

Cartesian coordinates of : PACN2_ 1

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.002450 | 0.002918 | -0.144599 |
| 6 | 0.002252 | 0.002620 | 1.307971 |
| 7 | 0.002083 | 0.002404 | 2.461249 |
| 1 | 0.802766 | -0.647380 | -0.508214 |
| 1 | 0.165595 | 1.021240 | -0.507933 |
| 1 | -0.960880 | -0.364871 | -0.508381 |
| 6 | 0.000965 | 0.002029 | 7.593521 |
| 6 | 0.001326 | 0.002065 | 6.140950 |
| 7 | 0.001600 | 0.002114 | 4.987672 |
| 1 | -0.963241 | -0.363913 | 7.956844 |
| 1 | 0.166007 | 1.019940 | 7.957152 |
| 1 | 0.799836 | -0.649954 | 7.957295 |
| 1 | 0.001857 | 0.002234 | 3.724461 |

Cartesian coordinates of : PACN2_ 2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.000661 | -1.285763 | -0.000001 |
| 6 | 2.049630 | 0.156033 | -0.000000 |
| 7 | 2.170710 | 1.300047 | -0.000001 |
| 1 | 1.451628 | -1.610543 | -0.889277 |
| 1 | 1.451623 | -1.610544 | 0.889273 |
| 1 | 3.021823 | -1.679870 | 0.000002 |
| 7 | -0.725943 | -0.037427 | 0.000003 |
| 6 | -1.886869 | 0.002615 | -0.000000 |
| 6 | -3.345361 | 0.052966 | -0.000001 |
| 1 | -3.751922 | -0.961447 | -0.001137 |
| 1 | -3.698922 | 0.579907 | -0.889741 |
| 1 | -3.698989 | 0.577942 | 0.890874 |
| 1 | 2.203021 | 2.311107 | -0.000000 |

Cartesian coordinates of : PACN2_ 3

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.475194 | -0.000157 | -0.000012 |
| 6 | 2.915238 | -0.000018 | 0.000025 |
| 7 | 4.066681 | 0.000087 | 0.000010 |
| 1 | 1.100613 | -1.012247 | -0.185283 |
| 1 | 1.100462 | 0.666294 | -0.783839 |
| 1 | 1.100464 | 0.345360 | 0.969097 |
| 6 | -4.053744 | 0.000010 | 0.000053 |
| 6 | -2.593815 | 0.000025 | -0.000022 |
| 7 | -1.432488 | 0.000083 | -0.000079 |
| 1 | -4.425967 | -0.243165 | -0.998186 |
| 1 | -4.425925 | 0.986097 | 0.288624 |
| 1 | -4.425898 | -0.742959 | 0.709739 |
| 1 | 5.079669 | 0.000268 | 0.000063 |

Cartesian coordinates of : PACN3_1

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.019295 | 1.282573 | 0.000046 |
| 1 | 4.981616 | 2.094647 | -0.730510 |
| 1 | 5.828241 | 0.596278 | -0.263176 |
| 1 | 5.205861 | 1.697559 | 0.993835 |
| 6 | 3.752144 | 0.566073 | -0.000023 |
| 7 | 2.746095 | -0.003372 | -0.000040 |
| 6 | -4.079954 | 2.335452 | 0.000031 |
| 1 | -5.115412 | 2.014556 | 0.137998 |
| 1 | -3.996492 | 2.867532 | -0.950799 |
| 1 | -3.806512 | 3.012502 | 0.813017 |
| 6 | -3.194952 | 1.174004 | 0.000011 |
| 7 | -2.491645 | 0.249877 | -0.000122 |
| 6 | -1.690643 | -2.688789 | 0.000059 |
| 6 | -0.473754 | -1.903221 | 0.000008 |
| 7 | 0.519035 | -1.321752 | -0.000030 |
| 1 | -1.435401 | -3.751962 | -0.000047 |
| 1 | -2.274120 | -2.428767 | -0.886899 |
| 1 | -2.273937 | -2.428914 | 0.887180 |
| 1 | 1.478944 | -0.743261 | -0.000048 |

Cartesian coordinates of : PACN3_2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.083416 | 2.333274 | 0.000044 |
| 1 | 3.494063 | 3.253431 | 0.001535 |
| 1 | 4.716837 | 2.317824 | -0.890309 |
| 1 | 4.718803 | 2.316213 | 0.888966 |
| 6 | 3.196667 | 1.173156 | -0.000026 |
| 7 | 2.492314 | 0.249825 | -0.000081 |
| 6 | -5.020835 | 1.282294 | 0.000052 |
| 1 | -4.984554 | 2.092745 | -0.732373 |
| 1 | -5.206380 | 1.699398 | 0.993145 |
| 1 | -5.829721 | 0.594950 | -0.260605 |
| 6 | -3.753279 | 0.566507 | -0.000024 |
| 7 | -2.746922 | -0.002396 | -0.000048 |
| 6 | 1.689511 | -2.688342 | 0.000051 |
| 6 | 0.472944 | -1.902277 | 0.000005 |
| 7 | -0.519662 | -1.320498 | -0.000030 |
| 1 | 2.273024 | -2.428599 | 0.887062 |
| 1 | 2.273021 | -2.428712 | -0.886994 |
| 1 | 1.433809 | -3.751406 | 0.000120 |
| 1 | -1.479556 | -0.742029 | -0.000047 |

Cartesian coordinates of : PACN3_3

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

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-----
 6      3.954765      -2.454935      0.000016
 1      3.744885      -3.053016      -0.890133
 1      3.744665      -3.053127      0.890038
 1      5.011739      -2.177393      0.000165
 6      3.125503      -1.253049      -0.000011
 7      2.466727      -0.296661      -0.000031
 6     -4.916842      -1.342153      -0.000009
 1     -4.961805      -1.976198      -0.889159
 1     -5.763394      -0.650759      -0.005411
 1     -4.966661      -1.968201      0.894532
 6     -3.671494      -0.588486      0.000003
 7     -2.682896      0.010626      0.000012
 6      1.669127      2.826660      -0.000004
 6      0.467140      2.019483      0.000008
 7     -0.501682      1.399004      0.000012
 1      2.524582      2.144780      -0.000390
 1      1.682882      3.454886      0.894988
 1      1.682488      3.455457      -0.894602
 1     -1.443620      0.787662      0.000013
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Cartesian coordinates of : PACN3_ 4

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Atomic number (AN) and Cartesian coordinates

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| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.070919 | 0.004784 | 0.033388 |
| 6 | -0.014845 | 0.000752 | 1.487279 |
| 7 | 0.029674 | -0.002426 | 2.641927 |
| 1 | -0.173132 | 1.032050 | -0.325938 |
| 1 | -0.929082 | -0.583762 | -0.301283 |
| 1 | 0.847140 | -0.430854 | -0.369375 |
| 6 | 0.447442 | -0.029305 | 13.405008 |
| 6 | 0.390073 | -0.025698 | 11.945721 |
| 7 | 0.344500 | -0.022830 | 10.785440 |
| 1 | 0.971944 | -0.921660 | 13.755303 |
| 1 | -0.564283 | -0.026449 | 13.817944 |
| 1 | 0.978652 | 0.857434 | 13.759434 |
| 7 | 0.128420 | -0.009160 | 5.204493 |
| 6 | 0.172807 | -0.012060 | 6.355703 |
| 6 | 0.228638 | -0.015660 | 7.802828 |
| 1 | -0.337080 | 0.829376 | 8.203842 |
| 1 | -0.198834 | -0.942521 | 8.194140 |
| 1 | 1.265418 | 0.063384 | 8.140129 |
| 1 | 0.084334 | -0.006196 | 4.060424 |

Cartesian coordinates of : PACN3_ 5

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Atomic number (AN) and Cartesian coordinates

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| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.225586 | 4.036563 | -0.001841 |
| 1 | -0.183889 | 4.409041 | 0.940375 |
| 1 | -0.389464 | 4.403645 | -0.827151 |
| 1 | 1.242092 | 4.419316 | -0.121591 |
| 6 | 0.238177 | 2.575434 | 0.001199 |
| 7 | 0.247572 | 1.413828 | 0.003794 |
| 6 | -3.982145 | -1.144746 | 0.001134 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.340587 | -1.032280 | -1.025346 |
| 1 | -4.278443 | -0.271091 | 0.587246 |
| 1 | -4.420222 | -2.043908 | 0.441903 |
| 6 | -2.532077 | -1.258820 | -0.000606 |
| 7 | -1.382113 | -1.349035 | -0.001937 |
| 6 | 3.749586 | -1.586526 | 0.000784 |
| 6 | 2.298060 | -1.547592 | -0.000528 |
| 7 | 1.148164 | -1.511492 | -0.001522 |
| 1 | 4.099008 | -2.125168 | 0.885644 |
| 1 | 4.136206 | -0.564040 | 0.017548 |
| 1 | 4.101301 | -2.096737 | -0.899882 |
| 1 | -0.044490 | -1.417762 | -0.001939 |

Cartesian coordinates of : PACN3_ 6

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.998499 | 1.075096 | -0.200249 |
| 1 | 5.003458 | 1.811212 | -1.007893 |
| 1 | 5.728089 | 0.293276 | -0.425324 |
| 1 | 5.281662 | 1.568369 | 0.732867 |
| 6 | 3.667496 | 0.489928 | -0.068892 |
| 7 | 2.608729 | 0.024062 | 0.035595 |
| 6 | -4.998394 | 1.075279 | -0.200295 |
| 1 | -5.704909 | 0.318651 | -0.550359 |
| 1 | -4.973313 | 1.899365 | -0.917539 |
| 1 | -5.334626 | 1.455567 | 0.767455 |
| 6 | -3.667541 | 0.489790 | -0.068877 |
| 7 | -2.608844 | 0.023767 | 0.035626 |
| 6 | -0.000023 | -0.789062 | 1.403705 |
| 6 | 0.000006 | -1.180640 | 0.016715 |
| 7 | 0.000035 | -1.541208 | -1.075350 |
| 1 | 0.909357 | -1.175307 | 1.872122 |
| 1 | -0.909260 | -1.175599 | 1.872160 |
| 1 | -0.000203 | 0.304337 | 1.440921 |
| 1 | 0.000054 | -1.808573 | -2.048153 |

