Supplementary Material

# Noble gas dimers confined inside $C_{70}$

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**Binding Energies**

$$BE = E_{Ng_n@C_{70}} + ZPE_{Ng_n@C_{70}} + BSSE_{Ng_n@C_{70}} - (E_{Ng_n} + ZPE_{Ng_n}) - (E_{C_{70}} + ZPE_{C_{70}})$$

Table 1: Contributions to the binding energy (BE) calculated at B97D3/6-31G(d) level of theory for the endohedral fullerenes studied in this work. All energy values in atomic units (a.u.), except in the case of BEs. $E_{C_{70}}$ = -2665.585494 a.u. and $ZPE_{C_{70}}$ = 0.429550 a.u.

| **Motif** | $\mathbf{E}_{complex}$ | $\mathbf{ZPE}_{complex}$ | $\mathbf{BSSE}_{complex}$ | $\mathbf{E}_{Ng_n}$ | $\mathbf{ZPE}_{Ng_n}$ | **BE (kcal/mol)** |
|---|---|---|---|---|---|---|
| $He@C_{70}$ | -2668.498732 | 0.430971 | 0.001040 | -2.908813 | | -1.23 |
| $Ne@C_{70}$ | -2794.444299 | 0.429896 | 0.004021 | -128.847789 | | -4.17 |
| $Ar@C_{70}$ | -3193.156068 | 0.430776 | 0.003438 | -527.549660 | | -10.20 |
| $He_2@C_{70}$ | -2671.408764 | 0.432488 | 0.003040 | -5.817715 | 0.000151 | 0.17 |
| $HeNe@C_{70}$ | -2797.355687 | 0.432476 | 0.009330 | -131.756816 | 0.000257 | -0.86 |
| $Ne_2@C_{70}$ | -2923.302470 | 0.431789 | 0.016306 | -257.696294 | 0.000228 | -1.48 |
| $HeAr@C_{70}$ | -3196.055542 | 0.432214 | 0.004742 | -530.458730 | 0.000163 | -2.56 |
| $NeAr@C_{70}$ | -3321.996425 | 0.431811 | 0.014239 | -656.398273 | 0.000129 | 2.33 |
| $Ar_2@C_{70}$ | -3720.664939 | 0.431632 | 0.007039 | -1055.100013 | 0.000099 | 18.57 |

Table 2: Contributions to the binding energy (BE) calculated at B97D3/BS1 (TZVP for Carbon atoms and aug-cc-pVDZ for Noble gas atoms) level of theory for the endohedral fullerenes studied in this work. All energy values in atomic units (a.u.), except in the case of BEs. $E_{C_{70}}$ = -2666.270756 a.u. and $ZPE_{C_{70}}$ = 0.429797 a.u.

| **Motif** | $\mathbf{E}_{complex}$ | $\mathbf{ZPE}_{complex}$ | $\mathbf{BSSE}_{complex}$ | $\mathbf{E}_{Ng_n}$ | $\mathbf{ZPE}_{Ng_n}$ | **BE (kcal/mol)** |
|---|---|---|---|---|---|---|
| He@$C_{70}$ | -2669.184752 | 0.430590 | 0.000455 | -2.910814 | | -1.21 |
| Ne@$C_{70}$ | -2795.159263 | 0.430328 | 0.001008 | -128.881437 | | -3.47 |
| Ar@$C_{70}$ | -3193.867588 | 0.430952 | 0.002255 | -527.577331 | | -10.10 |
| $He_2$@$C_{70}$ | -2672.095779 | 0.432740 | 0.001379 | -5.821706 | 0.000160 | 0.53 |
| HeNe@$C_{70}$ | -2798.067766 | 0.432280 | 0.002315 | -131.792349 | 0.000082 | 0.03 |
| $Ne_2$@$C_{70}$ | -2924.036914 | 0.431832 | 0.003546 | -257.763057 | 0.000085 | 1.50 |
| HeAr@$C_{70}$ | -3196.767517 | 0.432542 | 0.003206 | -530.488362 | 0.000123 | -1.61 |
| NeAr@$C_{70}$ | -3322.729145 | 0.432016 | 0.004492 | -656.459131 | 0.000091 | 4.62 |
| $Ar_2$@$C_{70}$ | -3721.402563 | 0.432115 | 0.005364 | -1055.155256 | 0.000091 | 19.48 |

Table 3: Contributions to the DF-DFT-SAPT interaction energy for the endohedral fullerenes studied in this work. All energy values in kcal/mol.

| **Guest/Component** | **Ne** | **Ar** | **$He_2$** | **HeNe** | **$Ne_2$** | **HeAr** | **NeAr** | **$Ar_2$** |
|---|---|---|---|---|---|---|---|---|
| $E^{(1)}_{elst}$ | -0.57 | -3.74 | -0.98 | -2.02 | -3.96 | -8.42 | -13.36 | -31.21 |
| $E^{(1)}_{exch}$ | 1.82 | 10.28 | 4.37 | 7.31 | 12.55 | 24.91 | 37.07 | 80.01 |
| $E^{(2)}_{ind}$ | -0.58 | -4.19 | -0.34 | -1.47 | -3.94 | -8.52 | -15.63 | -41.38 |
| $E^{(2)}_{exch-ind}$ | 0.60 | 4.13 | 0.34 | 1.51 | 4.07 | 8.36 | 15.53 | 40.09 |
| $E^{(2)}_{disp}$ | -3.90 | -16.57 | -5.73 | -8.83 | -12.74 | -24.82 | -31.06 | -54.77 |
| $E^{(2)}_{exch-disp}$ | 0.31 | 3.15 | 0.55 | 1.06 | 2.05 | 5.82 | 8.39 | 18.85 |
| $\delta E_{HF}$ | -0.06 | -0.37 | -0.25 | -0.35 | -0.42 | -1.08 | -1.21 | -1.93 |
| $E^{SAPT}_{int}$ | -2.37 | -7.32 | -2.04 | -2.78 | -2.39 | -3.74 | -0.28 | 9.66 |

## Optimized geometries for TSs at the B97D3/6-31G(d) level of theory

| TS $He_2$@C70 | | | |
|---|---|---|---|
| 6 | -3.227870 | 2.074198 | -1.269947 |
| 6 | -2.446831 | 3.006405 | -0.469370 |
| 6 | -3.978643 | 1.062320 | -0.648781 |
| 6 | -2.446911 | 2.898926 | 0.924438 |
| 6 | -1.206340 | 3.076012 | 1.661415 |
| 6 | 0.005873 | 3.450384 | 1.005550 |
| 6 | 1.217222 | 3.072199 | 1.660757 |
| 6 | -3.231508 | -0.567519 | -2.357496 |
| 6 | -2.448078 | 0.482100 | -2.991310 |
| 6 | -3.981021 | -0.286683 | -1.204218 |
| 6 | -2.446274 | 1.775859 | -2.459777 |
| 6 | -1.207139 | 2.532923 | -2.399667 |
| 6 | 0.003482 | 2.018676 | -2.951590 |
| 6 | 1.215754 | 2.529276 | -2.399731 |
| 6 | 0.005794 | 3.565928 | -0.466852 |
| 6 | -1.207207 | 3.296957 | -1.171705 |
| 6 | 1.217817 | 3.292658 | -1.171657 |
| 6 | -3.233617 | -2.418987 | -0.185547 |
| 6 | -2.453569 | -2.703386 | -1.380560 |
| 6 | -3.981532 | -1.232695 | -0.094677 |
| 6 | -2.451781 | -1.794045 | -2.442930 |
| 6 | -1.211745 | -1.504058 | -3.141016 |
| 6 | -0.002291 | -2.192039 | -2.826309 |
| 6 | 1.209115 | -1.506596 | -3.140226 |
| 6 | 0.001458 | 0.653653 | -3.510178 |
| 6 | -1.209690 | -0.098387 | -3.479028 |
| 6 | 1.210707 | -0.101202 | -3.478175 |
| 6 | -3.231964 | -0.922623 | 2.243993 |
| 6 | -2.452867 | -2.148187 | 2.141411 |
| 6 | -3.980562 | -0.467981 | 1.146697 |
| 6 | -2.454209 | -2.883941 | 0.952056 |
| 6 | -1.217068 | -3.469363 | 0.459504 |
| 6 | -0.003669 | -3.382143 | 1.207861 |
| 6 | 1.208955 | -3.466946 | 0.458972 |
| 6 | -0.003852 | -3.155072 | -1.708189 |
| 6 | -1.217121 | -3.357592 | -0.982895 |
| 6 | 1.209174 | -3.356072 | -0.982602 |
| 6 | -3.228075 | 1.855015 | 1.573050 |
| 6 | -2.445852 | 1.377202 | 2.702169 |
| 6 | -3.978566 | 0.950021 | 0.804545 |
| 6 | -2.448075 | 0.017708 | 3.030507 |
| 6 | -1.209764 | -0.631354 | 3.423636 |
| 6 | 0.001780 | 0.106733 | 3.569640 |
| 6 | 1.211518 | -0.634216 | 3.423419 |
| 6 | -0.002020 | -2.601146 | 2.460337 |
| 6 | -1.212045 | -1.968951 | 2.875386 |
| 6 | 1.209948 | -1.971577 | 2.874989 |

| | | | |
|---|---|---|---|
| 6 | 0.003640 | 1.540252 | 3.224187 |
| 6 | -1.206630 | 2.133588 | 2.758225 |
| 6 | 1.215455 | 2.130288 | 2.757806 |
| 6 | 3.233342 | -0.930263 | 2.243771 |
| 6 | 2.451863 | 0.011758 | 3.030535 |
| 6 | 2.452879 | 1.371021 | 2.701601 |
| 6 | 3.982732 | -0.477643 | 1.145913 |
| 6 | 3.229983 | -2.426161 | -0.186318 |
| 6 | 2.448846 | -2.887698 | 0.951374 |
| 6 | 2.450496 | -2.153397 | 2.141202 |
| 6 | 3.981729 | -1.242289 | -0.095585 |
| 6 | 3.232503 | -0.575137 | -2.358460 |
| 6 | 2.449208 | -1.799378 | -2.443491 |
| 6 | 2.448587 | -2.707908 | -1.380927 |
| 6 | 3.983242 | -0.296292 | -1.205277 |
| 6 | 3.236415 | 2.066334 | -1.271082 |
| 6 | 2.453737 | 1.770112 | -2.461040 |
| 6 | 2.451484 | 0.476228 | -2.992218 |
| 6 | 3.985124 | 1.052744 | -0.649910 |
| 6 | 3.236384 | 1.846902 | 1.572448 |
| 6 | 2.457568 | 2.892573 | 0.923841 |
| 6 | 2.457171 | 2.999593 | -0.469943 |
| 6 | 3.984813 | 0.940299 | 0.803694 |
| 2 | -0.200382 | -1.001265 | -0.033238 |
| 2 | -0.073855 | 0.977518 | -0.045497 |

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TS HeNe@C70

| | | | |
|---|---|---|---|
| 6 | 3.230580 | -1.909941 | -1.481133 |
| 6 | 2.451761 | -2.924664 | -0.784306 |
| 6 | 3.980301 | -0.967715 | -0.757591 |
| 6 | 2.451758 | -2.965094 | 0.612949 |
| 6 | 1.212274 | -3.225020 | 1.328139 |
| 6 | 0.000017 | -3.535042 | 0.637178 |
| 6 | -1.212239 | -3.225028 | 1.328143 |
| 6 | 3.231375 | 0.833629 | -2.284361 |
| 6 | 2.448234 | -0.144707 | -3.023437 |
| 6 | 3.980744 | 0.432615 | -1.167224 |
| 6 | 2.447472 | -1.487309 | -2.630770 |
| 6 | 1.210429 | -2.249212 | -2.651193 |
| 6 | 0.000002 | -1.679162 | -3.143618 |
| 6 | -1.210418 | -2.249223 | -2.651191 |
| 6 | 0.000015 | -3.491981 | -0.841019 |
| 6 | 1.211829 | -3.141506 | -1.512702 |
| 6 | -1.211805 | -3.141517 | -1.512699 |
| 6 | 3.230056 | 2.444609 | 0.069693 |
| 6 | 2.450736 | 2.854732 | -1.088398 |
| 6 | 3.980598 | 1.256476 | 0.035564 |
| 6 | 2.450798 | 2.062111 | -2.240522 |

| | | | |
|---|---|---|---|
| 6 | 1.210052 | 1.846508 | -2.963617 |
| 6 | -0.000017 | 2.498904 | -2.580559 |
| 6 | -1.210081 | 1.846497 | -2.963617 |
| 6 | -0.000005 | -0.262980 | -3.556587 |
| 6 | 1.209404 | 0.483377 | -3.445775 |
| 6 | -1.209421 | 0.483366 | -3.445774 |
| 6 | 3.231126 | 0.700016 | 2.326869 |
| 6 | 2.450158 | 1.928824 | 2.353458 |
| 6 | 3.981002 | 0.364403 | 1.188853 |
| 6 | 2.450411 | 2.786879 | 1.249346 |
| 6 | 1.213907 | 3.423870 | 0.821665 |
| 6 | -0.000008 | 3.259241 | 1.556864 |
| 6 | -1.213934 | 3.423871 | 0.821670 |
| 6 | -0.000027 | 3.344259 | -1.368956 |
| 6 | 1.213769 | 3.465503 | -0.624939 |
| 6 | -1.213813 | 3.465503 | -0.624943 |
| 6 | 3.230638 | -1.992489 | 1.367210 |
| 6 | 2.447864 | -1.637461 | 2.539855 |
| 6 | 3.980443 | -1.010026 | 0.699150 |
| 6 | 2.448365 | -0.319321 | 3.008719 |
| 6 | 1.209294 | 0.282882 | 3.466169 |
| 6 | 0.000011 | -0.468758 | 3.533975 |
| 6 | -1.209277 | 0.282871 | 3.466173 |
| 6 | -0.000001 | 2.344401 | 2.716643 |
| 6 | 1.209682 | 1.671432 | 3.062620 |
| 6 | -1.209678 | 1.671422 | 3.062624 |
| 6 | 0.000016 | -1.859336 | 3.041215 |
| 6 | 1.210614 | -2.399416 | 2.516056 |
| 6 | -1.210580 | -2.399425 | 2.516061 |
| 6 | -3.231115 | 0.699989 | 2.326879 |
| 6 | -2.448344 | -0.319341 | 3.008726 |
| 6 | -2.447836 | -1.637481 | 2.539866 |
| 6 | -3.980993 | 0.364369 | 1.188868 |
| 6 | -3.230073 | 2.444580 | 0.069704 |
| 6 | -2.450427 | 2.786862 | 1.249355 |
| 6 | -2.450160 | 1.928805 | 2.353466 |
| 6 | -3.980600 | 1.256440 | 0.035579 |
| 6 | -3.231388 | 0.833600 | -2.284348 |
| 6 | -2.450825 | 2.062090 | -2.240515 |
| 6 | -2.450770 | 2.854716 | -1.088393 |
| 6 | -3.980748 | 0.432580 | -1.167208 |
| 6 | -3.230565 | -1.909968 | -1.481121 |
| 6 | -2.447466 | -1.487329 | -2.630759 |
| 6 | -2.448242 | -0.144728 | -3.023427 |
| 6 | -3.980290 | -0.967749 | -0.757575 |
| 6 | -3.230611 | -1.992516 | 1.367222 |
| 6 | -2.451725 | -2.965111 | 0.612957 |
| 6 | -2.451736 | -2.924684 | -0.784297 |
| 6 | -3.980426 | -1.010059 | 0.699166 |
| 2 | -0.000415 | 1.192535 | 0.012740 |
| 10 | 0.000030 | -0.884665 | 0.011806 |

TS $Ne_2$@C70

| | | | |
|---|---|---|---|
| 6 | -3.227400 | 2.077052 | -1.262386 |
| 6 | -2.450883 | 3.015170 | -0.461973 |
| 6 | -3.976411 | 1.060319 | -0.646100 |
| 6 | -2.450827 | 2.902786 | 0.931378 |
| 6 | -1.211573 | 3.087387 | 1.670644 |
| 6 | -0.000070 | 3.482028 | 1.019039 |
| 6 | 1.211450 | 3.087424 | 1.670638 |
| 6 | -3.227249 | -0.566012 | -2.355819 |
| 6 | -2.444780 | 0.487665 | -2.983404 |
| 6 | -3.977351 | -0.288291 | -1.203912 |
| 6 | -2.444940 | 1.782286 | -2.450801 |
| 6 | -1.210422 | 2.547679 | -2.390584 |
| 6 | -0.000045 | 2.032926 | -2.941271 |
| 6 | 1.210315 | 2.547718 | -2.390584 |
| 6 | -0.000072 | 3.605581 | -0.459813 |
| 6 | -1.213295 | 3.320166 | -1.165068 |
| 6 | 1.213161 | 3.320203 | -1.165068 |
| 6 | -3.227076 | -2.425547 | -0.191891 |
| 6 | -2.448192 | -2.709891 | -1.386840 |
| 6 | -3.975795 | -1.238604 | -0.098453 |
| 6 | -2.446953 | -1.792923 | -2.443370 |
| 6 | -1.207263 | -1.499519 | -3.137124 |
| 6 | 0.000032 | -2.193243 | -2.826755 |
| 6 | 1.207302 | -1.499480 | -3.137129 |
| 6 | -0.000020 | 0.665308 | -3.497997 |
| 6 | -1.206821 | -0.091032 | -3.469380 |
| 6 | 1.206809 | -0.090991 | -3.469383 |
| 6 | -3.227536 | -0.933921 | 2.237296 |
| 6 | -2.448711 | -2.160656 | 2.132233 |
| 6 | -3.976621 | -0.475901 | 1.143261 |
| 6 | -2.449508 | -2.898363 | 0.943709 |
| 6 | -1.215290 | -3.495499 | 0.451381 |
| 6 | 0.000065 | -3.416513 | 1.203271 |
| 6 | 1.215413 | -3.495470 | 0.451388 |
| 6 | 0.000052 | -3.174301 | -1.719872 |
| 6 | -1.214958 | -3.376929 | -0.993378 |
| 6 | 1.215067 | -3.376896 | -0.993383 |
| 6 | -3.227364 | 1.849899 | 1.574125 |
| 6 | -2.443826 | 1.368587 | 2.698919 |
| 6 | -3.976215 | 0.943818 | 0.805499 |
| 6 | -2.444431 | 0.006751 | 3.022709 |
| 6 | -1.207398 | -0.643443 | 3.412847 |
| 6 | -0.000004 | 0.098248 | 3.559567 |
| 6 | 1.207416 | -0.643402 | 3.412845 |
| 6 | 0.000045 | -2.621815 | 2.452350 |
| 6 | -1.208206 | -1.982793 | 2.864678 |

| | | | |
|---|---|---|---|
| 6 | 1.208274 | -1.982752 | 2.864679 |
| 6 | -0.000032 | 1.534778 | 3.220107 |
| 6 | -1.209008 | 2.131216 | 2.758244 |
| 6 | 1.208923 | 2.131255 | 2.758240 |
| 6 | 3.227564 | -0.933811 | 2.237293 |
| 6 | 2.444425 | 0.006835 | 3.022705 |
| 6 | 2.443768 | 1.368669 | 2.698914 |
| 6 | 3.976629 | -0.475765 | 1.143256 |
| 6 | 3.227154 | -2.425442 | -0.191894 |
| 6 | 2.449609 | -2.898287 | 0.943709 |
| 6 | 2.448785 | -2.160575 | 2.132232 |
| 6 | 3.975827 | -1.238469 | -0.098458 |
| 6 | 3.227253 | -0.565903 | -2.355821 |
| 6 | 2.447003 | -1.792843 | -2.443374 |
| 6 | 2.448277 | -2.709813 | -1.386843 |
| 6 | 3.977347 | -0.288156 | -1.203917 |
| 6 | 3.227313 | 2.077161 | -1.262391 |
| 6 | 2.444861 | 1.782368 | -2.450803 |
| 6 | 2.444746 | 0.487748 | -2.983406 |
| 6 | 3.976361 | 1.060455 | -0.646106 |
| 6 | 3.227287 | 1.850008 | 1.574119 |
| 6 | 2.450712 | 2.902866 | 0.931373 |
| 6 | 2.450762 | 3.015250 | -0.461977 |
| 6 | 3.976172 | 0.943955 | 0.805493 |
| 10 | 0.000385 | -1.079356 | -0.010015 |
| 10 | -0.000162 | 1.068368 | -0.002835 |

