4.616604 | -0.482212 | 2.272806 |
| 14 | 6 | -5.972202 | -0.659105 | 2.073640 |
| 15 | 6 | -6.508894 | -0.151617 | 0.886187 |
| 16 | 1 | -7.574966 | -0.065913 | 0.701604 |
| 17 | 1 | -6.576455 | -1.086968 | 2.867247 |
| 18 | 8 | -7.021513 | 1.310268 | -1.725147 |
| 19 | 6 | -3.935966 | -0.753087 | 3.555601 |
| 20 | 6 | -2.665617 | 0.012417 | 3.474601 |
| 21 | 6 | -2.550762 | 0.661045 | 2.196127 |
| 22 | 6 | -2.012913 | 0.375089 | 4.639124 |
| 23 | 6 | -1.359372 | 1.603554 | 4.649742 |
| 24 | 6 | -1.367314 | 2.337718 | 3.480020 |
| 25 | 6 | -1.813845 | 1.878781 | 2.192936 |
| 26 | 1 | -0.979590 | 2.048485 | 5.562098 |
| 27 | 1 | -2.173486 | -0.209343 | 5.538799 |
| 28 | 8 | -4.394750 | -1.356396 | 4.508530 |
| 29 | 6 | -1.364844 | 3.820812 | 3.515469 |
| 30 | 6 | -1.883113 | 4.232216 | 2.192138 |
| 31 | 6 | -1.793190 | 3.108687 | 1.301317 |
| 32 | 6 | -2.404646 | 5.471535 | 1.880186 |
| 33 | 6 | -2.949337 | 5.616424 | 0.596859 |
| 34 | 6 | -2.640279 | 4.630902 | -0.317114 |
| 35 | 6 | -1.834150 | 3.468421 | -0.055729 |
| 36 | 1 | -2.448756 | 6.246771 | 2.638384 |
| 37 | 1 | -3.551623 | 6.468096 | 0.297340 |
| 38 | 8 | -1.087247 | 4.548991 | 4.453344 |
| 39 | 6 | -3.123411 | 4.537751 | -1.715226 |
| 40 | 6 | -2.252605 | 3.520142 | -2.356029 |
| 41 | 6 | -1.297928 | 3.030295 | -1.399030 |
| 42 | 8 | -4.003200 | 5.198349 | -2.238007 |
| 43 | 6 | -2.167607 | 3.394169 | -3.725492 |
| 44 | 6 | -0.999607 | 2.841052 | -4.241791 |
| 45 | 6 | 0.034806 | 2.597185 | -3.356231 |
| 46 | 6 | -0.018829 | 2.690739 | -1.925485 |
| 47 | 1 | -0.800443 | 2.775937 | -5.306985 |
| 48 | 1 | -2.941587 | 3.825839 | -4.352239 |
| 49 | 6 | 1.413980 | 2.779322 | -3.859973 |
| 50 | 6 | 2.183172 | 3.187121 | -2.664722 |
| 51 | 6 | 1.438404 | 2.915827 | -1.469738 |
| 52 | 8 | 1.788206 | 2.772905 | -5.019171 |
| 53 | 6 | 3.337036 | 3.946397 | -2.760648 |
| 54 | 6 | 3.748239 | 4.625456 | -1.610387 |
| 55 | 6 | 3.123428 | 4.276216 | -0.432165 |
| 56 | 6 | 2.142760 | 3.233583 | -0.287983 |

| | | | | |
|---|---|---|---|---|
| 57 | 1 | 3.795326 | 4.088461 | -3.733779 |
| 58 | 1 | 4.489540 | 5.418225 | -1.622980 |
| 59 | 6 | 3.143038 | 5.055727 | 0.834138 |
| 60 | 6 | 2.336197 | 4.264014 | 1.801392 |
| 61 | 6 | 2.043202 | 2.992773 | 1.190601 |
| 62 | 8 | 3.710157 | 6.113675 | 1.038154 |
| 63 | 6 | -2.048086 | -1.893962 | -2.077969 |
| 64 | 6 | -1.756604 | -2.248828 | -3.437856 |
| 65 | 6 | -1.831273 | -1.059759 | -4.312377 |
| 66 | 8 | -1.453224 | -0.944442 | -5.466312 |
| 67 | 6 | -2.042932 | -2.992940 | -1.190477 |
| 68 | 6 | -2.335616 | -4.264334 | -1.801077 |
| 69 | 6 | -2.166647 | -4.567996 | -3.133837 |