Cartesian coordinates of : PACN3_ 7

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.515275 | -0.017339 | -0.009770 |
| 6 | -4.055511 | -0.029536 | -0.004292 |
| 7 | -2.894113 | -0.039247 | 0.000071 |
| 1 | -5.895407 | -1.039341 | -0.082026 |
| 1 | -5.879383 | 0.559191 | -0.863724 |
| 1 | -5.887048 | 0.436561 | 0.912164 |
| 6 | -0.079692 | -1.211579 | 0.010860 |
| 6 | -0.038242 | 0.228451 | 0.009740 |
| 7 | 0.023829 | 1.376452 | 0.009228 |
| 1 | -0.621520 | -1.541426 | -0.880442 |
| 1 | -0.627350 | -1.540025 | 0.899101 |
| 1 | 0.954012 | -1.570894 | 0.014222 |
| 6 | 5.549685 | -0.036998 | -0.010051 |
| 6 | 4.089816 | -0.039706 | -0.003881 |
| 7 | 2.928325 | -0.042684 | 0.000870 |

| | | | |
|---|----------|-----------|-----------|
| 1 | 5.925991 | -0.700475 | 0.772515 |
| 1 | 5.921342 | 0.974414 | 0.171830 |
| 1 | 5.918183 | -0.383220 | -0.978837 |
| 1 | 0.080203 | 2.383810 | 0.008377 |

Cartesian coordinates of : PACN3_ 8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|------------|
| 6 | 0.000152 | 0.000734 | 0.042770 |
| 6 | 0.000597 | -0.000212 | 1.482059 |
| 7 | 0.000957 | -0.000971 | 2.633789 |
| 1 | 0.409314 | -0.942115 | -0.334876 |
| 1 | 0.612156 | 0.826987 | -0.333742 |
| 1 | -1.021364 | 0.118094 | -0.333701 |
| 6 | -0.000066 | 0.002170 | -5.448994 |
| 6 | -0.000179 | 0.002012 | -3.989956 |
| 7 | -0.000254 | 0.001870 | -2.827839 |
| 1 | 1.016148 | -0.107878 | -5.833700 |
| 1 | -0.412794 | 0.937280 | -5.833730 |
| 1 | -0.603453 | -0.822798 | -5.833909 |
| 1 | 0.001272 | -0.001636 | 3.646373 |
| 6 | -0.000935 | 0.005842 | -11.185276 |
| 1 | 0.423476 | -0.928715 | -11.560250 |
| 1 | 0.596350 | 0.841409 | -11.558390 |
| 1 | -1.023054 | 0.106061 | -11.558586 |
| 6 | -0.000408 | 0.004297 | -9.724267 |
| 7 | -0.000010 | 0.003117 | -8.563186 |

Cartesian coordinates of : PACN3_ 9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.070834 | 0.033112 | -0.000001 |
| 6 | -4.264993 | 0.835726 | 0.000001 |
| 7 | -5.221874 | 1.477051 | 0.000003 |
| 1 | -3.045121 | -0.604800 | 0.889621 |
| 1 | -2.182932 | 0.674412 | 0.000017 |
| 1 | -3.045106 | -0.604771 | -0.889643 |
| 6 | 1.685309 | -2.618971 | 0.000005 |
| 6 | 0.355771 | -2.019253 | -0.000005 |
| 7 | -0.710833 | -1.559916 | -0.000011 |
| 1 | 1.602560 | -3.708599 | 0.000090 |
| 1 | 2.233960 | -2.287231 | 0.884317 |
| 1 | 2.233912 | -2.287370 | -0.884390 |
| 1 | -6.063611 | 2.039488 | 0.000004 |
| 6 | 4.627420 | 2.104707 | -0.000009 |
| 1 | 4.597557 | 2.738492 | 0.889687 |
| 1 | 4.597221 | 2.738884 | -0.889414 |
| 1 | 5.562905 | 1.539854 | -0.000311 |
| 6 | 3.489729 | 1.187528 | 0.000005 |
| 7 | 2.586170 | 0.457800 | 0.000016 |

Cartesian coordinates of : PACN4_ 1

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Atomic number (AN) and Cartesian coordinates
AN      X      Y      Z
-----
6      -0.003240    -5.568770    -0.347885
1       0.850324    -6.048132     0.137914
1       0.066854    -5.716358    -1.428448
1      -0.927701    -6.021699     0.018956
6      -0.002236    -4.143529    -0.046177
7      -0.001460    -3.011936     0.193754
6       5.065221     1.989992    -0.979933
1       5.337590     3.033222    -0.802083
1       5.058906     1.803244    -2.056593
1       5.810729     1.343521    -0.510472
6       3.744704     1.717297    -0.418860
7       2.694817     1.500867     0.027551
6      -5.063092     1.994916    -0.979886
1      -5.824155     1.430404    -0.435613
1      -5.088737     1.704089    -2.032911
1      -5.287682     3.061406    -0.900499
6      -3.742853     1.720763    -0.418868
7      -2.693215     1.503177     0.027568
6       0.001080     2.076868     1.423226
6       0.000451     0.679389     1.051110
7      -0.000062    -0.440564     0.790918
1       0.907793     2.285470     1.995895
1      -0.905531     2.286325     1.995746
1       0.001445     2.672598     0.506940
1      -0.000600    -1.496461     0.536269
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Cartesian coordinates of : PACN4_2

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Atomic number (AN) and Cartesian coordinates
AN      X      Y      Z
-----
6      -0.451977     5.400790     0.000366
1      -1.506896     5.678288    -0.066299
1       0.085123     5.817095    -0.855532
1      -0.030033     5.806466     0.923265
6      -0.325507     3.949483    -0.000119
7      -0.224742     2.797172    -0.000490
6      -5.520293    -1.874955     0.001894
1      -5.948048    -1.366282     0.869287
1      -5.784173    -2.934478     0.046179
1      -5.941241    -1.442255    -0.908971
6      -4.067713    -1.723679     0.000925
7      -2.912662    -1.604128     0.000104
6       5.733464    -1.294717     0.002233
1       6.110611    -0.723653     0.854142
1       6.111296    -0.848899    -0.921131
1       6.097073    -2.322654     0.074916
6       4.273084    -1.281907     0.000742
7       3.111897    -1.272163    -0.000449
6       0.247472    -2.414791    -0.002544
6       0.129341    -0.973930    -0.001923
7       0.015693     0.170141    -0.001488
1       0.808198    -2.718216    -0.890322
1      -0.762266    -2.833841    -0.003280
1       0.807124    -2.719042     0.885630
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1 -0.085298 1.252558 -0.001063

Cartesian coordinates of : PACN4_ 3

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.198324 | 1.460648 | 2.384448 |
| 1 | -1.254862 | 1.919194 | 2.075763 |
| 1 | -2.130261 | 1.163769 | 3.433953 |
| 1 | -3.007590 | 2.186785 | 2.274357 |
| 6 | -2.457415 | 0.292227 | 1.549705 |
| 7 | -2.654834 | -0.636624 | 0.881971 |
| 6 | 4.747939 | -0.380892 | 0.887498 |
| 1 | 5.459477 | -0.520636 | 0.069820 |
| 1 | 5.048106 | -1.001465 | 1.735572 |
| 1 | 4.747018 | 0.668964 | 1.190731 |
| 6 | 3.413805 | -0.765489 | 0.447411 |
| 7 | 2.355441 | -1.072029 | 0.098650 |
| 6 | -0.069401 | 3.515598 | -1.860483 |
| 1 | 0.520053 | 3.408452 | -2.774435 |
| 1 | 0.309896 | 4.369199 | -1.293258 |
| 1 | -1.110974 | 3.704811 | -2.131599 |
| 6 | 0.026956 | 2.297895 | -1.057671 |
| 7 | 0.105051 | 1.329775 | -0.419599 |
| 6 | -2.379160 | -2.676246 | -1.326522 |
| 6 | -1.074720 | -2.185402 | -0.929871 |
| 7 | -0.021328 | -1.824111 | -0.643833 |
| 1 | -2.263358 | -3.427035 | -2.112512 |
| 1 | -2.978001 | -1.831819 | -1.676737 |
| 1 | -2.871031 | -3.101245 | -0.447822 |
| 1 | 0.983131 | -1.468076 | -0.331253 |

Cartesian coordinates of : PACN4_ 4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.345509 | -1.839204 | 0.007797 |
| 6 | 3.889305 | -1.732839 | 0.003555 |
| 7 | 2.731170 | -1.648326 | 0.000180 |
| 1 | 5.791411 | -0.841574 | 0.010381 |
| 1 | 5.682312 | -2.377249 | -0.881708 |
| 1 | 5.676968 | -2.379460 | 0.897969 |
| 6 | 0.011817 | -0.157386 | -0.004939 |
| 6 | -0.154835 | -1.586455 | -0.007756 |
| 7 | -0.313994 | -2.726050 | -0.010379 |
| 1 | 0.581970 | 0.141643 | -0.888766 |
| 1 | 0.578736 | 0.138446 | 0.882042 |
| 1 | -0.978449 | 0.306689 | -0.005798 |
| 6 | -5.728164 | -0.928458 | 0.007544 |
| 6 | -4.273399 | -1.053955 | 0.003568 |
| 7 | -3.116357 | -1.153405 | 0.000251 |
| 1 | -6.035085 | -0.180307 | 0.742538 |
| 1 | -6.184688 | -1.887413 | 0.264679 |
| 1 | -6.078092 | -0.621341 | -0.981077 |
| 1 | -0.456495 | -3.723567 | -0.012361 |
| 6 | 0.654689 | 5.444198 | 0.000082 |

| | | | |
|---|-----------|----------|-----------|
| 1 | 0.969869 | 5.786701 | 0.988754 |
| 1 | -0.297900 | 5.916448 | -0.252196 |
| 1 | 1.405000 | 5.743868 | -0.735676 |
| 6 | 0.507057 | 3.990964 | -0.000996 |
| 7 | 0.389546 | 2.835770 | -0.001754 |