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TS HeAr@C70

| | | | |
|---|---|---|---|
| 6 | 3.225424 | -1.948855 | -1.422747 |
| 6 | 2.450119 | -2.948962 | -0.699444 |
| 6 | 3.973481 | -0.983838 | -0.727922 |
| 6 | 2.450119 | -2.948966 | 0.699425 |
| 6 | 1.212781 | -3.196584 | 1.425142 |
| 6 | 0.000001 | -3.535439 | 0.742657 |
| 6 | -1.212780 | -3.196584 | 1.425142 |
| 6 | 3.224090 | 0.774006 | -2.302078 |
| 6 | 2.442303 | -0.226840 | -3.011220 |
| 6 | 3.974094 | 0.405026 | -1.176638 |
| 6 | 2.443357 | -1.560440 | -2.584499 |
| 6 | 1.210192 | -2.330225 | -2.587861 |
| 6 | 0.000000 | -1.773448 | -3.097718 |
| 6 | -1.210192 | -2.330225 | -2.587861 |
| 6 | 0.000000 | -3.535434 | -0.742679 |
| 6 | 1.212781 | -3.196575 | -1.425162 |
| 6 | -1.212780 | -3.196575 | -1.425162 |
| 6 | 3.224529 | 2.456517 | 0.000007 |
| 6 | 2.446873 | 2.838029 | -1.168686 |
| 6 | 3.972220 | 1.264703 | 0.000004 |

| | | | |
|---|---|---|---|
| 6 | 2.445544 | 2.005379 | -2.293355 |
| 6 | 1.206090 | 1.768669 | -3.008645 |
| 6 | 0.000000 | 2.440324 | -2.646503 |
| 6 | -1.206091 | 1.768669 | -3.008645 |
| 6 | 0.000000 | -0.363665 | -3.542375 |
| 6 | 1.205536 | 0.389486 | -3.451297 |
| 6 | -1.205537 | 0.389485 | -3.451297 |
| 6 | 3.224091 | 0.773992 | 2.302082 |
| 6 | 2.445544 | 2.005365 | 2.293367 |
| 6 | 3.974094 | 0.405019 | 1.176640 |
| 6 | 2.446873 | 2.838022 | 1.168703 |
| 6 | 1.216382 | 3.482430 | 0.726048 |
| 6 | 0.000000 | 3.341894 | 1.469634 |
| 6 | -1.216383 | 3.482430 | 0.726048 |
| 6 | -0.000001 | 3.341904 | -1.469614 |
| 6 | 1.216382 | 3.482435 | -0.726026 |
| 6 | -1.216383 | 3.482435 | -0.726026 |
| 6 | 3.225424 | -1.948864 | 1.422735 |
| 6 | 2.443357 | -1.560457 | 2.584489 |
| 6 | 3.973481 | -0.983843 | 0.727916 |
| 6 | 2.442304 | -0.226859 | 3.011219 |
| 6 | 1.205537 | 0.389464 | 3.451299 |
| 6 | 0.000000 | -0.363687 | 3.542373 |
| 6 | -1.205537 | 0.389464 | 3.451299 |
| 6 | 0.000000 | 2.440307 | 2.646517 |
| 6 | 1.206091 | 1.768650 | 3.008655 |
| 6 | -1.206091 | 1.768650 | 3.008655 |
| 6 | 0.000000 | -1.773468 | 3.097707 |
| 6 | 1.210193 | -2.330242 | 2.587847 |
| 6 | -1.210192 | -2.330242 | 2.587847 |
| 6 | -3.224091 | 0.773991 | 2.302083 |
| 6 | -2.442304 | -0.226860 | 3.011219 |
| 6 | -2.443357 | -1.560458 | 2.584490 |
| 6 | -3.974095 | 0.405018 | 1.176641 |
| 6 | -3.224530 | 2.456516 | 0.000008 |
| 6 | -2.446874 | 2.838022 | 1.168703 |
| 6 | -2.445545 | 2.005365 | 2.293367 |
| 6 | -3.972222 | 1.264702 | 0.000004 |
| 6 | -3.224091 | 0.774005 | -2.302078 |
| 6 | -2.445545 | 2.005379 | -2.293355 |
| 6 | -2.446874 | 2.838029 | -1.168685 |
| 6 | -3.974095 | 0.405026 | -1.176638 |
| 6 | -3.225424 | -1.948856 | -1.422747 |
| 6 | -2.443357 | -1.560441 | -2.584499 |
| 6 | -2.442304 | -0.226841 | -3.011221 |
| 6 | -3.973482 | -0.983839 | -0.727922 |
| 6 | -3.225424 | -1.948865 | 1.422735 |
| 6 | -2.450118 | -2.948967 | 0.699425 |
| 6 | -2.450118 | -2.948962 | -0.699444 |
| 6 | -3.973482 | -0.983844 | 0.727916 |
| 2 | 0.000001 | 1.525623 | 0.000004 |

| | | | |
|---|---|---|---|
| 18 | 0.000002 | -0.679700 | 0.000001 |

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TS NeAr@C70

| | | | |
|---|---|---|---|
| 6 | 3.219779 | -1.969599 | -1.419342 |
| 6 | 2.449618 | -2.979131 | -0.699788 |
| 6 | 3.966652 | -1.001224 | -0.727000 |
| 6 | 2.449618 | -2.979127 | 0.699806 |
| 6 | 1.213988 | -3.238666 | 1.428853 |
| 6 | 0.000000 | -3.594585 | 0.747358 |
| 6 | -1.213988 | -3.238666 | 1.428853 |
| 6 | 3.217545 | 0.759486 | -2.297154 |
| 6 | 2.435568 | -0.243505 | -3.001964 |
| 6 | 3.967684 | 0.389053 | -1.174460 |
| 6 | 2.437131 | -1.579935 | -2.578249 |
| 6 | 1.209015 | -2.358354 | -2.585687 |
| 6 | 0.000000 | -1.797247 | -3.092706 |
| 6 | -1.209015 | -2.358354 | -2.585687 |
| 6 | 0.000000 | -3.594589 | -0.747336 |
| 6 | 1.213988 | -3.238675 | -1.428833 |
| 6 | -1.213988 | -3.238675 | -1.428833 |
| 6 | 3.219198 | 2.445930 | -0.000007 |
| 6 | 2.444228 | 2.834391 | -1.168297 |
| 6 | 3.964852 | 1.250811 | -0.000004 |
| 6 | 2.441262 | 1.993811 | -2.288646 |
| 6 | 1.202545 | 1.757508 | -3.001925 |
| 6 | 0.000000 | 2.439253 | -2.644315 |
| 6 | -1.202545 | 1.757508 | -3.001925 |
| 6 | 0.000000 | -0.382495 | -3.531115 |
| 6 | 1.201428 | 0.374378 | -3.440567 |
| 6 | -1.201428 | 0.374378 | -3.440567 |
| 6 | 3.217545 | 0.759500 | 2.297149 |
| 6 | 2.441263 | 1.993825 | 2.288633 |
| 6 | 3.967684 | 0.389061 | 1.174458 |
| 6 | 2.444228 | 2.834399 | 1.168279 |
| 6 | 1.219925 | 3.498512 | 0.728819 |
| 6 | 0.000000 | 3.360330 | 1.475380 |
| 6 | -1.219924 | 3.498512 | 0.728819 |
| 6 | 0.000000 | 3.360320 | -1.475400 |
| 6 | 1.219925 | 3.498507 | -0.728840 |
| 6 | -1.219924 | 3.498507 | -0.728840 |
| 6 | 3.219779 | -1.969590 | 1.419355 |
| 6 | 2.437131 | -1.579919 | 2.578259 |
| 6 | 3.966652 | -1.001220 | 0.727006 |
| 6 | 2.435568 | -0.243486 | 3.001965 |
| 6 | 1.201428 | 0.374400 | 3.440564 |
| 6 | 0.000000 | -0.382472 | 3.531117 |
| 6 | -1.201428 | 0.374400 | 3.440564 |
| 6 | 0.000000 | 2.439270 | 2.644300 |

| | | | |
|---|---|---|---|
| 6 | 1.202545 | 1.757526 | 3.001914 |
| 6 | -1.202545 | 1.757527 | 3.001915 |
| 6 | 0.000000 | -1.797227 | 3.092717 |
| 6 | 1.209015 | -2.358337 | 2.585702 |
| 6 | -1.209015 | -2.358337 | 2.585701 |
| 6 | -3.217545 | 0.759501 | 2.297149 |
| 6 | -2.435568 | -0.243486 | 3.001965 |
| 6 | -2.437131 | -1.579919 | 2.578258 |
| 6 | -3.967684 | 0.389061 | 1.174458 |
| 6 | -3.219198 | 2.445931 | -0.000007 |
| 6 | -2.444228 | 2.834399 | 1.168280 |
| 6 | -2.441263 | 1.993826 | 2.288634 |
| 6 | -3.964853 | 1.250811 | -0.000004 |
| 6 | -3.217545 | 0.759486 | -2.297154 |
| 6 | -2.441262 | 1.993811 | -2.288646 |
| 6 | -2.444228 | 2.834392 | -1.168297 |
| 6 | -3.967684 | 0.389053 | -1.174461 |
| 6 | -3.219779 | -1.969599 | -1.419342 |
| 6 | -2.437131 | -1.579935 | -2.578249 |
| 6 | -2.435568 | -0.243505 | -3.001964 |
| 6 | -3.966652 | -1.001224 | -0.727000 |
| 6 | -3.219779 | -1.969590 | 1.419354 |
| 6 | -2.449618 | -2.979127 | 0.699806 |
| 6 | -2.449618 | -2.979131 | -0.699788 |
| 6 | -3.966652 | -1.001220 | 0.727006 |
| 10 | 0.000001 | 1.382339 | 0.000001 |
| 18 | -0.000001 | -0.898374 | 0.000000 |

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TS $Ar_2$@C70

| | | | |
|---|---|---|---|
| 6 | -3.205676 | 1.754775 | -1.678547 |
| 6 | -2.446288 | 2.874709 | -1.118789 |
| 6 | -3.950650 | 0.890893 | -0.861122 |
| 6 | -2.450058 | 3.091603 | 0.266013 |
| 6 | -1.222909 | 3.496049 | 0.960197 |
| 6 | -0.000541 | 3.782898 | 0.232363 |
| 6 | 1.221948 | 3.496342 | 0.960182 |
| 6 | -3.202978 | -1.088176 | -2.155332 |
| 6 | -2.419671 | -0.193929 | -2.987204 |
| 6 | -3.951279 | -0.552124 | -1.102934 |
| 6 | -2.420561 | 1.194004 | -2.758822 |
| 6 | -1.201762 | 1.972480 | -2.879471 |
| 6 | -0.000213 | 1.333746 | -3.293764 |
| 6 | 1.201180 | 1.972759 | -2.879469 |
| 6 | -0.000484 | 3.530281 | -1.265880 |
| 6 | -1.212059 | 3.038473 | -1.880332 |
| 6 | 1.211223 | 3.038764 | -1.880333 |
| 6 | -3.208164 | -2.428167 | 0.347039 |
| 6 | -2.444598 | -3.004789 | -0.753535 |

| | | | |
|---|---|---|---|
| 6 | -3.947974 | -1.237290 | 0.178907 |
| 6 | -2.437095 | -2.321834 | -1.979255 |
| 6 | -1.200134 | -2.201934 | -2.726480 |
| 6 | 0.000295 | -2.857501 | -2.294043 |
| 6 | 1.200576 | -2.201698 | -2.726504 |
| 6 | -0.000032 | -0.134962 | -3.526667 |
| 6 | -1.195021 | -0.878163 | -3.337635 |
| 6 | 1.195128 | -0.877905 | -3.337638 |
| 6 | -3.202123 | -0.413403 | 2.371800 |
| 6 | -2.429428 | -1.640488 | 2.537829 |
| 6 | -3.951577 | -0.209850 | 1.212269 |
| 6 | -2.435362 | -2.646935 | 1.557854 |
| 6 | -1.222466 | -3.397607 | 1.223622 |
| 6 | 0.000374 | -3.143389 | 1.942495 |
| 6 | 1.223256 | -3.397467 | 1.223654 |
| 6 | 0.000382 | -3.628784 | -0.997762 |
| 6 | -1.226792 | -3.633959 | -0.226275 |
| 6 | 1.227608 | -3.633856 | -0.226278 |
| 6 | -3.207530 | 2.172036 | 1.115572 |
| 6 | -2.426143 | 1.957403 | 2.316555 |
| 6 | -3.949277 | 1.104569 | 0.573528 |
| 6 | -2.422108 | 0.686358 | 2.917924 |
| 6 | -1.192327 | 0.137191 | 3.436825 |
| 6 | -0.000129 | 0.909988 | 3.419253 |
| 6 | 1.192253 | 0.137459 | 3.436811 |
| 6 | 0.000233 | -2.040656 | 2.956794 |
| 6 | -1.194424 | -1.301441 | 3.206883 |
| 6 | 1.194708 | -1.301183 | 3.206885 |
| 6 | -0.000305 | 2.267448 | 2.803876 |
| 6 | -1.211632 | 2.758940 | 2.226342 |
| 6 | 1.210890 | 2.759231 | 2.226327 |
| 6 | 3.202158 | -0.412678 | 2.371768 |
| 6 | 2.421885 | 0.686913 | 2.917889 |
| 6 | 2.425593 | 1.957966 | 2.316523 |
| 6 | 3.951538 | -0.208946 | 1.212229 |
| 6 | 3.208693 | -2.427507 | 0.347019 |
| 6 | 2.435974 | -2.646468 | 1.557859 |
| 6 | 2.429776 | -1.639966 | 2.537809 |
| 6 | 3.948171 | -1.236404 | 0.178876 |
| 6 | 3.203133 | -1.087469 | -2.155350 |
| 6 | 2.437568 | -2.321341 | -1.979279 |
| 6 | 2.445268 | -3.004352 | -0.753560 |
| 6 | 3.951301 | -0.551227 | -1.102958 |
| 6 | 3.205146 | 1.755520 | -1.678564 |
| 6 | 2.420160 | 1.194558 | -2.758828 |
| 6 | 2.419609 | -0.193386 | -2.987208 |
| 6 | 3.950327 | 0.891803 | -0.861151 |
| 6 | 3.206912 | 2.172788 | 1.115536 |
| 6 | 2.449209 | 3.092197 | 0.265991 |
| 6 | 2.445496 | 2.875295 | -1.118808 |
| 6 | 3.948910 | 1.105484 | 0.573492 |

| | | | |
|---|---|---|---|
| 18 | 0.000987 | -1.211130 | 0.003768 |
| 18 | -0.000024 | 1.213233 | 0.001892 |

**Optimized geometries for all minima at the B97D3/6-31G(d) level of theory**

| C70 | | | |
|---|---|---|---|
| 6 | -3.234661 | -1.953796 | -1.442092 |
| 6 | -2.452708 | -1.557681 | -2.603529 |
| 6 | -3.984951 | -0.998240 | -0.736803 |
| 6 | -2.453047 | -0.224808 | -3.026004 |
| 6 | -1.212379 | 0.392296 | -3.463036 |
| 6 | -0.000088 | -0.353520 | -3.557814 |
| 6 | 1.212229 | 0.392226 | -3.462995 |
| 6 | -3.234609 | -1.975114 | 1.412811 |
| 6 | -2.453280 | -2.957862 | 0.677189 |
| 6 | -3.984927 | -1.009170 | 0.721747 |
| 6 | -2.453085 | -2.947370 | -0.721078 |
| 6 | -1.212532 | -3.173062 | -1.443401 |
| 6 | -0.000226 | -3.492834 | -0.763212 |
| 6 | 1.212090 | -3.172942 | -1.443468 |
| 6 | -0.000200 | -1.759545 | -3.113399 |
| 6 | -1.212516 | -2.314849 | -2.606550 |
| 6 | 1.212098 | -2.314915 | -2.606372 |
| 6 | -3.234958 | 0.733466 | 2.315345 |
| 6 | -2.453122 | -0.269819 | 3.022601 |
| 6 | -3.984862 | 0.374754 | 1.182896 |
| 6 | -2.452633 | -1.596224 | 2.580202 |
| 6 | -1.212523 | -2.353476 | 2.571964 |
| 6 | -0.000037 | -1.805857 | 3.086706 |
| 6 | 1.212337 | -2.353570 | 2.571743 |
| 6 | -0.000210 | -3.503817 | 0.711296 |
| 6 | -1.212503 | -3.194235 | 1.396160 |
| 6 | 1.212204 | -3.194108 | 1.396131 |
| 6 | -3.235003 | 2.428800 | 0.018208 |
| 6 | -2.453025 | 2.790923 | 1.190827 |
| 6 | -3.985245 | 1.241100 | 0.009395 |
| 6 | -2.452825 | 1.960695 | 2.315770 |
| 6 | -1.212211 | 1.718592 | 3.032389 |
| 6 | 0.000099 | 2.377838 | 2.670939 |
| 6 | 1.212365 | 1.718388 | 3.032264 |
| 6 | -0.000002 | -0.406482 | 3.551678 |
| 6 | -1.212180 | 0.340657 | 3.468368 |
| 6 | 1.212305 | 0.340599 | 3.468133 |
| 6 | -3.235105 | 0.767861 | -2.304170 |
| 6 | -2.452940 | 1.994921 | -2.286292 |
| 6 | -3.984982 | 0.392504 | -1.177182 |
| 6 | -2.452923 | 2.808139 | -1.149046 |
| 6 | -1.212421 | 3.415263 | -0.697201 |
| 6 | 0.000109 | 3.274919 | -1.435308 |

| | | | |
|---|---|---|---|
| 6 | 1.212662 | 3.415046 | -0.697113 |
| 6 | 0.000094 | 3.252951 | 1.483943 |
| 6 | -1.212375 | 3.404477 | 0.747995 |
| 6 | 1.212614 | 3.404230 | 0.747854 |
| 6 | 0.000020 | 2.417138 | -2.634850 |
| 6 | -1.212244 | 1.763446 | -3.006398 |
| 6 | 1.212267 | 1.763235 | -3.006302 |
| 6 | 3.235427 | 2.428641 | 0.017983 |
| 6 | 2.453232 | 2.807981 | -1.149095 |
| 6 | 2.452987 | 1.994626 | -2.286274 |
| 6 | 3.985473 | 1.240795 | 0.009191 |
| 6 | 3.235310 | 0.733315 | 2.315328 |
| 6 | 2.453040 | 1.960444 | 2.315610 |
| 6 | 2.453228 | 2.790662 | 1.190737 |
| 6 | 3.985029 | 0.374591 | 1.182694 |
| 6 | 3.234632 | -1.975319 | 1.412840 |
| 6 | 2.452720 | -1.596402 | 2.580083 |
| 6 | 2.453168 | -0.270016 | 3.022462 |
| 6 | 3.984986 | -1.009349 | 0.721733 |
| 6 | 3.234544 | -1.954105 | -1.442141 |
| 6 | 2.452782 | -2.947377 | -0.721132 |
| 6 | 2.452973 | -2.957935 | 0.677091 |
| 6 | 3.984902 | -0.998545 | -0.736827 |
| 6 | 3.235204 | 0.767644 | -2.304322 |
| 6 | 2.452906 | -0.225050 | -3.026046 |
| 6 | 2.452473 | -1.557820 | -2.603551 |
| 6 | 3.985029 | 0.392049 | -1.177301 |

