

The Effect of Strain on the Aromatic Character of Infinitene

Maurizio D'Auria

*Dipartimento di Scienze, Università della Basilicata, V.le dell'Ateneo Lucano 10, 85100 Potenza;
maurizio.dauria@unibas.it; Tel. +39 0971 202480*

Infinitene

| Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|----|----|----|-----------|-------------|--------------|------------|------------|------------|
| 1 | C | | | | | | | 5.8226600 | -1.3308730 | -1.2907640 |
| 2 | C | 1 | | | 1.3570438 | | | 5.0647280 | -2.4296260 | -1.5354040 |
| 3 | C | 2 | 1 | | 1.4264695 | 120.8581740 | | 3.6529210 | -2.4044730 | -1.3329600 |
| 4 | C | 3 | 2 | 1 | 1.4280182 | 121.3991438 | -1.3596665 | 2.9925560 | -1.2378770 | -0.8408140 |
| 5 | C | 4 | 3 | 2 | 1.4777850 | 115.1531755 | -16.0697270 | 3.8773700 | -0.2298500 | -0.2204640 |
| 6 | C | 1 | 2 | 3 | 1.4225132 | 119.8393202 | 10.3567322 | 5.2524670 | -0.2122350 | -0.6221290 |
| 7 | C | 5 | 4 | 3 | 1.4431733 | 126.8155456 | -155.2286972 | 3.5066090 | 0.7566520 | 0.7654870 |
| 8 | C | 7 | 5 | 4 | 1.4151867 | 119.9558162 | -158.4424613 | 4.2964640 | 1.9187390 | 0.9341180 |
| 9 | C | 8 | 7 | 5 | 1.4157832 | 119.8197423 | -13.9897484 | 5.5905620 | 1.9793870 | 0.3630890 |
| 10 | C | 9 | 8 | 7 | 1.3662308 | 119.7238939 | -1.2886419 | 6.0784540 | 0.9045790 | -0.3249050 |
| 11 | C | 3 | 2 | 1 | 1.4239207 | 117.2936442 | 177.1788472 | 2.9236850 | -3.5796320 | -1.6717320 |
| 12 | C | 11 | 3 | 2 | 1.3563129 | 120.6481141 | -175.1324502 | 1.5694000 | -3.5977250 | -1.5998330 |
| 13 | C | 12 | 11 | 3 | 1.4227346 | 119.9405856 | 7.5667409 | 0.8559650 | -2.3945230 | -1.3400460 |
| 14 | C | 13 | 12 | 11 | 1.4236399 | 121.4070959 | -4.9956456 | 1.5348900 | -1.1779000 | -1.0474030 |
| 15 | C | 13 | 12 | 11 | 1.4216415 | 117.8857488 | 170.6539838 | -0.5591840 | -2.4185580 | -1.4736130 |
| 16 | C | 15 | 13 | 12 | 1.3599055 | 122.0877374 | -176.7046475 | -1.3192600 | -1.3027690 | -1.3103880 |
| 17 | C | 16 | 15 | 13 | 1.4224590 | 120.9821101 | 4.6879715 | -0.7175950 | -0.0322090 | -1.0934410 |
| 18 | C | 17 | 16 | 15 | 1.4366150 | 117.5566740 | 1.8118316 | 0.7175730 | 0.0322540 | -1.0934720 |
| 19 | C | 7 | 5 | 4 | 1.4510812 | 123.2310642 | 19.6358216 | 2.3187120 | 0.6477560 | 1.5917310 |
| 20 | C | 19 | 7 | 5 | 1.4455593 | 118.4833395 | -151.3791627 | 1.6894800 | 1.8628050 | 2.0579550 |
| 21 | C | 20 | 19 | 7 | 1.4364827 | 118.0511964 | -21.8826916 | 2.4835400 | 3.0588570 | 2.1070550 |
| 22 | C | 21 | 20 | 19 | 1.3565820 | 120.2660791 | 4.0508594 | 3.7597200 | 3.0516700 | 1.6470250 |
| 23 | C | 20 | 19 | 7 | 1.3851744 | 118.4621341 | 155.1197943 | 0.3410520 | 1.8289650 | 2.3730820 |
| 24 | C | 19 | 7 | 5 | 1.3844551 | 123.2080814 | 26.6798621 | 1.7346630 | -0.5626540 | 1.9241620 |
| 25 | C | 18 | 17 | 16 | 1.4224599 | 117.5565608 | 160.1836820 | 1.3192270 | 1.3028040 | -1.3105140 |
| 26 | C | 25 | 18 | 17 | 1.3599047 | 120.9822057 | 1.8130533 | 0.5591450 | 2.4185870 | -1.4737450 |
| 27 | C | 26 | 25 | 18 | 1.4216399 | 122.0877802 | 4.6871699 | -0.8559960 | 2.3945600 | -1.3401090 |
| 28 | C | 27 | 26 | 25 | 1.4236406 | 120.5624190 | -1.0173511 | -1.5349110 | 1.1779460 | -1.0474020 |
| 29 | C | 28 | 27 | 26 | 1.4734525 | 117.7634267 | 176.3408237 | -2.9925720 | 1.2379210 | -0.8407870 |
| 30 | C | 29 | 28 | 27 | 1.4280186 | 116.2579838 | 18.0437657 | -3.6529510 | 2.4045100 | -1.3329320 |
| 31 | C | 30 | 29 | 28 | 1.4239206 | 121.2907814 | -16.1312005 | 2.9237270 | 3.5796650 | -1.6717430 |
| 32 | C | 31 | 30 | 29 | 1.3563131 | 120.6481083 | 3.4084486 | -1.5694390 | 3.5977570 | -1.5998970 |
| 33 | C | 29 | 28 | 27 | 1.4777856 | 128.5658913 | -163.7897404 | 3.8773710 | 0.2298750 | -0.2204450 |
| 34 | C | 33 | 29 | 28 | 1.4326699 | 117.7346405 | -153.5456577 | -5.2524740 | 0.2122580 | -0.6220970 |
| 35 | C | 34 | 33 | 29 | 1.4225125 | 120.4536768 | -17.0169964 | -5.8226840 | 1.3309020 | -1.2907060 |
| 36 | C | 35 | 34 | 33 | 1.3570429 | 119.8393677 | -0.8398080 | -5.0647610 | 2.4296590 | -1.5353510 |
| 37 | C | 33 | 29 | 28 | 1.4431759 | 126.8155988 | 26.5849682 | -3.5065840 | -0.7566650 | 0.7654620 |
| 38 | C | 37 | 33 | 29 | 1.4151876 | 119.9556387 | -158.4418673 | -4.2964350 | -1.9187600 | 0.9340640 |
| 39 | C | 38 | 37 | 33 | 1.4157819 | 119.8199995 | -13.9894124 | -5.5905420 | -1.9793950 | 0.3630570 |
| 40 | C | 39 | 38 | 37 | 1.3662292 | 119.7238777 | -1.2883618 | -6.0784490 | -0.9045690 | -0.3248950 |
| 41 | C | 37 | 33 | 29 | 1.4510838 | 123.2313740 | 19.6370300 | -2.3186750 | -0.6477970 | 1.5916970 |
| 42 | C | 41 | 37 | 33 | 1.4455593 | 118.4832549 | -151.3799786 | -1.6894410 | -1.8628630 | 2.0578740 |
| 43 | C | 42 | 41 | 37 | 1.4364826 | 118.0514324 | -21.8823379 | -2.4834970 | -3.0589190 | 2.1069390 |
| 44 | C | 43 | 42 | 41 | 1.3565811 | 120.2659564 | 4.0506086 | -3.7596810 | -3.0517160 | 1.6469230 |
| 45 | C | 23 | 20 | 19 | 1.4122623 | 119.8759740 | 1.9571499 | -0.3741790 | 0.6152060 | 2.2745000 |