Cartesian coordinates of : PACN4_ 5

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.309227 | -0.996265 | -0.002498 |
| 6 | -2.207956 | -2.120108 | -0.002813 |
| 7 | -2.865086 | -3.066384 | -0.003187 |
| 1 | -0.271174 | -1.341997 | -0.003744 |
| 1 | -1.496269 | -0.381955 | 0.883041 |
| 1 | -1.497814 | -0.380223 | -0.886506 |
| 6 | 2.747788 | 2.722089 | -0.003892 |
| 6 | 1.589796 | 1.834407 | -0.003259 |
| 7 | 0.655168 | 1.145071 | -0.002791 |
| 1 | 2.418454 | 3.764071 | -0.005287 |
| 1 | 3.358826 | 2.524052 | -0.887245 |
| 1 | 3.358159 | 2.526196 | 0.880398 |
| 1 | -3.511065 | -3.842276 | -0.003409 |
| 6 | 6.726852 | -1.252587 | 0.004938 |
| 1 | 6.787130 | -1.943332 | -0.839677 |
| 1 | 6.851544 | -1.815049 | 0.933510 |
| 1 | 7.535621 | -0.522304 | -0.077319 |
| 6 | 5.434685 | -0.569981 | 0.002584 |
| 7 | 4.408210 | -0.026807 | 0.000767 |
| 6 | -6.169106 | 1.598951 | 0.005149 |
| 6 | -5.107378 | 0.597192 | 0.002852 |
| 7 | -4.262340 | -0.199367 | 0.001018 |
| 1 | -6.822292 | 1.446869 | 0.867931 |
| 1 | -6.760878 | 1.515964 | -0.909783 |
| 1 | -5.734626 | 2.600202 | 0.059079 |

Cartesian coordinates of : PACN4_ 6

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|------------|
| 6 | 0.000648 | -0.002020 | -0.006742 |
| 6 | -0.001062 | -0.004495 | 1.432342 |
| 7 | -0.002434 | -0.006482 | 2.584162 |
| 1 | 0.817558 | -0.625863 | -0.384242 |
| 1 | 0.133687 | 1.017949 | -0.382225 |
| 1 | -0.947943 | -0.396206 | -0.385968 |
| 6 | 0.005183 | 0.005457 | -5.488692 |
| 6 | 0.004230 | 0.003770 | -4.029956 |
| 7 | 0.003444 | 0.002383 | -2.867701 |
| 1 | 0.953550 | 0.386107 | -5.873875 |
| 1 | -0.797893 | 0.636893 | -5.874722 |
| 1 | -0.139367 | -1.005299 | -5.876164 |
| 1 | -0.003635 | -0.008221 | 3.596618 |
| 6 | 0.007402 | 0.009075 | -11.189749 |
| 1 | 0.618233 | -0.810073 | -11.575364 |
| 1 | 0.411694 | 0.947690 | -11.574920 |

| | | | |
|---|-----------|-----------|------------|
| 1 | -1.007313 | -0.110062 | -11.575713 |
| 6 | 0.006891 | 0.008602 | -9.729210 |
| 7 | 0.006488 | 0.008186 | -8.567431 |
| 6 | 0.012503 | 0.007644 | -16.975113 |
| 6 | 0.010825 | 0.008888 | -15.513940 |
| 7 | 0.009511 | 0.009830 | -14.352950 |
| 1 | -0.419305 | 0.938661 | -17.350497 |
| 1 | -0.577507 | -0.832702 | -17.349118 |
| 1 | 1.035630 | -0.084026 | -17.347908 |

Cartesian coordinates of : PACN5_ 1

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.806997 | -5.543345 | -0.006191 |
| 6 | -3.677162 | -4.088639 | -0.002735 |
| 7 | -3.574264 | -2.932053 | -0.000029 |
| 1 | -4.862456 | -5.823546 | 0.034156 |
| 1 | -3.294119 | -5.965698 | 0.861378 |
| 1 | -3.364910 | -5.955098 | -0.916755 |
| 6 | -4.388612 | 0.050657 | 0.007086 |
| 6 | -2.942517 | 0.015394 | 0.005516 |
| 7 | -1.792509 | 0.006758 | 0.004439 |
| 1 | -4.749878 | -0.475625 | 0.894138 |
| 1 | -4.751673 | -0.472374 | -0.881157 |
| 1 | -4.698945 | 1.098844 | 0.009161 |
| 6 | -3.188408 | 5.742753 | -0.006352 |
| 6 | -3.233230 | 4.282962 | -0.002475 |
| 7 | -3.269508 | 3.122396 | 0.000604 |
| 1 | -4.202852 | 6.146310 | -0.053404 |
| 1 | -2.625218 | 6.096645 | -0.873338 |
| 1 | -2.704799 | 6.103782 | 0.904622 |
| 1 | -0.685153 | -0.007306 | 0.003413 |
| 6 | 3.420184 | -0.074966 | 0.000477 |
| 1 | 3.807147 | 0.307200 | -0.946744 |
| 1 | 3.783157 | -1.096070 | 0.136774 |
| 1 | 3.812481 | 0.543549 | 0.810759 |
| 6 | 1.965238 | -0.049437 | 0.001440 |
| 7 | 0.808311 | -0.029410 | 0.002185 |
| 6 | 9.110597 | -0.194808 | -0.000501 |
| 6 | 7.650150 | -0.161129 | -0.000679 |
| 7 | 6.489365 | -0.134401 | -0.000790 |
| 1 | 9.481332 | -0.312743 | 1.020656 |
| 1 | 9.505721 | 0.735284 | -0.416326 |
| 1 | 9.464937 | -1.032824 | -0.605719 |

Cartesian coordinates of : PACN5_ 2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|-----------|
| 6 | 5.431563 | -1.645865 | -0.072871 |
| 1 | 6.215821 | -1.125950 | -0.628639 |
| 1 | 5.137650 | -2.541140 | -0.626331 |
| 1 | 5.826309 | -1.942287 | 0.902066 |
| 6 | 4.278288 | -0.766428 | 0.102334 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 3.361606 | -0.066218 | 0.242578 |
| 6 | -6.940340 | 0.177932 | -0.532119 |
| 1 | -7.124589 | 1.253076 | -0.465751 |
| 1 | -7.642226 | -0.349157 | 0.118933 |
| 1 | -7.088816 | -0.151030 | -1.563647 |
| 6 | -5.574405 | -0.112082 | -0.116983 |
| 7 | -4.490063 | -0.342662 | 0.212808 |
| 6 | 1.278510 | 0.689773 | -2.498763 |
| 1 | 2.190648 | 1.008966 | -1.985536 |
| 1 | 0.538305 | 1.492537 | -2.446594 |
| 1 | 1.505323 | 0.474238 | -3.545821 |
| 6 | 0.754863 | -0.502222 | -1.839076 |
| 7 | 0.338887 | -1.449115 | -1.310331 |
| 6 | 2.253078 | 3.217553 | 0.696662 |
| 1 | 2.178533 | 3.944453 | -0.116311 |
| 1 | 3.157003 | 2.615632 | 0.567596 |
| 1 | 2.310175 | 3.755498 | 1.646250 |
| 6 | 1.091574 | 2.333673 | 0.689481 |
| 7 | 0.175349 | 1.619409 | 0.677342 |
| 6 | 0.396508 | -1.459013 | 1.712632 |
| 6 | -0.942938 | -1.131719 | 1.275139 |
| 7 | -2.027882 | -0.899912 | 0.972943 |
| 1 | 1.085666 | -0.709817 | 1.307428 |
| 1 | 0.659527 | -2.440917 | 1.310145 |
| 1 | 0.425606 | -1.461596 | 2.805730 |
| 1 | -3.040429 | -0.662619 | 0.654486 |

 Cartesian coordinates of : PACN5_3

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -7.031583 | 1.476989 | 0.635208 |
| 1 | -7.457743 | 1.671346 | -0.352088 |
| 1 | -6.837412 | 2.430147 | 1.133054 |
| 1 | -7.752005 | 0.907201 | 1.227202 |
| 6 | -5.788631 | 0.721948 | 0.501465 |
| 7 | -4.800668 | 0.121258 | 0.395016 |
| 6 | 5.821481 | 0.499835 | 2.121611 |
| 1 | 6.740199 | 0.082723 | 1.701887 |
| 1 | 5.477428 | -0.142655 | 2.935847 |
| 1 | 6.034571 | 1.494339 | 2.521327 |
| 6 | 4.794565 | 0.588014 | 1.086122 |
| 7 | 3.978763 | 0.657925 | 0.261651 |
| 6 | 2.914232 | -2.655290 | -1.040993 |
| 1 | 3.039464 | -2.857013 | -2.107790 |
| 1 | 3.463268 | -3.410086 | -0.472351 |
| 1 | 3.317654 | -1.664530 | -0.810729 |
| 6 | 1.497922 | -2.703164 | -0.689175 |
| 7 | 0.371547 | -2.735874 | -0.408918 |
| 6 | 2.412053 | 3.199063 | -1.380060 |
| 1 | 2.392796 | 4.102452 | -0.765325 |
| 1 | 2.348101 | 3.477854 | -2.434829 |
| 1 | 3.337867 | 2.648013 | -1.194179 |
| 6 | 1.287362 | 2.344639 | -1.029876 |
| 7 | 0.389677 | 1.667875 | -0.758357 |
| 6 | -2.830782 | -2.249466 | 0.276479 |
| 6 | -2.070170 | -1.047789 | 0.015532 |
| 7 | -1.424631 | -0.119973 | -0.196677 |
| 1 | -2.135481 | -3.092799 | 0.223800 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -3.620924 | -2.337294 | -0.473199 |
| 1 | -3.291619 | -2.170408 | 1.264075 |
| 1 | -0.697670 | 0.673560 | -0.423570 |