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| | | | |
|---|---|---|---|
| 6 | 3.236264 | -1.097430 | -2.166476 |
| 6 | 2.454559 | -2.309430 | -1.968307 |
| 6 | 3.984832 | -0.559749 | -1.106597 |
| 6 | 2.454310 | -2.946337 | -0.723814 |
| 6 | 1.214097 | -3.481335 | -0.187207 |
| 6 | 0.001339 | -3.450709 | -0.938509 |
| 6 | -1.211462 | -3.482805 | -0.187165 |
| 6 | 3.235718 | 1.721945 | -1.713502 |
| 6 | 2.453448 | 1.158738 | -2.804073 |
| 6 | 3.984620 | 0.879935 | -0.874847 |
| 6 | 2.453652 | -0.221619 | -3.025635 |
| 6 | 1.213679 | -0.897390 | -3.367713 |
| 6 | 0.001428 | -0.172707 | -3.569222 |
| 6 | -1.210458 | -0.896861 | -3.365376 |
| 6 | 0.001549 | -2.779019 | -2.250486 |
| 6 | 1.213997 | -2.186737 | -2.715375 |
| 6 | -1.211024 | -2.186554 | -2.714301 |
| 6 | 3.235881 | 2.161860 | 1.107709 |
| 6 | 2.453823 | 3.025780 | 0.235509 |

| | | | |
|---|---|---|---|
| 6 | 3.985542 | 1.104666 | 0.566125 |
| 6 | 2.453869 | 2.810337 | -1.145902 |
| 6 | 1.213181 | 2.927089 | -1.893106 |
| 6 | 0.001357 | 3.344593 | -1.266117 |
| 6 | -1.210768 | 2.925982 | -1.891416 |
| 6 | 0.001088 | 1.282355 | -3.336269 |
| 6 | 1.213019 | 1.907364 | -2.916764 |
| 6 | -1.210672 | 1.906502 | -2.914914 |
| 6 | 3.237003 | -0.385436 | 2.398114 |
| 6 | 2.455040 | 0.710905 | 2.950407 |
| 6 | 3.985904 | -0.196498 | 1.224939 |
| 6 | 2.454244 | 1.958010 | 2.318223 |
| 6 | 1.213615 | 2.705013 | 2.198551 |
| 6 | 0.001409 | 2.238551 | 2.789431 |
| 6 | -1.210996 | 2.706073 | 2.199693 |
| 6 | 0.001202 | 3.572082 | 0.189978 |
| 6 | 1.213613 | 3.364691 | 0.913090 |
| 6 | -1.211238 | 3.365575 | 0.913842 |
| 6 | 3.235887 | -2.398575 | 0.374653 |
| 6 | 2.454603 | -2.585594 | 1.588168 |
| 6 | 3.985271 | -1.225012 | 0.191166 |
| 6 | 2.454811 | -1.599326 | 2.578953 |
| 6 | 1.213996 | -1.254775 | 3.251615 |
| 6 | 0.002028 | -1.960601 | 2.989895 |
| 6 | -1.209940 | -1.255294 | 3.252027 |
| 6 | 0.001743 | 0.923479 | 3.454886 |
| 6 | 1.213812 | 0.171578 | 3.479788 |
| 6 | -1.209967 | 0.171199 | 3.480242 |
| 6 | 0.001697 | -3.003443 | 1.948170 |
| 6 | 1.214240 | -3.258714 | 1.240389 |
| 6 | -1.211148 | -3.260810 | 1.240876 |
| 6 | -3.232115 | -0.386077 | 2.397705 |
| 6 | -2.450119 | -1.599871 | 2.578310 |
| 6 | -2.451310 | -2.587275 | 1.588587 |
| 6 | -3.981197 | -0.197010 | 1.225015 |
| 6 | -3.232826 | 2.161590 | 1.108740 |
| 6 | -2.451059 | 1.958091 | 2.319274 |
| 6 | -2.450819 | 0.710377 | 2.950352 |
| 6 | -3.982765 | 1.104452 | 0.567033 |
| 6 | -3.234613 | 1.722885 | -1.712852 |
| 6 | -2.452067 | 2.810861 | -1.144623 |
| 6 | -2.451920 | 3.026711 | 0.236804 |
| 6 | -3.982613 | 0.880087 | -0.874006 |
| 6 | -3.233700 | -1.097857 | -2.165407 |
| 6 | -2.450486 | -0.221388 | -3.023005 |
| 6 | -2.451630 | 1.159035 | -2.802750 |
| 6 | -3.982410 | -0.560130 | -1.105705 |
| 6 | -3.233106 | -2.399855 | 0.375109 |
| 6 | -2.452012 | -2.947873 | -0.723759 |
| 6 | -2.451932 | -2.309947 | -1.967713 |
| 6 | -3.982091 | -1.225785 | 0.191793 |

| | | | |
|---|---|---|---|
| 2 | -0.308732 | 0.022305 | -0.156743 |

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| | | | |
|---|---|---|---|
| 6 | 3.242133 | 2.244054 | -0.924186 |
| 6 | 2.460603 | 2.141454 | -2.147629 |
| 6 | 3.992553 | 1.146223 | -0.471856 |
| 6 | 2.461830 | 0.951074 | -2.880806 |
| 6 | 1.221959 | 0.457272 | -3.455879 |
| 6 | 0.008904 | 1.202872 | -3.365757 |
| 6 | -1.202709 | 0.454889 | -3.455741 |
| 6 | 3.241952 | 1.571065 | 1.850163 |
| 6 | 2.459226 | 2.702401 | 1.374931 |
| 6 | 3.992665 | 0.802388 | 0.945403 |
| 6 | 2.459249 | 3.031816 | 0.016376 |
| 6 | 1.218272 | 3.423926 | -0.629832 |
| 6 | 0.005967 | 3.568590 | 0.107907 |
| 6 | -1.205935 | 3.422321 | -0.630518 |
| 6 | 0.007457 | 2.456902 | -2.592472 |
| 6 | 1.218998 | 2.873988 | -1.965616 |
| 6 | -1.205098 | 2.871974 | -1.966213 |
| 6 | 3.244779 | -1.275749 | 2.067896 |
| 6 | 2.461639 | -0.474782 | 2.996878 |
| 6 | 3.993804 | -0.651861 | 1.056418 |
| 6 | 2.460424 | 0.919210 | 2.890385 |
| 6 | 1.219000 | 1.654008 | 3.064484 |
| 6 | 0.007188 | 0.995979 | 3.429847 |
| 6 | -1.205382 | 1.651645 | 3.063580 |
| 6 | 0.005951 | 3.222285 | 1.540407 |
| 6 | 1.218407 | 2.755325 | 2.129523 |
| 6 | -1.206119 | 2.753095 | 2.128999 |
| 6 | 3.245890 | -2.361668 | -0.572331 |
| 6 | 2.464075 | -2.998545 | 0.476900 |
| 6 | 3.994261 | -1.206526 | -0.292274 |
| 6 | 2.463721 | -2.467108 | 1.769831 |
| 6 | 1.222708 | -2.406814 | 2.523670 |
| 6 | 0.010759 | -2.959106 | 2.011889 |
| 6 | -1.202399 | -2.409265 | 2.523481 |
| 6 | 0.008220 | -0.472942 | 3.543017 |
| 6 | 1.221433 | -1.176807 | 3.281270 |
| 6 | -1.203650 | -1.179310 | 3.281242 |
| 6 | 3.244700 | -0.186524 | -2.421806 |
| 6 | 2.464013 | -1.382339 | -2.702768 |
| 6 | 3.993834 | -0.095418 | -1.236948 |
| 6 | 2.464277 | -2.447018 | -1.796892 |
| 6 | 1.223942 | -3.145628 | -1.505769 |
| 6 | 0.011794 | -2.831268 | -2.189261 |
| 6 | -1.200303 | -3.148345 | -1.506750 |
| 6 | 0.011599 | -3.519470 | 0.649188 |

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| 6 | 1.223949 | -3.486550 | -0.102244 |
| 6 | -1.200396 | -3.489067 | -0.102992 |
| 6 | 0.011236 | -1.708601 | -3.143499 |
| 6 | 1.223061 | -0.983336 | -3.345589 |
| 6 | -1.201618 | -0.985423 | -3.345830 |
| 6 | -3.223780 | -2.367301 | -0.574093 |
| 6 | -2.441653 | -2.451638 | -1.798493 |
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| 6 | -2.441482 | -3.002902 | 0.475575 |
| 6 | -3.975593 | -0.658850 | 1.054225 |
| 6 | -3.227306 | 1.564957 | 1.848034 |
| 6 | -2.445044 | 0.914356 | 2.888050 |
| 6 | -2.444896 | -0.479384 | 2.995908 |
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| 6 | -2.446128 | 3.027225 | 0.015146 |
| 6 | -2.445925 | 2.697367 | 1.373393 |
| 6 | -3.976797 | 1.139309 | -0.473855 |
| 6 | -3.225513 | -0.192371 | -2.423533 |
| 6 | -2.443938 | 0.946296 | -2.881729 |
| 6 | -2.444744 | 2.136319 | -2.147989 |
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| 10 | -0.373989 | 0.194143 | 0.037312 |

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| 6 | 2.455785 | -3.023882 | 0.246612 |
| 6 | 1.215927 | -3.362022 | 0.924904 |
| 6 | 0.003891 | -3.571531 | 0.201950 |
| 6 | -1.208011 | -3.362488 | 0.925184 |
| 6 | 3.237939 | 1.089394 | -2.170112 |
| 6 | 2.455668 | 0.210326 | -3.026313 |
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| 6 | 2.455318 | -1.168833 | -2.798962 |
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| 6 | 0.003675 | -1.295229 | -3.333702 |
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| 6 | 0.003770 | -3.350148 | -1.255459 |
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| 6 | -1.208081 | -2.934156 | -1.883185 |
| 6 | 3.237886 | 2.400623 | 0.365229 |
| 6 | 2.455769 | 2.943430 | -0.735490 |
| 6 | 3.987554 | 1.226383 | 0.186815 |

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| 6 | 2.455792 | 2.301258 | -1.977012 |
| 6 | 1.215722 | 2.175730 | -2.723890 |
| 6 | 0.003854 | 2.770565 | -2.262110 |
| 6 | -1.208140 | 2.176127 | -2.724018 |
| 6 | 0.003669 | 0.159117 | -3.573687 |
| 6 | 1.215646 | 0.884449 | -3.371967 |
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| 6 | 3.238204 | 0.394344 | 2.396119 |
| 6 | 2.456292 | 1.609184 | 2.572169 |
| 6 | 3.987949 | 0.201420 | 1.224248 |
| 6 | 2.456260 | 2.591767 | 1.577753 |
| 6 | 1.216222 | 3.263700 | 1.227592 |
| 6 | 0.004288 | 3.009449 | 1.936381 |
| 6 | -1.207788 | 3.264334 | 1.228056 |
| 6 | 0.003993 | 3.447789 | -0.952861 |
| 6 | 1.216018 | 3.481060 | -0.201004 |
| 6 | -1.207859 | 3.481708 | -0.200705 |
| 6 | 3.237709 | -2.156857 | 1.115327 |
| 6 | 2.456074 | -1.949393 | 2.325258 |
| 6 | 3.987675 | -1.101991 | 0.569886 |
| 6 | 2.455946 | -0.699734 | 2.951938 |
| 6 | 1.215836 | -0.159060 | 3.481729 |
| 6 | 0.004342 | -0.911823 | 3.458216 |
| 6 | -1.207052 | -0.159019 | 3.482128 |
| 6 | 0.004416 | 1.972425 | 2.984108 |
| 6 | 1.215938 | 1.266721 | 3.247082 |
| 6 | -1.207076 | 1.266799 | 3.247265 |
| 6 | 0.004183 | -2.229999 | 2.798209 |
| 6 | 1.215985 | -2.698102 | 2.208428 |
| 6 | -1.207697 | -2.698376 | 2.208780 |
| 6 | -3.229196 | 0.394578 | 2.396772 |
| 6 | -2.447218 | -0.699704 | 2.952581 |
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| 6 | -3.229309 | 2.401070 | 0.365913 |
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| 6 | -3.229505 | 1.089517 | -2.169442 |
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| 6 | -2.447689 | 2.944115 | -0.735067 |
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| 6 | -3.229728 | -1.727329 | -1.706266 |
| 6 | -2.447793 | -1.168963 | -2.799148 |
| 6 | -2.448186 | 0.210426 | -3.026545 |
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| 6 | -3.229101 | -2.156774 | 1.115770 |
| 6 | -2.447969 | -3.024459 | 0.246921 |
| 6 | -2.448075 | -2.813950 | -1.135132 |
| 6 | -3.978639 | -1.101743 | 0.570428 |
| 18 | -0.096334 | -0.002209 | -0.004194 |

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| 6 | 2.453781 | 2.503131 | -1.715568 |
| 6 | 3.985772 | 1.214973 | -0.252536 |
| 6 | 2.453776 | 1.468120 | -2.655429 |
| 6 | 1.212675 | 1.089210 | -3.309774 |
| 6 | 0.000203 | 1.806513 | -3.084044 |
| 6 | -1.212153 | 1.089064 | -3.310052 |
| 6 | 3.236237 | 1.205553 | 2.109328 |
| 6 | 2.453639 | 2.405075 | 1.850117 |
| 6 | 3.985520 | 0.615758 | 1.077554 |
| 6 | 2.453736 | 2.979275 | 0.575468 |
| 6 | 1.212466 | 3.484640 | 0.013107 |
| 6 | -0.000298 | 3.491663 | 0.765082 |
| 6 | -1.212909 | 3.484509 | 0.012883 |
| 6 | 0.000025 | 2.898245 | -2.094331 |
| 6 | 1.212619 | 3.190618 | -1.401058 |
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| 6 | 3.235892 | -1.633062 | 1.798142 |
| 6 | 2.453246 | -1.016177 | 2.858864 |
| 6 | 3.985215 | -0.834065 | 0.918516 |
| 6 | 2.453477 | 0.373510 | 3.011469 |
| 6 | 1.212376 | 1.064818 | 3.318083 |
| 6 | -0.000272 | 0.351968 | 3.558194 |
| 6 | -1.213012 | 1.064646 | 3.318041 |
| 6 | -0.000392 | 2.886324 | 2.108155 |
| 6 | 1.212326 | 2.318705 | 2.601217 |
| 6 | -1.213085 | 2.318541 | 2.601073 |
| 6 | 3.235891 | -2.214227 | -0.997265 |
| 6 | 2.453694 | -3.033105 | -0.082903 |
| 6 | 3.985977 | -1.131227 | -0.509356 |
| 6 | 2.453453 | -2.748327 | 1.285790 |
| 6 | 1.212535 | -2.826829 | 2.037894 |
| 6 | 0.000204 | -3.276383 | 1.434204 |
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| 6 | -0.000164 | -1.112697 | 3.396684 |
| 6 | 1.212258 | -1.757263 | 3.008971 |
| 6 | -1.212435 | -1.757450 | 3.008851 |
| 6 | 3.236038 | 0.264671 | -2.414008 |
| 6 | 2.453751 | -0.857994 | -2.909937 |
| 6 | 3.985790 | 0.135254 | -1.233048 |
| 6 | 2.453854 | -2.072021 | -2.216494 |
| 6 | 1.212912 | -2.811891 | -2.058838 |
| 6 | 0.000485 | -2.375872 | -2.671821 |
| 6 | -1.211945 | -2.811960 | -2.058954 |
| 6 | 0.000391 | -3.575055 | -0.008972 |
| 6 | 1.212931 | -3.405527 | -0.741697 |

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| 6 | -1.212051 | -3.405579 | -0.741821 |
| 6 | 0.000452 | -1.096630 | -3.403405 |
| 6 | 1.212817 | -0.346822 | -3.467160 |
| 6 | -1.212002 | -0.346973 | -3.467428 |
| 6 | -3.235138 | -2.214517 | -0.997679 |
| 6 | -2.452930 | -2.072186 | -2.216784 |
| 6 | -2.452958 | -0.858258 | -2.910381 |
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| 6 | -2.453198 | -2.748652 | 1.285522 |
| 6 | -2.453005 | -3.033325 | -0.083224 |
| 6 | -3.985468 | -0.834668 | 0.917974 |
| 6 | -3.236747 | 1.205109 | 2.108971 |
| 6 | -2.454025 | 0.373177 | 3.011374 |
| 6 | -2.453529 | -1.016503 | 2.858655 |
| 6 | -3.985426 | 0.615104 | 1.076875 |
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| 6 | -2.454178 | 2.404650 | 1.849640 |
| 6 | -3.985223 | 1.214230 | -0.253156 |
| 6 | -3.235482 | 0.264279 | -2.414537 |
| 6 | -2.453429 | 1.467833 | -2.655914 |
| 6 | -2.453743 | 2.502855 | -1.716069 |
| 6 | -3.985639 | 0.134666 | -1.233759 |
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| 2 | -1.158577 | 0.011728 | 0.004020 |

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| 6 | 2.475234 | 2.329345 | -1.945549 |
| 6 | 1.233502 | 2.212305 | -2.691787 |
| 6 | 0.021004 | 2.799592 | -2.222067 |
| 6 | -1.191708 | 2.212002 | -2.690787 |
| 6 | 3.258014 | 0.360781 | 2.401124 |
| 6 | 2.475714 | 1.572840 | 2.593837 |
| 6 | 4.007503 | 0.184056 | 1.226093 |
| 6 | 2.475632 | 2.569333 | 1.613356 |
| 6 | 1.234328 | 3.243783 | 1.271891 |
| 6 | 0.021780 | 2.978395 | 1.975594 |
| 6 | -1.190953 | 3.243320 | 1.272068 |
| 6 | 0.021294 | 3.458463 | -0.904235 |
| 6 | 1.234196 | 3.481266 | -0.152854 |
| 6 | -1.191294 | 3.480745 | -0.152457 |
| 6 | 3.257506 | -2.172859 | 1.084967 |
| 6 | 2.475279 | -1.981370 | 2.297499 |
| 6 | 4.007578 | -1.110310 | 0.553754 |