| | | | | | | | | | | |
|----|---|----|----|----|-----------|-------------|--------------|------------|------------|------------|
| 46 | C | 24 | 19 | 7 | 1.4058110 | 120.0534229 | -156.2022876 | 0.3742160 | -0.6152720 | 2.2744760 |
| 47 | C | 41 | 37 | 33 | 1.3844564 | 123.2082969 | 26.6799151 | -1.7346260 | 0.5626010 | 1.9241770 |
| 48 | C | 42 | 41 | 37 | 1.3851741 | 118.4622438 | 155.1206984 | -0.3410140 | -1.8290350 | 2.3730050 |
| 49 | H | 1 | 2 | 3 | 1.0844792 | 121.2575412 | -173.2800171 | 6.8770770 | -1.3070100 | -1.5432130 |
| 50 | H | 2 | 1 | 6 | 1.0845294 | 120.9260077 | -173.8570423 | 5.5046230 | -3.3283090 | -1.9538120 |
| 51 | H | 9 | 8 | 7 | 1.0847092 | 119.2730516 | -178.4528716 | 6.1982090 | 2.8642670 | 0.5191230 |
| 52 | H | 10 | 9 | 8 | 1.0846706 | 120.7124702 | -173.8942214 | 7.1018950 | 0.8948670 | -0.6840490 |
| 53 | H | 11 | 3 | 2 | 1.0845981 | 118.2988170 | 5.5937733 | 3.4795320 | -4.4598580 | -1.9760170 |
| 54 | H | 12 | 11 | 3 | 1.0844720 | 121.1635311 | -177.3474687 | 1.0080130 | -4.5003500 | -1.8147570 |
| 55 | H | 15 | 13 | 12 | 1.0846585 | 118.0298530 | 2.7993502 | -1.0317930 | -3.3628140 | -1.7216160 |
| 56 | H | 16 | 15 | 13 | 1.0788590 | 119.2439223 | 179.7679704 | -2.3896220 | -1.3726120 | -1.4260770 |
| 57 | H | 21 | 20 | 19 | 1.0848257 | 118.7689052 | -174.6797102 | 2.0502170 | 3.9559750 | 2.5363070 |
| 58 | H | 22 | 21 | 20 | 1.0850148 | 120.5323546 | -176.4382909 | 4.3821580 | 3.9360820 | 1.7344520 |
| 59 | H | 23 | 20 | 19 | 1.0853692 | 119.8568752 | -170.6869823 | -0.1891770 | 2.7534340 | 2.5786070 |
| 60 | H | 24 | 19 | 7 | 1.0827906 | 120.1613609 | 12.8787588 | 2.2657420 | -1.4896220 | 1.7477510 |
| 61 | H | 25 | 18 | 17 | 1.0788582 | 119.5922369 | -173.2504795 | 2.3895820 | 1.3726420 | -1.4262630 |
| 62 | H | 26 | 25 | 18 | 1.0846594 | 119.8805240 | -174.8077778 | 1.0317440 | 3.3628330 | -1.7218090 |
| 63 | H | 31 | 30 | 29 | 1.0845981 | 118.2988279 | -175.8663214 | -3.4795840 | 4.4598840 | -1.9760300 |
| 64 | H | 32 | 31 | 30 | 1.0844716 | 121.1635776 | -177.3483167 | -1.0080580 | 4.5003750 | -1.8148640 |
| 65 | H | 35 | 34 | 33 | 1.0844795 | 118.8053873 | -177.2928892 | -6.8771040 | 1.3070330 | -1.5431430 |
| 66 | H | 36 | 35 | 34 | 1.0845299 | 120.9259538 | -173.8580404 | -5.5046660 | 3.3283400 | -1.9537540 |
| 67 | H | 39 | 38 | 37 | 1.0847098 | 119.2730758 | -178.4528979 | -6.1981820 | -2.8642840 | 0.5190710 |
| 68 | H | 40 | 39 | 38 | 1.0846713 | 120.7124861 | -173.8946692 | -7.1018950 | -0.8948520 | -0.6840270 |
| 69 | H | 43 | 42 | 41 | 1.0848246 | 118.7689455 | -174.6797466 | -2.0501690 | -3.9560500 | 2.5361560 |
| 70 | H | 44 | 43 | 42 | 1.0850150 | 120.5322820 | -176.4381657 | -4.3821170 | -3.9361320 | 1.7343260 |
| 71 | H | 47 | 41 | 37 | 1.0827898 | 120.1613653 | 12.8782335 | -2.2657070 | 1.4895750 | 1.7478080 |
| 72 | H | 48 | 42 | 41 | 1.0853696 | 119.8568899 | -170.6870902 | 0.1892150 | -2.7535120 | 2.5784960 |