| 70 | 6 | -1.744405 | -3.527634 | -3.966906 |
| 71 | 1 | -1.540688 | -3.668643 | -5.022542 |
| 72 | 1 | -2.411039 | -5.557778 | -3.505772 |
| 73 | 6 | -2.142683 | -3.233484 | 0.288122 |
| 74 | 6 | -3.123294 | -4.276168 | 0.432381 |
| 75 | 6 | -3.142461 | -5.056002 | -0.833760 |
| 76 | 8 | -3.709435 | -6.114044 | -1.037668 |
| 77 | 6 | -1.438489 | -2.915463 | 1.469898 |
| 78 | 6 | -2.183373 | -3.186497 | 2.664840 |
| 79 | 6 | -3.337309 | -3.945707 | 2.760753 |
| 80 | 6 | -3.748333 | -4.625059 | 1.610596 |
| 81 | 1 | -4.489631 | -5.417826 | 1.623316 |
| 82 | 1 | -3.795746 | -4.087565 | 3.733844 |
| 83 | 6 | 0.018808 | -2.690719 | 1.925682 |
| 84 | 6 | -0.034826 | -2.597333 | 3.356420 |
| 85 | 6 | -1.414082 | -2.778983 | 3.860132 |
| 86 | 8 | -1.788320 | -2.772411 | 5.019318 |
| 87 | 6 | 1.297828 | -3.030454 | 1.399137 |
| 88 | 6 | 2.252391 | -3.520591 | 2.356102 |
| 89 | 6 | 2.167366 | -3.394927 | 3.725591 |
| 90 | 6 | 0.999479 | -2.841657 | 4.241974 |
| 91 | 1 | 0.800287 | -2.776669 | 5.307172 |
| 92 | 1 | 2.941260 | -3.826887 | 4.352243 |
| 93 | 6 | 1.834131 | -3.468279 | 0.055733 |
| 94 | 6 | 2.640353 | -4.630754 | 0.316950 |
| 95 | 6 | 3.123235 | -4.538058 | 1.715136 |
| 96 | 8 | 4.002884 | -5.198884 | 2.237886 |
| 97 | 6 | 1.793226 | -3.108339 | -1.301279 |
| 98 | 6 | 1.883400 | -4.231751 | -2.192254 |
| 99 | 6 | 2.405115 | -5.471046 | -1.880506 |
| 100 | 6 | 2.949676 | -5.616073 | -0.597161 |
| 101 | 1 | 3.552027 | -6.467703 | -0.297658 |
| 102 | 1 | 2.449418 | -6.246108 | -2.638868 |
| 103 | 6 | 1.813591 | -1.878349 | -2.192852 |
| 104 | 6 | 1.366987 | -2.337245 | -3.479893 |
| 105 | 6 | 1.364988 | -3.820337 | -3.515528 |
| 106 | 8 | 1.087511 | -4.548537 | -4.453420 |
| 107 | 6 | 2.048172 | 1.893687 | 2.077975 |
| 108 | 6 | 1.756737 | 2.248413 | 3.437906 |
| 109 | 6 | 1.744847 | 3.527160 | 3.967125 |
| 110 | 6 | 2.167341 | 4.567522 | 3.134199 |
| 111 | 1 | 2.411995 | 5.557185 | 3.506277 |
| 112 | 1 | 1.541259 | 3.668082 | 5.022800 |
| 113 | 6 | 2.690379 | 0.490748 | 2.142174 |
| 114 | 6 | 2.624963 | 0.098894 | 3.519286 |
| 115 | 6 | 1.831205 | 1.059202 | 4.312291 |
| 116 | 8 | 1.453068 | 0.943780 | 5.466178 |
| 117 | 6 | 3.650956 | -0.217837 | 1.377756 |
| 118 | 6 | 4.662795 | -0.909586 | 2.133398 |
| 119 | 6 | 4.601539 | -1.220840 | 3.472853 |

| | | | | |
|---|---|---|---|---|
| 120 | 6 | 3.487911 | -0.760683 | 4.174985 |
| 121 | 1 | 3.358987 | -0.917560 | 5.241358 |
| 122 | 1 | 5.435021 | -1.728047 | 3.948749 |
| 123 | 6 | 4.174601 | -0.154075 | -0.029040 |
| 124 | 6 | 5.605607 | -0.234184 | 0.081128 |
| 125 | 6 | 5.933010 | -0.901186 | 1.362918 |
