

# Theoretical investigations on the healing of mono- vacancies in single-walled carbon nanotubes by adsorption of carbon monoxide

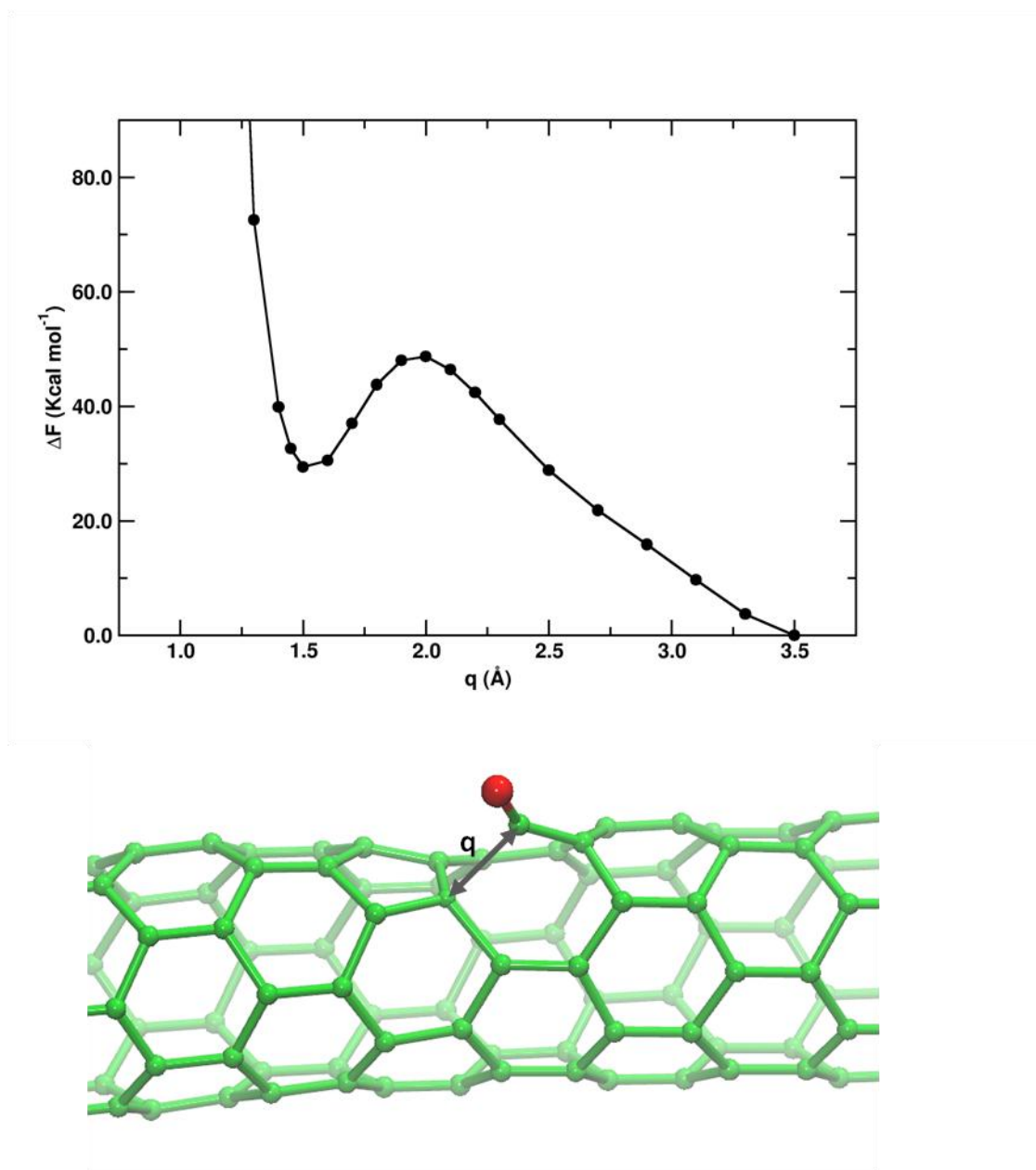
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06123 Perugia, Italy.

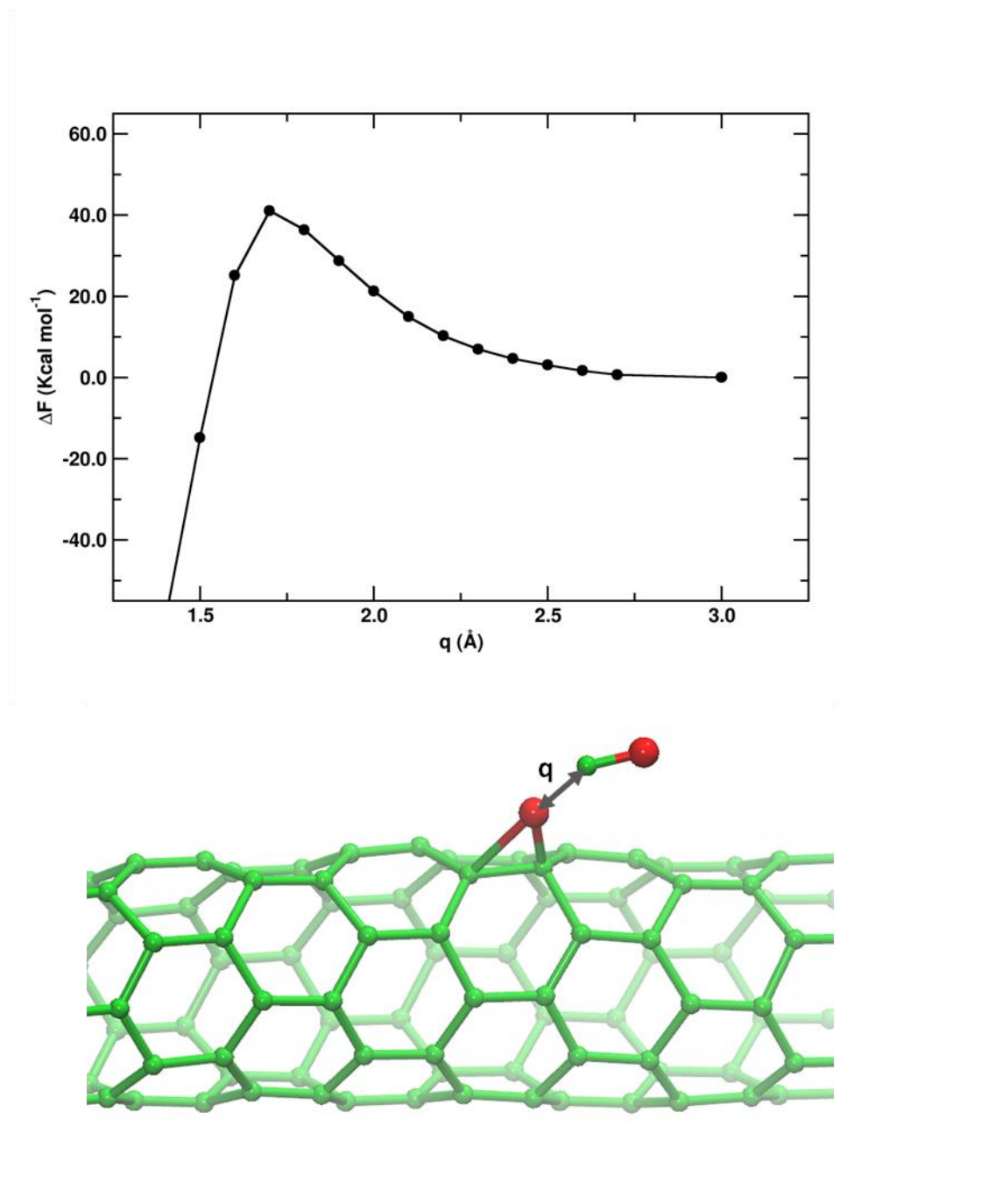
## Supporting Information

Pages S2 – S4: Free energy profiles obtained by integration of the potential of mean force along selected reaction coordinates.