Infinitene PBE0

| Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|----|----|----|-----------|-------------|--------------|------------|------------|------------|
| 1 | C | | | | | | | 5.8330750 | -1.3457110 | -1.2952630 |
| 2 | C | 1 | | | 1.3667533 | | | 5.0688160 | -2.4558680 | -1.5221420 |
| 3 | C | 2 | 1 | | 1.4288903 | 120.8676206 | | 3.6555220 | -2.4281210 | -1.3134370 |
| 4 | C | 3 | 2 | 1 | 1.4376074 | 121.3364253 | -1.5298771 | 2.9944090 | -1.2472010 | -0.8285940 |
| 5 | C | 4 | 3 | 2 | 1.4771648 | 115.1237519 | -16.0630569 | 3.8835420 | -0.2338470 | -0.2247960 |
| 6 | C | 1 | 2 | 3 | 1.4248695 | 119.7797749 | 10.597256 | 5.2649250 | -0.2183480 | -0.6345730 |
| 7 | C | 5 | 4 | 3 | 1.4455176 | 126.5674687 | -155.2465757 | 3.5127560 | 0.7644080 | 0.7527140 |
| 8 | C | 7 | 5 | 4 | 1.4245757 | 120.0198463 | -158.2545249 | 4.3032260 | 1.9395450 | 0.9064220 |
| 9 | C | 8 | 7 | 5 | 1.4206337 | 119.7004024 | -14.0090807 | 5.5991110 | 1.9969060 | 0.3271190 |
| 10 | C | 9 | 8 | 7 | 1.3743367 | 119.7288752 | -1.4117627 | 6.0909580 | 0.9078820 | -0.3517880 |
| 11 | C | 3 | 2 | 1 | 1.4269150 | 117.4301675 | 177.0574336 | 2.9204070 | -3.6083110 | -1.6341300 |
| 12 | C | 11 | 3 | 2 | 1.3653343 | 120.6226606 | -175.1461841 | 1.5574970 | -3.6220350 | -1.5539700 |
| 13 | C | 12 | 11 | 3 | 1.4260134 | 119.9182318 | 7.6889336 | 0.8472880 | -2.4102900 | -1.3074110 |
| 14 | C | 13 | 12 | 11 | 1.4329043 | 121.4051347 | -5.3668837 | 1.5356120 | -1.1852130 | -1.0270340 |
| 15 | C | 13 | 12 | 11 | 1.4247011 | 117.9155563 | 170.1062551 | -0.5706930 | -2.4285530 | -1.4444130 |
| 16 | C | 15 | 13 | 12 | 1.3690663 | 122.0872005 | -176.8899525 | -1.3309060 | -1.3005510 | -1.2893960 |
| 17 | C | 16 | 15 | 13 | 1.4254380 | 120.9619800 | 4.4717036 | -0.7220900 | -0.0296970 | -1.0745780 |
| 18 | C | 17 | 16 | 15 | 1.4453854 | 117.6069412 | 2.1599853 | 0.7220730 | 0.0297340 | -1.0745980 |
| 19 | C | 7 | 5 | 4 | 1.4503538 | 122.9987935 | 19.6410224 | 2.3260520 | 0.6576520 | 1.5796740 |
| 20 | C | 19 | 7 | 5 | 1.4512655 | 118.5785767 | -151.6870002 | 1.6913480 | 1.8774140 | 2.0438970 |
| 21 | C | 20 | 19 | 7 | 1.4363047 | 118.1252074 | -21.3973573 | 2.4777300 | 3.0788040 | 2.0790610 |
| 22 | C | 21 | 20 | 19 | 1.3675077 | 120.2664238 | 3.7686101 | 3.7627050 | 3.0754320 | 1.6111880 |
| 23 | C | 20 | 19 | 7 | 1.3942346 | 118.3386864 | 155.1768911 | 0.3345530 | 1.8376330 | 2.3623540 |
| 24 | C | 19 | 7 | 5 | 1.3928876 | 122.9922141 | 26.3029066 | 1.7430840 | -0.5618740 | 1.9158890 |
| 25 | C | 18 | 17 | 16 | 1.4254371 | 117.6068108 | 160.4142138 | 1.3308800 | 1.3005820 | -1.2894710 |
| 26 | C | 25 | 18 | 17 | 1.3690671 | 120.9620631 | 2.1608425 | 0.5706620 | 2.4285820 | -1.4444850 |
| 27 | C | 26 | 25 | 18 | 1.4247013 | 122.0872507 | 4.4710784 | -0.8473150 | 2.4103230 | -1.3074390 |
| 28 | C | 27 | 26 | 25 | 1.4329043 | 120.5225835 | -1.3754891 | -1.5356300 | 1.1852490 | -1.0270270 |
| 29 | C | 28 | 27 | 26 | 1.4735344 | 117.7718277 | 176.9099033 | -2.9944230 | 1.2472310 | -0.8285710 |
| 30 | C | 29 | 28 | 27 | 1.4376071 | 116.3856019 | 17.8530222 | -3.6555480 | 2.4281480 | -1.3134040 |
| 31 | C | 30 | 29 | 28 | 1.4269157 | 121.2180005 | -16.1615065 | -2.9204420 | 3.6083390 | -1.6341170 |
| 32 | C | 31 | 30 | 29 | 1.3653342 | 120.6226986 | 3.4432376 | -1.5575300 | 3.6220650 | -1.5539930 |
| 33 | C | 29 | 28 | 27 | 1.4771656 | 128.4683082 | -163.9581511 | -3.8835430 | 0.2338590 | -0.2247820 |
| 34 | C | 33 | 29 | 28 | 1.4409644 | 117.9153847 | -153.4843965 | -5.2649300 | 0.2183590 | -0.6345480 |
| 35 | C | 34 | 33 | 29 | 1.4248686 | 120.3715220 | -17.0137003 | -5.8330960 | 1.3457280 | -1.2952120 |