| 126 | 8 | 7.021552 | -1.310422 | 1.724840 |
| 127 | 6 | 3.691058 | -0.101923 | -1.348105 |
| 128 | 6 | 2.550533 | -0.660645 | -2.196110 |
| 129 | 6 | 2.665286 | -0.011966 | -3.474561 |
| 130 | 6 | 3.935743 | 0.753378 | -3.555652 |
| 131 | 6 | 4.616513 | 0.482295 | -2.272955 |
| 132 | 6 | 5.972124 | 0.659108 | -2.073876 |
| 133 | 6 | 6.508859 | 0.151557 | -0.886450 |
| 134 | 1 | 6.576351 | 1.086982 | -2.867495 |
| 135 | 1 | 7.574933 | 0.065739 | -0.701933 |
| 136 | 8 | 4.394518 | 1.356769 | -4.508533 |
| 137 | 6 | 1.358862 | -1.603048 | -4.649601 |
| 138 | 6 | 2.012406 | -0.374591 | -4.639017 |
| 139 | 1 | 2.172907 | 0.209842 | -5.538707 |
| 140 | 1 | 0.979051 | -2.048019 | -5.561929 |

**Table S31.** The optimized Cartesian coordinates of the [30]circulene ketone in the ground singlet state calculated at the B3LYP/6-31(d) level of theory

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 5.082984 | 2.630809 | 0.448697 |
| 2 | 6 | 5.347434 | 3.402551 | -0.781778 |
| 3 | 6 | 4.233019 | 3.076494 | -1.697079 |
| 4 | 6 | 3.448179 | 2.013086 | -1.113306 |
| 5 | 6 | 3.739911 | 2.104428 | 0.371697 |
| 6 | 6 | 5.915206 | 2.604953 | 1.543885 |
| 7 | 6 | 5.376338 | 2.058168 | 2.706536 |
| 8 | 6 | 4.011730 | 1.845070 | 2.712200 |
| 9 | 6 | 3.084890 | 2.006392 | 1.622198 |
| 10 | 1 | 6.916897 | 3.017103 | 1.476950 |
| 11 | 1 | 5.938300 | 1.897024 | 3.620368 |
| 12 | 6 | 4.180547 | 3.522698 | -2.996297 |
| 13 | 6 | 3.316369 | 2.835159 | -3.841219 |
| 14 | 6 | 2.761145 | 1.663581 | -3.362692 |
| 15 | 6 | 2.901841 | 1.093072 | -2.052028 |
| 16 | 1 | 3.175584 | 3.090492 | -4.885923 |
| 17 | 1 | 4.835254 | 4.323944 | -3.323388 |
| 18 | 6 | 1.687964 | 2.197710 | 2.287757 |
| 19 | 6 | 1.874060 | 1.757085 | 3.645201 |
| 20 | 6 | 3.299826 | 1.539065 | 3.953473 |
| 21 | 6 | 1.015757 | 1.913166 | 4.714616 |
| 22 | 6 | -0.073194 | 2.746530 | 4.534967 |
| 23 | 6 | -0.238044 | 3.297936 | 3.280555 |
| 24 | 6 | 0.510490 | 2.997231 | 2.085255 |
| 25 | 1 | 1.322801 | 1.548007 | 5.689449 |
| 26 | 1 | -0.709279 | 3.077646 | 5.347264 |
| 27 | 6 | 0.010660 | 4.030770 | 1.059917 |
| 28 | 6 | -0.528125 | 5.114834 | 1.840242 |
| 29 | 6 | -0.926520 | 4.601603 | 3.158597 |
| 30 | 8 | 3.791817 | 1.306504 | 5.046216 |
| 31 | 8 | 6.293664 | 4.138447 | -1.002292 |
| 32 | 8 | -1.601650 | 5.178166 | 3.993559 |
| 33 | 6 | -0.649869 | 6.435020 | 1.463639 |

| | | | | |
|---|---|---|---|---|
| 34 | 6 | -0.143225 | 6.765119 | 0.204129 |
| 35 | 6 | 0.130369 | 5.704456 | -0.629771 |
| 36 | 6 | -0.026317 | 4.302591 | -0.322464 |
| 37 | 6 | 0.703468 | 5.817432 | -1.982336 |
| 38 | 6 | 0.521503 | 4.482655 | -2.590440 |