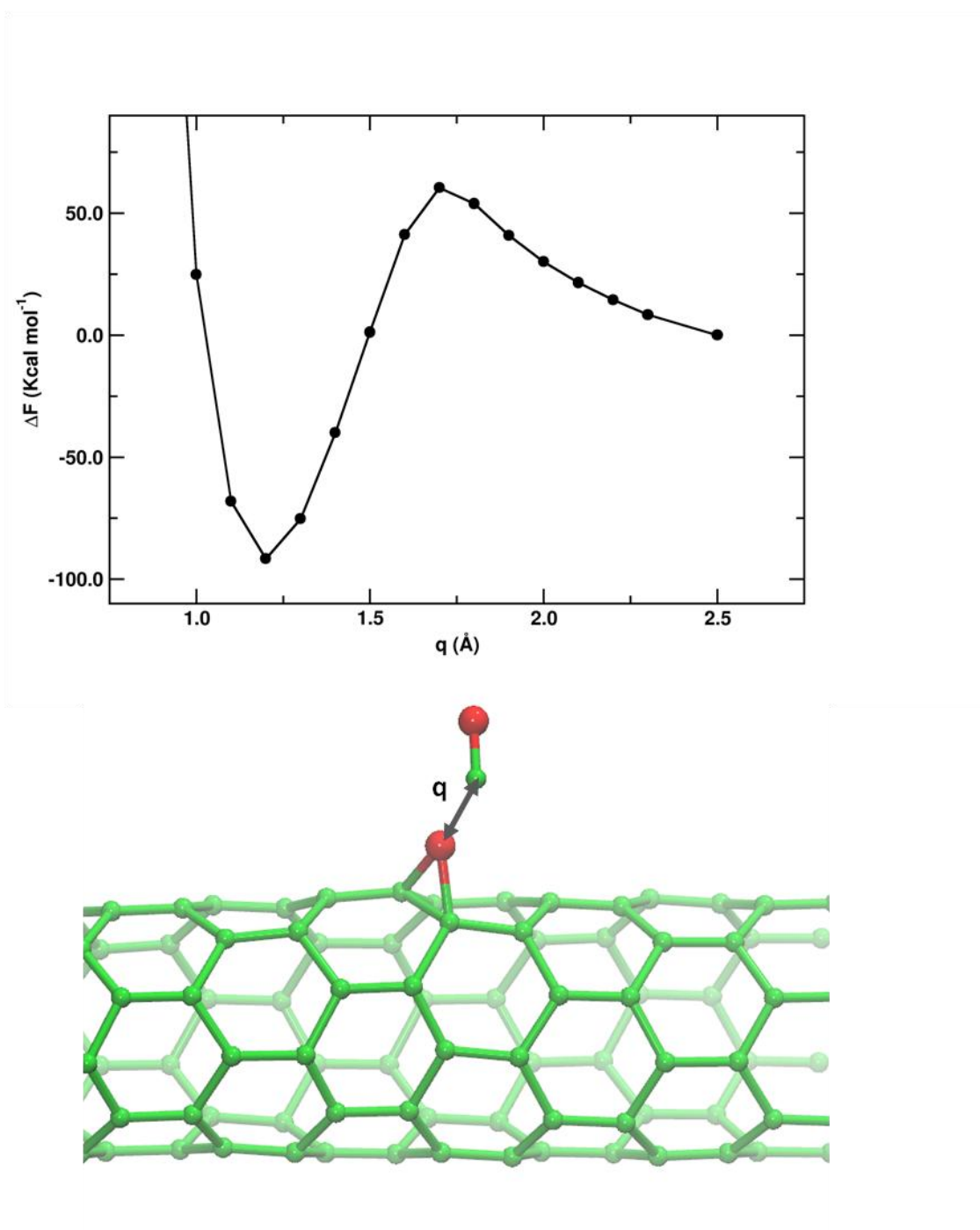
Pages S5 – S20: Cartesian coordinates of structures **1** – **6** and structures (free energy maxima) of presumed transition states **TS1** – **TS3**.



**Figure S10.** Free energy profile derived by integration of the potential of mean force along the reaction coordinate  $q$  (corresponding to the path leading from structure **2** to structure **TS1**).



**Figure S11.** Free energy profile derived by integration of the potential of mean force along the reaction coordinate  $q$  (corresponding to the path leading from structure **4** to structure **TS2**).



**Figure S12.** Free energy profile derived by integration of the potential of mean force along the reaction coordinate  $q$  (corresponding to the path leading from structure **5** to structure **TS3**).

## Cartesian coordinates

### Structure 1

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|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.418734  | -0.008422 | 0.059064  |
| C | 2.154673  | 1.251664  | 3.610784  |
| C | 2.115264  | 1.229036  | 2.190882  |
| C | 1.203826  | 2.114975  | 1.482536  |
| C | 1.194283  | 2.108989  | 0.059098  |
| C | 0.012209  | 2.432415  | 3.650525  |
| C | -0.008976 | 2.440316  | 2.220842  |
| C | -1.240983 | 2.140974  | 1.500558  |
| C | -1.246893 | 2.143801  | 0.074138  |
| C | -2.123295 | 1.240220  | 3.665370  |
| C | -2.134268 | 1.249290  | 2.243135  |
| C | -2.425144 | 0.018602  | 1.498818  |
| C | -2.424372 | 0.019082  | 0.071041  |
| C | -2.086229 | -1.204021 | 3.653887  |
| C | -2.069729 | -1.194592 | 2.220936  |
| C | -1.199095 | -2.112017 | 1.498047  |
| C | -1.197944 | -2.111998 | 0.071582  |
| C | 0.011503  | -2.455854 | 3.664864  |
| C | 0.014488  | -2.469636 | 2.242956  |
| C | 1.231056  | -2.134440 | 1.500671  |
| C | 1.230695  | -2.141377 | 0.073519  |
| C | 2.107456  | -1.193853 | 3.650582  |
| C | 2.104156  | -1.215844 | 2.220685  |
| C | 2.428362  | -0.002804 | 1.482401  |
| C | 2.484588  | 0.031195  | 4.335723  |
| C | 2.312771  | 1.343212  | 6.386237  |
| C | 1.309213  | 2.124684  | 5.767472  |
| C | 1.262092  | 2.147105  | 4.335491  |
| C | 0.135747  | 2.052326  | 7.976631  |
| C | 0.090491  | 2.238224  | 6.558950  |
| C | -1.155942 | 2.037760  | 5.836586  |
| C | -1.189892 | 2.097185  | 4.406921  |
| C | -2.131077 | 1.192528  | 7.964496  |
| C | -2.125810 | 1.198543  | 6.552744  |
| C | -2.465274 | -0.015531 | 5.810904  |
| C | -2.444740 | 0.000203  | 4.386311  |
| C | -2.148206 | -1.239893 | 7.979807  |
| C | -2.138429 | -1.234319 | 6.541418  |
| C | -1.249468 | -2.130475 | 5.809750  |
| C | -1.225555 | -2.120420 | 4.386457  |
| C | -0.034092 | -2.439300 | 7.964029  |
| C | -0.026352 | -2.437799 | 6.552649  |
| C | 1.182408  | -2.009525 | 5.836549  |
| C | 1.217607  | -2.068677 | 4.406305  |
| C | 1.837870  | -0.896421 | 7.976486  |
| C | 1.976797  | -1.028990 | 6.558653  |
| C | 2.488331  | 0.083348  | 5.767640  |
| C | 2.010938  | 0.308335  | 8.797600  |
| C | 2.160677  | 1.255067  | 12.355954 |
| C | 2.168873  | 1.260051  | 10.955661 |
| C | 1.251662  | 2.058872  | 10.169088 |
| C | 1.265146  | 1.599276  | 8.797963  |
| C | 0.013345  | 2.439908  | 12.294027 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.029829  | 2.405479  | 10.851805 |
| C | -1.188486 | 2.064597  | 10.120425 |
| C | -1.134613 | 1.978521  | 8.703412  |
| C | -2.131464 | 1.243581  | 12.279313 |
| C | -2.127771 | 1.226135  | 10.860176 |
| C | -2.465510 | -0.009904 | 10.135889 |
| C | -2.485743 | -0.023673 | 8.710555  |
| C | -2.078960 | -1.200388 | 12.303037 |
| C | -2.103567 | -1.214199 | 10.868770 |
| C | -1.245089 | -2.133644 | 10.135170 |
| C | -1.266837 | -2.144094 | 8.711170  |
| C | 0.010575  | -2.465718 | 12.278814 |
| C | -0.003100 | -2.453360 | 10.859670 |
| C | 1.189366  | -2.050483 | 10.120367 |
| C | 1.141213  | -1.960555 | 8.702690  |
| C | 2.114545  | -1.196721 | 12.293614 |
| C | 2.092198  | -1.164724 | 10.851188 |
| C | 2.402585  | 0.066833  | 10.168416 |
| C | 2.451511  | 0.004366  | 13.046638 |
| C | 2.091814  | 1.215199  | 16.609708 |
| C | 2.098001  | 1.218673  | 15.190919 |
| C | 1.203695  | 2.118510  | 14.469362 |
| C | 1.222123  | 2.131379  | 13.046855 |
| C | -0.023987 | 2.444022  | 16.611505 |
| C | -0.020401 | 2.442656  | 15.181551 |
| C | -1.237904 | 2.142535  | 14.440873 |
| C | -1.220541 | 2.132799  | 13.013097 |
| C | -2.147712 | 1.255925  | 16.603415 |
| C | -2.142584 | 1.253956  | 15.182724 |
| C | -2.422331 | 0.017754  | 14.452262 |
| C | -2.425577 | 0.015065  | 13.024232 |
| C | -2.061263 | -1.189988 | 16.616385 |
| C | -2.061361 | -1.190270 | 15.180932 |
| C | -1.198269 | -2.110458 | 14.451386 |
| C | -1.202517 | -2.111975 | 13.024723 |
| C | 0.013804  | -2.485328 | 16.603213 |
| C | 0.014640  | -2.480034 | 15.182455 |
| C | 1.233838  | -2.133242 | 14.440821 |
| C | 1.233899  | -2.113556 | 13.012153 |
| C | 2.100545  | -1.231236 | 16.611401 |
| C | 2.100767  | -1.227567 | 15.181183 |
| C | 2.431265  | -0.005289 | 14.469018 |