| | | | | | | | | | | |
|----|---|----|----|----|-----------|-------------|--------------|------------|------------|------------|
| 36 | C | 35 | 34 | 33 | 1.3667535 | 119.7797630 | -1.0500207 | -5.0688450 | 2.4558910 | -1.5220900 |
| 37 | C | 33 | 29 | 28 | 1.4455186 | 126.5674725 | 26.5438196 | -3.5127360 | -0.7644220 | 0.7526950 |
| 38 | C | 37 | 33 | 29 | 1.4245773 | 120.0197285 | -158.2542916 | -4.3032010 | -1.9395670 | 0.9063820 |
| 39 | C | 38 | 37 | 33 | 1.4206332 | 119.7004981 | -14.0087521 | -5.5990920 | -1.9969200 | 0.3270930 |
| 40 | C | 39 | 38 | 37 | 1.3743362 | 119.7289343 | -1.4117184 | -6.0909530 | -0.9078830 | -0.3517820 |
| 41 | C | 37 | 33 | 29 | 1.4503548 | 122.9989493 | 19.6416419 | -2.3260230 | -0.6576830 | 1.5796460 |
| 42 | C | 41 | 37 | 33 | 1.4512666 | 118.5785388 | -151.6877352 | -1.6913150 | -1.8774560 | 2.0438380 |
| 43 | C | 42 | 41 | 37 | 1.4363038 | 118.1253058 | -21.3968314 | -2.4776920 | -3.0788490 | 2.0789750 |
| 44 | C | 43 | 42 | 41 | 1.3675071 | 120.2664756 | 3.7682796 | -3.7626700 | -3.0754700 | 1.6111120 |
| 45 | C | 23 | 20 | 19 | 1.4159167 | 119.8781470 | 1.6524477 | -0.3780530 | 0.6182280 | 2.2620340 |
| 46 | C | 24 | 19 | 7 | 1.4093341 | 119.9792860 | -155.9332499 | 0.3780810 | -0.6182720 | 2.2620230 |
| 47 | C | 41 | 37 | 33 | 1.3928887 | 122.9923469 | 26.3027223 | -1.7430550 | 0.5618360 | 1.9158910 |
| 48 | C | 42 | 41 | 37 | 1.3942336 | 118.3387980 | 155.1779373 | -0.3345230 | -1.8376800 | 2.3623040 |
| 49 | H | 1 | 2 | 3 | 1.0931469 | 121.3317982 | -172.9853229 | 6.8937380 | -1.3222410 | -1.5587270 |
| 50 | H | 2 | 1 | 6 | 1.0932705 | 120.9940027 | -173.5544390 | 5.5095510 | -3.3686710 | -1.9317560 |
| 51 | H | 9 | 8 | 7 | 1.0933397 | 119.1900317 | -178.5940602 | 6.2077680 | 2.8938790 | 0.4698350 |
| 52 | H | 10 | 9 | 8 | 1.0933618 | 120.7800437 | -173.6611006 | 7.1220740 | 0.8940020 | -0.7151710 |
| 53 | H | 11 | 3 | 2 | 1.0933387 | 118.2349719 | 5.3552075 | 3.4780210 | -4.4989350 | -1.9361980 |
| 54 | H | 12 | 11 | 3 | 1.0931697 | 121.2527571 | -177.3681975 | 0.9866170 | -4.5321410 | -1.7560170 |
| 55 | H | 15 | 13 | 12 | 1.0934211 | 117.9863316 | 2.4534987 | -1.0500730 | -3.3796390 | -1.6917990 |
| 56 | H | 16 | 15 | 13 | 1.0883930 | 119.3546683 | 179.6236187 | -2.4107170 | -1.3641310 | -1.4100820 |
| 57 | H | 21 | 20 | 19 | 1.0934362 | 118.7811934 | -175.2566945 | 2.0350320 | 3.9856460 | 2.5000820 |
| 58 | H | 22 | 21 | 20 | 1.0937014 | 120.5517839 | -176.3546011 | 4.3853640 | 3.9711360 | 1.6898830 |
| 59 | H | 23 | 20 | 19 | 1.0941315 | 119.7716673 | -170.5896159 | -0.2034460 | 2.7685470 | 2.5650360 |
| 60 | H | 24 | 19 | 7 | 1.0920993 | 120.0643385 | 13.2189876 | 2.2857580 | -1.4937540 | 1.7433040 |
| 61 | H | 25 | 18 | 17 | 1.0883923 | 119.5072681 | -172.9842027 | 2.4106860 | 1.3641620 | -1.4101950 |
| 62 | H | 26 | 25 | 18 | 1.0934211 | 119.9231894 | -174.8599186 | 1.0500350 | 3.3796630 | -1.6919040 |
| 63 | H | 31 | 30 | 29 | 1.0933382 | 118.2349623 | -176.0559530 | -3.4780640 | 4.4989590 | -1.9361800 |
| 64 | H | 32 | 31 | 30 | 1.0931691 | 121.2527854 | -177.3686825 | -0.9866560 | 4.5321690 | -1.7560630 |
| 65 | H | 35 | 34 | 33 | 1.0931467 | 118.7937624 | -177.5589024 | -6.8937610 | 1.3222550 | -1.5586670 |
| 66 | H | 36 | 35 | 34 | 1.0932712 | 120.9939991 | -173.5551053 | -5.5095890 | 3.3686950 | -1.9316940 |
| 67 | H | 39 | 38 | 37 | 1.0933396 | 119.1899839 | -178.5940852 | -6.2077420 | -2.8939000 | 0.4697940 |
| 68 | H | 40 | 39 | 38 | 1.0933613 | 120.7800641 | -173.6612960 | -7.1220720 | -0.8940010 | -0.7151550 |
| 69 | H | 43 | 42 | 41 | 1.0934368 | 118.7811796 | -175.2567161 | -2.0349890 | -3.9857000 | 2.4999730 |
| 70 | H | 44 | 43 | 42 | 1.0937017 | 120.5518316 | -176.3544772 | -4.3853260 | -3.9711780 | 1.6897890 |
| 71 | H | 47 | 41 | 37 | 1.0920985 | 120.0643475 | 13.2186392 | -2.2857310 | 1.4937190 | 1.7433340 |
| 72 | H | 48 | 42 | 41 | 1.0941321 | 119.7716692 | -170.5901551 | 0.2034760 | -2.7685980 | 2.5649710 |