| 39 | 6 | -0.152104 | 3.603310 | -1.664711 |
| 40 | 8 | 1.178637 | 6.811768 | -2.504348 |
| 41 | 1 | -1.055321 | 7.158250 | 2.163648 |
| 42 | 1 | 0.000000 | 7.782722 | -0.144439 |
| 43 | 6 | 0.698076 | 4.289890 | -3.939892 |
| 44 | 6 | 0.132476 | 3.144468 | -4.484287 |
| 45 | 6 | -0.686737 | 2.395222 | -3.661901 |
| 46 | 6 | -0.976323 | 2.604294 | -2.268196 |
| 47 | 1 | 1.192712 | 5.054590 | -4.530311 |
| 48 | 1 | 0.198281 | 2.880169 | -5.532933 |
| 49 | 6 | -2.397549 | 1.966532 | -2.052028 |
| 50 | 6 | -2.821276 | 1.559431 | -3.362692 |
| 51 | 6 | -1.707791 | 1.571092 | -4.321073 |
| 52 | 8 | -1.702659 | 1.138334 | -5.461288 |
| 53 | 6 | -4.113504 | 1.454480 | -3.841219 |
| 54 | 6 | -5.141020 | 1.859111 | -2.996297 |
| 55 | 6 | -4.780832 | 2.127655 | -1.697079 |
| 56 | 6 | -3.467473 | 1.979668 | -1.113306 |
| 57 | 1 | -4.264237 | 1.204890 | -4.885923 |
| 58 | 1 | -6.162272 | 2.025481 | -3.323388 |
| 59 | 6 | -5.620412 | 2.929738 | -0.781778 |
| 60 | 6 | -4.819839 | 3.086589 | 0.448697 |
| 61 | 6 | -3.692444 | 2.186645 | 0.371697 |
| 62 | 6 | -5.213559 | 3.820242 | 1.543885 |
| 63 | 6 | -4.470595 | 3.626962 | 2.706536 |
| 64 | 6 | -3.603743 | 2.551725 | 2.712200 |
| 65 | 6 | -3.280031 | 1.668397 | 1.622198 |
| 66 | 1 | -6.071336 | 4.481657 | 1.476950 |
| 67 | 1 | -4.612021 | 4.194207 | 3.620368 |
| 68 | 8 | -6.730832 | 3.381249 | -1.002292 |
| 69 | 6 | -2.747254 | 0.362965 | 2.287757 |
| 70 | 6 | -2.458711 | 0.744441 | 3.645201 |
| 71 | 6 | -2.982782 | 2.088200 | 3.953473 |
| 72 | 8 | -3.027374 | 2.630558 | 5.046216 |
| 73 | 6 | -2.850923 | -1.056519 | 2.085255 |
| 74 | 6 | -2.737074 | -1.855120 | 3.280555 |
| 75 | 6 | -2.341967 | -1.436653 | 4.534967 |
| 76 | 6 | -2.164729 | -0.076912 | 4.714616 |
| 77 | 1 | -2.002013 | 0.371576 | 5.689449 |
| 78 | 1 | -2.310681 | -2.153076 | 5.347264 |
| 79 | 6 | -3.496079 | -2.006153 | 1.059917 |
| 80 | 6 | -4.165514 | -3.014787 | 1.840242 |
| 81 | 6 | -3.521845 | -3.103191 | 3.158597 |
| 82 | 8 | -3.683599 | -3.976153 | 3.993559 |
| 83 | 6 | -5.247956 | -3.780313 | 1.463639 |
| 84 | 6 | -5.787152 | -3.506596 | 0.204129 |
| 85 | 6 | -5.005388 | -2.739326 | -0.629771 |
| 86 | 6 | -3.712995 | -2.174086 | -0.322464 |
| 87 | 1 | -6.740035 | -3.891361 | -0.144439 |
| 88 | 1 | -5.671566 | -4.493060 | 2.163648 |
| 89 | 6 | -5.389778 | -2.299495 | -1.982336 |
| 90 | 6 | -4.142845 | -1.789693 | -2.590440 |
| 91 | 6 | -3.044506 | -1.933381 | -1.664711 |
| 92 | 8 | -6.488483 | -2.385154 | -2.504348 |
| 93 | 6 | -4.064192 | -1.540393 | -3.939892 |
| 94 | 6 | -2.789427 | -1.457507 | -4.484287 |
| 95 | 6 | -1.730954 | -1.792343 | -3.661901 |