## Structure 2

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|   |           |           |          |
|---|-----------|-----------|----------|
| C | 2.447807  | -0.138223 | 0.054473 |
| C | 2.367669  | 1.179260  | 3.585773 |
| C | 2.309129  | 1.150041  | 2.190423 |
| C | 1.382182  | 2.042196  | 1.470914 |
| C | 1.364946  | 2.038726  | 0.054520 |
| C | 0.186321  | 2.301476  | 3.643990 |
| C | 0.164399  | 2.328971  | 2.208986 |
| C | -1.075690 | 2.082797  | 1.499321 |
| C | -1.087350 | 2.102345  | 0.065626 |
| C | -2.039490 | 1.266458  | 3.658581 |
| C | -2.051100 | 1.283538  | 2.230187 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.507473 | 0.111313  | 1.483357  |
| C | -2.500725 | 0.117941  | 0.056498  |
| C | -2.312939 | -1.150283 | 3.633190  |
| C | -2.293632 | -1.141407 | 2.210674  |
| C | -1.424714 | -2.068379 | 1.482706  |
| C | -1.414926 | -2.065597 | 0.055519  |
| C | -0.222487 | -2.392276 | 3.658767  |
| C | -0.214628 | -2.411788 | 2.229792  |
| C | 1.011362  | -2.114117 | 1.498417  |
| C | 1.020860  | -2.134154 | 0.064386  |
| C | 1.944397  | -1.237614 | 3.644390  |
| C | 1.954108  | -1.272260 | 2.209053  |
| C | 2.460292  | -0.127618 | 1.471011  |
| C | 2.522314  | -0.098734 | 4.331609  |
| C | 2.740586  | 1.365947  | 6.249911  |
| C | 1.506502  | 2.068464  | 5.741993  |
| C | 1.443290  | 2.076009  | 4.331277  |
| C | 0.310771  | 1.971703  | 7.964666  |
| C | 0.296792  | 2.090516  | 6.530790  |
| C | -0.967387 | 1.943353  | 5.821951  |
| C | -1.018652 | 2.014397  | 4.390530  |
| C | -2.017566 | 1.234625  | 7.957001  |
| C | -2.011525 | 1.225887  | 6.537591  |
| C | -2.544425 | 0.081753  | 5.800066  |
| C | -2.535287 | 0.092278  | 4.376479  |
| C | -2.345688 | -1.162851 | 7.968630  |
| C | -2.352521 | -1.167625 | 6.541696  |
| C | -1.473565 | -2.077415 | 5.800640  |
| C | -1.458609 | -2.078677 | 4.377060  |
| C | -0.236893 | -2.348533 | 7.957778  |
| C | -0.239745 | -2.341758 | 6.538728  |
| C | 0.961795  | -1.940290 | 5.822906  |
| C | 0.988705  | -2.025822 | 4.391348  |
| C | 1.752015  | -0.930733 | 7.964317  |
| C | 1.839430  | -1.017701 | 6.530928  |
| C | 2.553787  | -0.041690 | 5.742023  |
| C | 2.087195  | 0.219826  | 8.810193  |
| C | 2.285164  | 1.142855  | 12.360273 |
| C | 2.300421  | 1.151316  | 10.969550 |
| C | 1.417470  | 1.995606  | 10.176453 |
| C | 1.428857  | 1.544789  | 8.811212  |
| C | 0.174300  | 2.386755  | 12.299011 |
| C | 0.196602  | 2.356894  | 10.853124 |
| C | -1.015840 | 2.030293  | 10.113982 |
| C | -0.955540 | 1.928569  | 8.681630  |
| C | -2.033671 | 1.306572  | 12.276449 |
| C | -2.022546 | 1.285284  | 10.844042 |
| C | -2.524601 | 0.106254  | 10.125805 |
| C | -2.547066 | 0.091518  | 8.704618  |
| C | -2.260297 | -1.119433 | 12.287843 |
| C | -2.287075 | -1.132343 | 10.866294 |
| C | -1.442236 | -2.069116 | 10.126469 |
| C | -1.467786 | -2.079649 | 8.705740  |
| C | -0.187081 | -2.400804 | 12.275241 |
| C | -0.198423 | -2.379074 | 10.843735 |
| C | 1.001658  | -2.024022 | 10.113479 |
| C | 0.955918  | -1.915478 | 8.681572  |
| C | 2.005765  | -1.290483 | 12.297429 |
| C | 1.993663  | -1.253331 | 10.851568 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.440858  | -0.061357 | 10.175157 |
| C | 2.470953  | -0.134328 | 13.053660 |
| C | 2.245676  | 1.119414  | 16.602806 |
| C | 2.241582  | 1.118756  | 15.198116 |
| C | 1.360714  | 2.044517  | 14.472072 |
| C | 1.377642  | 2.059236  | 13.054610 |
| C | 0.141099  | 2.361662  | 16.621377 |
| C | 0.141183  | 2.371790  | 15.185509 |
| C | -1.082212 | 2.118538  | 14.447659 |
| C | -1.066808 | 2.118509  | 13.009646 |
| C | -2.058428 | 1.303788  | 16.608038 |
| C | -2.054334 | 1.309814  | 15.177577 |
| C | -2.485942 | 0.126878  | 14.443324 |
| C | -2.483726 | 0.129954  | 13.015533 |
| C | -2.260836 | -1.124177 | 16.600650 |
| C | -2.253684 | -1.119180 | 15.175255 |
| C | -1.399446 | -2.053543 | 14.442088 |
| C | -1.397032 | -2.051175 | 13.014634 |
| C | -0.202062 | -2.426737 | 16.606136 |
| C | -0.195079 | -2.424099 | 15.175667 |
| C | 1.035811  | -2.134594 | 14.445594 |
| C | 1.044246  | -2.120245 | 13.007677 |
| C | 1.968080  | -1.308749 | 16.620346 |
| C | 1.976187  | -1.312398 | 15.184179 |
| C | 2.449828  | -0.141249 | 14.471228 |
| C | 3.937214  | 1.959425  | 6.413099  |
| O | 4.972622  | 2.473953  | 6.656880  |