[12]-Circulene

| Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|----|----|----|-----------|-------------|--------------|------------|------------|------------|
| 1 | C | | | | | | | 4.7133380 | -0.0034680 | 0.7319270 |
| 2 | C | 1 | | | 1.4638830 | | | 4.7133120 | -0.0034580 | -0.7319560 |
| 3 | C | 2 | 1 | | 1.4046868 | 118.7657952 | | 4.5603930 | 1.2183560 | -1.4079230 |
| 4 | C | 3 | 2 | 1 | 1.4047029 | 120.5468957 | -15.9413678 | 4.0834870 | 2.3535220 | -0.7317950 |
| 5 | C | 4 | 3 | 2 | 1.4638530 | 118.7710019 | 15.9370331 | 4.0834110 | 2.3534510 | 0.7320580 |
| 6 | C | 1 | 2 | 3 | 1.4046552 | 118.7720824 | 0.0069725 | 4.5603070 | 1.2182170 | 1.4080360 |
| 7 | C | 1 | 6 | 5 | 1.4047638 | 120.8540202 | -149.4099248 | 4.5588600 | -1.2252120 | 1.4078260 |
| 8 | C | 7 | 1 | 6 | 1.4047019 | 120.5531461 | 149.3928687 | 4.0802960 | -2.3597330 | 0.7317890 |
| 9 | C | 8 | 7 | 1 | 1.4638950 | 118.7672469 | 15.9502750 | 4.0802330 | -2.3596800 | -0.7321060 |
| 10 | C | 9 | 8 | 7 | 1.4046780 | 118.7635450 | -0.004881 | 4.5587380 | -1.2250850 | -1.4080110 |
| 11 | C | 4 | 3 | 2 | 1.4046773 | 120.8502535 | -149.4180281 | 3.3403990 | 3.3353290 | -1.4078080 |
| 12 | C | 11 | 4 | 3 | 1.4047154 | 120.5492319 | 149.4088079 | 2.3597800 | 4.0800850 | -0.7318270 |
| 13 | C | 12 | 11 | 4 | 1.4638360 | 118.7661646 | 15.9429378 | 2.3596540 | 4.0799560 | 0.7320090 |
| 14 | C | 5 | 4 | 3 | 1.4046692 | 118.7650675 | -165.6674974 | 3.3403060 | 3.3352680 | 1.4080210 |
| 15 | C | 12 | 11 | 4 | 1.4047222 | 120.8549699 | -149.3948167 | 1.2252290 | 4.5586600 | -1.4078480 |
| 16 | C | 15 | 12 | 11 | 1.4047505 | 120.5512013 | 149.3870756 | 0.0035050 | 4.7130220 | -0.7319140 |
| 17 | C | 16 | 15 | 12 | 1.4638540 | 118.7641157 | 15.9536040 | 0.0034480 | 4.7129370 | 0.7319400 |
| 18 | C | 13 | 12 | 11 | 1.4046872 | 118.7677613 | -165.6551001 | 1.2251130 | 4.5585310 | 1.4079740 |
| 19 | C | 8 | 7 | 1 | 1.4047235 | 120.8518651 | -149.3928895 | 3.3355560 | -3.3403420 | 1.4078190 |
| 20 | C | 9 | 8 | 7 | 1.4047352 | 118.7626408 | -165.6561374 | 3.3354630 | -3.3403470 | -1.4080430 |
| 21 | C | 16 | 15 | 12 | 1.4046881 | 120.8530941 | -149.3870992 | -1.2182060 | 4.5598610 | -1.4080150 |
| 22 | C | 21 | 16 | 15 | 1.4046516 | 120.5490387 | 149.4235552 | -2.3534410 | 4.0831370 | -0.7319810 |
| 23 | C | 22 | 16 | 16 | 1.4638120 | 118.7709347 | 15.9221854 | -2.3535050 | 4.0831740 | 0.7318310 |
| 24 | C | 17 | 16 | 15 | 1.4046686 | 118.7697104 | -165.6643654 | -1.2183280 | 4.5600140 | 1.4079370 |
| 25 | C | 19 | 8 | 7 | 1.4046981 | 120.5456739 | 149.3830688 | 2.3535560 | -4.0832370 | 0.7318310 |
| 26 | C | 20 | 9 | 8 | 1.4046676 | 120.5471400 | 15.9703320 | 2.3534740 | -4.0831670 | -0.7320200 |
| 27 | C | 26 | 20 | 9 | 1.4046776 | 120.8580929 | 149.3971628 | 1.2181800 | -4.5599320 | -1.4079800 |
| 28 | C | 27 | 26 | 20 | 1.4046761 | 120.5503306 | -149.4420721 | -0.0035070 | -4.7130290 | -0.7318460 |