Cartesian coordinates of : PACN5_ 4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.217294 | 0.640347 | -0.161296 |
| 1 | 5.618087 | 0.994435 | -1.114503 |
| 1 | 5.907599 | -0.089209 | 0.269600 |
| 1 | 5.111084 | 1.486782 | 0.521866 |
| 6 | 3.917367 | 0.019963 | -0.379019 |
| 7 | 2.884551 | -0.471551 | -0.554135 |
| 6 | 0.933947 | -1.077104 | 2.529245 |
| 1 | 1.009135 | -0.897649 | 3.604729 |
| 1 | 1.888550 | -1.472388 | 2.169345 |
| 1 | 0.143189 | -1.809898 | 2.341091 |
| 6 | 0.613980 | 0.164759 | 1.829648 |
| 7 | 0.353718 | 1.139431 | 1.252751 |
| 6 | -3.238016 | 0.741859 | 1.510752 |
| 1 | -3.828777 | 0.674954 | 2.427632 |
| 1 | -3.888956 | 1.028000 | 0.680486 |
| 1 | -2.457185 | 1.499277 | 1.634301 |
| 6 | -2.609090 | -0.542410 | 1.220728 |
| 7 | -2.092699 | -1.558096 | 0.992782 |
| 6 | -1.136472 | 3.329727 | -0.952136 |
| 1 | -0.627210 | 3.829050 | -1.780243 |
| 1 | -0.471492 | 3.287936 | -0.084945 |
| 1 | -2.035057 | 3.898751 | -0.699190 |
| 6 | -1.497397 | 1.968126 | -1.334081 |
| 7 | -1.785244 | 0.880462 | -1.623333 |
| 6 | -1.788922 | -2.364516 | -1.956371 |
| 6 | -0.520371 | -1.841685 | -1.499589 |
| 7 | 0.509474 | -1.445493 | -1.173715 |
| 1 | -1.650876 | -2.846258 | -2.928389 |
| 1 | -2.475922 | -1.516377 | -2.038999 |
| 1 | -2.163780 | -3.074379 | -1.214424 |
| 1 | 1.479093 | -1.040688 | -0.896093 |

Cartesian coordinates of : PACN5_ 5

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.778476 | -5.560125 | 0.000830 |
| 6 | -0.511972 | -4.124032 | 0.000635 |
| 7 | -0.300402 | -2.982426 | 0.000409 |
| 1 | -1.854526 | -5.739592 | 0.063947 |
| 1 | -0.289409 | -6.030551 | 0.857346 |
| 1 | -0.396804 | -6.010739 | -0.918619 |
| 6 | -1.095139 | 0.043960 | -0.000334 |
| 6 | 0.345291 | -0.060258 | -0.000259 |
| 7 | 1.493661 | -0.125265 | -0.000220 |
| 1 | -1.495592 | -0.457693 | 0.883769 |
| 1 | -1.495512 | -0.457551 | -0.884556 |
| 1 | -1.369957 | 1.101458 | -0.000274 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.446473 | 5.652496 | 0.000873 |
| 6 | 0.373477 | 4.193665 | 0.000560 |
| 7 | 0.315161 | 3.034044 | 0.000307 |
| 1 | -0.560882 | 6.076000 | 0.002855 |
| 1 | 0.975574 | 6.000269 | -0.889748 |
| 1 | 0.978831 | 5.999727 | 0.889761 |
| 1 | 2.565394 | -0.191519 | -0.000203 |
| 6 | 6.762743 | -0.469227 | -0.000607 |
| 1 | 7.153424 | -0.146980 | -0.968988 |
| 1 | 7.062411 | -1.504101 | 0.182244 |
| 1 | 7.175029 | 0.169021 | 0.784809 |
| 6 | 5.308736 | -0.371487 | -0.000364 |
| 7 | 4.154363 | -0.293974 | -0.000241 |
| 6 | -6.776871 | 0.465324 | -0.000172 |
| 6 | -5.321627 | 0.335914 | -0.000677 |
| 7 | -4.165087 | 0.233237 | -0.000951 |
| 1 | -7.164679 | 0.319962 | 1.011069 |
| 1 | -7.219115 | -0.284233 | -0.661002 |
| 1 | -7.063849 | 1.459835 | -0.350447 |

 Cartesian coordinates of : PACN5_ 6

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.297565 | -4.919806 | -0.530428 |
| 1 | 3.617832 | -4.854053 | -1.573119 |
| 1 | 2.548360 | -5.709819 | -0.437342 |
| 1 | 4.160221 | -5.173852 | 0.090387 |
| 6 | 2.732485 | -3.643338 | -0.100604 |
| 7 | 2.283333 | -2.628739 | 0.241384 |
| 6 | 3.277849 | 4.930314 | -0.534536 |
| 1 | 3.940218 | 5.327393 | 0.238590 |
| 1 | 2.473695 | 5.647678 | -0.715621 |
| 1 | 3.849016 | 4.795737 | -1.456368 |
| 6 | 2.718277 | 3.651888 | -0.103331 |
| 7 | 2.273580 | 2.635670 | 0.239672 |
| 6 | -4.676887 | -0.004369 | 3.056502 |
| 1 | -5.287278 | 0.892335 | 2.924208 |
| 1 | -4.288640 | -0.019912 | 4.077857 |
| 1 | -5.303482 | -0.886455 | 2.903332 |
| 6 | -3.571387 | -0.003211 | 2.100698 |
| 7 | -2.692777 | -0.002273 | 1.341227 |
| 6 | -3.781676 | -0.008288 | -3.641419 |
| 1 | -4.365524 | -0.926431 | -3.540131 |
| 1 | -3.371953 | 0.047634 | -4.652875 |
| 1 | -4.432398 | 0.852448 | -3.468778 |
| 6 | -2.696560 | -0.006464 | -2.668343 |
| 7 | -1.836285 | -0.004980 | -1.895730 |
| 6 | 1.868019 | 0.003283 | 1.819030 |
| 6 | 0.874126 | 0.001029 | 0.767467 |
| 7 | 0.057388 | -0.000812 | -0.039502 |
| 1 | 2.857598 | 0.005396 | 1.356730 |
| 1 | 1.743759 | -0.902094 | 2.417567 |
| 1 | 1.739853 | 0.908252 | 2.417363 |
| 1 | -0.728821 | -0.002535 | -0.781370 |

 Cartesian coordinates of : PACN5_ 7

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.419796 | 4.912955 | 0.507171 |
| 1 | -3.739539 | 4.827001 | 1.548547 |
| 1 | -4.283245 | 5.177319 | -0.108238 |
| 1 | -2.671916 | 5.705760 | 0.428308 |
| 6 | -2.853621 | 3.645636 | 0.052574 |
| 7 | -2.403975 | 2.638155 | -0.309167 |
| 6 | 3.541168 | 0.261568 | 3.731974 |
| 1 | 4.172102 | 1.135734 | 3.553447 |
| 1 | 4.157183 | -0.640229 | 3.694392 |
| 1 | 3.083944 | 0.343824 | 4.721031 |
| 6 | 2.502162 | 0.189501 | 2.712396 |
| 7 | 1.678341 | 0.132389 | 1.903077 |
| 6 | -2.861204 | -5.213977 | 0.630721 |
| 1 | -1.993004 | -5.856710 | 0.795621 |
| 1 | -3.519973 | -5.688483 | -0.100738 |
| 1 | -3.402536 | -5.097750 | 1.572823 |
| 6 | -2.429551 | -3.908217 | 0.138825 |
| 7 | -2.086897 | -2.870180 | -0.252474 |
| 6 | 4.736497 | 0.137366 | -2.932366 |
| 1 | 5.508173 | -0.543204 | -2.564296 |
| 1 | 5.149896 | 1.147512 | -2.985896 |
| 1 | 4.438602 | -0.176586 | -3.935779 |
| 6 | 3.581277 | 0.115925 | -2.037571 |
| 7 | 2.663030 | 0.099200 | -1.326710 |
| 6 | -1.823057 | -0.109120 | -1.990979 |
| 6 | -0.885311 | -0.044084 | -0.892494 |
| 7 | -0.124411 | 0.008265 | -0.034300 |
| 1 | -2.371353 | -1.051452 | -1.908489 |
| 1 | -1.269267 | -0.070621 | -2.932924 |
| 1 | -2.495470 | 0.749125 | -1.909140 |
| 1 | 0.622417 | 0.058637 | 0.746846 |

Cartesian coordinates of : PACN5_ 8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.739313 | -0.557598 | -0.000715 |
| 6 | 2.288651 | -0.719793 | -0.000577 |
| 7 | 1.134040 | -0.850385 | -0.000458 |
| 1 | 4.235002 | -1.530719 | 0.007389 |
| 1 | 4.065081 | -0.000835 | 0.880576 |
| 1 | 4.066469 | -0.014850 | -0.890197 |
| 6 | -1.532661 | -2.332941 | -0.000400 |
| 6 | -1.812107 | -0.914690 | -0.000295 |
| 7 | -2.059151 | 0.208078 | -0.000203 |
| 1 | -0.939668 | -2.569633 | 0.886698 |
| 1 | -0.939792 | -2.569530 | -0.887608 |
| 1 | -2.487977 | -2.864209 | -0.000361 |
| 6 | -7.336289 | -2.431324 | 0.000756 |
| 6 | -5.907904 | -2.126846 | 0.000346 |
| 7 | -4.772096 | -1.885441 | 0.000078 |
| 1 | -7.486804 | -3.511215 | -0.072381 |
| 1 | -7.821511 | -1.947092 | -0.850225 |
| 1 | -7.794476 | -2.071012 | 0.925059 |
| 1 | -2.271340 | 1.270008 | -0.000122 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -3.016957 | 5.379604 | 0.000079 |
| 1 | -3.320867 | 5.699877 | -0.999601 |
| 1 | -2.107589 | 5.912673 | 0.288483 |
| 1 | -3.812836 | 5.613638 | 0.711464 |
| 6 | -2.764887 | 3.944632 | 0.000057 |
| 7 | -2.564367 | 2.805397 | -0.000020 |
| 6 | 9.476741 | -0.177200 | 0.001063 |
| 6 | 8.016556 | -0.228239 | 0.000271 |
| 7 | 6.856189 | -0.268816 | -0.000320 |
| 1 | 9.846825 | -0.077545 | 1.024413 |
| 1 | 9.821335 | 0.677994 | -0.585475 |
| 1 | 9.883109 | -1.093011 | -0.435166 |