### Structure 3

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|   |           |           |          |
|---|-----------|-----------|----------|
| C | 2.278628  | 0.225186  | 8.681107 |
| C | 3.153353  | 1.120446  | 7.788575 |
| C | 2.444904  | -0.197060 | 0.045351 |
| C | 2.279628  | 1.033152  | 3.600784 |
| C | 2.231037  | 1.038396  | 2.184857 |
| C | 1.353214  | 1.967570  | 1.486123 |
| C | 1.336887  | 1.983738  | 0.061648 |
| C | 0.190648  | 2.295474  | 3.668651 |
| C | 0.164592  | 2.341579  | 2.234359 |
| C | -1.079198 | 2.125787  | 1.512907 |
| C | -1.095675 | 2.136309  | 0.077548 |
| C | -2.040234 | 1.305242  | 3.666942 |
| C | -2.046300 | 1.316215  | 2.236690 |
| C | -2.486574 | 0.135290  | 1.492048 |
| C | -2.490345 | 0.135711  | 0.065042 |
| C | -2.268964 | -1.112551 | 3.639515 |
| C | -2.248880 | -1.110770 | 2.212419 |
| C | -1.393785 | -2.043700 | 1.485050 |
| C | -1.391516 | -2.042463 | 0.054239 |
| C | -0.194012 | -2.401817 | 3.658774 |
| C | -0.191255 | -2.425341 | 2.219705 |
| C | 1.036758  | -2.195230 | 1.483815 |
| C | 1.039526  | -2.192473 | 0.046821 |
| C | 2.028634  | -1.388323 | 3.624456 |
| C | 2.019893  | -1.395821 | 2.202095 |
| C | 2.460881  | -0.209139 | 1.462474 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.561618  | -0.211964 | 4.314947  |
| C | 2.553851  | 1.125812  | 6.391859  |
| C | 1.479837  | 1.895796  | 5.806935  |
| C | 1.409415  | 1.911609  | 4.364872  |
| C | 0.217096  | 1.984747  | 7.995150  |
| C | 0.250768  | 2.132196  | 6.566434  |
| C | -0.998018 | 2.007054  | 5.840971  |
| C | -1.035108 | 2.061076  | 4.406944  |
| C | -2.089445 | 1.271403  | 7.965822  |
| C | -2.053367 | 1.272037  | 6.543835  |
| C | -2.536408 | 0.114225  | 5.800010  |
| C | -2.521982 | 0.119358  | 4.375063  |
| C | -2.356738 | -1.130033 | 7.966843  |
| C | -2.326574 | -1.130581 | 6.535185  |
| C | -1.438079 | -2.034293 | 5.801349  |
| C | -1.415812 | -2.038159 | 4.375155  |
| C | -0.248625 | -2.325813 | 7.957260  |
| C | -0.220518 | -2.342707 | 6.534507  |
| C | 1.022605  | -2.058831 | 5.827210  |
| C | 1.038058  | -2.131126 | 4.385052  |
| C | 1.819862  | -1.030988 | 7.942394  |
| C | 1.972843  | -1.210398 | 6.541475  |
| C | 2.617872  | -0.163389 | 5.718639  |
| C | 2.262096  | 1.126286  | 12.353983 |
| C | 2.278897  | 1.119915  | 10.951637 |
| C | 1.305739  | 1.890827  | 10.189355 |
| C | 1.272266  | 1.490040  | 8.836635  |
| C | 0.133806  | 2.389196  | 12.305578 |
| C | 0.125023  | 2.356191  | 10.869137 |
| C | -1.104765 | 2.085668  | 10.131404 |
| C | -1.063674 | 2.000361  | 8.706534  |
| C | -2.082334 | 1.328227  | 12.292632 |
| C | -2.097850 | 1.315034  | 10.861920 |
| C | -2.568041 | 0.130577  | 10.132641 |
| C | -2.592159 | 0.111949  | 8.702606  |
| C | -2.280665 | -1.094706 | 12.295182 |
| C | -2.304824 | -1.102170 | 10.867706 |
| C | -1.450799 | -2.022399 | 10.124089 |
| C | -1.475435 | -2.036133 | 8.700021  |
| C | -0.192368 | -2.356751 | 12.266627 |
| C | -0.202415 | -2.323114 | 10.831503 |
| C | 0.993219  | -1.991633 | 10.099221 |
| C | 0.938064  | -1.902666 | 8.671442  |
| C | 2.018541  | -1.289798 | 12.270987 |
| C | 2.014696  | -1.234605 | 10.823084 |
| C | 2.517133  | -0.057426 | 10.155417 |
| C | 2.473481  | -0.140591 | 13.041873 |
| C | 2.188341  | 1.052249  | 16.610196 |
| C | 2.187097  | 1.069945  | 15.191588 |
| C | 1.332555  | 2.015183  | 14.468056 |
| C | 1.342544  | 2.034814  | 13.049214 |
| C | 0.133420  | 2.376864  | 16.623217 |
| C | 0.124008  | 2.389266  | 15.190685 |
| C | -1.104201 | 2.142832  | 14.460163 |
| C | -1.105661 | 2.138396  | 13.023152 |
| C | -2.063793 | 1.329953  | 16.620438 |
| C | -2.068496 | 1.331165  | 15.191155 |
| C | -2.496534 | 0.143320  | 14.457204 |
| C | -2.512583 | 0.142151  | 13.027941 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.241784 | -1.100087 | 16.610339 |
| C | -2.242074 | -1.098092 | 15.181485 |
| C | -1.393090 | -2.027240 | 14.439681 |
| C | -1.398866 | -2.018517 | 13.009464 |
| C | -0.192583 | -2.426326 | 16.594296 |
| C | -0.188074 | -2.417004 | 15.156608 |
| C | 1.043215  | -2.159704 | 14.423984 |
| C | 1.046151  | -2.113656 | 12.985637 |
| C | 2.005594  | -1.383949 | 16.597442 |
| C | 2.005395  | -1.364332 | 15.170265 |
| C | 2.443248  | -0.167964 | 14.463861 |
| O | 4.164556  | 1.746122  | 8.093924  |