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| 6 | 2.475856 | -0.741039 | 2.942266 |
| 6 | 1.234666 | -0.207362 | 3.478417 |
| 6 | 0.021826 | -0.958435 | 3.443806 |
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| 6 | 0.021906 | 1.928267 | 3.008951 |
| 6 | 1.234691 | 1.220885 | 3.263502 |
| 6 | -1.190838 | 1.220823 | 3.263243 |
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| 6 | 3.257244 | 1.119609 | -2.155870 |
| 6 | 2.474444 | 0.252134 | -3.023732 |
| 6 | 4.007204 | 0.571688 | -1.101828 |
| 6 | 2.474598 | -1.130475 | -2.816455 |
| 6 | 1.233304 | -1.877112 | -2.936236 |
| 6 | 0.020550 | -1.248733 | -3.348940 |
| 6 | -1.192115 | -1.876526 | -2.935178 |
| 6 | 0.020765 | -3.328580 | -1.300633 |
| 6 | 1.233426 | -2.906670 | -1.922906 |
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| 6 | 0.020585 | 0.208359 | -3.566716 |
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| 6 | -1.191768 | 0.930197 | -3.355991 |
| 6 | -3.215622 | -1.703418 | -1.729967 |
| 6 | -2.433241 | -1.129869 | -2.814804 |
| 6 | -2.433055 | 0.252435 | -3.022152 |
| 6 | -3.966258 | -0.870403 | -0.883684 |
| 6 | -3.215464 | -2.172283 | 1.086007 |
| 6 | -2.432744 | -3.026393 | 0.205242 |
| 6 | -2.433113 | -2.797107 | -1.173454 |
| 6 | -3.966084 | -1.109943 | 0.555187 |
| 6 | -3.214807 | 0.361088 | 2.401705 |
| 6 | -2.432332 | -0.740472 | 2.942202 |
| 6 | -2.432340 | -1.980629 | 2.297734 |
| 6 | -3.965434 | 0.184445 | 1.227420 |
| 6 | -3.215238 | 2.395724 | 0.399238 |
| 6 | -2.432254 | 2.569042 | 1.613722 |
| 6 | -2.431978 | 1.572637 | 2.593887 |
| 6 | -3.965252 | 1.223925 | 0.204230 |
| 6 | -3.215731 | 1.119797 | -2.154388 |
| 6 | -2.433182 | 2.328974 | -1.944241 |
| 6 | -2.432802 | 2.953468 | -0.693804 |
| 6 | -3.965909 | 0.572051 | -1.100452 |
| 2 | 1.271518 | 0.000173 | 0.005914 |

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| 10 | -1.142690 | 0.000381 | -0.004731 |

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| 6 | 2.453429 | -3.022853 | 0.255226 |
| 6 | 1.211947 | -3.355722 | 0.933938 |
| 6 | -0.001326 | -3.566685 | 0.213161 |
| 6 | -1.213794 | -3.354800 | 0.934835 |
| 6 | 3.236561 | 1.081667 | -2.174048 |
| 6 | 2.452610 | 0.200063 | -3.026322 |
| 6 | 3.988578 | 0.552099 | -1.111855 |
| 6 | 2.452454 | -1.178151 | -2.795725 |
| 6 | 1.210680 | -1.925850 | -2.902775 |
| 6 | -0.002110 | -1.304707 | -3.326193 |
| 6 | -1.215113 | -1.924941 | -2.901911 |
| 6 | -0.002014 | -3.349170 | -1.243677 |
| 6 | 1.210811 | -2.937619 | -1.872573 |
| 6 | -1.215143 | -2.936599 | -1.871609 |
| 6 | 3.239336 | 2.400898 | 0.356886 |
| 6 | 2.455621 | 2.939550 | -0.745134 |
| 6 | 3.990704 | 1.226383 | 0.181800 |
| 6 | 2.454761 | 2.294384 | -1.984869 |
| 6 | 1.212490 | 2.165332 | -2.728587 |
| 6 | 0.000020 | 2.760634 | -2.269052 |
| 6 | -1.213344 | 2.165929 | -2.727538 |
| 6 | -0.001598 | 0.148087 | -3.569509 |
| 6 | 1.211561 | 0.872587 | -3.371909 |
| 6 | -1.214136 | 0.873421 | -3.371172 |
| 6 | 3.239079 | 0.400728 | 2.393682 |
| 6 | 2.456344 | 1.615560 | 2.565355 |
| 6 | 3.990766 | 0.204051 | 1.222789 |
| 6 | 2.456927 | 2.595510 | 1.568743 |
| 6 | 1.214997 | 3.263657 | 1.215958 |
| 6 | 0.002155 | 3.011363 | 1.923963 |
| 6 | -1.211058 | 3.264319 | 1.216792 |
| 6 | 0.001059 | 3.440663 | -0.962333 |
| 6 | 1.214448 | 3.476592 | -0.212321 |
| 6 | -1.211613 | 3.477414 | -0.211451 |
| 6 | 3.237432 | -2.154313 | 1.120923 |
| 6 | 2.454666 | -1.941975 | 2.329509 |
| 6 | 3.989956 | -1.101970 | 0.572239 |
| 6 | 2.455644 | -0.691094 | 2.952751 |
| 6 | 1.214337 | -0.148413 | 3.479250 |
| 6 | 0.001200 | -0.899232 | 3.457956 |
| 6 | -1.211340 | -0.147570 | 3.480340 |
| 6 | 0.002129 | 1.978724 | 2.974391 |

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| 6 | -1.210855 | 1.276384 | 3.241102 |
| 6 | 0.000295 | -2.217690 | 2.800995 |
| 6 | 1.212681 | -2.688270 | 2.214332 |
| 6 | -1.212944 | -2.687309 | 2.215197 |
| 6 | -3.236412 | 0.403090 | 2.396201 |
| 6 | -2.453479 | -0.689248 | 2.954681 |
| 6 | -2.454199 | -1.940079 | 2.331354 |
| 6 | -3.989008 | 0.206945 | 1.225816 |
| 6 | -3.236493 | 2.402993 | 0.359420 |
| 6 | -2.452774 | 2.596705 | 1.570482 |
| 6 | -2.452634 | 1.617352 | 2.567464 |
| 6 | -3.988858 | 1.229133 | 0.184867 |
| 6 | -3.238329 | 1.083927 | -2.171965 |
| 6 | -2.454663 | 2.295741 | -1.982689 |
| 6 | -2.453646 | 2.941303 | -0.743219 |
| 6 | -3.989935 | 0.554972 | -1.109023 |
| 6 | -3.239456 | -1.731184 | -1.699796 |
| 6 | -2.456431 | -1.176422 | -2.794209 |
| 6 | -2.455802 | 0.201880 | -3.025195 |
| 6 | -3.990643 | -0.883821 | -0.867694 |
| 6 | -3.238231 | -2.151888 | 1.123497 |
| 6 | -2.455646 | -3.021008 | 0.257108 |
| 6 | -2.456313 | -2.814950 | -1.125075 |
| 6 | -3.990175 | -1.098966 | 0.575334 |
| 10 | 1.224371 | -0.002680 | -0.002899 |
| 10 | -1.223038 | -0.007022 | -0.002632 |

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| 6 | 2.480683 | 2.494991 | 1.723820 |
| 6 | 1.237343 | 3.182356 | 1.414052 |
| 6 | 0.024810 | 2.886726 | 2.106389 |
| 6 | -1.189031 | 3.183504 | 1.417010 |
| 6 | 3.269117 | -2.214862 | 0.985583 |
| 6 | 2.485100 | -2.078458 | 2.204362 |
| 6 | 4.025532 | -1.131869 | 0.503597 |
| 6 | 2.484353 | -0.868165 | 2.902707 |
| 6 | 1.241549 | -0.361320 | 3.461328 |
| 6 | 0.029216 | -1.110926 | 3.394232 |
| 6 | -1.184250 | -0.363799 | 3.465946 |
| 6 | 0.026480 | 1.791787 | 3.091869 |
| 6 | 1.240399 | 1.074403 | 3.311388 |
| 6 | -1.185775 | 1.073014 | 3.316218 |
| 6 | 3.266930 | -1.621257 | -1.805063 |
| 6 | 2.483480 | -2.738154 | -1.297884 |

| | | | |
|---|---|---|---|
| 6 | 4.023744 | -0.827951 | -0.924409 |
| 6 | 2.484758 | -3.029031 | 0.068679 |
| 6 | 1.242787 | -3.404877 | 0.725025 |
| 6 | 0.029103 | -3.572544 | -0.006975 |
| 6 | -1.184078 | -3.410614 | 0.726979 |
| 6 | 0.029770 | -2.387568 | 2.659558 |
| 6 | 1.243181 | -2.817895 | 2.043936 |
| 6 | -1.183502 | -2.822370 | 2.046513 |
| 6 | 3.263599 | 1.215684 | -2.102743 |
| 6 | 2.479709 | 0.388463 | -3.008063 |
| 6 | 4.021755 | 0.623669 | -1.077068 |
| 6 | 2.481265 | -1.001052 | -2.862046 |
| 6 | 1.239029 | -1.741035 | -3.014528 |
| 6 | 0.024942 | -1.096857 | -3.399254 |
| 6 | -1.187564 | -1.744729 | -3.016621 |
| 6 | 0.028020 | -3.267153 | -1.448108 |
| 6 | 1.240654 | -2.814001 | -2.048921 |
| 6 | -1.185923 | -2.818496 | -2.050055 |
| 6 | 3.264358 | 2.376135 | 0.502995 |
| 6 | 2.478524 | 2.981211 | -0.562527 |
| 6 | 4.022456 | 1.217637 | 0.256445 |
| 6 | 2.478031 | 2.412407 | -1.838512 |
| 6 | 1.235360 | 2.329184 | -2.588452 |
| 6 | 0.021940 | 2.894942 | -2.093901 |
| 6 | -1.191198 | 2.329991 | -2.589516 |
| 6 | 0.023346 | 0.368039 | -3.553875 |
| 6 | 1.236366 | 1.079478 | -3.310619 |
| 6 | -1.190485 | 1.079342 | -3.312525 |
| 6 | 0.022347 | 3.494766 | -0.748426 |
| 6 | 1.236146 | 3.483330 | 0.002215 |
| 6 | -1.190437 | 3.485476 | 0.004113 |
| 6 | -3.214981 | 1.213021 | -2.101492 |
| 6 | -2.432631 | 2.412298 | -1.837112 |
| 6 | -2.432676 | 2.981901 | -0.559824 |
| 6 | -3.963865 | 0.617827 | -1.071879 |
| 6 | -3.211407 | -1.627629 | -1.803403 |
| 6 | -2.429685 | -1.005025 | -2.862191 |
| 6 | -2.431612 | 0.385643 | -3.008277 |
| 6 | -3.962130 | -0.833615 | -0.919831 |
| 6 | -3.209905 | -2.222990 | 0.990093 |
| 6 | -2.426666 | -3.036679 | 0.070781 |
| 6 | -2.427254 | -2.744840 | -1.296732 |
| 6 | -3.961148 | -1.137596 | 0.507615 |
| 6 | -3.210940 | 0.250819 | 2.419314 |
| 6 | -2.426188 | -0.873782 | 2.908541 |
| 6 | -2.425982 | -2.084843 | 2.209324 |
| 6 | -3.961353 | 0.126199 | 1.237690 |
| 6 | -3.214058 | 2.374530 | 0.508425 |
| 6 | -2.430092 | 2.493714 | 1.729621 |
| 6 | -2.428516 | 1.454139 | 2.664992 |
| 6 | -3.963014 | 1.211080 | 0.261627 |

| | | | |
|---|---|---|---|
| 2 | 1.692826 | -0.028891 | 0.019091 |
| 18 | -0.816321 | 0.002667 | -0.011136 |

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NeAr@C70

| | | | |
|---|---|---|---|
| 6 | 3.251585 | 0.454473 | 2.383980 |
| 6 | 2.464839 | 1.671061 | 2.528485 |
| 6 | 4.013214 | 0.232865 | 1.221350 |
| 6 | 2.464693 | 2.627210 | 1.510254 |
| 6 | 1.220500 | 3.285355 | 1.143042 |
| 6 | 0.006222 | 3.050156 | 1.855795 |
| 6 | -1.208043 | 3.289572 | 1.144434 |
| 6 | 3.251753 | -2.126892 | 1.168644 |
| 6 | 2.465029 | -1.887942 | 2.370169 |
| 6 | 4.013290 | -1.089444 | 0.598858 |
| 6 | 2.464921 | -0.624210 | 2.964922 |
| 6 | 1.220748 | -0.071796 | 3.477843 |
| 6 | 0.006713 | -0.822521 | 3.474618 |
| 6 | -1.207408 | -0.072108 | 3.482490 |
| 6 | 0.006302 | 2.041809 | 2.928923 |
| 6 | 1.220577 | 1.345377 | 3.208346 |
| 6 | -1.207714 | 1.346622 | 3.212675 |
| 6 | 3.251849 | -1.768959 | -1.661745 |
| 6 | 2.465126 | -2.837832 | -1.063010 |
| 6 | 4.013054 | -0.906007 | -0.850970 |
| 6 | 2.465166 | -3.013179 | 0.322630 |
| 6 | 1.221054 | -3.330441 | 1.006751 |
| 6 | 0.006837 | -3.559183 | 0.291800 |
| 6 | -1.207320 | -3.335425 | 1.008434 |
| 6 | 0.006791 | -2.154786 | 2.847398 |
| 6 | 1.220901 | -2.635497 | 2.270973 |
| 6 | -1.207203 | -2.639408 | 2.273877 |
| 6 | 3.251497 | 1.033647 | -2.195206 |
| 6 | 2.464792 | 0.134043 | -3.027030 |
| 6 | 4.013319 | 0.529511 | -1.124522 |
| 6 | 2.464763 | -1.237963 | -2.765451 |
| 6 | 1.220607 | -1.986315 | -2.855670 |
| 6 | 0.006479 | -1.376701 | -3.293747 |
| 6 | -1.207463 | -1.989159 | -2.859277 |
| 6 | 0.006815 | -3.374455 | -1.169101 |
| 6 | 1.220892 | -2.974066 | -1.804251 |
| 6 | -1.207223 | -2.977893 | -1.806635 |
| 6 | 3.251903 | 2.408002 | 0.305080 |
| 6 | 2.464415 | 2.920147 | -0.807380 |
| 6 | 4.013111 | 1.233385 | 0.156251 |
| 6 | 2.464526 | 2.247814 | -2.031449 |
| 6 | 1.220342 | 2.102029 | -2.771051 |
| 6 | 0.005957 | 2.706766 | -2.327083 |
| 6 | -1.208256 | 2.104698 | -2.774997 |

| | | | |
|---|---|---|---|
| 6 | 0.006323 | 0.069676 | -3.570067 |
| 6 | 1.220644 | 0.797193 | -3.385964 |
| 6 | -1.208078 | 0.798230 | -3.390374 |
| 6 | 0.005958 | 3.416619 | -1.036996 |
| 6 | 1.220296 | 3.466572 | -0.288048 |
| 6 | -1.208295 | 3.471580 | -0.288267 |
| 6 | -3.236002 | 1.034743 | -2.198273 |
| 6 | -2.451770 | 2.251575 | -2.034513 |
| 6 | -2.451851 | 2.925049 | -0.809059 |
| 6 | -3.989432 | 0.528705 | -1.123645 |
| 6 | -3.235190 | -1.771706 | -1.663569 |
| 6 | -2.451272 | -1.240093 | -2.770330 |
| 6 | -2.451527 | 0.133569 | -3.031959 |
| 6 | -3.988645 | -0.906185 | -0.850115 |
| 6 | -3.235438 | -2.131051 | 1.170681 |
| 6 | -2.450840 | -3.018920 | 0.323069 |
| 6 | -2.450734 | -2.842920 | -1.064216 |
| 6 | -3.988813 | -1.089837 | 0.598778 |
| 6 | -3.235383 | 0.454216 | 2.387646 |
| 6 | -2.450875 | -0.626291 | 2.969960 |
| 6 | -2.450924 | -1.891536 | 2.374533 |
| 6 | -3.989035 | 0.231807 | 1.221046 |
| 6 | -3.236080 | 2.410596 | 0.305702 |
| 6 | -2.451360 | 2.630739 | 1.513102 |
| 6 | -2.451337 | 1.673407 | 2.532465 |
| 6 | -3.989425 | 1.232071 | 0.156663 |
| 10 | 1.535201 | 0.004285 | -0.004209 |
| 18 | -1.029844 | 0.004231 | -0.003562 |