Cartesian coordinates of : PACN5_9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.803223 | -1.817751 | 1.714802 |
| 1 | -4.531729 | -2.544972 | 1.347676 |
| 1 | -3.967617 | -0.857299 | 1.218600 |
| 1 | -3.936873 | -1.697267 | 2.792704 |
| 6 | -2.448333 | -2.277187 | 1.426583 |
| 7 | -1.368515 | -2.634083 | 1.193359 |
| 6 | -3.568901 | 0.030603 | -3.161859 |
| 1 | -3.701859 | -1.019454 | -3.433676 |
| 1 | -2.967661 | 0.521922 | -3.930836 |
| 1 | -4.548979 | 0.512026 | -3.118151 |
| 6 | -2.902782 | 0.132476 | -1.864768 |
| 7 | -2.373949 | 0.214608 | -0.833355 |
| 6 | -1.080146 | 4.761238 | 1.050934 |
| 1 | -0.593009 | 5.449922 | 0.356239 |
| 1 | -0.849780 | 5.062470 | 2.075839 |
| 1 | -2.161491 | 4.800699 | 0.898649 |
| 6 | -0.600211 | 3.405072 | 0.817514 |
| 7 | -0.219374 | 2.328867 | 0.633275 |
| 6 | 6.473774 | 0.228095 | -0.462891 |
| 1 | 6.786996 | 0.691186 | 0.476014 |
| 1 | 6.575596 | 0.956562 | -1.271002 |
| 1 | 7.123100 | -0.625837 | -0.671088 |
| 6 | 5.085670 | -0.214872 | -0.361991 |
| 7 | 3.982325 | -0.567713 | -0.281523 |
| 6 | 1.451416 | -2.600808 | 0.012775 |
| 6 | 0.973772 | -1.243767 | 0.163866 |
| 7 | 0.604255 | -0.161079 | 0.272654 |
| 1 | 2.463953 | -2.562299 | -0.396270 |
| 1 | 0.763875 | -3.142880 | -0.640994 |
| 1 | 1.441440 | -3.080250 | 0.995064 |
| 1 | 0.244628 | 0.852670 | 0.400565 |

Cartesian coordinates of : PACN5_10

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.776270 | -6.392971 | -0.000766 |
| 6 | -3.537066 | -4.956179 | -0.000290 |
| 7 | -3.347331 | -3.815304 | 0.000041 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -3.270766 | -6.849967 | 0.853620 |
| 1 | -3.389725 | -6.829518 | -0.925086 |
| 1 | -4.849563 | -6.586850 | 0.068793 |
| 6 | 2.789939 | -0.253255 | 0.000944 |
| 6 | 1.333560 | -0.155101 | 0.000635 |
| 7 | 0.174333 | -0.076579 | 0.000358 |
| 1 | 3.140568 | -0.784990 | -0.886229 |
| 1 | 3.139744 | -0.791899 | 0.884267 |
| 1 | 3.242383 | 0.740754 | 0.005037 |
| 7 | -2.932935 | -1.219998 | 0.000345 |
| 6 | -2.722028 | -0.088467 | 0.000332 |
| 6 | -2.534788 | 1.345178 | 0.000320 |
| 1 | -1.961321 | 1.635154 | 0.884069 |
| 1 | -1.962136 | 1.635250 | -0.883926 |
| 1 | -3.503247 | 1.850921 | 0.000772 |
| 1 | -3.099385 | -2.299223 | 0.000273 |
| 6 | -2.532221 | 7.012550 | -0.000703 |
| 6 | -2.541546 | 5.551863 | -0.000292 |
| 7 | -2.548981 | 4.390811 | 0.000078 |
| 1 | -1.592754 | 7.379853 | -0.420916 |
| 1 | -2.634839 | 7.386805 | 1.020820 |
| 1 | -3.362183 | 7.390916 | -0.602468 |
| 6 | 8.536138 | -0.549735 | -0.001073 |
| 6 | 7.075892 | -0.500147 | -0.000063 |
| 7 | 5.915484 | -0.460693 | 0.000712 |
| 1 | 8.925317 | -0.126251 | 0.928088 |
| 1 | 8.929145 | 0.023915 | -0.844053 |
| 1 | 8.875110 | -1.584946 | -0.088079 |

Cartesian coordinates of : PACN5_11

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|------------|
| 6 | -0.000841 | 0.001375 | 0.007138 |
| 6 | -0.000675 | 0.001468 | 1.456630 |
| 7 | -0.000530 | 0.001526 | 2.609914 |
| 1 | 0.619700 | -0.814295 | -0.372119 |
| 1 | 0.395200 | 0.946597 | -0.372235 |
| 1 | -1.017542 | -0.128276 | -0.371978 |
| 6 | 0.001869 | 0.002385 | -5.583933 |
| 6 | 0.000627 | 0.001856 | -4.124052 |
| 7 | -0.000313 | 0.001446 | -2.962189 |
| 1 | 1.011523 | 0.162885 | -5.968120 |
| 1 | -0.641336 | 0.796443 | -5.969322 |
| 1 | -0.363584 | -0.951753 | -5.969718 |
| 1 | -0.000362 | 0.001553 | 3.813252 |
| 6 | 0.011750 | 0.007320 | -11.347205 |
| 1 | 0.843027 | -0.596117 | -11.720030 |
| 1 | 0.120343 | 1.028898 | -11.719679 |
| 1 | -0.925619 | -0.409471 | -11.723732 |
| 6 | 0.008546 | 0.005579 | -9.886108 |
| 7 | 0.006043 | 0.004213 | -8.725087 |
| 6 | 0.000217 | 0.001537 | 7.748697 |
| 6 | -0.000002 | 0.001549 | 6.296357 |
| 7 | -0.000173 | 0.001560 | 5.141130 |
| 1 | -1.014325 | -0.142186 | 8.127746 |
| 1 | 0.383116 | 0.952051 | 8.127566 |
| 1 | 0.632038 | -0.805267 | 8.127516 |
| 6 | 0.003578 | 0.003393 | 13.402294 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.002460 | 0.002467 | 11.941637 |
| 7 | 0.001594 | 0.001770 | 10.780531 |
| 1 | -0.404376 | -0.938788 | 13.776423 |
| 1 | -0.608180 | 0.828405 | 13.775416 |
| 1 | 1.024156 | 0.121311 | 13.774613 |

Cartesian coordinates of : PACN5_12

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 7.253010 | -2.130912 | 0.016122 |
| 6 | 5.805300 | -1.940876 | 0.008797 |
| 7 | 4.654021 | -1.789747 | 0.002967 |
| 1 | 7.755581 | -1.160607 | 0.019926 |
| 1 | 7.560288 | -2.687308 | -0.872775 |
| 1 | 7.551000 | -2.689461 | 0.906830 |
| 6 | 2.024385 | -0.132349 | -0.007095 |
| 6 | 1.765135 | -1.547540 | -0.010773 |
| 7 | 1.540097 | -2.675916 | -0.014178 |
| 1 | 2.614505 | 0.129484 | -0.889522 |
| 1 | 2.607064 | 0.126152 | 0.881245 |
| 1 | 1.064262 | 0.391572 | -0.009973 |
| 6 | -3.719728 | -0.607205 | -0.003451 |
| 6 | -2.272318 | -0.793682 | -0.005417 |
| 7 | -1.119857 | -0.943002 | -0.007163 |
| 1 | -4.006516 | 0.169299 | 0.709016 |
| 1 | -4.227260 | -1.532708 | 0.276912 |
| 1 | -4.070876 | -0.310618 | -0.994172 |
| 1 | 1.319352 | -3.658810 | -0.016836 |
| 6 | 3.016618 | 5.421707 | 0.000286 |
| 1 | 3.326574 | 5.753570 | 0.994223 |
| 1 | 2.089050 | 5.931722 | -0.271006 |
| 1 | 3.792457 | 5.688734 | -0.721430 |
| 6 | 2.809795 | 3.975689 | -0.001118 |
| 7 | 2.645224 | 2.826309 | -0.002144 |
| 6 | -9.424263 | 0.065062 | 0.009787 |
| 6 | -7.972821 | -0.102120 | 0.005937 |
| 7 | -6.819370 | -0.234955 | 0.002918 |
| 1 | -9.796816 | 0.073935 | 1.037046 |
| 1 | -9.896866 | -0.758121 | -0.531640 |
| 1 | -9.693283 | 1.007703 | -0.473111 |

Cartesian coordinates of : PACN5_13

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|----------|-----------|
| 6 | 2.922518 | 5.594164 | 0.021270 |
| 6 | 3.096009 | 4.144468 | 0.010262 |
| 7 | 3.233716 | 2.991533 | 0.001555 |
| 1 | 1.858752 | 5.841540 | -0.015038 |
| 1 | 3.420437 | 6.035594 | -0.845533 |
| 1 | 3.354752 | 6.014142 | 0.932820 |
| 6 | 2.157726 | 0.082508 | -0.014935 |
| 6 | 3.595434 | 0.125122 | -0.018929 |
| 7 | 4.746211 | 0.134042 | -0.022932 |
| 1 | 1.776247 | 0.605540 | -0.896129 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 1.781645 | 0.597046 | 0.873558 |
| 1 | 1.840004 | -0.963870 | -0.018633 |
| 6 | 3.666091 | -5.490016 | 0.021328 |
| 6 | 3.629537 | -4.030352 | 0.009593 |
| 7 | 3.600244 | -2.869494 | 0.000282 |
| 1 | 2.651243 | -5.886583 | 0.104747 |
| 1 | 4.256091 | -5.841397 | 0.871358 |
| 1 | 4.117298 | -5.859094 | -0.902961 |
| 1 | 5.753606 | 0.138150 | -0.025546 |
| 6 | -3.442306 | -0.050377 | -0.005113 |
| 1 | -3.831794 | 0.103126 | 1.003604 |
| 1 | -3.793595 | -1.020416 | -0.363409 |
| 1 | -3.857353 | 0.724047 | -0.653768 |
| 6 | -1.983176 | 0.002443 | -0.007702 |
| 7 | -0.822055 | 0.044530 | -0.009588 |
| 6 | -9.202926 | -0.268004 | 0.004434 |
| 6 | -7.742973 | -0.209775 | 0.002035 |
| 7 | -6.582840 | -0.163495 | 0.000160 |
| 1 | -9.570744 | -0.387798 | 1.026445 |
| 1 | -9.544458 | -1.114304 | -0.596631 |
| 1 | -9.614663 | 0.653376 | -0.414698 |