## Structure 4

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|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.460357  | -0.302499 | 8.515884  |
| C | 2.525654  | 1.031236  | 7.801465  |
| C | 2.417331  | -0.323143 | -0.122235 |
| C | 2.369521  | 0.965363  | 3.438857  |
| C | 2.344202  | 0.954775  | 2.036452  |
| C | 1.504370  | 1.917173  | 1.299392  |
| C | 1.498134  | 1.916853  | -0.122635 |
| C | 0.317326  | 2.296691  | 3.467960  |
| C | 0.310994  | 2.308390  | 2.028875  |
| C | -0.940442 | 2.164956  | 1.309754  |
| C | -0.943787 | 2.173037  | -0.122216 |
| C | -1.982718 | 1.440501  | 3.461379  |
| C | -1.983185 | 1.448706  | 2.036953  |
| C | -2.527569 | 0.309332  | 1.301280  |
| C | -2.524329 | 0.312341  | -0.121892 |
| C | -2.406341 | -0.956124 | 3.453075  |
| C | -2.397577 | -0.952294 | 2.030831  |
| C | -1.604438 | -1.940693 | 1.302394  |
| C | -1.600855 | -1.939822 | -0.122305 |
| C | -0.426556 | -2.375724 | 3.462594  |
| C | -0.422272 | -2.382260 | 2.036555  |
| C | 0.826786  | -2.186267 | 1.310192  |
| C | 0.829079  | -2.192982 | -0.122439 |
| C | 1.832356  | -1.418112 | 3.467898  |
| C | 1.835436  | -1.431494 | 2.029402  |
| C | 2.422893  | -0.320466 | 1.299052  |
| C | 2.446906  | -0.311583 | 4.186966  |
| C | 2.528169  | 1.031645  | 6.315435  |
| C | 1.544427  | 1.934046  | 5.600204  |
| C | 1.527103  | 1.928144  | 4.186122  |
| C | 0.333684  | 2.235225  | 7.780038  |
| C | 0.335411  | 2.234927  | 6.334129  |
| C | -0.917481 | 2.109045  | 5.622149  |
| C | -0.926216 | 2.131648  | 4.191287  |
| C | -1.985538 | 1.424960  | 7.767200  |
| C | -1.984556 | 1.424990  | 6.345950  |
| C | -2.550131 | 0.296273  | 5.610857  |
| C | -2.543258 | 0.300846  | 4.187896  |
| C | -2.425012 | -0.964155 | 7.768788  |
| C | -2.424908 | -0.963774 | 6.344841  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.627549 | -1.946314 | 5.612118  |
| C | -1.619949 | -1.945380 | 4.187548  |
| C | -0.437796 | -2.365076 | 7.768675  |
| C | -0.437662 | -2.364134 | 6.345840  |
| C | 0.806872  | -2.129245 | 5.623076  |
| C | 0.815473  | -2.152451 | 4.191606  |
| C | 1.802564  | -1.360078 | 7.780277  |
| C | 1.803496  | -1.359507 | 6.335395  |
| C | 2.463768  | -0.302444 | 5.600417  |
| C | 2.341156  | 0.956976  | 12.078153 |
| C | 2.365398  | 0.966542  | 10.676056 |
| C | 1.522588  | 1.928460  | 9.929232  |
| C | 1.540860  | 1.933579  | 8.515097  |
| C | 0.307254  | 2.309361  | 12.086101 |
| C | 0.312860  | 2.297229  | 10.647149 |
| C | -0.930160 | 2.132143  | 9.923038  |
| C | -0.919745 | 2.109732  | 8.491515  |
| C | -1.986194 | 1.448362  | 12.077906 |
| C | -1.986114 | 1.439896  | 10.653200 |
| C | -2.544858 | 0.299790  | 9.926330  |
| C | -2.550591 | 0.295739  | 8.502699  |
| C | -2.398336 | -0.952604 | 12.084303 |
| C | -2.406864 | -0.956881 | 10.661584 |
| C | -1.620947 | -1.946232 | 9.927122  |
| C | -1.627941 | -1.947170 | 8.502185  |
| C | -0.423574 | -2.382670 | 12.079343 |
| C | -0.428216 | -2.376851 | 10.653085 |
| C | 0.813783  | -2.153449 | 9.924144  |
| C | 0.806188  | -2.130656 | 8.492288  |
| C | 1.832165  | -1.429075 | 12.086250 |
| C | 1.828947  | -1.417004 | 10.647963 |
| C | 2.443094  | -0.310774 | 9.929234  |
| C | 2.419921  | -0.318161 | 12.815489 |
| C | 2.322107  | 0.946872  | 16.382318 |
| C | 2.321362  | 0.947400  | 14.975037 |
| C | 1.496929  | 1.917677  | 14.236651 |
| C | 1.501609  | 1.919274  | 12.814732 |
| C | 0.304500  | 2.323585  | 16.398190 |
| C | 0.303594  | 2.323758  | 14.959350 |
| C | -0.945375 | 2.173029  | 14.236949 |
| C | -0.943698 | 2.165134  | 12.805258 |
| C | -1.985921 | 1.458643  | 16.391261 |
| C | -1.986683 | 1.458546  | 14.967101 |
| C | -2.525714 | 0.312217  | 14.237161 |
| C | -2.529205 | 0.308629  | 12.814014 |
| C | -2.385054 | -0.946343 | 16.390415 |
| C | -2.385588 | -0.946278 | 14.968582 |
| C | -1.601640 | -1.939760 | 14.237948 |
| C | -1.605613 | -1.940939 | 12.813473 |
| C | -0.418374 | -2.389187 | 16.392398 |
| C | -0.418913 | -2.389202 | 14.966717 |
| C | 0.827916  | -2.192084 | 14.237799 |
| C | 0.824938  | -2.184841 | 12.805601 |
| C | 1.839482  | -1.444516 | 16.397817 |
| C | 1.838802  | -1.443643 | 14.959952 |
| C | 2.415755  | -0.322025 | 14.236212 |
| O | 3.690637  | 1.510364  | 7.062125  |

## Structure 5

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|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.407230  | -0.156877 | 0.040710  |
| C | 2.330499  | 1.069844  | 3.607059  |
| C | 2.310638  | 1.082229  | 2.204136  |
| C | 1.462671  | 2.060526  | 1.477043  |
| C | 1.438107  | 2.070547  | 0.072845  |
| C | 0.270957  | 2.333740  | 3.657383  |
| C | 0.238582  | 2.344764  | 2.226528  |
| C | -0.993278 | 2.048374  | 1.519967  |
| C | -1.021297 | 2.053780  | 0.081344  |
| C | -1.933726 | 1.248952  | 3.675716  |
| C | -1.965177 | 1.258112  | 2.248886  |
| C | -2.465182 | 0.093953  | 1.512148  |
| C | -2.484480 | 0.094585  | 0.088432  |
| C | -2.269070 | -1.167760 | 3.651518  |
| C | -2.273503 | -1.163129 | 2.231509  |
| C | -1.443937 | -2.114595 | 1.481210  |
| C | -1.448614 | -2.106013 | 0.056655  |
| C | -0.231153 | -2.494634 | 3.636096  |
| C | -0.231815 | -2.486355 | 2.205432  |
| C | 0.991078  | -2.189001 | 1.459621  |
| C | 0.989133  | -2.164798 | 0.030142  |
| C | 1.928873  | -1.368646 | 3.613778  |
| C | 1.929293  | -1.353317 | 2.178277  |
| C | 2.409929  | -0.180521 | 1.468107  |
| C | 2.415683  | -0.211214 | 4.316264  |
| C | 2.475865  | 1.050824  | 6.420526  |
| C | 1.584929  | 2.066070  | 5.779139  |
| C | 1.522919  | 2.055643  | 4.371904  |
| C | 0.273823  | 2.416818  | 8.008251  |
| C | 0.344044  | 2.325968  | 6.559605  |
| C | -0.878492 | 1.993656  | 5.839197  |
| C | -0.922237 | 2.009634  | 4.397513  |
| C | -1.922358 | 1.242075  | 7.970408  |
| C | -1.894597 | 1.235570  | 6.546909  |
| C | -2.429480 | 0.089059  | 5.810854  |
| C | -2.436332 | 0.085777  | 4.393150  |
| C | -2.287820 | -1.159847 | 7.958037  |
| C | -2.273809 | -1.166897 | 6.538628  |
| C | -1.442240 | -2.127689 | 5.801237  |
| C | -1.441252 | -2.131169 | 4.378284  |
| C | -0.227046 | -2.438328 | 7.960697  |
| C | -0.226648 | -2.474999 | 6.534991  |
| C | 1.000013  | -2.187409 | 5.799258  |
| C | 0.998859  | -2.203466 | 4.363158  |
| C | 1.927270  | -1.250145 | 7.953184  |
| C | 1.942032  | -1.335058 | 6.511532  |
| C | 2.434682  | -0.222860 | 5.737845  |
| C | 2.486500  | -0.087512 | 8.645375  |
| C | 2.288812  | 1.205530  | 12.280279 |
| C | 2.307748  | 1.263265  | 10.874837 |
| C | 1.399042  | 2.260128  | 10.232245 |
| C | 1.445977  | 2.486842  | 8.860586  |
| C | 0.143012  | 2.366859  | 12.337732 |
| C | 0.133933  | 2.386148  | 10.913884 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.040222 | 2.069809  | 10.141668 |
| C | -0.959897 | 2.041688  | 8.700163  |
| C | -2.047616 | 1.277637  | 12.287734 |
| C | -2.033253 | 1.275536  | 10.854452 |
| C | -2.502254 | 0.103264  | 10.117040 |
| C | -2.467368 | 0.096739  | 8.694647  |
| C | -2.317297 | -1.145184 | 12.274181 |
| C | -2.312608 | -1.147444 | 10.853056 |
| C | -1.455524 | -2.085820 | 10.115232 |
| C | -1.449344 | -2.100801 | 8.694643  |
| C | -0.239797 | -2.406810 | 12.262455 |
| C | -0.232002 | -2.400245 | 10.841874 |
| C | 0.980164  | -2.041651 | 10.108606 |
| C | 0.984709  | -2.070822 | 8.682870  |
| C | 1.895279  | -1.203491 | 12.256864 |
| C | 1.890047  | -1.160741 | 10.814888 |
| C | 2.406214  | -0.003695 | 10.091831 |
| C | 2.399702  | -0.073454 | 12.998056 |
| C | 2.287974  | 1.120883  | 16.581022 |
| C | 2.283203  | 1.146765  | 15.178350 |
| C | 1.408389  | 2.099413  | 14.449937 |
| C | 1.400080  | 2.119965  | 13.045163 |
| C | 0.190367  | 2.354689  | 16.613517 |
| C | 0.170174  | 2.359590  | 15.182758 |
| C | -1.060554 | 2.062765  | 14.473121 |
| C | -1.074918 | 2.063140  | 13.038315 |
| C | -2.015513 | 1.267370  | 16.620995 |
| C | -2.036470 | 1.270077  | 15.193189 |
| C | -2.512632 | 0.102563  | 14.445784 |
| C | -2.519747 | 0.103679  | 13.017880 |
| C | -2.293503 | -1.151920 | 16.597419 |
| C | -2.302705 | -1.148191 | 15.173823 |
| C | -1.458729 | -2.087113 | 14.423601 |
| C | -1.461245 | -2.082455 | 13.001850 |
| C | -0.239289 | -2.456906 | 16.566759 |
| C | -0.238076 | -2.436831 | 15.140886 |
| C | 0.984288  | -2.110556 | 14.406759 |
| C | 0.981809  | -2.078714 | 12.977681 |
| C | 1.920612  | -1.306910 | 16.571770 |
| C | 1.918554  | -1.277460 | 15.133838 |
| C | 2.404264  | -0.106528 | 14.426506 |
| C | 2.709338  | 1.067658  | 7.790501  |
| O | 2.725465  | 2.351655  | 8.329573  |