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$Ar_2$@C70

| | | | |
|---|---|---|---|
| 6 | 3.257928 | -0.615500 | -2.351510 |
| 6 | 2.466822 | -1.839608 | -2.410133 |
| 6 | 4.024696 | -0.315044 | -1.205829 |
| 6 | 2.466889 | -2.725073 | -1.328920 |
| 6 | 1.217995 | -3.352332 | -0.916252 |
| 6 | 0.000756 | -3.163251 | -1.640033 |
| 6 | -1.216456 | -3.352626 | -0.916309 |
| 6 | 3.257225 | 2.046695 | -1.312833 |
| 6 | 2.465922 | 1.724074 | -2.494681 |
| 6 | 4.024312 | 1.049968 | -0.673367 |
| 6 | 2.466193 | 0.422131 | -3.002592 |
| 6 | 1.217372 | -0.164275 | -3.471270 |
| 6 | 0.000090 | 0.582367 | -3.515409 |
| 6 | -1.216908 | -0.164698 | -3.471413 |
| 6 | 0.000609 | -2.231384 | -2.777958 |
| 6 | 1.217733 | -1.559004 | -3.106184 |
| 6 | -1.216753 | -1.559411 | -3.106307 |
| 6 | 3.257389 | 1.881094 | 1.540117 |

| | | | |
|---|---|---|---|
| 6 | 2.465488 | 2.904944 | 0.868081 |
| 6 | 4.024339 | 0.965046 | 0.789511 |
| 6 | 2.465590 | 2.986186 | -0.526901 |
| 6 | 1.216635 | 3.251045 | -1.229030 |
| 6 | -0.000675 | 3.522666 | -0.531994 |
| 6 | -1.217861 | 3.250710 | -1.229128 |
| 6 | -0.000242 | 1.952467 | -2.980725 |
| 6 | 1.216807 | 2.472452 | -2.442490 |
| 6 | -1.217543 | 2.472104 | -2.442565 |
| 6 | 3.257814 | -0.883054 | 2.264211 |
| 6 | 2.466270 | 0.072266 | 3.031165 |
| 6 | 4.024606 | -0.452319 | 1.160850 |
| 6 | 2.466001 | 1.424211 | 2.677155 |
| 6 | 1.216861 | 2.173950 | 2.712230 |
| 6 | -0.000487 | 1.595160 | 3.186205 |
| 6 | -1.218007 | 2.173559 | 2.712131 |
| 6 | -0.000691 | 3.438555 | 0.936354 |
| 6 | 1.216701 | 3.086954 | 1.596525 |
| 6 | -1.218036 | 3.086594 | 1.596430 |
| 6 | 3.258185 | -2.426157 | -0.140761 |
| 6 | 2.466729 | -2.860117 | 1.004981 |
| 6 | 4.024919 | -1.243619 | -0.072315 |
| 6 | 2.466527 | -2.105358 | 2.180972 |
| 6 | 1.217717 | -1.907304 | 2.905046 |
| 6 | 0.000350 | -2.537581 | 2.501876 |
| 6 | -1.217288 | -1.907702 | 2.904999 |
| 6 | -0.000202 | 0.172116 | 3.558113 |
| 6 | 1.217422 | -0.564343 | 3.429085 |
| 6 | -1.217552 | -0.564739 | 3.429066 |
| 6 | 0.000594 | -3.332016 | 1.264067 |
| 6 | 1.217881 | -3.435738 | 0.523117 |
| 6 | -1.216560 | -3.436091 | 0.523030 |
| 6 | -3.257720 | -0.884169 | 2.263978 |
| 6 | -2.465960 | -2.106203 | 2.180847 |
| 6 | -2.465643 | -2.860925 | 1.004825 |
| 6 | -4.024579 | -0.453694 | 1.160537 |
| 6 | -3.258269 | 1.879991 | 1.539809 |
| 6 | -2.466862 | 1.423376 | 2.676976 |
| 6 | -2.466641 | 0.071436 | 3.031062 |
| 6 | -4.024853 | 0.963691 | 0.789129 |
| 6 | -3.258245 | 2.045812 | -1.313217 |
| 6 | -2.466898 | 2.985565 | -0.527139 |
| 6 | -2.466757 | 2.904244 | 0.867878 |
| 6 | -4.025110 | 1.048693 | -0.673818 |
| 6 | -3.257329 | -0.616657 | -2.351745 |
| 6 | -2.465935 | 0.421293 | -3.002670 |
| 6 | -2.466359 | 1.723251 | -2.494797 |
| 6 | -4.024515 | -0.316455 | -1.206252 |
| 6 | -3.256950 | -2.427098 | -0.140993 |
| 6 | -2.465498 | -2.725821 | -1.329056 |
| 6 | -2.465722 | -1.840435 | -2.410266 |

| | | | |
|---|---|---|---|
| 6 | -4.024146 | -1.244918 | -0.072653 |
| 18 | 1.338137 | -0.000200 | 0.001564 |
| 18 | -1.338175 | 0.000218 | 0.001488 |

**Optimized geometries for TSs at the B97D3/BS1 (TZVP for Carbon atoms and aug-cc-pVDZ for Noble gas atoms) level of theory**

| | | | |
|---|---|---|---|
| TS He2@C70 | | | |
| 6 | -3.223391 | 1.960608 | -1.421431 |
| 6 | -2.444952 | 2.950046 | -0.695857 |
| 6 | -3.969611 | 1.002141 | -0.727223 |
| 6 | -2.444950 | 2.949897 | 0.696510 |
| 6 | -1.208144 | 3.184796 | 1.416913 |
| 6 | 0.000037 | 3.509070 | 0.737352 |
| 6 | 1.208215 | 3.184783 | 1.416914 |
| 6 | -3.223434 | -0.748513 | -2.301119 |
| 6 | -2.443051 | 0.248375 | -3.012208 |
| 6 | -3.969865 | -0.382383 | -1.176723 |
| 6 | -2.442994 | 1.573469 | -2.582504 |
| 6 | -1.207380 | 2.331962 | -2.579454 |
| 6 | 0.000011 | 1.780511 | -3.088437 |
| 6 | 1.207416 | 2.331946 | -2.579463 |
| 6 | 0.000034 | 3.509220 | -0.736586 |
| 6 | -1.208148 | 3.185099 | -1.416213 |
| 6 | 1.208208 | 3.185087 | -1.416222 |
| 6 | -3.223390 | -2.422743 | -0.000262 |
| 6 | -2.444260 | -2.795456 | -1.167683 |
| 6 | -3.969352 | -1.238579 | -0.000129 |
| 6 | -2.444092 | -1.974600 | -2.292680 |
| 6 | -1.206929 | -1.738054 | -3.009375 |
| 6 | -0.000031 | -2.397066 | -2.645953 |
| 6 | 1.206880 | -1.738077 | -3.009379 |
| 6 | -0.000005 | 0.380167 | -3.541025 |
| 6 | -1.206671 | -0.365640 | -3.452587 |
| 6 | 1.206647 | -0.365663 | -3.452591 |
| 6 | -3.223422 | -0.749022 | 2.300965 |
| 6 | -2.444074 | -1.975108 | 2.292247 |
| 6 | -3.969857 | -0.382643 | 1.176653 |
| 6 | -2.444251 | -2.795718 | 1.167074 |
| 6 | -1.208995 | -3.412548 | 0.721023 |
| 6 | -0.000022 | -3.269698 | 1.458298 |
| 6 | 1.208927 | -3.412547 | 0.721024 |
| 6 | -0.000041 | -3.269363 | -1.459017 |
| 6 | -1.209004 | -3.412380 | -0.721773 |
| 6 | 1.208917 | -3.412382 | -0.721778 |
| 6 | -3.223383 | 1.960293 | 1.421869 |
| 6 | -2.442978 | 1.572899 | 2.582853 |
| 6 | -3.969604 | 1.001980 | 0.727455 |
| 6 | -2.443031 | 0.247710 | 3.012265 |
| 6 | -1.206650 | -0.366406 | 3.452501 |
| 6 | 0.000015 | 0.379383 | 3.541091 |
| 6 | 1.206667 | -0.366428 | 3.452495 |
| 6 | -0.000010 | -2.397662 | 2.645425 |
| 6 | -1.206909 | -1.738724 | 3.008992 |

| | | | |
|---|---|---|---|
| 6 | 1.206901 | -1.738746 | 3.008985 |
| 6 | 0.000028 | 1.779830 | 3.088818 |
| 6 | -1.207367 | 2.331395 | 2.579963 |
| 6 | 1.207428 | 2.331378 | 2.579961 |
| 6 | 3.223427 | -0.749081 | 2.300950 |
| 6 | 2.443056 | 0.247666 | 3.012252 |
| 6 | 2.443025 | 1.572857 | 2.582842 |
| 6 | 3.969860 | -0.382716 | 1.176633 |
| 6 | 3.223346 | -2.422807 | -0.000278 |
| 6 | 2.444207 | -2.795758 | 1.167061 |
| 6 | 2.444060 | -1.975154 | 2.292239 |
| 6 | 3.969332 | -1.238654 | -0.000149 |
| 6 | 3.223410 | -0.748573 | -2.301136 |
| 6 | 2.444044 | -1.974647 | -2.292694 |
| 6 | 2.444196 | -2.795498 | -1.167694 |
| 6 | 3.969854 | -0.382457 | -1.176744 |
| 6 | 3.223423 | 1.960550 | -1.421447 |
| 6 | 2.443014 | 1.573426 | -2.582516 |
| 6 | 2.443040 | 0.248330 | -3.012217 |
| 6 | 3.969630 | 1.002069 | -0.727244 |
| 6 | 3.223432 | 1.960237 | 1.421854 |
| 6 | 2.445014 | 2.949859 | 0.696500 |
| 6 | 2.445008 | 2.950008 | -0.695869 |
| 6 | 3.969632 | 1.001907 | 0.727435 |
| 2 | -0.000890 | -1.002543 | 0.000251 |
| 2 | 0.000604 | 0.980164 | 0.000496 |

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TS HeNe@C70

| | | | |
|---|---|---|---|
| 6 | 3.221319 | -2.032727 | -1.297206 |
| 6 | 2.444208 | -2.977853 | -0.512772 |
| 6 | 3.967501 | -1.032787 | -0.663732 |
| 6 | 2.444099 | -2.891878 | 0.877110 |
| 6 | 1.207515 | -3.083405 | 1.611540 |
| 6 | -0.000595 | -3.452737 | 0.953351 |
| 6 | -1.208564 | -3.083050 | 1.611601 |
| 6 | 3.221747 | 0.618918 | -2.340791 |
| 6 | 2.440977 | -0.420129 | -2.988089 |
| 6 | 3.968277 | 0.322111 | -1.196970 |
| 6 | 2.441003 | -1.717628 | -2.479561 |
| 6 | 1.206960 | -2.477748 | -2.431842 |
| 6 | -0.000228 | -1.957892 | -2.974123 |
| 6 | -1.207644 | -2.477374 | -2.431940 |
| 6 | -0.000601 | -3.544221 | -0.519964 |
| 6 | 1.208295 | -3.260579 | -1.218698 |
| 6 | -1.209374 | -3.260291 | -1.218805 |
| 6 | 3.221450 | 2.431966 | -0.148366 |
| 6 | 2.443483 | 2.734582 | -1.336071 |
| 6 | 3.967769 | 1.249472 | -0.076033 |

| | | | |
|---|---|---|---|
| 6 | 2.442667 | 1.843819 | -2.406865 |
| 6 | 1.205831 | 1.563628 | -3.106172 |
| 6 | 0.000669 | 2.246060 | -2.783577 |
| 6 | -1.204770 | 1.564092 | -3.106169 |
| 6 | 0.000075 | -0.585370 | -3.508308 |
| 6 | 1.205325 | 0.165853 | -3.464341 |
| 6 | -1.204863 | 0.166337 | -3.464393 |
| 6 | 3.222373 | 0.903073 | 2.249739 |
| 6 | 2.444094 | 2.127411 | 2.166050 |
| 6 | 3.968104 | 0.467248 | 1.150520 |
| 6 | 2.444374 | 2.879614 | 0.993619 |
| 6 | 1.210916 | 3.475459 | 0.511506 |
| 6 | 0.000867 | 3.379846 | 1.257143 |
| 6 | -1.209109 | 3.475738 | 0.511483 |
| 6 | 0.000863 | 3.197191 | -1.656747 |
| 6 | 1.210950 | 3.385706 | -0.930028 |
| 6 | -1.209164 | 3.386029 | -0.930025 |
| 6 | 3.221307 | -1.857231 | 1.539189 |
| 6 | 2.440347 | -1.397991 | 2.672519 |
| 6 | 3.967279 | -0.942767 | 0.787750 |
| 6 | 2.441022 | -0.048522 | 3.019138 |
| 6 | 1.205629 | 0.592434 | 3.420101 |
| 6 | 0.000084 | -0.147343 | 3.555806 |
| 6 | -1.205156 | 0.592906 | 3.420086 |
| 6 | 0.000664 | 2.574910 | 2.493030 |
| 6 | 1.206511 | 1.935967 | 2.894534 |
| 6 | -1.205457 | 1.936431 | 2.894512 |
| 6 | -0.000220 | -1.574175 | 3.192183 |
| 6 | 1.206573 | -2.157623 | 2.719044 |
| 6 | -1.207239 | -2.157218 | 2.719089 |
| 6 | -3.221764 | 0.904351 | 2.249693 |
| 6 | -2.440807 | -0.047566 | 3.019095 |
| 6 | -2.440681 | -1.397045 | 2.672489 |
| 6 | -3.967657 | 0.468845 | 1.150449 |
| 6 | -3.220118 | 2.433209 | -0.148434 |
| 6 | -2.442850 | 2.880476 | 0.993556 |
| 6 | -2.442944 | 2.128338 | 2.166001 |
| 6 | -3.966976 | 1.251058 | -0.076119 |
| 6 | -3.221119 | 0.620192 | -2.340870 |
| 6 | -2.441515 | 1.844756 | -2.406909 |
| 6 | -2.441967 | 2.735463 | -1.336096 |
| 6 | -3.967819 | 0.323704 | -1.197068 |
| 6 | -3.221771 | -2.031443 | -1.297251 |
| 6 | -2.441292 | -1.716649 | -2.479571 |
| 6 | -2.440755 | -0.419167 | -2.988138 |
| 6 | -3.967527 | -1.031178 | -0.663805 |
| 6 | -3.221769 | -1.855955 | 1.539114 |
| 6 | -2.445017 | -2.890976 | 0.877075 |
| 6 | -2.445150 | -2.976991 | -0.512833 |
| 6 | -3.967327 | -0.941166 | 0.787664 |
| 2 | 0.004656 | 1.226605 | -0.015813 |

| | | | |
|---|---|---|---|
| 10 | -0.007722 | -0.821631 | -0.019096 |

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TS Ne2@C70

| | | | |
|---|---|---|---|
| 6 | -3.217987 | 1.964385 | -1.418349 |
| 6 | -2.444191 | 2.962447 | -0.696292 |
| 6 | -3.963375 | 1.003275 | -0.726426 |
| 6 | -2.444178 | 2.962390 | 0.696546 |
| 6 | -1.208905 | 3.207721 | 1.419679 |
| 6 | 0.000007 | 3.547729 | 0.741151 |
| 6 | 1.208924 | 3.207727 | 1.419675 |
| 6 | -3.217401 | -0.750041 | -2.296641 |
| 6 | -2.436739 | 0.248450 | -3.003952 |
| 6 | -3.963885 | -0.382483 | -1.174739 |
| 6 | -2.436995 | 1.575899 | -2.576619 |
| 6 | -1.206002 | 2.342005 | -2.577207 |
| 6 | -0.000030 | 1.786681 | -3.083852 |
| 6 | 1.205953 | 2.342006 | -2.577226 |
| 6 | -0.000013 | 3.547795 | -0.740876 |
| 6 | -1.208928 | 3.207832 | -1.419422 |
| 6 | 1.208901 | 3.207840 | -1.419439 |
| 6 | -3.218270 | -2.427065 | -0.000070 |
| 6 | -2.441849 | -2.806089 | -1.167121 |
| 6 | -3.962526 | -1.240106 | -0.000020 |
| 6 | -2.440309 | -1.978854 | -2.288651 |
| 6 | -1.203940 | -1.743078 | -3.004168 |
| 6 | -0.000050 | -2.410863 | -2.644696 |
| 6 | 1.203845 | -1.743091 | -3.004182 |
| 6 | -0.000040 | 0.382010 | -3.531369 |
| 6 | -1.202991 | -0.367044 | -3.443508 |
| 6 | 1.202904 | -0.367055 | -3.443522 |
| 6 | -3.217366 | -0.750217 | 2.296626 |
| 6 | -2.440272 | -1.979031 | 2.288535 |
| 6 | -3.963869 | -0.382572 | 1.174765 |
| 6 | -2.441828 | -2.806183 | 1.166943 |
| 6 | -1.211400 | -3.440154 | 0.723388 |
| 6 | -0.000006 | -3.299743 | 1.463464 |
| 6 | 1.211368 | -3.440172 | 0.723386 |
| 6 | -0.000052 | -3.299617 | -1.463702 |
| 6 | -1.211421 | -3.440092 | -0.723636 |
| 6 | 1.211345 | -3.440116 | -0.723644 |
| 6 | -3.217967 | 1.964277 | 1.418540 |
| 6 | -2.436959 | 1.575702 | 2.576771 |
| 6 | -3.963367 | 1.003221 | 0.726555 |
| 6 | -2.436695 | 0.248220 | 3.004001 |
| 6 | -1.202942 | -0.367308 | 3.443500 |
| 6 | 0.000009 | 0.381741 | 3.531406 |
| 6 | 1.202953 | -0.367315 | 3.443486 |
| 6 | -0.000005 | -2.411065 | 2.644517 |

| | | | |
|---|---|---|---|
| 6 | -1.203894 | -1.743310 | 3.004055 |
| 6 | 1.203890 | -1.743317 | 3.004041 |
| 6 | 0.000013 | 1.786444 | 3.083990 |
| 6 | -1.205967 | 2.341808 | 2.577402 |
| 6 | 1.205989 | 2.341809 | 2.577395 |
| 6 | 3.217356 | -0.750238 | 2.296585 |
| 6 | 2.436702 | 0.248205 | 3.003970 |
| 6 | 2.436972 | 1.575689 | 2.576743 |
| 6 | 3.963844 | -0.382600 | 1.174714 |
| 6 | 3.218219 | -2.427092 | -0.000107 |
| 6 | 2.441798 | -2.806205 | 1.166917 |
| 6 | 2.440258 | -1.979047 | 2.288506 |
| 6 | 3.962477 | -1.240134 | -0.000070 |
| 6 | 3.217321 | -0.750066 | -2.296676 |
| 6 | 2.440219 | -1.978874 | -2.288676 |
| 6 | 2.441774 | -2.806115 | -1.167148 |
| 6 | 3.963825 | -0.382512 | -1.174787 |
| 6 | 3.217944 | 1.964362 | -1.418385 |
| 6 | 2.436933 | 1.575883 | -2.576645 |
| 6 | 2.436660 | 0.248432 | -3.003977 |
| 6 | 3.963333 | 1.003247 | -0.726474 |
| 6 | 3.217966 | 1.964256 | 1.418501 |
| 6 | 2.444180 | 2.962380 | 0.696521 |
| 6 | 2.444171 | 2.962438 | -0.696320 |
| 6 | 3.963348 | 1.003193 | 0.726506 |
| 10 | 0.000310 | -1.072406 | -0.000038 |
| 10 | 0.000417 | 1.061224 | -0.000073 |