Cartesian coordinates of : PACN6_1

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.064499 | -0.272705 | 2.691389 |
| 1 | -4.056396 | 0.585407 | 3.367969 |
| 1 | -4.569304 | -1.108217 | 3.182591 |
| 1 | -4.604666 | -0.008950 | 1.778276 |
| 6 | -2.697728 | -0.648535 | 2.344926 |
| 7 | -1.611436 | -0.948871 | 2.064860 |
| 6 | 1.907135 | -1.491430 | 2.043062 |
| 1 | 0.873863 | -1.157484 | 2.183400 |
| 1 | 2.328683 | -1.764806 | 3.013751 |
| 1 | 1.911127 | -2.368634 | 1.388722 |
| 6 | 2.705429 | -0.432618 | 1.430923 |
| 7 | 3.340482 | 0.404714 | 0.934001 |
| 6 | -5.533801 | 1.238898 | -2.340022 |
| 1 | -6.433768 | 0.619647 | -2.368070 |
| 1 | -5.164897 | 1.374394 | -3.359692 |
| 1 | -5.786589 | 2.216205 | -1.921546 |
| 6 | -4.509901 | 0.594106 | -1.521393 |
| 7 | -3.696014 | 0.080525 | -0.870416 |
| 6 | 3.342714 | 3.847438 | 0.445946 |
| 1 | 4.057172 | 3.107639 | 0.820116 |
| 1 | 3.091750 | 4.553033 | 1.241618 |
| 1 | 3.778597 | 4.389689 | -0.396621 |
| 6 | 2.149698 | 3.134765 | 0.017265 |
| 7 | 1.214964 | 2.537865 | -0.313253 |
| 6 | 4.508624 | -1.578206 | -1.820749 |
| 1 | 4.805921 | -0.767187 | -1.149424 |
| 1 | 4.650602 | -1.263241 | -2.857493 |
| 1 | 5.132517 | -2.454372 | -1.627460 |
| 6 | 3.105177 | -1.901813 | -1.583754 |
| 7 | 1.988544 | -2.148098 | -1.378684 |
| 6 | -1.105870 | -2.068150 | -0.813108 |
| 6 | -0.558380 | -0.733928 | -0.706561 |
| 7 | -0.121589 | 0.328226 | -0.636817 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.688504 | -2.670795 | -0.001550 |
| 1 | -0.807094 | -2.493838 | -1.774182 |
| 1 | -2.192636 | -1.998625 | -0.715945 |
| 1 | 0.377368 | 1.302674 | -0.529835 |

Cartesian coordinates of : PACN6_ 2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.415373 | 0.724035 | 3.582973 |
| 1 | 3.436603 | 0.017291 | 4.416031 |
| 1 | 3.632905 | 1.728496 | 3.954030 |
| 1 | 4.160844 | 0.436034 | 2.835328 |
| 6 | 2.109498 | 0.700736 | 2.942480 |
| 7 | 1.085897 | 0.671313 | 2.403300 |
| 6 | -5.380407 | 3.435600 | 0.852930 |
| 1 | -5.271932 | 3.574560 | 1.931353 |
| 1 | -6.374349 | 3.031858 | 0.645080 |
| 1 | -5.280134 | 4.404472 | 0.357603 |
| 6 | -4.356630 | 2.516584 | 0.362395 |
| 7 | -3.543063 | 1.786006 | -0.028080 |
| 6 | 2.024395 | -1.902864 | -1.326745 |
| 1 | 2.671232 | -2.716882 | -1.663732 |
| 1 | 1.667781 | -1.341863 | -2.196405 |
| 1 | 1.163143 | -2.323814 | -0.798310 |
| 6 | 2.767393 | -1.002555 | -0.448708 |
| 7 | 3.354141 | -0.277841 | 0.245182 |
| 6 | -2.316494 | -5.289131 | 0.482855 |
| 1 | -3.329669 | -5.105622 | 0.848821 |
| 1 | -1.718956 | -5.718174 | 1.290934 |
| 1 | -2.360602 | -6.001977 | -0.344217 |
| 6 | -1.716472 | -4.037058 | 0.029771 |
| 7 | -1.239663 | -3.041367 | -0.331200 |
| 6 | 3.563620 | 2.505830 | -1.998464 |
| 1 | 4.088594 | 2.012420 | -1.175259 |
| 1 | 3.409096 | 3.559382 | -1.752842 |
| 1 | 4.169473 | 2.437823 | -2.905414 |
| 6 | 2.277900 | 1.846837 | -2.206088 |
| 7 | 1.259968 | 1.308753 | -2.359609 |
| 6 | -1.681354 | -0.125541 | -1.921457 |
| 6 | -1.013296 | 0.111310 | -0.662973 |
| 7 | -0.464877 | 0.292378 | 0.331803 |
| 1 | -2.692879 | 0.283393 | -1.849763 |
| 1 | -1.707237 | -1.205554 | -2.093971 |
| 1 | -1.108135 | 0.382113 | -2.703064 |
| 1 | 0.116255 | 0.468646 | 1.240207 |

Cartesian coordinates of : PACN6_ 3

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|----------|----------|
| 6 | 0.109870 | 1.433324 | 1.936529 |
| 1 | 0.470095 | 1.834128 | 2.887299 |
| 1 | -0.979947 | 1.344227 | 1.961233 |
| 1 | 0.375082 | 2.121585 | 1.127410 |
| 6 | 0.692628 | 0.117266 | 1.688771 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 1.150734 | -0.928689 | 1.472339 |
| 6 | 1.649202 | -3.918720 | -0.185358 |
| 1 | 1.206645 | -4.849975 | 0.178658 |
| 1 | 2.012397 | -3.329441 | 0.661449 |
| 1 | 2.484523 | -4.163152 | -0.846326 |
| 6 | 0.649103 | -3.137907 | -0.906921 |
| 7 | -0.155291 | -2.510783 | -1.463053 |
| 6 | -1.801496 | -2.903080 | 1.547249 |
| 1 | -1.960556 | -3.635653 | 0.751663 |
| 1 | -2.407205 | -3.173729 | 2.415693 |
| 1 | -0.743599 | -2.895400 | 1.828589 |
| 6 | -2.175418 | -1.575339 | 1.070837 |
| 7 | -2.472936 | -0.513804 | 0.702657 |
| 6 | -4.081458 | 2.602922 | 0.599570 |
| 1 | -4.931864 | 2.842505 | -0.043692 |
| 1 | -4.036118 | 3.334519 | 1.410226 |
| 1 | -4.213854 | 1.600734 | 1.017362 |
| 6 | -2.843678 | 2.630231 | -0.173325 |
| 7 | -1.854343 | 2.632612 | -0.782642 |
| 6 | 5.348847 | 2.065770 | 0.442150 |
| 1 | 5.351823 | 3.126033 | 0.707059 |
| 1 | 6.105966 | 1.885697 | -0.325193 |
| 1 | 5.584685 | 1.470606 | 1.327822 |
| 6 | 4.036830 | 1.689647 | -0.068010 |
| 7 | 2.996365 | 1.390210 | -0.476331 |
| 6 | -1.631928 | 0.040783 | -2.555443 |
| 6 | -0.359385 | 0.382357 | -1.962631 |
| 7 | 0.667276 | 0.661213 | -1.525999 |
| 1 | -2.312999 | -0.232262 | -1.742775 |
| 1 | -1.487920 | -0.815245 | -3.219441 |
| 1 | -2.013509 | 0.915034 | -3.089376 |
| 1 | 1.615030 | 0.940945 | -1.096960 |

Cartesian coordinates of : PACN6_ 4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.119880 | -1.781718 | -0.573538 |
| 1 | -2.926605 | -1.103125 | -0.865881 |
| 1 | -2.486855 | -2.811224 | -0.580704 |
| 1 | -1.288741 | -1.698026 | -1.280557 |
| 6 | -1.651138 | -1.424698 | 0.761940 |
| 7 | -1.266746 | -1.117620 | 1.815120 |
| 6 | -3.953133 | 0.879887 | 2.874402 |
| 1 | -3.083215 | 0.301284 | 3.198357 |
| 1 | -4.865299 | 0.367855 | 3.190789 |
| 1 | -3.924085 | 1.870506 | 3.334953 |
| 6 | -3.931445 | 1.005012 | 1.419858 |
| 7 | -3.907106 | 1.097216 | 0.261862 |
| 6 | 1.792483 | -5.233599 | -1.171705 |
| 1 | 1.327722 | -5.485626 | -2.128059 |
| 1 | 1.445127 | -5.936461 | -0.410461 |
| 1 | 2.876994 | -5.324263 | -1.270633 |
| 6 | 1.439835 | -3.868503 | -0.789260 |
| 7 | 1.161658 | -2.782302 | -0.485579 |
| 6 | -3.403729 | 2.484861 | -2.741568 |
| 1 | -4.201851 | 2.205350 | -2.047832 |
| 1 | -3.585304 | 2.037579 | -3.721974 |
| 1 | -3.364835 | 3.572461 | -2.841612 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -2.145112 | 1.996736 | -2.199346 |
| 7 | -1.147016 | 1.607714 | -1.761446 |
| 6 | 5.969553 | 3.252984 | 0.053021 |
| 1 | 5.760270 | 4.236163 | 0.481606 |
| 1 | 6.148428 | 3.363104 | -1.019341 |
| 1 | 6.867665 | 2.844749 | 0.522966 |
| 6 | 4.837367 | 2.358806 | 0.280658 |
| 7 | 3.937298 | 1.648069 | 0.462066 |
| 6 | 2.107258 | -0.583748 | 1.598127 |
| 6 | 1.365714 | 0.099680 | 0.563089 |
| 7 | 0.735395 | 0.634759 | -0.236797 |
| 1 | 1.430833 | -1.309036 | 2.061141 |
| 1 | 2.461538 | 0.153997 | 2.321769 |
| 1 | 2.961615 | -1.087778 | 1.140591 |
| 1 | 0.005586 | 1.073444 | -0.925775 |