| | | | | | | | | | | |
|----|---|----|----|----|-----------|-------------|--------------|------------|------------|------------|
| 29 | C | 28 | 27 | 26 | 1.4638370 | 118.7707609 | -15.9217806 | -0.0034500 | -4.7129640 | 0.7319910 |
| 30 | C | 25 | 19 | 8 | 1.4046704 | 120.8522362 | -149.4023768 | 1.2183700 | -4.5599940 | 1.4079630 |
| 31 | C | 28 | 27 | 26 | 1.4047422 | 120.8489342 | 149.4191340 | -1.2251870 | -4.5585910 | -1.4078250 |
| 32 | C | 31 | 28 | 27 | 1.4047154 | 120.5515470 | -149.3965872 | -2.3597830 | -4.0801300 | -0.7318130 |
| 33 | C | 32 | 31 | 28 | 1.4638540 | 118.7670098 | -15.9418707 | -2.3597320 | -4.0799910 | 0.7320410 |
| 34 | C | 33 | 32 | 31 | 1.4047444 | 118.7667891 | 0.0020452 | -1.2250460 | -4.5582940 | 1.4080740 |
| 35 | C | 32 | 31 | 28 | 1.4047086 | 120.8538315 | 149.3949036 | -3.3404320 | -3.3354410 | -1.4078100 |
| 36 | C | 35 | 32 | 31 | 1.4046977 | 120.5485690 | -149.3799701 | -4.0834060 | -2.3534780 | -0.7318560 |
| 37 | C | 36 | 35 | 32 | 1.4638090 | 118.7666716 | -15.9631815 | -4.0834400 | -2.3534320 | 0.7319530 |
| 38 | C | 33 | 32 | 31 | 1.4046930 | 118.7659125 | 165.6520539 | -3.3403810 | -3.3352860 | 1.4079880 |
| 39 | C | 36 | 35 | 32 | 1.4046653 | 120.8534274 | 149.4012783 | -4.5602160 | -1.2183200 | -1.4079870 |
| 40 | C | 39 | 36 | 35 | 1.4046894 | 120.5472463 | -149.4354587 | -4.7133280 | 0.0034490 | -0.7319770 |
| 41 | C | 40 | 39 | 36 | 1.4638630 | 118.7693412 | -15.9302554 | -4.7134120 | 0.0034930 | 0.7318860 |
| 42 | C | 37 | 36 | 35 | 1.4046821 | 118.7703538 | 165.6773759 | -4.5603850 | -1.2182480 | 1.4079800 |
| 43 | C | 40 | 39 | 36 | 1.4047286 | 120.8518569 | 149.4128481 | -4.5588220 | 1.2250820 | -1.4079970 |
| 44 | C | 43 | 40 | 39 | 1.4047260 | 120.5510284 | -149.3907586 | -4.0802700 | 2.3596730 | -0.7320190 |
| 45 | C | 44 | 43 | 40 | 1.4638520 | 118.7656435 | -15.9512570 | -4.0803170 | 2.3597130 | 0.7318330 |
| 46 | C | 45 | 44 | 43 | 1.4047141 | 118.7657576 | -0.0021800 | -4.5589510 | 1.2251880 | 1.4078390 |
| 47 | C | 44 | 43 | 40 | 1.4047043 | 120.8552294 | 149.3896539 | -3.3354300 | 3.3402130 | -1.4079990 |
| 48 | C | 23 | 22 | 21 | 1.4046860 | 118.7668870 | -165.6722977 | -3.3355150 | 3.3403050 | 1.4078080 |
| 49 | H | 3 | 2 | 1 | 1.0857062 | 118.6354107 | -178.9318316 | 4.5430440 | 1.2137850 | -2.4934810 |
| 50 | H | 6 | 1 | 7 | 1.0856999 | 118.6402729 | 13.5848673 | 4.5429290 | 1.2135940 | 2.4935870 |
| 51 | H | 7 | 1 | 6 | 1.0857051 | 118.6262688 | -13.5941210 | 4.5416710 | -1.2205560 | 2.4933850 |
| 52 | H | 10 | 9 | 8 | 1.0857045 | 118.6403374 | -178.9320990 | 4.5414520 | -1.2202220 | -2.4935670 |
| 53 | H | 11 | 4 | 3 | 1.0857123 | 118.6405469 | -13.5959042 | 3.3279630 | 3.3229920 | -2.4933790 |
| 54 | H | 14 | 5 | 4 | 1.0857166 | 118.6377799 | 178.9485065 | 3.3277150 | 3.3228010 | 2.4935930 |
| 55 | H | 15 | 12 | 11 | 1.0857249 | 118.6442835 | -13.6343084 | 1.2207110 | 4.5421530 | -2.4934380 |
| 56 | H | 18 | 13 | 12 | 1.0857032 | 118.6409299 | 178.9373423 | 1.2202920 | 4.5412500 | 2.4935290 |
| 57 | H | 19 | 8 | 7 | 1.0857346 | 118.6303826 | -13.6097736 | 3.3232600 | -3.3278390 | 2.4934120 |
| 58 | H | 20 | 9 | 8 | 1.0857137 | 118.6313554 | 178.9551719 | 3.3230360 | -3.3278780 | -2.4936140 |
| 59 | H | 21 | 16 | 15 | 1.0856964 | 118.6354899 | -13.5766966 | -1.2134960 | 4.5423530 | -2.4935600 |
| 60 | H | 24 | 17 | 16 | 1.0856990 | 118.6381543 | 178.9348877 | -1.2137760 | 4.5426750 | 2.4934880 |
| 61 | H | 27 | 26 | 20 | 1.0856965 | 118.6353591 | 13.5573824 | 1.2134350 | -4.5424900 | -2.4935260 |
| 62 | H | 30 | 25 | 19 | 1.0856958 | 118.6344375 | -13.5652648 | 1.2138330 | -4.5426010 | 2.4935100 |
| 63 | H | 31 | 28 | 27 | 1.0856994 | 118.6246201 | 13.5796529 | -3.3279370 | -3.3230680 | -2.4933780 |
| 64 | H | 34 | 33 | 32 | 1.0857040 | 118.6378994 | 178.9091879 | -1.2203920 | -4.5411650 | -2.4933740 |
| 65 | H | 35 | 32 | 31 | 1.0857104 | 118.6318992 | 13.6096827 | -1.2201350 | -4.5405590 | 2.4936220 |
| 66 | H | 38 | 33 | 32 | 1.0857106 | 118.6331166 | -178.9543077 | -3.3278830 | -3.3228080 | 2.4935550 |
| 67 | H | 39 | 36 | 35 | 1.0856955 | 118.6356548 | 13.5642854 | -4.5427920 | -1.2137450 | -2.4935330 |
| 68 | H | 42 | 37 | 36 | 1.0856954 | 118.6351534 | -178.9302279 | -4.5430470 | -1.2136110 | 2.4935270 |
| 69 | H | 43 | 40 | 39 | 1.0857001 | 118.6264234 | 13.5933179 | -4.5415400 | 1.2202950 | -2.4935490 |
| 70 | H | 46 | 45 | 44 | 1.0857016 | 118.6393728 | 178.9335802 | -4.5417460 | 1.2204580 | 2.4933940 |
| 71 | H | 47 | 44 | 43 | 1.0857093 | 118.6338129 | 13.6112452 | -3.3229800 | 3.3277190 | -2.4935650 |
| 72 | H | 48 | 23 | 22 | 1.0857107 | 118.6376743 | 178.9478632 | -3.3231150 | 3.3278090 | 2.4933760 |