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TS HeAr@C70

| | | | |
|---|---|---|---|
| 6 | 3.216864 | 1.943189 | 1.418818 |
| 6 | 2.443168 | 2.940924 | 0.696661 |
| 6 | 3.961695 | 0.982069 | 0.726409 |
| 6 | 2.443168 | 2.940927 | -0.696644 |
| 6 | 1.208930 | 3.187319 | -1.421101 |
| 6 | 0.000017 | 3.523942 | -0.741008 |
| 6 | -1.208900 | 3.187327 | -1.421098 |
| 6 | 3.215459 | -0.771246 | 2.295452 |
| 6 | 2.435513 | 0.227428 | 3.003599 |
| 6 | 3.962234 | -0.403847 | 1.174296 |
| 6 | 2.436620 | 1.555634 | 2.578370 |
| 6 | 1.206404 | 2.323700 | 2.581564 |
| 6 | 0.000006 | 1.769225 | 3.089901 |
| 6 | -1.206385 | 2.323710 | 2.581562 |
| 6 | 0.000017 | 3.523940 | 0.741030 |
| 6 | 1.208931 | 3.187314 | 1.421121 |
| 6 | -1.208900 | 3.187322 | 1.421118 |
| 6 | 3.215782 | -2.448608 | -0.000009 |
| 6 | 2.439922 | -2.828929 | 1.166427 |

| | | | |
|---|---|---|---|
| 6 | 3.960423 | -1.261544 | -0.000005 |
| 6 | 2.438546 | -2.000058 | 2.286865 |
| 6 | 1.202420 | -1.763630 | 3.001039 |
| 6 | -0.000021 | -2.432705 | 2.640564 |
| 6 | -1.202455 | -1.763616 | 3.001039 |
| 6 | -0.000004 | 0.362433 | 3.534249 |
| 6 | 1.201875 | -0.387783 | 3.442882 |
| 6 | -1.201892 | -0.387769 | 3.442882 |
| 6 | 3.215459 | -0.771234 | -2.295459 |
| 6 | 2.438548 | -2.000048 | -2.286881 |
| 6 | 3.962234 | -0.403840 | -1.174301 |
| 6 | 2.439924 | -2.828925 | -1.166448 |
| 6 | 1.212250 | -3.471279 | -0.724218 |
| 6 | -0.000027 | -3.331058 | -1.464964 |
| 6 | -1.212306 | -3.471260 | -0.724218 |
| 6 | -0.000027 | -3.331054 | 1.464935 |
| 6 | 1.212249 | -3.471277 | 0.724192 |
| 6 | -1.212305 | -3.471264 | 0.724192 |
| 6 | 3.216864 | 1.943196 | -1.418808 |
| 6 | 2.436620 | 1.555647 | -2.578361 |
| 6 | 3.961695 | 0.982073 | -0.726404 |
| 6 | 2.435513 | 0.227444 | -3.003598 |
| 6 | 1.201875 | -0.387766 | -3.442885 |
| 6 | -0.000003 | 0.362451 | -3.534246 |
| 6 | -1.201891 | -0.387752 | -3.442885 |
| 6 | -0.000021 | -2.432698 | -2.640586 |
| 6 | 1.202421 | -1.763616 | -3.001054 |
| 6 | -1.202455 | -1.763602 | -3.001054 |
| 6 | 0.000006 | 1.769239 | -3.089888 |
| 6 | 1.206403 | 2.323711 | -2.581549 |
| 6 | -1.206384 | 2.323722 | -2.581546 |
| 6 | -3.215484 | -0.771196 | -2.295461 |
| 6 | -2.435522 | 0.227472 | -3.003599 |
| 6 | -2.436611 | 1.555674 | -2.578360 |
| 6 | -3.962252 | -0.403794 | -1.174301 |
| 6 | -3.215828 | -2.448570 | -0.000009 |
| 6 | -2.439972 | -2.828895 | -1.166448 |
| 6 | -2.438586 | -2.000019 | -2.286883 |
| 6 | -3.960454 | -1.261497 | -0.000005 |
| 6 | -3.215483 | -0.771209 | 2.295454 |
| 6 | -2.438584 | -2.000030 | 2.286866 |
| 6 | -2.439971 | -2.828900 | 1.166427 |
| 6 | -3.962252 | -0.403800 | 1.174296 |
| 6 | -3.216851 | 1.943225 | 1.418818 |
| 6 | -2.436612 | 1.555661 | 2.578369 |
| 6 | -2.435523 | 0.227456 | 3.003598 |
| 6 | -3.961694 | 0.982115 | 0.726408 |
| 6 | -3.216851 | 1.943233 | -1.418808 |
| 6 | -2.443140 | 2.940951 | -0.696643 |
| 6 | -2.443140 | 2.940948 | 0.696660 |
| 6 | -3.961694 | 0.982118 | -0.726405 |

| | | | |
|---|---|---|---|
| 2 | 0.000060 | -1.527121 | -0.000074 |
| 18 | 0.000136 | 0.670208 | 0.000034 |

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TS NeAr@C70

| | | | |
|---|---|---|---|
| 6 | 3.210514 | 1.962629 | 1.415094 |
| 6 | 2.442503 | 2.970693 | 0.696970 |
| 6 | 3.954073 | 0.998021 | 0.725392 |
| 6 | 2.442501 | 2.970681 | -0.696981 |
| 6 | 1.210177 | 3.230011 | -1.425051 |
| 6 | 0.000101 | 3.585696 | -0.746245 |
| 6 | -1.209994 | 3.230057 | -1.425039 |
| 6 | 3.208419 | -0.758225 | 2.290390 |
| 6 | 2.428144 | 0.242621 | 2.993842 |
| 6 | 3.955132 | -0.389352 | 1.172044 |
| 6 | 2.429681 | 1.573766 | 2.571480 |
| 6 | 1.205020 | 2.351142 | 2.579137 |
| 6 | 0.000043 | 1.791948 | 3.084311 |
| 6 | -1.204898 | 2.351199 | 2.579127 |
| 6 | 0.000100 | 3.585717 | 0.746237 |
| 6 | 1.210181 | 3.230040 | 1.425045 |
| 6 | -1.209998 | 3.230086 | 1.425032 |
| 6 | 3.210380 | -2.439842 | 0.000005 |
| 6 | 2.437743 | -2.827573 | 1.166468 |
| 6 | 3.952617 | -1.249181 | 0.000004 |
| 6 | 2.434215 | -1.990463 | 2.282604 |
| 6 | 1.199067 | -1.754842 | 2.995645 |
| 6 | -0.000100 | -2.434531 | 2.640594 |
| 6 | -1.199222 | -1.754771 | 2.995648 |
| 6 | -0.000007 | 0.379788 | 3.522586 |
| 6 | 1.197602 | -0.374260 | 3.432188 |
| 6 | -1.197665 | -0.374189 | 3.432188 |
| 6 | 3.208421 | -0.758250 | -2.290384 |
| 6 | 2.434223 | -1.990495 | -2.282602 |
| 6 | 3.955133 | -0.389364 | -1.172041 |
| 6 | 2.437754 | -2.827601 | -1.166461 |
| 6 | 1.215738 | -3.488957 | -0.727207 |
| 6 | -0.000132 | -3.351386 | -1.471313 |
| 6 | -1.216006 | -3.488878 | -0.727197 |
| 6 | -0.000136 | -3.351329 | 1.471308 |
| 6 | 1.215729 | -3.488926 | 0.727209 |
| 6 | -1.216017 | -3.488903 | 0.727223 |
| 6 | 3.210513 | 1.962613 | -1.415102 |
| 6 | 2.429679 | 1.573736 | -2.571482 |
| 6 | 3.954074 | 0.998014 | -0.725396 |
| 6 | 2.428143 | 0.242588 | -2.993840 |
| 6 | 1.197604 | -0.374301 | -3.432185 |
| 6 | -0.000005 | 0.379746 | -3.522581 |
| 6 | -1.197663 | -0.374228 | -3.432185 |

| | | | |
|---|---|---|---|
| 6 | -0.000096 | -2.434584 | -2.640607 |
| 6 | 1.199073 | -1.754886 | -2.995649 |
| 6 | -1.199220 | -1.754811 | -2.995648 |
| 6 | 0.000044 | 1.791904 | -3.084304 |
| 6 | 1.205016 | 2.351103 | -2.579135 |
| 6 | -1.204893 | 2.351161 | -2.579125 |
| 6 | -3.208509 | -0.758055 | -2.290384 |
| 6 | -2.428165 | 0.242734 | -2.993842 |
| 6 | -2.429610 | 1.573877 | -2.571479 |
| 6 | -3.955199 | -0.389124 | -1.172040 |
| 6 | -3.210583 | -2.439651 | 0.000012 |
| 6 | -2.437975 | -2.827446 | -1.166453 |
| 6 | -2.434386 | -1.990344 | -2.282597 |
| 6 | -3.952741 | -1.248941 | 0.000007 |
| 6 | -3.208511 | -0.758033 | 2.290392 |
| 6 | -2.434388 | -1.990322 | 2.282608 |
| 6 | -2.437984 | -2.827453 | 1.166482 |
| 6 | -3.955202 | -0.389113 | 1.172047 |
| 6 | -3.210421 | 1.962815 | 1.415093 |
| 6 | -2.429614 | 1.573906 | 2.571478 |
| 6 | -2.428168 | 0.242764 | 2.993844 |
| 6 | -3.954049 | 0.998260 | 0.725393 |
| 6 | -3.210420 | 1.962800 | -1.415101 |
| 6 | -2.442335 | 2.970806 | -0.696978 |
| 6 | -2.442336 | 2.970817 | 0.696966 |
| 6 | -3.954049 | 0.998252 | -0.725396 |
| 10 | 0.000072 | -1.366335 | -0.000257 |
| 18 | 0.000407 | 0.909282 | 0.000122 |

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TS Ar2@C70

| | | | |
|---|---|---|---|
| 6 | -3.197017 | 1.748101 | -1.675369 |
| 6 | -2.438728 | 2.865582 | -1.117019 |
| 6 | -3.938813 | 0.888730 | -0.859969 |
| 6 | -2.442604 | 3.082749 | 0.261832 |
| 6 | -1.218499 | 3.486172 | 0.954525 |
| 6 | -0.000035 | 3.770885 | 0.229538 |
| 6 | 1.218464 | 3.486173 | 0.954510 |
| 6 | -3.194916 | -1.085915 | -2.148640 |
| 6 | -2.413250 | -0.194685 | -2.980084 |
| 6 | -3.939674 | -0.551426 | -1.100402 |
| 6 | -2.413899 | 1.187969 | -2.753325 |
| 6 | -1.197806 | 1.964110 | -2.874387 |
| 6 | -0.000056 | 1.327936 | -3.287243 |
| 6 | 1.197707 | 1.964116 | -2.874431 |
| 6 | -0.000034 | 3.516996 | -1.265629 |
| 6 | -1.207814 | 3.027468 | -1.877252 |
| 6 | 1.207740 | 3.027478 | -1.877297 |
| 6 | -3.199901 | -2.420070 | 0.347933 |

| | | | |
|---|---|---|---|
| 6 | -2.438154 | -2.995809 | -0.750260 |
| 6 | -3.936370 | -1.233705 | 0.179405 |
| 6 | -2.430477 | -2.317019 | -1.971841 |
| 6 | -1.196938 | -2.197550 | -2.717751 |
| 6 | -0.000070 | -2.849582 | -2.286373 |
| 6 | 1.196812 | -2.197573 | -2.717771 |
| 6 | -0.000064 | -0.138138 | -3.519113 |
| 6 | -1.191743 | -0.877567 | -3.329451 |
| 6 | 1.191613 | -0.877582 | -3.329471 |
| 6 | -3.193773 | -0.409720 | 2.365461 |
| 6 | -2.422706 | -1.634249 | 2.532328 |
| 6 | -3.939757 | -0.208037 | 1.210196 |
| 6 | -2.428878 | -2.637003 | 1.556406 |
| 6 | -1.218615 | -3.385413 | 1.222870 |
| 6 | 0.000029 | -3.131484 | 1.938489 |
| 6 | 1.218619 | -3.385393 | 1.222829 |
| 6 | -0.000086 | -3.617345 | -0.991522 |
| 6 | -1.223117 | -3.622482 | -0.223250 |
| 6 | 1.223028 | -3.622456 | -0.223257 |
| 6 | -3.198652 | 2.166442 | 1.111024 |
| 6 | -2.419137 | 1.953242 | 2.309682 |
| 6 | -3.937355 | 1.102969 | 0.571335 |
| 6 | -2.415287 | 0.687863 | 2.910322 |
| 6 | -1.188881 | 0.140274 | 3.428841 |
| 6 | 0.000016 | 0.909550 | 3.411293 |
| 6 | 1.188918 | 0.140275 | 3.428821 |
| 6 | 0.000020 | -2.031551 | 2.951706 |
| 6 | -1.191184 | -1.295407 | 3.200163 |
| 6 | 1.191224 | -1.295406 | 3.200152 |
| 6 | 0.000007 | 2.263165 | 2.794170 |
| 6 | -1.207264 | 2.752329 | 2.218563 |
| 6 | 1.207261 | 2.752333 | 2.218536 |
| 6 | 3.193790 | -0.409717 | 2.365402 |
| 6 | 2.415313 | 0.687870 | 2.910277 |
| 6 | 2.419142 | 1.953245 | 2.309631 |
| 6 | 3.939733 | -0.208040 | 1.210113 |
| 6 | 3.199881 | -2.420095 | 0.347878 |
| 6 | 2.428896 | -2.637022 | 1.556377 |
| 6 | 2.422730 | -1.634246 | 2.532282 |
| 6 | 3.936324 | -1.233718 | 0.179326 |
| 6 | 3.194810 | -1.085935 | -2.148701 |
| 6 | 2.430377 | -2.317043 | -1.971881 |
| 6 | 2.438085 | -2.995834 | -0.750295 |
| 6 | 3.939583 | -0.551438 | -1.100479 |
| 6 | 3.196927 | 1.748091 | -1.675434 |
| 6 | 2.413790 | 1.187956 | -2.753374 |
| 6 | 2.413127 | -0.194701 | -2.980125 |
| 6 | 3.938728 | 0.888715 | -0.860051 |
| 6 | 3.198628 | 2.166445 | 1.110954 |
| 6 | 2.442571 | 3.082766 | 0.261782 |
| 6 | 2.438671 | 2.865597 | -1.117081 |

| | | | |
|---|---|---|---|
| 6 | 3.937307 | 1.102961 | 0.571251 |
| 18 | 0.000238 | -1.208366 | 0.004866 |
| 18 | 0.000323 | 1.209633 | 0.002576 |

**Optimized geometries for all minima at the B97D3/BS1 (TZVP for Carbon atoms and aug-cc-pVDZ for Noble gas atoms) level of theory**

| C70 | | | |
|---|---|---|---|
| 6 | -3.226068 | 2.389158 | 0.394186 |
| 6 | -2.445979 | 2.564431 | 1.606411 |
| 6 | -3.972509 | 1.221394 | 0.201541 |
| 6 | -2.445957 | 1.573372 | 2.584780 |
| 6 | -1.208462 | 1.222822 | 3.253561 |
| 6 | -0.000007 | 1.928246 | 2.999707 |
| 6 | 1.208445 | 1.222807 | 3.253551 |
| 6 | -3.226054 | 1.113169 | -2.150389 |
| 6 | -2.445978 | 2.320221 | -1.942414 |
| 6 | -3.972483 | 0.569083 | -1.099294 |
| 6 | -2.445955 | 2.944470 | -0.697567 |
| 6 | -1.208502 | 3.472401 | -0.157538 |
| 6 | -0.000014 | 3.448681 | -0.906849 |
| 6 | 1.208484 | 3.472376 | -0.157510 |
| 6 | -0.000016 | 2.974653 | 1.966622 |
| 6 | -1.208511 | 3.237835 | 1.264635 |
| 6 | 1.208492 | 3.237822 | 1.264596 |
| 6 | -3.226088 | -1.701153 | -1.723181 |
| 6 | -2.445962 | -1.130308 | -2.806907 |
| 6 | -3.972597 | -0.869747 | -0.880943 |
| 6 | -2.446013 | 0.246518 | -3.016014 |
| 6 | -1.208550 | 0.923242 | -3.351283 |
| 6 | -0.000006 | 0.203240 | -3.560111 |
| 6 | 1.208535 | 0.923263 | -3.351255 |
| 6 | -0.000016 | 2.789446 | -2.221246 |
| 6 | -1.208485 | 2.203171 | -2.688454 |
| 6 | 1.208478 | 2.203130 | -2.688446 |
| 6 | -3.226173 | -2.164721 | 1.085453 |
| 6 | -2.446033 | -3.018930 | 0.207650 |
| 6 | -3.972687 | -1.106747 | 0.554949 |
| 6 | -2.446010 | -2.792150 | -1.166348 |
| 6 | -1.208494 | -2.901858 | -1.913549 |
| 6 | -0.000005 | -3.323323 | -1.293469 |
| 6 | 1.208487 | -2.901826 | -1.913547 |
| 6 | -0.000011 | -1.250513 | -3.339272 |
| 6 | -1.208434 | -1.875917 | -2.925936 |
| 6 | 1.208435 | -1.875913 | -2.925900 |
| 6 | -3.226131 | 0.363459 | 2.394047 |
| 6 | -2.446007 | -0.735368 | 2.935206 |
| 6 | -3.972637 | 0.185763 | 1.223980 |
| 6 | -2.445995 | -1.972090 | 2.295025 |

| | | | |
|---|---|---|---|
| 6 | -1.208490 | -2.716552 | 2.168345 |
| 6 | -0.000006 | -2.256950 | 2.760524 |
| 6 | 1.208486 | -2.716544 | 2.168317 |
| 6 | -0.000010 | -3.562568 | 0.157471 |
| 6 | -1.208492 | -3.362733 | 0.880005 |
| 6 | 1.208491 | -3.362695 | 0.880020 |
| 6 | -0.000010 | -0.951149 | 3.436667 |
| 6 | -1.208465 | -0.202171 | 3.469999 |
| 6 | 1.208459 | -0.202155 | 3.469973 |
| 6 | 3.226195 | -2.164715 | 1.085474 |
| 6 | 2.446018 | -1.972092 | 2.295031 |
| 6 | 2.446001 | -0.735356 | 2.935188 |
| 6 | 3.972695 | -1.106739 | 0.554953 |
| 6 | 3.226116 | -1.701160 | -1.723188 |
| 6 | 2.446024 | -2.792137 | -1.166335 |
| 6 | 2.446035 | -3.018928 | 0.207641 |
| 6 | 3.972599 | -0.869742 | -0.880931 |
| 6 | 3.226069 | 1.113166 | -2.150400 |
| 6 | 2.446045 | 0.246518 | -3.016007 |
| 6 | 2.445956 | -1.130296 | -2.806903 |
| 6 | 3.972498 | 0.569079 | -1.099297 |
| 6 | 3.226080 | 2.389174 | 0.394179 |
| 6 | 2.445965 | 2.944457 | -0.697567 |
| 6 | 2.445974 | 2.320230 | -1.942407 |
| 6 | 3.972516 | 1.221397 | 0.201541 |
| 6 | 3.226144 | 0.363455 | 2.394060 |
| 6 | 2.445958 | 1.573386 | 2.584773 |
| 6 | 2.445983 | 2.564425 | 1.606420 |
| 6 | 3.972638 | 0.185785 | 1.223973 |

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| 6 | -2.447832 | -2.392748 | 1.852053 |
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| 6 | -0.001644 | -2.765105 | 2.251309 |
| 6 | 1.207068 | -3.096600 | 1.578998 |
| 6 | -3.228627 | 2.261395 | 0.865143 |
| 6 | -2.448062 | 2.189704 | 2.087793 |
| 6 | -3.975210 | 1.156066 | 0.441801 |
| 6 | -2.447946 | 1.022496 | 2.847205 |
| 6 | -1.210447 | 0.544788 | 3.432460 |
| 6 | -0.002085 | 1.287036 | 3.325158 |
| 6 | 1.206356 | 0.544958 | 3.432682 |
| 6 | -0.001859 | -1.621540 | 3.175145 |
| 6 | -1.210367 | -0.894563 | 3.358219 |
| 6 | 1.206521 | -0.894399 | 3.358437 |