Cartesian coordinates of : PACN6_ 5

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.403678 | 2.484600 | 2.741791 |
| 1 | 3.364648 | 3.572171 | 2.842108 |
| 1 | 4.201734 | 2.205373 | 2.047865 |
| 1 | 3.585463 | 2.037104 | 3.722059 |
| 6 | 2.145047 | 1.996432 | 2.199640 |
| 7 | 1.146941 | 1.607374 | 1.761795 |
| 6 | -5.969347 | 3.253317 | -0.053092 |
| 1 | -6.830844 | 2.920578 | -0.637230 |
| 1 | -5.707352 | 4.270402 | -0.354769 |
| 1 | -6.237355 | 3.254344 | 1.006277 |
| 6 | -4.837370 | 2.358780 | -0.280358 |
| 7 | -3.937473 | 1.647741 | -0.461438 |
| 6 | 2.120139 | -1.781626 | 0.573098 |
| 1 | 1.289068 | -1.698212 | 1.280230 |
| 1 | 2.926772 | -1.102934 | 0.865468 |
| 1 | 2.487308 | -2.811063 | 0.580040 |
| 6 | 1.651177 | -1.424456 | -0.762263 |
| 7 | 1.266612 | -1.117264 | -1.815347 |
| 6 | -1.791588 | -5.234213 | 1.171214 |
| 1 | -1.443968 | -5.936902 | 0.409931 |
| 1 | -2.876087 | -5.325169 | 1.270010 |
| 1 | -1.326870 | -5.486228 | 2.127592 |
| 6 | -1.439242 | -3.868987 | 0.788960 |
| 7 | -1.161297 | -2.782683 | 0.485434 |
| 6 | 3.952414 | 0.880921 | -2.874663 |
| 1 | 4.864572 | 0.369026 | -3.191293 |
| 1 | 3.923208 | 1.871624 | -3.335025 |
| 1 | 3.082494 | 0.302302 | -3.198588 |
| 6 | 3.930951 | 1.005772 | -1.420092 |
| 7 | 3.906796 | 1.097760 | -0.262075 |
| 6 | -2.107460 | -0.583930 | -1.597763 |
| 6 | -1.365872 | 0.099417 | -0.562703 |
| 7 | -0.735527 | 0.634443 | 0.237199 |
| 1 | -2.461722 | 0.153874 | -2.321355 |
| 1 | -2.961832 | -1.087950 | -1.140244 |
| 1 | -1.431072 | -1.309212 | -2.060838 |
| 1 | -0.005700 | 1.073109 | 0.926168 |

Cartesian coordinates of : PACN6_ 6

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Atomic number (AN) and Cartesian coordinates
AN      X      Y      Z
-----
6      -4.856100    1.117401    1.889964
1      -3.967392    1.695756    2.158530
1      -5.188178    0.537100    2.754402
1      -5.655561    1.801087    1.593653
6      -4.529774    0.222599    0.783243
7      -4.260832   -0.483846   -0.099110
6       5.891450   -2.210345    1.077594
1       6.062164   -2.809886    0.180076
1       5.612858   -2.873954    1.899901
1       6.816026   -1.690074    1.339692
6       4.825261   -1.241266    0.836263
7       3.978009   -0.469621    0.644948
6       3.919312    1.686580   -2.214798
1       3.934281    1.255797   -3.219021
1       4.573879    1.103182   -1.561881
1       4.280950    2.716606   -2.264697
6       2.561704    1.658330   -1.679387
7       1.482608    1.636805   -1.249641
6      -1.955331    1.689714   -1.692239
1      -0.988253    1.493194   -2.162993
1      -2.390900    2.592459   -2.128058
1      -2.633749    0.847225   -1.856556
6      -1.754923    1.871564   -0.258479
7      -1.594963    1.997454    0.886210
6      -3.375921   -3.372737   -1.506037
1      -3.172412   -3.581335   -2.559268
1      -4.220027   -2.682982   -1.416086
1      -3.605486   -4.307766   -0.988913
6      -2.215891   -2.744877   -0.892980
7      -1.296266   -2.242333   -0.402969
6       1.503115    1.391670    1.920264
6       0.870681    0.244841    1.307623
7       0.347630   -0.665560    0.836561
1       1.371440    1.342060    3.004412
1       1.010640    2.284383    1.522250
1       2.563767    1.381389    1.654988
1      -0.298841   -1.395387    0.311385
-----

```

Cartesian coordinates of : PACN6_ 7