## Structure 6

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|   |           |           |          |
|---|-----------|-----------|----------|
| C | 2.442365  | -0.000001 | 0.006530 |
| C | 2.115413  | 1.221196  | 3.589645 |
| C | 2.115415  | 1.221197  | 2.163905 |
| C | 1.221261  | 2.115296  | 1.432465 |
| C | 1.221183  | 2.115266  | 0.006545 |
| C | 0.000000  | 2.442523  | 3.589770 |
| C | 0.000000  | 2.442525  | 2.163779 |
| C | -1.221261 | 2.115297  | 1.432464 |
| C | -1.221183 | 2.115268  | 0.006545 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.115413 | 1.221197  | 3.589645  |
| C | -2.115416 | 1.221198  | 2.163905  |
| C | -2.442549 | -0.000001 | 1.432438  |
| C | -2.442366 | -0.000001 | 0.006530  |
| C | -2.115413 | -1.221198 | 3.589645  |
| C | -2.115416 | -1.221199 | 2.163905  |
| C | -1.221260 | -2.115297 | 1.432464  |
| C | -1.221183 | -2.115268 | 0.006546  |
| C | 0.000000  | -2.442523 | 3.589770  |
| C | 0.000001  | -2.442525 | 2.163780  |
| C | 1.221261  | -2.115296 | 1.432464  |
| C | 1.221182  | -2.115265 | 0.006545  |
| C | 2.115411  | -1.221197 | 3.589646  |
| C | 2.115414  | -1.221198 | 2.163906  |
| C | 2.442548  | 0.000000  | 1.432439  |
| C | 2.442550  | -0.000001 | 4.321111  |
| C | 2.115131  | 1.221168  | 7.904960  |
| C | 2.115132  | 1.221170  | 6.478907  |
| C | 1.221182  | 2.115264  | 5.747003  |
| C | 1.221261  | 2.115296  | 4.321085  |
| C | 0.000001  | 2.442491  | 7.905012  |
| C | 0.000000  | 2.442495  | 6.478854  |
| C | -1.221182 | 2.115265  | 5.747004  |
| C | -1.221261 | 2.115298  | 4.321087  |
| C | -2.115132 | 1.221171  | 7.904960  |
| C | -2.115132 | 1.221170  | 6.478907  |
| C | -2.442360 | 0.000000  | 5.747018  |
| C | -2.442551 | 0.000000  | 4.321110  |
| C | -2.115132 | -1.221170 | 7.904960  |
| C | -2.115132 | -1.221171 | 6.478907  |
| C | -1.221181 | -2.115264 | 5.747003  |
| C | -1.221260 | -2.115297 | 4.321086  |
| C | 0.000000  | -2.442490 | 7.905012  |
| C | 0.000001  | -2.442494 | 6.478854  |
| C | 1.221182  | -2.115264 | 5.747004  |
| C | 1.221260  | -2.115297 | 4.321087  |
| C | 2.115131  | -1.221169 | 7.904961  |
| C | 2.115132  | -1.221170 | 6.478908  |
| C | 2.442360  | -0.000001 | 5.747019  |
| C | 2.442364  | 0.000000  | 8.636848  |
| C | 2.115413  | 1.221196  | 12.219963 |
| C | 2.115416  | 1.221197  | 10.794223 |
| C | 1.221261  | 2.115295  | 10.062782 |
| C | 1.221183  | 2.115264  | 8.636864  |
| C | 0.000001  | 2.442523  | 12.220087 |
| C | 0.000000  | 2.442525  | 10.794096 |
| C | -1.221260 | 2.115295  | 10.062782 |
| C | -1.221184 | 2.115267  | 8.636864  |
| C | -2.115414 | 1.221197  | 12.219963 |
| C | -2.115416 | 1.221197  | 10.794223 |
| C | -2.442549 | 0.000000  | 10.062756 |
| C | -2.442366 | 0.000001  | 8.636848  |
| C | -2.115413 | -1.221198 | 12.219963 |
| C | -2.115415 | -1.221199 | 10.794223 |
| C | -1.221260 | -2.115296 | 10.062782 |
| C | -1.221182 | -2.115265 | 8.636864  |
| C | 0.000000  | -2.442523 | 12.220086 |
| C | 0.000001  | -2.442525 | 10.794097 |
| C | 1.221261  | -2.115295 | 10.062783 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.221183  | -2.115266 | 8.636865  |
| C | 2.115412  | -1.221197 | 12.219964 |
| C | 2.115415  | -1.221197 | 10.794224 |
| C | 2.442549  | 0.000000  | 10.062756 |
| C | 2.442551  | 0.000000  | 12.951429 |
| C | 2.115132  | 1.221170  | 16.535282 |
| C | 2.115134  | 1.221171  | 15.109227 |
| C | 1.221183  | 2.115266  | 14.377322 |
| C | 1.221261  | 2.115298  | 12.951403 |
| C | 0.000001  | 2.442496  | 16.535335 |
| C | 0.000001  | 2.442497  | 15.109174 |
| C | -1.221183 | 2.115267  | 14.377323 |
| C | -1.221261 | 2.115299  | 12.951404 |
| C | -2.115133 | 1.221171  | 16.535282 |
| C | -2.115134 | 1.221171  | 15.109227 |
| C | -2.442362 | 0.000000  | 14.377337 |
| C | -2.442552 | 0.000000  | 12.951428 |
| C | -2.115134 | -1.221173 | 16.535282 |
| C | -2.115135 | -1.221172 | 15.109227 |
| C | -1.221182 | -2.115266 | 14.377322 |
| C | -1.221261 | -2.115298 | 12.951404 |
| C | 0.000000  | -2.442495 | 16.535334 |
| C | 0.000000  | -2.442496 | 15.109174 |
| C | 1.221183  | -2.115266 | 14.377323 |
| C | 1.221261  | -2.115298 | 12.951405 |
| C | 2.115133  | -1.221171 | 16.535282 |
| C | 2.115134  | -1.221172 | 15.109227 |
| C | 2.442362  | 0.000000  | 14.377338 |