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| 6 | -3.227911 | 1.521874 | -1.884025 |
| 6 | -2.447535 | 2.662445 | -1.437504 |
| 6 | -3.974562 | 0.777950 | -0.963678 |
| 6 | -2.448178 | 3.024540 | -0.092985 |
| 6 | -1.210503 | 3.433552 | 0.542165 |
| 6 | -0.001767 | 3.560805 | -0.196542 |
| 6 | 1.206818 | 3.434117 | 0.542439 |
| 6 | -0.002096 | 2.519483 | 2.522948 |
| 6 | -1.210497 | 2.917929 | 1.887884 |
| 6 | 1.206396 | 2.918191 | 1.888110 |
| 6 | -3.227710 | -1.320957 | -2.030103 |
| 6 | -2.447054 | -0.544145 | -2.977036 |
| 6 | -3.974673 | -0.675641 | -1.038407 |
| 6 | -2.447277 | 0.846496 | -2.905648 |
| 6 | -1.209678 | 1.577076 | -3.097730 |
| 6 | -0.001071 | 0.913603 | -3.446736 |
| 6 | 1.207340 | 1.577383 | -3.097852 |
| 6 | -0.001484 | 3.178472 | -1.616171 |
| 6 | -1.209820 | 2.697473 | -2.191523 |
| 6 | 1.207046 | 2.697836 | -2.191533 |
| 6 | -3.227787 | -2.338718 | 0.628268 |
| 6 | -2.447087 | -2.999100 | -0.403009 |
| 6 | -3.974822 | -1.196012 | 0.320894 |
| 6 | -2.447242 | -2.501435 | -1.703401 |
| 6 | -1.209483 | -2.458587 | -2.457547 |
| 6 | -0.000955 | -2.995852 | -1.934391 |
| 6 | 1.207664 | -2.458591 | -2.457313 |
| 6 | -0.000903 | -0.554780 | -3.522230 |
| 6 | -1.209366 | -1.250501 | -3.243043 |
| 6 | 1.207589 | -1.250449 | -3.242922 |
| 6 | -0.001169 | -3.521103 | -0.560963 |
| 6 | -1.209707 | -3.470977 | 0.186966 |
| 6 | 1.207169 | -3.470629 | 0.187200 |
| 6 | 3.225382 | -1.320652 | -2.029504 |
| 6 | 2.445261 | -2.501422 | -1.702993 |
| 6 | 2.444823 | -2.999079 | -0.402512 |
| 6 | 3.971179 | -0.675038 | -1.037297 |
| 6 | 3.224908 | 1.522373 | -1.883395 |
| 6 | 2.444997 | 0.846900 | -2.905554 |
| 6 | 2.445111 | -0.543835 | -2.976909 |
| 6 | 3.971102 | 0.778424 | -0.962808 |
| 6 | 3.224547 | 2.261859 | 0.865652 |
| 6 | 2.444676 | 3.025261 | -0.092561 |
| 6 | 2.444463 | 2.663072 | -1.437163 |
| 6 | 3.970902 | 1.156517 | 0.442553 |
| 6 | 3.224309 | -0.124023 | 2.418194 |
| 6 | 2.443896 | 1.022866 | 2.847733 |
| 6 | 2.443909 | 2.190059 | 2.088271 |
| 6 | 3.970885 | -0.063199 | 1.236468 |
| 6 | 3.224884 | -2.338403 | 0.629077 |
| 6 | 2.444602 | -2.392485 | 1.852728 |

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| 6 | 2.444236 | -1.309277 | 2.727804 |
| 6 | 3.971223 | -1.195333 | 0.321837 |
| 2 | 0.330542 | -0.009715 | 0.061597 |

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| 6 | 2.449374 | 2.932109 | 0.746652 |
| 6 | 3.976152 | 0.988751 | 0.744586 |
| 6 | 2.449481 | 2.956249 | -0.645423 |
| 6 | 1.212165 | 3.198618 | -1.361060 |
| 6 | 0.003815 | 3.501961 | -0.675382 |
| 6 | -1.204371 | 3.198868 | -1.361455 |
| 6 | 3.229591 | -0.788127 | 2.288929 |
| 6 | 2.449306 | 0.195431 | 3.019028 |
| 6 | 3.976184 | -0.402993 | 1.170229 |
| 6 | 2.449274 | 1.526855 | 2.611787 |
| 6 | 1.211867 | 2.282207 | 2.621075 |
| 6 | 0.003551 | 1.723657 | 3.121292 |
| 6 | -1.204682 | 2.282374 | 2.621081 |
| 6 | 0.003691 | 3.476379 | 0.795064 |
| 6 | 1.211918 | 3.149418 | 1.470013 |
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| 6 | 3.229816 | -2.420887 | -0.042446 |
| 6 | 2.449529 | -2.811450 | 1.118483 |
| 6 | 3.976361 | -1.237877 | -0.021861 |
| 6 | 2.449409 | -2.012720 | 2.258944 |
| 6 | 1.211941 | -1.788187 | 2.980064 |
| 6 | 0.003736 | -2.436715 | 2.603419 |
| 6 | -1.204544 | -1.788388 | 2.980110 |
| 6 | 0.003553 | 0.317328 | 3.551302 |
| 6 | 1.211871 | -0.425488 | 3.449168 |
| 6 | -1.204671 | -0.425619 | 3.449268 |
| 6 | 3.229978 | -0.708132 | -2.315851 |
| 6 | 2.449769 | -1.932968 | -2.328410 |
| 6 | 3.976379 | -0.362099 | -1.184302 |
| 6 | 2.449737 | -2.770822 | -1.216415 |
| 6 | 1.212350 | -3.387647 | -0.780190 |
| 6 | 0.004134 | -3.230067 | -1.513466 |
| 6 | -1.204196 | -3.388095 | -0.780480 |
| 6 | 0.003868 | -3.280413 | 1.398798 |
| 6 | 1.212217 | -3.412650 | 0.660803 |
| 6 | -1.204309 | -3.413034 | 0.660611 |
| 6 | 3.229809 | 1.983150 | -1.389336 |
| 6 | 2.449679 | 1.616611 | -2.558204 |
| 6 | 3.976242 | 1.014002 | -0.710563 |
| 6 | 2.449758 | 0.300149 | -3.011408 |
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| 6 | 0.004208 | 0.440535 | -3.539891 |

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| 6 | -1.203977 | -0.305590 | -3.463707 |
| 6 | 0.004231 | -2.344987 | -2.688015 |
| 6 | 1.212468 | -1.683669 | -3.041667 |
| 6 | -1.203962 | -1.683877 | -3.042136 |
| 6 | 0.004098 | 1.831201 | -3.061370 |
| 6 | 1.212296 | 2.371887 | -2.541537 |
| 6 | -1.204224 | 2.372098 | -2.542031 |
| 6 | -3.221396 | -0.708350 | -2.316434 |
| 6 | -2.441294 | 0.300012 | -3.011997 |
| 6 | -2.441415 | 1.616541 | -2.558807 |
| 6 | -3.967817 | -0.362344 | -1.184969 |
| 6 | -3.221624 | -2.421171 | -0.043046 |
| 6 | -2.441417 | -2.771132 | -1.216932 |
| 6 | -2.441272 | -1.933242 | -2.328952 |
| 6 | -3.967939 | -1.238086 | -0.022581 |
| 6 | -3.221918 | -0.788337 | 2.288382 |
| 6 | -2.441713 | -2.012928 | 2.258533 |
| 6 | -2.441623 | -2.811741 | 1.118088 |
| 6 | -3.968089 | -0.403231 | 1.169467 |
| 6 | -3.221965 | 1.933643 | 1.455944 |
| 6 | -2.441906 | 1.526758 | 2.611448 |
| 6 | -2.441954 | 0.195296 | 3.018723 |
| 6 | -3.968051 | 0.988468 | 0.743840 |
| 6 | -3.221649 | 1.982987 | -1.389960 |
| 6 | -2.441693 | 2.956293 | -0.645916 |
| 6 | -2.441781 | 2.932084 | 0.746223 |
| 6 | -3.967850 | 1.013708 | -0.711257 |
| 10 | -0.166776 | 0.005644 | 0.031691 |

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| 6 | 3.971429 | 1.227938 | -0.158015 |
| 6 | 2.444973 | 1.664581 | -2.527132 |
| 6 | 1.208056 | 1.338468 | -3.209264 |
| 6 | 0.000283 | 2.035642 | -2.931168 |
| 6 | -1.207502 | 1.338534 | -3.209377 |
| 6 | 3.224767 | 1.035757 | 2.188074 |
| 6 | 2.444783 | 2.249613 | 2.023498 |
| 6 | 3.971317 | 0.529693 | 1.118836 |
| 6 | 2.444868 | 2.917707 | 0.801912 |
| 6 | 1.208116 | 3.466011 | 0.280954 |
| 6 | 0.000293 | 3.417123 | 1.029919 |
| 6 | -1.207539 | 3.466080 | 0.280978 |
| 6 | 0.000307 | 3.045248 | -1.860949 |
| 6 | 1.208196 | 3.282261 | -1.148948 |
| 6 | -1.207571 | 3.282355 | -1.148936 |
| 6 | 3.224822 | -1.761110 | 1.660994 |

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| 6 | 2.444880 | -1.229434 | 2.764667 |
| 6 | 3.971309 | -0.900451 | 0.849317 |
| 6 | 2.444908 | 0.138819 | 3.022590 |
| 6 | 1.208030 | 0.803730 | 3.382863 |
| 6 | 0.000170 | 0.076291 | 3.567111 |
| 6 | -1.207631 | 0.803811 | 3.382840 |
| 6 | 0.000259 | 2.711127 | 2.320900 |
| 6 | 1.208065 | 2.106934 | 2.766376 |
| 6 | -1.207595 | 2.106999 | 2.766319 |
| 6 | 3.224713 | -2.123848 | -1.161592 |
| 6 | 2.444788 | -3.009395 | -0.315038 |
| 6 | 3.971209 | -1.085976 | -0.593996 |
| 6 | 2.444786 | -2.831901 | 1.065886 |
| 6 | 1.207967 | -2.969198 | 1.809553 |
| 6 | 0.000110 | -3.369735 | 1.174783 |
| 6 | -1.207747 | -2.969187 | 1.809534 |
| 6 | 0.000126 | -1.369491 | 3.294793 |
| 6 | 1.207958 | -1.979834 | 2.858103 |
| 6 | -1.207712 | -1.979862 | 2.858139 |
| 6 | 3.224902 | 0.448473 | -2.379249 |
| 6 | 2.444892 | -0.630315 | -2.959604 |
| 6 | 3.971373 | 0.229351 | -1.216606 |
| 6 | 2.444820 | -1.888802 | -2.363918 |
| 6 | 1.208033 | -2.638601 | -2.264634 |
| 6 | 0.000182 | -2.158769 | -2.841613 |
| 6 | -1.207705 | -2.638616 | -2.264686 |
| 6 | 0.000114 | -3.557649 | -0.284560 |
| 6 | 1.208000 | -3.330436 | -0.999891 |
| 6 | -1.207773 | -3.330540 | -0.999970 |
| 6 | 0.000211 | -0.828784 | -3.470683 |
| 6 | 1.208011 | -0.078259 | -3.476305 |
| 6 | -1.207552 | -0.078218 | -3.476435 |
| 6 | -3.224347 | -2.123714 | -1.161654 |
| 6 | -2.444427 | -1.888711 | -2.363976 |
| 6 | -2.444409 | -0.630211 | -2.959614 |
| 6 | -3.970742 | -1.085775 | -0.594057 |
| 6 | -3.224553 | -1.761005 | 1.660935 |
| 6 | -2.444557 | -2.831848 | 1.065832 |
| 6 | -2.444545 | -3.009370 | -0.315099 |
| 6 | -3.970992 | -0.900286 | 0.849252 |
| 6 | -3.224314 | 1.035913 | 2.187984 |
| 6 | -2.444478 | 0.138931 | 3.022440 |
| 6 | -2.444521 | -1.229312 | 2.764522 |
| 6 | -3.970927 | 0.529882 | 1.118772 |
| 6 | -3.224163 | 2.401285 | -0.308922 |
| 6 | -2.444362 | 2.917895 | 0.801907 |
| 6 | -2.444353 | 2.249811 | 2.023505 |
| 6 | -3.970955 | 1.228129 | -0.158084 |
| 6 | -3.224390 | 0.448616 | -2.379298 |
| 6 | -2.444298 | 1.664605 | -2.527049 |
| 6 | -2.444455 | 2.620167 | -1.514374 |

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| 6 | -3.970946 | 0.229535 | -1.216687 |
| 18 | -0.004947 | -0.003315 | 0.003524 |

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| 6 | -2.446598 | 0.415219 | 2.996877 |
| 6 | -3.974818 | 0.629884 | 1.065996 |
| 6 | -2.446414 | -0.970846 | 2.865796 |
| 6 | -1.208453 | -1.708608 | 3.026444 |
| 6 | 0.000136 | -1.060752 | 3.403395 |
| 6 | 1.208895 | -1.708328 | 3.026449 |
| 6 | -3.227600 | 2.362767 | -0.527845 |
| 6 | -2.447097 | 2.978882 | 0.531074 |
| 6 | -3.974856 | 1.208193 | -0.269915 |
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| 6 | -1.209049 | 2.350578 | 2.559994 |
| 6 | -0.000413 | 2.909766 | 2.060706 |
| 6 | 1.208348 | 2.350766 | 2.559963 |
| 6 | -0.000073 | 0.403134 | 3.541780 |
| 6 | -1.208802 | 1.109942 | 3.292987 |
| 6 | 1.208479 | 1.110190 | 3.293018 |
| 6 | -3.227104 | 0.227884 | -2.410368 |
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| 6 | -3.974444 | 0.116252 | -1.232695 |
| 6 | -2.447002 | 2.469625 | -1.748225 |
| 6 | -1.209147 | 3.161098 | -1.444372 |
| 6 | -0.000396 | 2.858862 | -2.130099 |
| 6 | 1.208246 | 3.161303 | -1.444328 |
| 6 | -0.000506 | 3.494109 | 0.711309 |
| 6 | -1.209220 | 3.475365 | -0.037993 |
| 6 | 1.208197 | 3.475568 | -0.037984 |
| 6 | -3.226986 | -2.222485 | -0.961927 |
| 6 | -2.446212 | -2.098121 | -2.180469 |
| 6 | -3.974362 | -1.136935 | -0.491893 |
| 6 | -2.446271 | -0.899604 | -2.888858 |
| 6 | -1.208528 | -0.396964 | -3.452603 |
| 6 | 0.000192 | -1.142546 | -3.376881 |
| 6 | 1.208737 | -0.396729 | -3.452629 |
| 6 | -0.000210 | 1.756003 | -3.102616 |
| 6 | -1.208787 | 1.037683 | -3.316935 |
| 6 | 1.208543 | 1.037906 | -3.316865 |
| 6 | -3.227089 | -1.601998 | 1.816024 |
| 6 | -2.446343 | -2.722595 | 1.321354 |
| 6 | -3.974400 | -0.819543 | 0.928799 |
| 6 | -2.446289 | -3.026102 | -0.037406 |
| 6 | -1.208281 | -3.406741 | -0.689473 |
| 6 | 0.000459 | -3.565188 | 0.043021 |
| 6 | 1.209171 | -3.406447 | -0.689460 |

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| 6 | 0.000353 | -2.408437 | -2.628681 |
| 6 | -1.208301 | -2.834192 | -2.011866 |
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| 6 | 0.000411 | -3.244528 | 1.478080 |
| 6 | -1.208369 | -2.789457 | 2.073470 |
| 6 | 1.209078 | -2.789169 | 2.073468 |
| 6 | 3.227636 | -2.221751 | -0.961915 |
| 6 | 2.447082 | -3.025514 | -0.037392 |
| 6 | 2.447047 | -2.722011 | 1.321368 |
| 6 | 3.974764 | -1.136024 | -0.491856 |
| 6 | 3.227146 | 0.228525 | -2.410320 |
| 6 | 2.446688 | -0.899120 | -2.888977 |
| 6 | 2.446891 | -2.097620 | -2.180514 |
| 6 | 3.974581 | 0.117145 | -1.232691 |
| 6 | 3.226911 | 2.363474 | -0.527829 |
| 6 | 2.446232 | 2.470034 | -1.748079 |
| 6 | 2.446375 | 1.425796 | -2.668854 |
| 6 | 3.974410 | 1.209065 | -0.269890 |
| 6 | 3.227155 | 1.232686 | 2.084235 |
| 6 | 2.446294 | 2.426151 | 1.808685 |
| 6 | 2.446125 | 2.979197 | 0.531022 |
| 6 | 3.974590 | 0.630718 | 1.066022 |
| 6 | 3.227580 | -1.601280 | 1.816079 |
| 6 | 2.446697 | -0.970300 | 2.865841 |
| 6 | 2.446508 | 0.415761 | 2.996980 |
| 6 | 3.974794 | -0.818689 | 0.928870 |
| 2 | -1.142313 | -0.003187 | -0.001140 |
| 2 | 1.142089 | 0.002351 | -0.000148 |

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| 6 | 2.462802 | 3.023391 | 0.119225 |
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| 6 | 2.463020 | 2.756663 | -1.247134 |
| 6 | 1.224658 | 2.843530 | -1.996718 |
| 6 | 0.015591 | 3.282410 | -1.389632 |
| 6 | -1.193286 | 2.843970 | -1.997318 |
| 6 | 3.243867 | -0.293098 | 2.403409 |
| 6 | 2.462558 | 0.820913 | 2.911832 |
| 6 | 3.992422 | -0.149775 | 1.229507 |
| 6 | 2.462528 | 2.037973 | 2.235932 |
| 6 | 1.224192 | 2.777794 | 2.087024 |
| 6 | 0.015214 | 2.335881 | 2.691921 |
| 6 | -1.193726 | 2.778236 | 2.087278 |
| 6 | 0.015380 | 3.564254 | 0.053245 |
| 6 | 1.224315 | 3.385867 | 0.780979 |
| 6 | -1.193669 | 3.386352 | 0.780935 |
| 6 | 3.244394 | -2.376204 | 0.463903 |