Dodecacene

| Tag | Symbol | NA | NB | NC | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|----|----|----|-----------|-------------|--------------|-------------|------------|------------|
| 1 | C | | | | | | | -14.0619090 | -0.6703140 | 0.0834890 |
| 2 | C | 1 | | | 1.3406771 | | - | 14.0619590 | 0.6703630 | 0.0840980 |
| 3 | C | 2 | 1 | | 1.3416124 | 119.7998156 | | -12.8979090 | 1.3371570 | 0.0668580 |
| 4 | C | 3 | 2 | 1 | 1.3459817 | 120.6598955 | -0.0090035 | -11.7269980 | 0.6735920 | 0.0490930 |
| 5 | C | 4 | 3 | 2 | 1.3472751 | 119.5359892 | -0.0002828 | -11.7270460 | -0.6736830 | 0.0486720 |
| 6 | C | 1 | 2 | 3 | 1.3416214 | 119.8084909 | 0.0047457 | -12.8979010 | -1.3371860 | 0.0657410 |
| 7 | C | 4 | 3 | 2 | 1.3451565 | 121.1370640 | -179.9720552 | -10.5543380 | 1.3324030 | 0.0322830 |
| 8 | C | 7 | 4 | 3 | 1.3452663 | 121.3135653 | 179.9345901 | -9.3819930 | 0.6727990 | 0.0158120 |
| 9 | C | 8 | 7 | 4 | 1.3455680 | 119.3638785 | 0.0311494 | -9.3819360 | -0.6727690 | 0.0155150 |
| 10 | C | 5 | 4 | 3 | 1.3450446 | 119.3170625 | -179.9624222 | -10.5544140 | -1.3323100 | 0.0316520 |
| 11 | C | 8 | 7 | 4 | 1.3453458 | 121.3096122 | -179.9156631 | -8.2091900 | 1.3317830 | 0.0006920 |
| 12 | C | 11 | 8 | 7 | 1.3452590 | 121.3388666 | 179.8816665 | -7.0364840 | 0.6727810 | -0.0134100 |
| 13 | C | 12 | 11 | 8 | 1.3455761 | 119.3302003 | 0.0749023 | -7.0365330 | -0.6727950 | -0.0139050 |
| 14 | C | 9 | 8 | 7 | 1.3452743 | 119.3374399 | -179.9572852 | -8.2092680 | -1.3318360 | -0.0000860 |
| 15 | C | 12 | 11 | 8 | 1.3452114 | 121.3347853 | -179.8651553 | -5.8638130 | 1.3317820 | -0.0258240 |
| 16 | C | 15 | 12 | 11 | 1.3452810 | 121.3370357 | 179.8453889 | -4.6910290 | 0.6728150 | -0.0368260 |
| 17 | C | 16 | 15 | 12 | 1.3455680 | 119.3280443 | 0.0848894 | -4.6910730 | -0.6727530 | -0.0371210 |