## Structure TS1

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|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.201196  | 0.222068  | 8.823973  |
| C | 3.185912  | 1.256338  | 7.424028  |
| C | 2.274165  | -0.395934 | -0.040854 |
| C | 2.183752  | 0.973111  | 3.462210  |
| C | 2.089012  | 0.886308  | 2.054708  |
| C | 1.105729  | 1.741363  | 1.430457  |
| C | 1.055107  | 1.809434  | 0.008164  |
| C | -0.053436 | 2.045873  | 3.604477  |
| C | -0.104271 | 1.982378  | 2.192199  |
| C | -1.340101 | 1.724574  | 1.449553  |
| C | -1.361357 | 1.722784  | 0.022299  |
| C | -2.232051 | 0.956326  | 3.648824  |
| C | -2.273022 | 0.897574  | 2.244747  |
| C | -2.596001 | -0.373002 | 1.530006  |
| C | -2.573329 | -0.406944 | 0.116944  |
| C | -2.149196 | -1.464603 | 3.679531  |
| C | -2.188220 | -1.531882 | 2.251545  |
| C | -1.389367 | -2.452422 | 1.494507  |
| C | -1.356067 | -2.491948 | 0.056250  |
| C | -0.040184 | -2.658482 | 3.622255  |
| C | -0.095069 | -2.715445 | 2.175773  |
| C | 1.066132  | -2.379143 | 1.430568  |
| C | 1.034037  | -2.456670 | -0.020286 |
| C | 2.110584  | -1.494988 | 3.512310  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.052212  | -1.569335 | 2.129265  |
| C | 2.412256  | -0.379226 | 1.333930  |
| C | 2.556426  | -0.253967 | 4.184146  |
| C | 2.476077  | 1.091831  | 6.202692  |
| C | 1.286694  | 1.782343  | 5.670115  |
| C | 1.222184  | 1.805841  | 4.255871  |
| C | 0.180435  | 1.683445  | 7.965855  |
| C | 0.106773  | 1.805056  | 6.524426  |
| C | -1.160760 | 1.748266  | 5.891562  |
| C | -1.245390 | 1.785163  | 4.421168  |
| C | -2.125015 | 0.909776  | 7.913976  |
| C | -2.164468 | 0.978585  | 6.551348  |
| C | -2.561842 | -0.223283 | 5.863884  |
| C | -2.548842 | -0.220840 | 4.405637  |
| C | -2.078311 | -1.393263 | 7.904146  |
| C | -2.035631 | -1.416565 | 6.495146  |
| C | -1.165071 | -2.333235 | 5.828347  |
| C | -1.230733 | -2.367573 | 4.389688  |
| C | 0.116052  | -2.507417 | 7.898150  |
| C | 0.127653  | -2.586761 | 6.504249  |
| C | 1.280364  | -2.256364 | 5.805118  |
| C | 1.245813  | -2.338925 | 4.366832  |
| C | 1.993605  | -1.072860 | 7.874516  |
| C | 2.132579  | -1.234826 | 6.450404  |
| C | 2.706009  | -0.207332 | 5.578279  |
| C | 2.157097  | 1.048256  | 12.365450 |
| C | 2.143925  | 1.000653  | 10.995256 |
| C | 1.143164  | 1.701160  | 10.219516 |
| C | 1.197574  | 1.316374  | 8.848470  |
| C | -0.064170 | 2.138861  | 12.320007 |
| C | -0.045719 | 2.092187  | 10.905463 |
| C | -1.202947 | 1.713173  | 10.142383 |
| C | -1.062171 | 1.636852  | 8.689265  |
| C | -2.224894 | 0.968733  | 12.285590 |
| C | -2.198096 | 0.943136  | 10.867137 |
| C | -2.566734 | -0.307336 | 10.049886 |
| C | -2.541555 | -0.287846 | 8.662179  |
| C | -2.166110 | -1.461366 | 12.210101 |
| C | -2.181988 | -1.456953 | 10.781196 |
| C | -1.169744 | -2.236875 | 10.017732 |
| C | -1.142569 | -2.287225 | 8.596743  |
| C | 0.006903  | -2.654873 | 12.216713 |
| C | 0.012711  | -2.531132 | 10.788464 |
| C | 1.248810  | -2.214290 | 10.100538 |
| C | 1.250223  | -2.034457 | 8.648368  |
| C | 2.179216  | -1.480679 | 12.296425 |
| C | 2.182176  | -1.420530 | 10.895935 |
| C | 2.561448  | -0.136835 | 10.192440 |
| C | 2.446762  | -0.223172 | 13.043161 |
| C | 1.914358  | 0.857971  | 16.600863 |
| C | 1.989085  | 0.920941  | 15.203687 |
| C | 1.139194  | 1.829172  | 14.503345 |
| C | 1.174430  | 1.920568  | 13.052219 |
| C | -0.159630 | 2.025073  | 16.602800 |
| C | -0.178419 | 2.088765  | 15.179631 |
| C | -1.356879 | 1.740917  | 14.463566 |
| C | -1.267384 | 1.813677  | 13.034591 |
| C | -2.288433 | 0.814285  | 16.600640 |
| C | -2.254035 | 0.881404  | 15.212739 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.546355 | -0.326600 | 14.454564 |
| C | -2.565411 | -0.289589 | 12.993354 |
| C | -2.212683 | -1.607911 | 16.623085 |
| C | -2.185208 | -1.537007 | 15.168798 |
| C | -1.313827 | -2.393393 | 14.390717 |
| C | -1.201166 | -2.269454 | 12.934952 |
| C | -0.147479 | -2.805927 | 16.542907 |
| C | -0.094996 | -2.731443 | 15.086174 |
| C | 1.156583  | -2.409875 | 14.413273 |
| C | 1.226980  | -2.348959 | 12.967039 |
| C | 1.904004  | -1.560299 | 16.510671 |
| C | 2.026117  | -1.545162 | 15.145500 |
| C | 2.407314  | -0.285006 | 14.452319 |
| O | 4.254352  | 1.560330  | 7.862004  |

## Structure TS2

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|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 3.832181  | 1.510364  | 6.783950  |
| C | 5.255359  | 1.798442  | 5.890391  |
| C | 2.451212  | -0.398634 | 8.526392  |
| C | 2.423732  | 0.923216  | 7.867715  |
| C | 2.401390  | -0.575233 | -0.120503 |
| C | 2.303250  | 0.836243  | 3.438877  |
| C | 2.267941  | 0.743516  | 2.021982  |
| C | 1.507827  | 1.684353  | 1.319433  |
| C | 1.485133  | 1.664636  | -0.101242 |
| C | 0.378028  | 2.281780  | 3.479196  |
| C | 0.388201  | 2.238899  | 2.023907  |
| C | -0.867251 | 2.088415  | 1.319903  |
| C | -0.907654 | 2.066436  | -0.074081 |
| C | -1.884458 | 1.435329  | 3.431999  |
| C | -1.949995 | 1.383368  | 2.042554  |
| C | -2.443633 | 0.226367  | 1.302676  |
| C | -2.440767 | 0.238649  | -0.113535 |
| C | -2.305126 | -1.039559 | 3.470048  |
| C | -2.280416 | -1.083487 | 2.025452  |
| C | -1.563876 | -2.097094 | 1.311119  |
| C | -1.498656 | -2.037149 | -0.155479 |
| C | -0.404814 | -2.602411 | 3.442403  |
| C | -0.404706 | -2.591720 | 2.035541  |
| C | 0.912837  | -2.417537 | 1.327156  |
| C | 0.897003  | -2.439543 | -0.077330 |
| C | 1.849660  | -1.569302 | 3.495088  |
| C | 1.949038  | -1.644776 | 2.029783  |
| C | 2.465008  | -0.509693 | 1.306259  |
| C | 2.384446  | -0.445416 | 4.212746  |
| C | 2.675654  | 1.055501  | 6.342312  |
| C | 1.626073  | 1.917157  | 5.576018  |
| C | 1.524219  | 1.785352  | 4.189910  |
| C | 0.471373  | 2.298002  | 7.776825  |
| C | 0.432377  | 2.248332  | 6.314009  |
| C | -0.863903 | 2.231141  | 5.600172  |
| C | -0.901422 | 2.205301  | 4.168590  |
| C | -1.835442 | 1.500297  | 7.793234  |
| C | -1.838967 | 1.441987  | 6.376041  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -2.342524 | 0.283432  | 5.619177  |
| C | -2.312703 | 0.253211  | 4.179294  |
| C | -2.347634 | -0.952690 | 7.757789  |
| C | -2.346011 | -0.978340 | 6.336355  |
| C | -1.587593 | -1.993335 | 5.571601  |
| C | -1.598409 | -2.061483 | 4.193619  |
| C | -0.510752 | -2.530741 | 7.774601  |
| C | -0.509029 | -2.488087 | 6.350216  |
| C | 0.787876  | -2.245771 | 5.617052  |
| C | 0.820188  | -2.389416 | 4.194866  |
| C | 1.755380  | -1.470655 | 7.797144  |
| C | 1.717214  | -1.399895 | 6.324014  |
| C | 2.482857  | -0.348339 | 5.611699  |
| C | 2.324522  | 0.713708  | 12.101837 |
| C | 2.356173  | 0.799103  | 10.694448 |
| C | 1.595749  | 1.874509  | 9.979213  |
| C | 1.626275  | 1.910522  | 8.553269  |
| C | 0.375407  | 2.200345  | 12.130309 |
| C | 0.448357  | 2.313195  | 10.707277 |
| C | -0.837585 | 2.207365  | 9.974487  |
| C | -0.786355 | 2.259631  | 8.519422  |
| C | -1.967123 | 1.552858  | 12.087646 |
| C | -1.926009 | 1.474982  | 10.682821 |
| C | -2.420379 | 0.313017  | 9.883800  |
| C | -2.410432 | 0.351198  | 8.492487  |
| C | -2.310597 | -0.896691 | 12.061840 |
| C | -2.286389 | -0.928039 | 10.653277 |
| C | -1.618105 | -1.975763 | 9.922706  |
| C | -1.633261 | -1.967839 | 8.522944  |
| C | -0.454746 | -2.508429 | 12.076341 |
| C | -0.487408 | -2.486768 | 10.666352 |
| C | 0.783245  | -2.354317 | 9.940462  |
| C | 0.797863  | -2.326492 | 8.468728  |
| C | 1.796967  | -1.655929 | 12.029752 |
| C | 1.839930  | -1.608445 | 10.609396 |
| C | 2.394567  | -0.450884 | 9.941465  |
| C | 2.401587  | -0.563685 | 12.793866 |
| C | 2.309323  | 0.650062  | 16.383862 |
| C | 2.317641  | 0.670475  | 15.000778 |
| C | 1.495689  | 1.648427  | 14.282907 |
| C | 1.508014  | 1.688412  | 12.858458 |
| C | 0.332065  | 2.140126  | 16.441971 |
| C | 0.374505  | 2.127609  | 15.009279 |
| C | -0.869832 | 2.082151  | 14.259630 |
| C | -0.886857 | 2.198561  | 12.853102 |
| C | -1.990260 | 1.458553  | 16.395001 |
| C | -2.019486 | 1.487209  | 15.007786 |
| C | -2.525861 | 0.290351  | 14.258744 |
| C | -2.456782 | 0.308716  | 12.834432 |
| C | -2.270000 | -0.988828 | 16.393095 |
| C | -2.257728 | -0.963471 | 14.975086 |
| C | -1.504301 | -1.976152 | 14.206145 |
| C | -1.534441 | -1.935245 | 12.803758 |
| C | -0.335566 | -2.524436 | 16.363895 |
| C | -0.322132 | -2.541642 | 14.938961 |
| C | 0.893086  | -2.485950 | 14.182236 |
| C | 0.817590  | -2.436704 | 12.759761 |
| C | 1.903248  | -1.705440 | 16.414107 |
| C | 1.908305  | -1.738593 | 14.923518 |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 2.408317 | -0.560155 | 14.204505 |
| O | 5.969547 | 0.781409  | 5.928285  |