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| 6 | 2.463030 | -2.515622 | 1.680520 |
| 6 | 3.992865 | -1.215363 | 0.237435 |
| 6 | 2.462815 | -1.496793 | 2.629247 |
| 6 | 1.224312 | -1.126627 | 3.286624 |
| 6 | 0.015452 | -1.838674 | 3.053268 |
| 6 | -1.193540 | -1.126909 | 3.286967 |
| 6 | 0.015227 | 1.050638 | 3.405617 |
| 6 | 1.224184 | 0.303495 | 3.461043 |
| 6 | -1.193671 | 0.303460 | 3.461507 |
| 6 | 3.244582 | -1.175286 | -2.116572 |
| 6 | 2.463417 | -2.375558 | -1.873223 |
| 6 | 3.993063 | -0.601041 | -1.082619 |
| 6 | 2.463394 | -2.963089 | -0.611083 |
| 6 | 1.224881 | -3.474017 | -0.055966 |
| 6 | 0.015991 | -3.472297 | -0.805274 |
| 6 | -1.193035 | -3.474680 | -0.056199 |
| 6 | 0.015664 | -2.914676 | 2.051485 |
| 6 | 1.224710 | -3.197989 | 1.358047 |
| 6 | -1.193198 | -3.198655 | 1.358068 |
| 6 | 3.244416 | 1.650165 | -1.771850 |
| 6 | 2.463205 | 1.047701 | -2.838070 |
| 6 | 3.993025 | 0.844257 | -0.906333 |
| 6 | 2.463312 | -0.334221 | -3.006698 |
| 6 | 1.224990 | -1.020271 | -3.321136 |
| 6 | 0.016043 | -0.307213 | -3.550950 |
| 6 | -1.192842 | -1.020598 | -3.322008 |
| 6 | 0.016102 | -2.851940 | -2.138101 |
| 6 | 1.225060 | -2.279847 | -2.621826 |
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| 6 | 0.015914 | 1.152061 | -3.372841 |
| 6 | 1.224778 | 1.789083 | -2.978350 |
| 6 | -1.193096 | 1.789312 | -2.979152 |
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| 6 | -2.431356 | 1.047683 | -2.839332 |
| 6 | -3.959191 | -0.601426 | -1.083251 |
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| 6 | -2.431327 | -2.963885 | -0.611723 |
| 6 | -2.431225 | -2.376443 | -1.874149 |
| 6 | -3.959475 | -1.215728 | 0.236673 |
| 6 | -3.212689 | -0.293440 | 2.403493 |
| 6 | -2.431755 | -1.497377 | 2.629350 |
| 6 | -2.431585 | -2.516445 | 1.680514 |
| 6 | -3.959555 | -0.150164 | 1.228715 |
| 6 | -3.212731 | 2.195613 | 1.021363 |
| 6 | -2.431986 | 2.038347 | 2.236288 |
| 6 | -2.431995 | 0.821005 | 2.912297 |
| 6 | -3.959524 | 1.122626 | 0.521966 |
| 6 | -3.212367 | 1.650256 | -1.772919 |
| 6 | -2.431671 | 2.757135 | -1.247838 |
| 6 | -2.431856 | 3.023870 | 0.118791 |

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| 6 | -3.959295 | 0.843716 | -0.906932 |
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| 10 | -0.943144 | -0.001821 | 0.004017 |

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| 6 | 2.448474 | 2.470959 | 1.746367 |
| 6 | 3.979974 | 0.657752 | 1.050462 |
| 6 | 2.448569 | 2.991290 | 0.455072 |
| 6 | 1.209325 | 3.471397 | -0.126277 |
| 6 | -0.000236 | 3.508494 | 0.621456 |
| 6 | -1.209677 | 3.471269 | -0.126437 |
| 6 | 3.230656 | -1.554824 | 1.856705 |
| 6 | 2.448481 | -0.897049 | 2.889465 |
| 6 | 3.980109 | -0.795360 | 0.950159 |
| 6 | 2.448399 | 0.491810 | 2.985341 |
| 6 | 1.209101 | 1.192947 | 3.262329 |
| 6 | -0.000290 | 0.493010 | 3.528540 |
| 6 | -1.209735 | 1.192832 | 3.262204 |
| 6 | -0.000319 | 2.959090 | 1.984643 |
| 6 | 1.209105 | 2.413844 | 2.497935 |
| 6 | -1.209771 | 2.413712 | 2.497770 |
| 6 | 3.231124 | -2.246053 | -0.904914 |
| 6 | 2.449026 | -3.025180 | 0.039779 |
| 6 | 3.980549 | -1.149067 | -0.462806 |
| 6 | 2.448836 | -2.687175 | 1.390284 |
| 6 | 1.209480 | -2.734076 | 2.142676 |
| 6 | 0.000102 | -3.203922 | 1.559479 |
| 6 | -1.209424 | -2.734156 | 2.142498 |
| 6 | -0.000181 | -0.973239 | 3.427547 |
| 6 | 1.209306 | -1.629710 | 3.067517 |
| 6 | -1.209548 | -1.629824 | 3.067361 |
| 6 | 3.230978 | 0.166931 | -2.415689 |
| 6 | 2.449124 | -0.972402 | -2.864805 |
| 6 | 3.980369 | 0.085522 | -1.235773 |
| 6 | 2.449193 | -2.152442 | -2.125954 |
| 6 | 1.209862 | -2.882465 | -1.937974 |
| 6 | 0.000415 | -2.472785 | -2.564668 |
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| 6 | 0.000268 | -3.560744 | 0.133626 |
| 6 | 1.209805 | -3.421039 | -0.601971 |
| 6 | -1.209162 | -3.421159 | -0.602144 |
| 6 | 3.230664 | 2.349411 | -0.587712 |
| 6 | 2.448804 | 2.424371 | -1.810076 |
| 6 | 3.980313 | 1.202238 | -0.300539 |
| 6 | 2.448979 | 1.357089 | -2.704036 |
| 6 | 1.209733 | 0.952551 | -3.340318 |
| 6 | 0.000179 | 1.675078 | -3.144344 |

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| 6 | -1.209261 | 0.952432 | -3.340501 |
| 6 | 0.000378 | -1.227223 | -3.344712 |
| 6 | 1.209821 | -0.484470 | -3.439498 |
| 6 | -1.209137 | -0.484595 | -3.439681 |
| 6 | 0.000023 | 2.801835 | -2.200665 |
| 6 | 1.209421 | 3.121433 | -1.523549 |
| 6 | -1.209520 | 3.121295 | -1.523716 |
| 6 | -3.230547 | 0.166584 | -2.416164 |
| 6 | -2.448664 | 1.356828 | -2.704412 |
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| 6 | -3.980087 | 0.085103 | -1.236332 |
| 6 | -3.230480 | -2.246348 | -0.905382 |
| 6 | -2.448416 | -2.152642 | -2.126302 |
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| 6 | -3.980087 | -1.149449 | -0.463355 |
| 6 | -3.230715 | -1.555131 | 1.856280 |
| 6 | -2.448634 | -2.687348 | 1.389913 |
| 6 | -2.448508 | -3.025403 | 0.039421 |
| 6 | -3.980205 | -0.795765 | 0.949655 |
| 6 | -3.231007 | 1.285062 | 2.052426 |
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| 6 | -2.448815 | -0.897306 | 2.889205 |
| 6 | -3.980347 | 0.657385 | 1.049980 |
| 6 | -3.230842 | 2.349083 | -0.588177 |
| 6 | -2.448974 | 2.991054 | 0.454744 |
| 6 | -2.449045 | 2.470744 | 1.746056 |
| 6 | -3.980352 | 1.201807 | -0.301091 |
| 10 | 1.196624 | 0.000481 | -0.000591 |
| 10 | -1.197941 | -0.000309 | -0.000074 |

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| 6 | 2.474425 | 1.430318 | 2.663677 |
| 6 | 4.011693 | 0.121545 | 1.232201 |
| 6 | 2.473108 | 2.472586 | 1.741691 |
| 6 | 1.233151 | 3.161702 | 1.437622 |
| 6 | 0.024319 | 2.861662 | 2.124815 |
| 6 | -1.185490 | 3.163450 | 1.440003 |
| 6 | 3.260071 | -2.217381 | 0.963882 |
| 6 | 2.477362 | -2.091374 | 2.181416 |
| 6 | 4.012562 | -1.133974 | 0.492753 |
| 6 | 2.476657 | -0.892281 | 2.887610 |
| 6 | 1.237001 | -0.390346 | 3.449834 |
| 6 | 0.028240 | -1.136842 | 3.377854 |
| 6 | -1.181508 | -0.392391 | 3.454588 |
| 6 | 0.025734 | 1.760421 | 3.098963 |
| 6 | 1.235663 | 1.043006 | 3.311484 |
| 6 | -1.182772 | 1.042345 | 3.316329 |

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| 6 | 3.258000 | -1.601557 | -1.813747 |
| 6 | 2.476256 | -2.720862 | -1.317004 |
| 6 | 4.011144 | -0.818541 | -0.929750 |
| 6 | 2.477221 | -3.021967 | 0.041572 |
| 6 | 1.238346 | -3.401796 | 0.693972 |
| 6 | 0.028787 | -3.564821 | -0.036917 |
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| 6 | 0.028950 | -2.403743 | 2.631984 |
| 6 | 1.238381 | -2.827236 | 2.014318 |
| 6 | -1.180217 | -2.832612 | 2.017563 |
| 6 | 3.255069 | 1.230333 | -2.086344 |
| 6 | 2.472571 | 0.411959 | -2.996416 |
| 6 | 4.009476 | 0.631697 | -1.069377 |
| 6 | 2.474024 | -0.973240 | -2.863142 |
| 6 | 1.235237 | -1.711341 | -3.021482 |
| 6 | 0.025258 | -1.066543 | -3.400687 |
| 6 | -1.183222 | -1.715220 | -3.023781 |
| 6 | 0.027896 | -3.246759 | -1.472402 |
| 6 | 1.236621 | -2.789977 | -2.067409 |
| 6 | -1.181972 | -2.794844 | -2.068808 |
| 6 | 3.255390 | 2.364793 | 0.522397 |
| 6 | 2.471607 | 2.977441 | -0.536338 |
| 6 | 4.009808 | 1.212718 | 0.266657 |
| 6 | 2.471497 | 2.422556 | -1.812460 |
| 6 | 1.232020 | 2.345253 | -2.562327 |
| 6 | 0.022468 | 2.905187 | -2.065138 |
| 6 | -1.186545 | 2.346015 | -2.564392 |
| 6 | 0.023911 | 0.396912 | -3.541767 |
| 6 | 1.232667 | 1.104178 | -3.292835 |
| 6 | -1.185707 | 1.103735 | -3.295494 |
| 6 | 0.022564 | 3.491635 | -0.716810 |
| 6 | 1.232225 | 3.473130 | 0.031598 |
| 6 | -1.186361 | 3.475266 | 0.032674 |
| 6 | -3.204957 | 1.226708 | -2.086069 |
| 6 | -2.424943 | 2.421935 | -1.812612 |
| 6 | -2.424880 | 2.977467 | -0.535322 |
| 6 | -3.951505 | 0.625388 | -1.065972 |
| 6 | -3.202390 | -1.608198 | -1.812772 |
| 6 | -2.422239 | -0.977922 | -2.864256 |
| 6 | -2.423475 | 0.408468 | -2.997893 |
| 6 | -3.950013 | -0.824344 | -0.926214 |
| 6 | -3.200680 | -2.224310 | 0.967284 |
| 6 | -2.419550 | -3.029337 | 0.043413 |
| 6 | -2.420300 | -2.727913 | -1.316315 |
| 6 | -3.949094 | -1.139479 | 0.495644 |
| 6 | -3.202043 | 0.229633 | 2.412443 |
| 6 | -2.419801 | -0.897030 | 2.892381 |
| 6 | -2.419209 | -2.097229 | 2.185826 |
| 6 | -3.949815 | 0.115492 | 1.234675 |
| 6 | -3.204953 | 2.362595 | 0.525479 |
| 6 | -2.423415 | 2.471798 | 1.745819 |

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| 6 | -2.421982 | 1.428610 | 2.668704 |
| 6 | -3.951308 | 1.206246 | 0.269618 |
| 2 | 1.680594 | -0.025731 | 0.021388 |
| 18 | -0.811813 | 0.009697 | -0.002423 |

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| 6 | -4.000831 | -0.313114 | -1.201192 |
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| 6 | -0.008136 | 1.957067 | -2.975239 |
| 6 | 1.202121 | 2.476281 | -2.436243 |
| 6 | -3.244318 | -2.417801 | -0.145216 |
| 6 | -2.458961 | -2.715231 | -1.331638 |
| 6 | -4.000633 | -1.239492 | -0.074595 |
| 6 | -2.459098 | -1.831411 | -2.406457 |
| 6 | -1.217684 | -1.550832 | -3.104460 |
| 6 | -0.007014 | -2.225040 | -2.780817 |
| 6 | 1.203262 | -1.551806 | -3.107725 |
| 6 | -0.007678 | 0.589221 | -3.512128 |
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| 6 | 1.202935 | -0.157511 | -3.470035 |
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| 6 | -4.001082 | -0.454348 | 1.154593 |
| 6 | -2.459174 | -2.854822 | 0.997310 |
| 6 | -1.217556 | -3.431856 | 0.515089 |
| 6 | -0.007107 | -3.332373 | 1.256666 |
| 6 | 1.203439 | -3.435119 | 0.515710 |
| 6 | -0.006863 | -3.158382 | -1.645855 |
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| 6 | 1.203554 | -3.348913 | -0.922322 |
| 6 | -3.245864 | 1.869496 | 1.537644 |
| 6 | -2.460581 | 1.412935 | 2.672473 |
| 6 | -4.001538 | 0.957376 | 0.787681 |
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| 6 | -1.218642 | -0.570736 | 3.422645 |
| 6 | -0.008279 | 0.165390 | 3.557284 |
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| 6 | -1.218225 | -1.910566 | 2.896753 |
| 6 | 1.202760 | -1.911945 | 2.900135 |
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| 6 | -2.460707 | 2.978164 | -0.518726 |
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| 6 | -2.460827 | 2.894890 | 0.870364 |
| 6 | -1.219449 | 3.078742 | 1.600022 |

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| 6 | -0.008903 | 3.434496 | 0.941880 |
| 6 | 1.201565 | 3.082530 | 1.602064 |
| 6 | -0.008640 | 1.587540 | 3.187578 |
| 6 | -1.219294 | 2.164479 | 2.711679 |
| 6 | 1.201674 | 2.167487 | 2.714691 |
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| 6 | -1.219220 | 3.247799 | -1.221002 |
| 6 | 1.201802 | 3.251813 | -1.222249 |
| 6 | 3.225815 | 1.872493 | 1.539367 |
| 6 | 2.442414 | 2.899251 | 0.871510 |
| 6 | 2.442537 | 2.982588 | -0.518674 |
| 6 | 3.976855 | 0.958815 | 0.787993 |
| 6 | 3.226547 | -0.884773 | 2.256075 |
| 6 | 2.442931 | 0.067529 | 3.026190 |
| 6 | 2.442579 | 1.415432 | 2.675838 |
| 6 | 3.977324 | -0.452266 | 1.154791 |
| 6 | 3.227190 | -2.418304 | -0.144774 |
| 6 | 2.443977 | -2.856843 | 0.999039 |
| 6 | 2.443632 | -2.107108 | 2.172749 |
| 6 | 3.977697 | -1.237081 | -0.073862 |
| 6 | 3.226932 | -0.608917 | -2.345150 |
| 6 | 2.444005 | -1.832447 | -2.408615 |
| 6 | 2.444171 | -2.717059 | -1.332925 |
| 6 | 3.977576 | -0.311069 | -1.200006 |
| 6 | 3.226118 | 2.043016 | -1.304318 |
| 6 | 2.443045 | 1.724969 | -2.487365 |
| 6 | 2.443454 | 0.428543 | -2.996164 |
| 6 | 3.977042 | 1.046094 | -0.667314 |
| 10 | -1.500189 | 0.003401 | 0.000939 |
| 18 | 1.038715 | -0.000213 | 0.000371 |

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| 6 | 2.458951 | 2.991798 | 0.440691 |
| 6 | 1.213399 | 3.463588 | -0.142027 |
| 6 | 0.000042 | 3.503718 | 0.602629 |
| 6 | -1.213022 | 3.463684 | -0.142452 |
| 6 | 3.247804 | -1.547482 | 1.865999 |
| 6 | 2.458109 | -0.883153 | 2.892468 |
| 6 | 4.011281 | -0.794275 | 0.958087 |
| 6 | 2.458191 | 0.505773 | 2.981713 |
| 6 | 1.212527 | 1.205635 | 3.250184 |
| 6 | -0.000702 | 0.509572 | 3.517995 |
| 6 | -1.213778 | 1.205754 | 3.249767 |
| 6 | -0.000285 | 2.961460 | 1.966715 |
| 6 | 1.212773 | 2.421066 | 2.481205 |

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| 6 | 3.248496 | -2.252519 | -0.894514 |
| 6 | 2.458796 | -3.023768 | 0.054354 |
| 6 | 4.011684 | -1.156098 | -0.458666 |
| 6 | 2.458497 | -2.679377 | 1.402871 |
| 6 | 1.212663 | -2.718705 | 2.151222 |
| 6 | -0.000450 | -3.188670 | 1.571754 |
| 6 | -1.213760 | -2.718595 | 2.150785 |
| 6 | -0.000735 | -0.955329 | 3.423756 |
| 6 | 1.212463 | -1.611551 | 3.069301 |
| 6 | -1.213857 | -1.611447 | 3.068884 |
| 6 | 3.248893 | 0.155283 | -2.418083 |
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| 6 | 4.011952 | 0.079585 | -1.240542 |
| 6 | 2.459209 | -2.161740 | -2.114132 |
| 6 | 1.213526 | -2.885904 | -1.920527 |
| 6 | 0.000451 | -2.480161 | -2.546658 |
| 6 | -1.212896 | -2.885780 | -1.920959 |
| 6 | -0.000144 | -3.551899 | 0.149426 |
| 6 | 1.213235 | -3.417147 | -0.583962 |
| 6 | -1.213211 | -3.417018 | -0.584400 |
| 6 | 3.248660 | 2.348250 | -0.599032 |
| 6 | 2.459360 | 2.414364 | -1.820287 |
| 6 | 4.011860 | 1.205059 | -0.306988 |
| 6 | 2.459500 | 1.343153 | -2.708891 |
| 6 | 1.213950 | 0.935046 | -3.337876 |
| 6 | 0.000746 | 1.655782 | -3.145641 |
| 6 | -1.212429 | 0.935135 | -3.338274 |
| 6 | 0.000666 | -1.239649 | -3.331502 |
| 6 | 1.213868 | -0.500279 | -3.429818 |
| 6 | -1.212429 | -0.500173 | -3.430229 |
| 6 | 0.000585 | 2.785699 | -2.208573 |
| 6 | 1.213650 | 3.107618 | -1.535492 |
| 6 | -1.212713 | 3.107684 | -1.535904 |
| 6 | -3.247746 | 0.155531 | -2.419184 |
| 6 | -2.458162 | 1.343307 | -2.709703 |
| 6 | -2.458337 | 2.414511 | -1.821132 |
| 6 | -4.011329 | 0.079896 | -1.241994 |
| 6 | -3.248193 | -2.252197 | -0.895715 |
| 6 | -2.458410 | -2.161491 | -2.114998 |
| 6 | -2.458196 | -0.985372 | -2.859160 |
| 6 | -4.011573 | -1.155782 | -0.460139 |
| 6 | -3.248765 | -1.547234 | 1.864851 |
| 6 | -2.459295 | -2.679158 | 1.401972 |
| 6 | -2.458985 | -3.023515 | 0.053448 |
| 6 | -4.011850 | -0.793956 | 0.956641 |
| 6 | -3.248779 | 1.296218 | 2.047523 |
| 6 | -2.459425 | 0.505998 | 2.980864 |
| 6 | -2.459414 | -0.882950 | 2.891637 |
| 6 | -4.011956 | 0.665298 | 1.050426 |
| 6 | -3.248143 | 2.348467 | -0.600205 |

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| 6 | -2.459138 | 2.477960 | 1.733207 |
| 6 | -4.011582 | 1.205362 | -0.308455 |
| 18 | 1.332486 | 0.000519 | -0.000962 |
| 18 | -1.332818 | -0.000850 | 0.000591 |