| | | | | | | | | | | |
|----|---|----|----|----|-----------|-------------|--------------|-------------|------------|------------|
| 18 | C | 17 | 16 | 15 | 1.3452316 | 119.3337684 | 0.0146597 | -5.8637940 | -1.3317410 | -0.0267090 |
| 19 | C | 16 | 15 | 12 | 1.3452438 | 121.3397049 | -179.8152573 | -3.5182650 | 1.3317760 | -0.0455360 |
| 20 | C | 19 | 16 | 15 | 1.3452279 | 121.3334491 | 179.7700600 | -2.3455650 | 0.6727070 | -0.0519260 |
| 21 | C | 20 | 19 | 16 | 1.3454590 | 119.3344588 | 0.1205108 | -2.3456030 | -0.6727520 | -0.0520250 |
| 22 | C | 21 | 20 | 19 | 1.3452552 | 119.3372411 | 0.0089392 | -3.5183330 | -1.3318260 | -0.0459150 |
| 23 | C | 20 | 19 | 16 | 1.3453333 | 121.3258736 | -179.7707920 | -1.1727850 | 1.3318670 | -0.0560390 |
| 24 | C | 23 | 20 | 19 | 1.3452776 | 121.3235198 | 179.7352964 | -0.0000510 | 0.6727270 | -0.0571200 |
| 25 | C | 24 | 23 | 20 | 1.3455510 | 119.3411825 | 0.1461733 | 0.0000160 | -0.6728240 | -0.0570180 |
| 26 | C | 25 | 24 | 23 | 1.3452237 | 119.3293978 | 0.0038598 | -1.1727410 | -1.3318130 | -0.0559160 |
| 27 | C | 24 | 23 | 20 | 1.3453271 | 121.3267094 | -179.7303271 | 1.1727660 | 1.3318200 | -0.0558240 |
| 28 | C | 27 | 24 | 23 | 1.3452483 | 121.3318869 | 179.7457106 | 2.3455280 | 0.6728010 | -0.0518050 |
| 29 | C | 28 | 27 | 24 | 1.3455550 | 119.3315913 | 0.1355268 | 2.3454920 | -0.6727540 | -0.0518000 |
| 30 | C | 29 | 28 | 27 | 1.3452257 | 119.3396424 | -0.0005725 | 1.1728070 | -1.3318640 | -0.0558020 |
| 31 | C | 28 | 27 | 24 | 1.3452264 | 121.3340279 | -179.7600521 | 3.5182660 | 1.3318020 | -0.0456970 |
| 32 | C | 31 | 28 | 27 | 1.3452844 | 121.3348061 | 179.7703365 | 4.6910440 | 0.6727820 | -0.0370720 |
| 33 | C | 32 | 31 | 28 | 1.3455470 | 119.3353097 | 0.1156508 | 4.6911130 | -0.6727650 | -0.0368700 |
| 34 | C | 33 | 32 | 31 | 1.3453041 | 119.3284912 | 0.0137360 | 3.5183090 | -1.3317780 | -0.0455790 |
| 35 | C | 32 | 31 | 28 | 1.3452471 | 121.3362947 | -179.7903246 | 5.8637870 | 1.3317640 | -0.0267590 |
| 36 | C | 35 | 32 | 31 | 1.3453310 | 121.3360447 | 179.8002587 | 7.0365670 | 0.6727170 | -0.0141280 |
| 37 | C | 36 | 35 | 32 | 1.3455331 | 119.3317191 | 0.0909319 | 7.0365430 | -0.6728160 | -0.0136240 |
| 38 | C | 37 | 36 | 35 | 1.3452255 | 119.3324561 | 0.0186032 | 5.8638440 | -1.3317940 | -0.0261410 |
| 39 | C | 36 | 35 | 32 | 1.3452073 | 121.3326239 | -179.8251242 | 8.2091990 | 1.3317510 | -0.0003090 |
| 40 | C | 39 | 36 | 35 | 1.3452779 | 121.3378597 | 179.8455216 | 9.3819560 | 0.6728380 | 0.0154200 |
| 41 | C | 40 | 39 | 36 | 1.3456341 | 119.3265442 | 0.0702833 | 9.3819330 | -0.6727960 | 0.0159290 |
| 42 | C | 41 | 40 | 39 | 1.3452342 | 119.3329348 | -0.0003916 | 8.2092650 | -1.3317900 | 0.0007080 |
| 43 | C | 40 | 39 | 36 | 1.3452712 | 121.3148772 | -179.8808236 | 10.5543480 | 1.3323750 | 0.0316260 |
| 44 | C | 43 | 40 | 39 | 1.3451608 | 121.3198807 | 179.9303120 | 11.7270410 | 0.6736220 | 0.0487520 |
| 45 | C | 44 | 43 | 40 | 1.3472321 | 119.3215983 | 0.0174362 | 11.7270180 | -0.6736100 | 0.0493300 |
| 46 | C | 45 | 44 | 43 | 1.3450885 | 119.3251119 | 0.0134732 | 10.5544100 | -1.3323740 | 0.0324950 |
| 47 | C | 44 | 43 | 40 | 1.3459010 | 121.1372894 | -179.9507076 | 12.8978590 | 1.3372030 | 0.0659240 |
| 48 | C | 47 | 44 | 43 | 1.3416831 | 120.6563835 | 179.9705526 | 14.0619560 | 0.6703580 | 0.0835170 |
| 49 | C | 48 | 47 | 44 | 1.3406341 | 119.8023902 | 0.0065361 | 14.0619330 | -0.6702760 | 0.0839090 |
| 50 | C | 49 | 48 | 47 | 1.3416670 | 119.8105512 | -0.0101087 | 12.8979190 | -1.3372490 | 0.0669130 |
| 51 | H | 1 | 2 | 3 | 1.1029458 | 120.0044974 | 179.9968764 | -15.0169150 | -1.2219040 | 0.0976830 |
| 52 | H | 2 | 1 | 6 | 1.1029115 | 120.0092717 | -179.9823487 | -15.0169280 | 1.2219310 | 0.0989550 |
| 53 | H | 3 | 2 | 1 | 1.1034895 | 118.4069405 | -179.9860850 | -12.9247670 | 2.4403190 | 0.0679990 |
| 54 | H | 6 | 1 | 2 | 1.1035621 | 118.4130884 | 179.9814379 | -12.9247260 | -2.4404220 | 0.0659570 |
| 55 | H | 7 | 4 | 3 | 1.1038545 | 119.2798478 | -0.0164512 | -10.5552030 | 2.4362570 | 0.0328380 |
| 56 | H | 10 | 5 | 4 | 1.1038263 | 119.2762216 | 179.9750254 | -10.5552340 | -2.4361360 | 0.0317380 |
| 57 | H | 11 | 8 | 7 | 1.1037663 | 119.3255489 | -0.0176714 | -8.2092470 | 2.4355490 | 0.0015320 |
| 58 | H | 14 | 9 | 8 | 1.1037180 | 119.3338332 | 179.9699440 | -8.2092840 | -2.4355540 | 0.0001760 |
| 59 | H | 15 | 12 | 11 | 1.1038796 | 119.3350827 | -0.0167215 | -5.8637630 | 2.4356610 | -0.0246920 |
| 60 | H | 18 | 17 | 16 | 1.1038220 | 119.3330176 | -179.9756987 | -5.8638120 | -2.4355630 | -0.0265430 |
| 61 | H | 19 | 16 | 15 | 1.1038653 | 119.3322986 | -0.0646690 | -3.5182220 | 2.4356410 | -0.0447030 |
| 62 | H | 22 | 21 | 20 | 1.1038012 | 119.3360787 | -179.9555004 | -3.5183380 | -2.4356270 | -0.0452490 |
| 63 | H | 23 | 20 | 19 | 1.1037612 | 119.3399631 | -0.0696502 | -1.1727440 | 2.4356280 | -0.0553020 |
| 64 | H | 26 | 25 | 24 | 1.1037923 | 119.3322791 | -179.9534814 | -1.1727410 | -2.4356050 | -0.0550510 |
| 65 | H | 27 | 24 | 23 | 1.1038622 | 119.3317730 | -0.0747459 | 1.1727060 | 2.4356820 | -0.0550890 |
| 66 | H | 30 | 29 | 28 | 1.1037923 | 119.3431373 | -179.9485425 | 1.1727070 | -2.4356560 | -0.0549340 |
| 67 | H | 31 | 28 | 27 | 1.1038622 | 119.3350347 | -0.0606005 | 3.5183060 | 2.4356640 | -0.0449650 |
| 68 | H | 34 | 33 | 32 | 1.1037923 | 119.3310983 | -179.9583396 | 3.5183100 | -2.4355700 | -0.0447140 |
| 69 | H | 35 | 32 | 31 | 1.1038441 | 119.3331032 | -0.0643725 | 5.8638180 | 2.4356080 | -0.0264260 |
| 70 | H | 38 | 37 | 36 | 1.1037884 | 119.3309629 | -179.9671766 | 5.8638470 | -2.4355820 | -0.0251760 |
| 71 | H | 39 | 36 | 35 | 1.1038310 | 119.3359998 | -0.0573673 | 8.2092210 | 2.4355820 | -0.0002760 |
| 72 | H | 42 | 41 | 40 | 1.1037973 | 119.3318199 | -179.9793258 | 8.2092630 | -2.4355870 | 0.0014730 |
| 73 | H | 43 | 40 | 39 | 1.1038264 | 119.4055689 | -0.0300890 | 10.5552680 | 2.4362010 | 0.0315370 |
| 74 | H | 46 | 45 | 44 | 1.1038015 | 119.2827407 | -179.9904458 | 10.5552050 | -2.4361750 | 0.0331410 |
| 75 | H | 47 | 44 | 43 | 1.1034803 | 120.9339164 | -0.0160994 | 12.9246930 | 2.4403570 | 0.0661120 |
| 76 | H | 48 | 47 | 44 | 1.1029696 | 120.1891860 | -179.9918232 | 15.0169770 | 1.2219710 | 0.0976560 |
| 77 | H | 49 | 48 | 47 | 1.1029569 | 120.0063815 | -179.9912654 | 15.0169420 | -1.2218730 | 0.0984890 |
| 78 | H | 50 | 49 | 48 | 1.1033934 | 118.4166500 | -179.9799772 | 12.9247330 | -2.4403160 | 0.0679710 |