## Structure TS3

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|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 3.720653  | -0.870981 | 7.893187  |
| C | 5.207076  | -1.413241 | 7.267734  |
| C | 0.836685  | -1.867754 | -0.129883 |
| C | 1.772531  | -1.030260 | 3.436305  |
| C | 1.759011  | -1.042064 | 2.016182  |
| C | 2.213931  | 0.152409  | 1.282632  |
| C | 2.228806  | 0.202811  | -0.121140 |
| C | 2.078351  | 1.363884  | 3.436675  |
| C | 1.966747  | 1.363870  | 2.023406  |
| C | 1.044049  | 2.259517  | 1.316961  |
| C | 1.014878  | 2.325719  | -0.115437 |
| C | -0.108515 | 2.442377  | 3.492462  |
| C | -0.170207 | 2.469413  | 2.036828  |
| C | -1.424983 | 2.190237  | 1.330340  |
| C | -1.472624 | 2.209197  | -0.088065 |
| C | -2.239772 | 1.179237  | 3.501024  |
| C | -2.284060 | 1.277810  | 2.049604  |
| C | -2.767542 | 0.107383  | 1.340378  |
| C | -2.798549 | 0.106708  | -0.127395 |
| C | -2.522424 | -1.203854 | 3.478897  |
| C | -2.483155 | -1.165333 | 2.076671  |
| C | -1.593209 | -2.053015 | 1.288849  |
| C | -1.642604 | -2.094369 | -0.115960 |
| C | -0.357109 | -2.315943 | 3.494525  |
| C | -0.360356 | -2.290598 | 2.041866  |
| C | 0.815235  | -1.851646 | 1.294270  |
| C | 0.877859  | -1.921513 | 4.179641  |
| C | 2.049300  | -1.208024 | 6.252267  |
| C | 2.338305  | 0.031301  | 5.578094  |
| C | 2.236150  | 0.090194  | 4.144432  |
| C | 2.017905  | 1.278050  | 7.759644  |
| C | 2.070606  | 1.270048  | 6.327033  |
| C | 1.078359  | 2.085658  | 5.608538  |
| C | 1.102789  | 2.180364  | 4.206532  |
| C | -0.163212 | 2.347058  | 7.800929  |
| C | -0.163156 | 2.386087  | 6.357205  |
| C | -1.371093 | 1.992871  | 5.666620  |
| C | -1.362116 | 2.062497  | 4.235347  |
| C | -2.279465 | 1.181801  | 7.813386  |
| C | -2.353568 | 1.135796  | 6.399041  |
| C | -2.684988 | -0.057847 | 5.675898  |
| C | -2.733241 | -0.030519 | 4.229056  |
| C | -2.397278 | -1.266863 | 7.812820  |
| C | -2.487705 | -1.292358 | 6.397944  |
| C | -1.532919 | -2.191936 | 5.699502  |
| C | -1.615330 | -2.148468 | 4.252305  |
| C | -0.112418 | -2.154855 | 7.867685  |
| C | -0.227738 | -2.307914 | 6.416972  |
| C | 0.937590  | -1.971058 | 5.602683  |
| C | 1.148243  | -1.978581 | 8.526835  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 1.917871  | -1.045004 | 12.168156 |
| C | 2.074394  | -1.127425 | 10.737067 |
| C | 2.440765  | 0.131459  | 10.027056 |
| C | 2.559185  | 0.119898  | 8.533522  |
| C | 2.009612  | 1.426350  | 12.141055 |
| C | 1.960252  | 1.318989  | 10.714302 |
| C | 1.053467  | 2.126421  | 9.950014  |
| C | 1.051848  | 2.047462  | 8.483926  |
| C | -0.161857 | 2.564531  | 12.094534 |
| C | -0.202420 | 2.520880  | 10.616065 |
| C | -1.383885 | 2.099060  | 9.946486  |
| C | -1.397564 | 2.038212  | 8.504918  |
| C | -2.267500 | 1.387102  | 12.125911 |
| C | -2.384214 | 1.355692  | 10.665907 |
| C | -2.701710 | 0.085896  | 9.970391  |
| C | -2.715770 | -0.006977 | 8.568221  |
| C | -2.301121 | -1.072779 | 12.143248 |
| C | -2.390259 | -1.182807 | 10.719108 |
| C | -1.396711 | -1.971473 | 10.006517 |
| C | -1.365570 | -2.015219 | 8.564154  |
| C | -0.182168 | -2.211933 | 12.136539 |
| C | -0.161290 | -2.259649 | 10.675668 |
| C | 1.082570  | -1.900729 | 9.951888  |
| C | 0.967390  | -1.878639 | 12.918507 |
| C | 1.759341  | -0.961110 | 16.474194 |
| C | 1.731772  | -0.993499 | 15.038105 |
| C | 2.210633  | 0.159837  | 14.312504 |
| C | 2.262340  | 0.143147  | 12.891295 |
| C | 1.916212  | 1.416231  | 16.456051 |
| C | 1.900691  | 1.405950  | 15.015153 |
| C | 0.936660  | 2.259959  | 14.286098 |
| C | 1.015136  | 2.297043  | 12.892953 |
| C | -0.243278 | 2.536474  | 16.481688 |
| C | -0.234259 | 2.610313  | 15.033598 |
| C | -1.420509 | 2.259964  | 14.247247 |
| C | -1.417538 | 2.272320  | 12.840166 |
| C | -2.407693 | 1.356441  | 16.464228 |
| C | -2.340071 | 1.374097  | 15.029054 |
| C | -2.656892 | 0.169937  | 14.341237 |
| C | -2.623461 | 0.144175  | 12.860483 |
| C | -2.481268 | -1.141031 | 16.463003 |
| C | -2.404750 | -1.095053 | 15.020691 |
| C | -1.461129 | -1.977558 | 14.311821 |
| C | -1.423013 | -1.956056 | 12.870202 |
| C | -0.357579 | -2.284094 | 16.450407 |
| C | -0.270218 | -2.338612 | 15.029946 |
| C | 0.948205  | -1.899913 | 14.326868 |
| C | 2.255547  | -1.229497 | 7.725054  |
| O | 6.228084  | -0.816179 | 7.269965  |