| 96 | 6 | -1.767223 | -2.147667 | -2.268196 |

| | | | | |
|---|---|---|---|---|
| 97 | 1 | -4.973759 | -1.494376 | -4.530311 |
| 98 | 1 | -2.593440 | -1.268368 | -5.532933 |
| 99 | 6 | -0.504292 | -3.059604 | -2.052028 |
| 100 | 6 | 0.060131 | -3.223013 | -3.362692 |
| 101 | 6 | -0.506710 | -2.264537 | -4.321073 |
| 102 | 8 | -0.134497 | -2.043713 | -5.461288 |
| 103 | 6 | 2.743546 | -0.456626 | -2.268196 |
| 104 | 6 | 2.417692 | -0.602879 | -3.661901 |
| 105 | 6 | 2.214501 | 0.693445 | -4.321073 |
| 106 | 8 | 1.837156 | 0.905379 | -5.461288 |
| 107 | 6 | 2.656951 | -1.686961 | -4.484287 |
| 108 | 6 | 3.366116 | -2.749497 | -3.939892 |
| 109 | 6 | 3.621342 | -2.692962 | -2.590440 |
| 110 | 6 | 3.196610 | -1.669930 | -1.664711 |
| 111 | 1 | 2.395158 | -1.611801 | -5.532933 |
| 112 | 1 | 3.781047 | -3.560214 | -4.530311 |
| 113 | 6 | 3.739311 | -2.128504 | -0.322464 |
| 114 | 6 | 4.875020 | -2.965131 | -0.629771 |
| 115 | 6 | 4.686310 | -3.517937 | -1.982336 |
| 116 | 6 | 3.485420 | -2.024617 | 1.059917 |
| 117 | 6 | 2.340433 | -1.940713 | 2.085255 |
| 118 | 6 | 2.975118 | -1.442816 | 3.280555 |
| 119 | 6 | 4.448365 | -1.498412 | 3.158597 |
| 120 | 6 | 4.693639 | -2.100047 | 1.840242 |
| 121 | 6 | 5.897826 | -2.654707 | 1.463639 |
| 122 | 6 | 5.930378 | -3.258523 | 0.204129 |
| 123 | 1 | 6.740035 | -3.891361 | -0.144439 |
| 124 | 1 | 6.726887 | -2.665190 | 2.163648 |
| 125 | 8 | 5.309846 | -4.426614 | -2.504348 |
| 126 | 8 | 5.285248 | -1.202014 | 3.993559 |
| 127 | 6 | 1.059290 | -2.560675 | 2.287757 |
| 128 | 6 | 0.584650 | -2.501526 | 3.645201 |
| 129 | 6 | 1.148972 | -1.836255 | 4.714616 |
| 130 | 6 | 2.415162 | -1.309877 | 4.534967 |
| 131 | 1 | 3.019959 | -0.924570 | 5.347264 |
| 132 | 1 | 0.679213 | -1.919582 | 5.689449 |
| 133 | 6 | 0.195141 | -3.674789 | 1.622198 |
| 134 | 6 | -0.407987 | -4.396795 | 2.712200 |
| 135 | 6 | -0.317043 | -3.627266 | 3.953473 |
| 136 | 8 | -0.764443 | -3.937062 | 5.046216 |
| 137 | 6 | -0.047468 | -4.291072 | 0.371697 |
| 138 | 6 | -0.263145 | -5.717398 | 0.448697 |
| 139 | 6 | -0.701647 | -6.425195 | 1.543885 |
| 140 | 6 | -0.905744 | -5.685129 | 2.706536 |
| 141 | 1 | -1.326279 | -6.091231 | 3.620368 |
| 142 | 1 | -0.845561 | -7.498760 | 1.476950 |
| 143 | 6 | 0.019294 | -3.992753 | -1.113306 |
| 144 | 6 | 0.547812 | -5.204149 | -1.697079 |
| 145 | 6 | 0.272979 | -6.332289 | -0.781778 |
| 146 | 8 | 0.437169 | -7.519696 | -1.002292 |
| 147 | 6 | 0.797135 | -4.289639 | -3.841219 |
| 148 | 6 | 0.960473 | -5.381809 | -2.996297 |
| 149 | 1 | 1.327018 | -6.349425 | -3.323388 |
| 150 | 1 | 1.088653 | -4.295382 | -4.885923 |