```

-----
Atomic number (AN) and Cartesian coordinates
AN      X      Y      Z
-----
6       2.197509    2.750331    2.770389
1       2.767445    2.206079    3.527509
1       1.133949    2.717792    3.020598
1       2.535203    3.789498    2.750190
6       2.392711    2.136729    1.460582
7       2.545832    1.649815    0.416645
6      -3.509558    1.511838    2.381145
1      -4.013583    0.976162    1.572514
1      -3.967882    2.496313    2.503845
1      -3.618514    0.950468    3.312393
6      -2.095909    1.657673    2.047401
-----

```

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.971290 | 1.774619 | 1.779722 |
| 6 | -5.093515 | -0.710045 | -2.509063 |
| 1 | -5.731035 | -1.437261 | -2.000280 |
| 1 | -4.632436 | -1.187937 | -3.376955 |
| 1 | -5.709265 | 0.126008 | -2.849715 |
| 6 | -4.058866 | -0.228461 | -1.597003 |
| 7 | -3.236338 | 0.155061 | -0.871495 |
| 6 | 1.306241 | -5.511091 | 1.795391 |
| 1 | 1.497767 | -6.197296 | 0.966729 |
| 1 | 0.487418 | -5.901979 | 2.404361 |
| 1 | 2.205739 | -5.430918 | 2.410737 |
| 6 | 0.949096 | -4.197961 | 1.273012 |
| 7 | 0.666582 | -3.155585 | 0.857321 |
| 6 | 4.451292 | 0.794801 | -2.371237 |
| 1 | 4.504643 | 1.217547 | -1.364352 |
| 1 | 4.764711 | 1.547632 | -3.098765 |
| 1 | 5.120088 | -0.066548 | -2.441768 |
| 6 | 3.075952 | 0.384769 | -2.636114 |
| 7 | 1.979001 | 0.061168 | -2.839505 |
| 6 | -0.292152 | 1.535265 | -1.363469 |
| 6 | -0.056570 | 0.260982 | -0.724809 |
| 7 | 0.122066 | -0.758287 | -0.224289 |
| 1 | -0.329262 | 1.372417 | -2.443717 |
| 1 | 0.549863 | 2.188609 | -1.115503 |
| 1 | -1.231732 | 1.942469 | -0.983623 |
| 1 | 0.328534 | -1.705583 | 0.219674 |

Cartesian coordinates of : PACN6_ 8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.757943 | 5.328053 | 0.306800 |
| 1 | 1.804417 | 5.383331 | -0.003257 |
| 1 | 0.661666 | 5.724088 | 1.320854 |
| 1 | 0.147501 | 5.928734 | -0.372023 |
| 6 | 0.309733 | 3.941521 | 0.278403 |
| 7 | -0.045745 | 2.840020 | 0.258335 |
| 6 | -6.661431 | -0.356422 | 0.008791 |
| 1 | -7.151113 | -1.304888 | 0.242827 |
| 1 | -6.881516 | -0.089958 | -1.027863 |
| 1 | -7.057774 | 0.419721 | 0.668019 |
| 6 | -5.218254 | -0.481210 | 0.196269 |
| 7 | -4.071033 | -0.581022 | 0.345547 |
| 6 | 3.968529 | -0.419844 | 2.098936 |
| 1 | 3.984422 | 0.167772 | 3.020302 |
| 1 | 4.128760 | 0.239674 | 1.241487 |
| 1 | 4.767386 | -1.164716 | 2.144348 |
| 6 | 2.675739 | -1.080949 | 1.949007 |
| 7 | 1.649519 | -1.608792 | 1.815594 |
| 6 | 2.914696 | -2.886124 | -1.105558 |
| 1 | 3.306906 | -3.445281 | -1.958584 |
| 1 | 2.991433 | -3.498495 | -0.203399 |
| 1 | 3.498927 | -1.970297 | -0.969522 |
| 6 | 1.519404 | -2.526434 | -1.336682 |
| 7 | 0.412741 | -2.224918 | -1.522611 |
| 6 | 0.757425 | 0.941529 | -2.728462 |
| 1 | 1.241289 | 1.083553 | -3.698124 |
| 1 | 0.120235 | 1.805944 | -2.519428 |
| 1 | 0.143786 | 0.036005 | -2.762188 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 1.762302 | 0.800051 | -1.677717 |
| 7 | 2.545182 | 0.679756 | -0.827402 |
| 6 | -1.472446 | -2.197900 | 0.925930 |
| 6 | -1.082021 | -0.830601 | 0.673338 |
| 7 | -0.766059 | 0.262260 | 0.503923 |
| 1 | -2.244206 | -2.199129 | 1.699692 |
| 1 | -0.578099 | -2.741203 | 1.244154 |
| 1 | -1.870899 | -2.617551 | -0.001073 |
| 1 | -0.475061 | 1.281560 | 0.385742 |

Cartesian coordinates of : PACN6_9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.274810 | -5.589485 | 0.009950 |
| 6 | -2.129451 | -4.136078 | 0.006543 |
| 7 | -2.014112 | -2.980837 | 0.003788 |
| 1 | -3.332773 | -5.858364 | 0.059944 |
| 1 | -1.759437 | -6.014265 | 0.874853 |
| 1 | -1.844512 | -6.009842 | -0.902330 |
| 6 | -2.962476 | 0.007661 | -0.002994 |
| 6 | -1.517698 | -0.015553 | -0.002525 |
| 7 | -0.367278 | -0.016557 | -0.002331 |
| 1 | -3.334579 | -0.514331 | 0.881582 |
| 1 | -3.334115 | -0.516798 | -0.886304 |
| 1 | -3.296470 | 1.047874 | -0.004448 |
| 6 | -1.657265 | 5.704956 | 0.010252 |
| 6 | -1.702004 | 4.244953 | 0.006068 |
| 7 | -1.737806 | 3.084497 | 0.002757 |
| 1 | -2.670394 | 6.108720 | 0.078512 |
| 1 | -1.192416 | 6.067100 | -0.910002 |
| 1 | -1.076325 | 6.058491 | 0.865600 |
| 1 | 0.721699 | -0.022830 | -0.002097 |
| 6 | 4.876112 | -0.064906 | -0.001528 |
| 1 | 5.262336 | 0.368802 | -0.926516 |
| 1 | 5.245621 | -1.089317 | 0.081492 |
| 1 | 5.263778 | 0.512462 | 0.840632 |
| 6 | 3.420335 | -0.048434 | -0.001687 |
| 7 | 2.262964 | -0.035448 | -0.001828 |
| 6 | -8.669155 | 0.117520 | -0.008062 |
| 6 | -7.209045 | 0.065817 | -0.006806 |
| 7 | -6.048709 | 0.024959 | -0.005699 |
| 1 | -9.049850 | -0.045584 | 1.003180 |
| 1 | -9.070170 | -0.656288 | -0.667248 |
| 1 | -9.008329 | 1.094398 | -0.361312 |
| 6 | 10.579905 | -0.146327 | -0.003429 |
| 1 | 10.950704 | -0.272275 | -1.023607 |
| 1 | 10.969492 | 0.790409 | 0.402602 |
| 1 | 10.940095 | -0.975858 | 0.609975 |
| 6 | 9.119223 | -0.121926 | -0.002416 |
| 7 | 7.958318 | -0.102571 | -0.001646 |

Cartesian coordinates of : PACN6_10

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.694741 | -0.076641 | 5.964317 |
| 1 | -1.728835 | -0.271967 | 6.258546 |
| 1 | -0.386532 | 0.894322 | 6.359652 |
| 1 | -0.050236 | -0.854800 | 6.380405 |
| 6 | -0.588352 | -0.073394 | 4.510024 |
| 7 | -0.504179 | -0.070770 | 3.355618 |
| 6 | -5.781252 | -1.179177 | -1.559629 |
| 1 | -6.054760 | -2.119097 | -1.073992 |
| 1 | -5.991638 | -1.258606 | -2.629005 |
| 1 | -6.386211 | -0.372477 | -1.138483 |
| 6 | -4.362327 | -0.902147 | -1.348862 |
| 7 | -3.234832 | -0.682063 | -1.181071 |
| 6 | 2.168855 | -5.156336 | -1.099220 |
| 1 | 1.430198 | -5.958054 | -1.023125 |
| 1 | 2.894106 | -5.264648 | -0.289054 |
| 1 | 2.689827 | -5.244921 | -2.055728 |
| 6 | 1.506943 | -3.856881 | -1.008665 |
| 7 | 0.979257 | -2.825337 | -0.936893 |
| 6 | -0.201215 | 5.588333 | -1.178307 |
| 1 | 0.409992 | 5.996841 | -0.369825 |
| 1 | -1.204276 | 6.017423 | -1.115959 |
| 1 | 0.244578 | 5.868318 | -2.135929 |
| 6 | -0.272211 | 4.133253 | -1.066266 |
| 7 | -0.330236 | 2.977205 | -0.977396 |
| 6 | 5.339715 | 1.016492 | -0.488168 |
| 1 | 5.805748 | 0.294170 | 0.186514 |
| 1 | 5.502392 | 2.023484 | -0.096229 |
| 1 | 5.812001 | 0.938939 | -1.470593 |
| 6 | 3.907749 | 0.747300 | -0.599358 |
| 7 | 2.770180 | 0.533668 | -0.688439 |
| 6 | -0.244130 | -0.072829 | -1.954711 |
| 6 | -0.306042 | -0.073123 | -0.513648 |
| 7 | -0.357486 | -0.071531 | 0.634273 |
| 1 | 0.795039 | 0.120561 | -2.234513 |
| 1 | -0.903890 | 0.716754 | -2.320260 |
| 1 | -0.569082 | -1.053706 | -2.307360 |
| 1 | -0.405299 | -0.069840 | 1.687257 |

Cartesian coordinates of : PACN6_11

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.987446 | 3.852731 | -1.138424 |
| 1 | -4.264158 | 4.028532 | -2.180880 |
| 1 | -3.577900 | 4.775708 | -0.720696 |
| 1 | -4.882630 | 3.575475 | -0.576395 |
| 6 | -2.994707 | 2.783591 | -1.058588 |
| 7 | -2.205656 | 1.934373 | -0.995502 |
| 6 | 4.562157 | -3.572548 | -1.041666 |
| 1 | 4.947724 | -3.574977 | -2.064157 |
| 1 | 4.323659 | -4.598558 | -0.750871 |
| 1 | 5.334087 | -3.184469 | -0.372644 |
| 6 | 3.364762 | -2.739222 | -0.961001 |
| 7 | 2.412513 | -2.078294 | -0.896964 |
| 6 | -0.000030 | 0.146618 | 5.974590 |
| 1 | 0.000660 | -0.862501 | 6.393839 |
| 1 | -0.890960 | 0.677567 | 6.318660 |
| 1 | 0.890202 | 0.678766 | 6.318615 |
| 6 | -0.000019 | 0.075256 | 4.518150 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.000010 | 0.018320 | 3.362083 |
| 6 | -4.562251 | -3.572477 | -1.041684 |
| 1 | -4.323883 | -4.598339 | -0.750262 |
| 1 | -4.947436 | -3.575434 | -2.064317 |
| 1 | -5.334422 | -3.184031 | -0.373153 |
| 6 | -3.364868 | -2.739134 | -0.961009 |
| 7 | -2.412629 | -2.078193 | -0.896963 |
| 6 | 3.987592 | 3.852595 | -1.138369 |
| 1 | 3.577619 | 4.775886 | -0.721756 |
| 1 | 4.265239 | 4.027571 | -2.180715 |
| 1 | 4.882280 | 3.575839 | -0.575307 |
| 6 | 2.994837 | 2.783466 | -1.058571 |
| 7 | 2.205774 | 1.934258 | -0.995513 |
| 6 | -0.000013 | -0.347592 | -1.941956 |
| 6 | -0.000007 | -0.246517 | -0.503209 |
| 7 | -0.000004 | -0.159317 | 0.642538 |
| 1 | -0.000049 | -1.406580 | -2.207633 |
| 1 | 0.903463 | 0.147394 | -2.306784 |
| 1 | -0.903452 | 0.147462 | -2.306781 |
| 1 | -0.000004 | -0.083928 | 1.693918 |

Cartesian coordinates of : PACN6_12

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.152019 | -0.021561 | -0.002379 |
| 6 | -0.302662 | -0.015749 | -0.002760 |
| 7 | -1.459784 | -0.011279 | -0.003010 |
| 1 | 1.531856 | -0.675890 | -0.790096 |
| 1 | 1.532559 | -0.378722 | 0.957080 |
| 1 | 1.538473 | 0.985467 | -0.173921 |
| 6 | -5.958498 | -5.582766 | 0.005632 |
| 6 | -5.871706 | -4.124850 | 0.002989 |
| 7 | -5.802986 | -2.965753 | 0.000909 |
| 1 | -7.004851 | -5.894072 | -0.042954 |
| 1 | -5.511527 | -5.981352 | 0.919663 |
| 1 | -5.426502 | -5.989673 | -0.857796 |
| 7 | -4.052810 | -0.005718 | -0.003713 |
| 6 | -5.202963 | -0.009155 | -0.004023 |
| 6 | -6.649552 | 0.011057 | -0.004592 |
| 1 | -7.006135 | -0.518612 | -0.891482 |
| 1 | -7.006754 | -0.515989 | 0.883613 |
| 1 | -6.970894 | 1.055923 | -0.006121 |
| 1 | -2.939632 | -0.007277 | -0.003384 |
| 6 | 6.806035 | -0.047363 | -0.001726 |
| 6 | 5.345780 | -0.038818 | -0.001885 |
| 7 | 4.184008 | -0.031984 | -0.002009 |
| 1 | 7.195917 | 0.728100 | 0.661167 |
| 1 | 7.192619 | 0.135496 | -1.006666 |
| 1 | 7.185744 | -1.012503 | 0.340489 |
| 6 | -5.460077 | 5.715554 | 0.005796 |
| 6 | -5.515863 | 4.256130 | 0.002734 |
| 7 | -5.560785 | 3.095891 | 0.000302 |
| 1 | -4.951837 | 6.071553 | -0.893676 |
| 1 | -4.915236 | 6.066436 | 0.885636 |
| 1 | -6.472254 | 6.126865 | 0.027809 |
| 6 | 12.582696 | -0.080390 | 0.003840 |
| 1 | 12.955645 | -0.522747 | -0.923190 |
| 1 | 12.962459 | 0.940895 | 0.087001 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 12.952028 | -0.665742 | 0.849487 |
| 6 | 11.121574 | -0.071977 | 0.001578 |
| 7 | 9.960588 | -0.065275 | -0.000174 |

Cartesian coordinates of : PACN6_13

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|------------|-----------|-----------|
| 6 | -3.887694 | -0.251035 | 0.000804 |
| 6 | -2.428359 | -0.206716 | -0.000131 |
| 7 | -1.267120 | -0.171659 | -0.000847 |
| 1 | -4.303310 | 0.755917 | -0.077059 |
| 1 | -4.258994 | -0.703867 | 0.922673 |
| 1 | -4.256096 | -0.839089 | -0.842539 |
| 6 | 1.528434 | 1.170588 | -0.003877 |
| 6 | 1.680985 | -0.265361 | -0.003723 |
| 7 | 1.827024 | -1.406206 | -0.003730 |
| 1 | 0.962235 | 1.473844 | 0.879927 |
| 1 | 0.961819 | 1.473666 | -0.887475 |
| 1 | 2.519862 | 1.629574 | -0.004093 |
| 6 | 7.325892 | 0.678185 | 0.011991 |
| 6 | 5.879171 | 0.476745 | 0.007415 |
| 7 | 4.729166 | 0.317006 | 0.003838 |
| 1 | 7.553674 | 1.745428 | -0.044803 |
| 1 | 7.776193 | 0.173390 | -0.846210 |
| 1 | 7.756729 | 0.272007 | 0.930412 |
| 1 | 1.945465 | -2.470284 | -0.003686 |
| 6 | 2.346079 | -6.668332 | -0.004000 |
| 1 | 2.677979 | -7.008260 | -0.988116 |
| 1 | 1.380820 | -7.125113 | 0.227951 |
| 1 | 3.078186 | -6.972544 | 0.748094 |
| 6 | 2.215180 | -5.216825 | -0.003822 |
| 7 | 2.110882 | -4.064544 | -0.003741 |
| 6 | 0.882318 | 6.834829 | -0.004112 |
| 6 | 1.073292 | 5.386372 | -0.004607 |
| 7 | 1.225238 | 4.235326 | -0.004931 |
| 1 | 0.579062 | 7.171483 | 0.990289 |
| 1 | 0.107157 | 7.109892 | -0.723548 |
| 1 | 1.814274 | 7.334910 | -0.278860 |
| 6 | -9.652816 | -0.376255 | 0.004488 |
| 1 | -10.028969 | -0.202780 | -1.006733 |
| 1 | -10.017144 | -1.344346 | 0.356925 |
| 1 | -10.034291 | 0.407261 | 0.663825 |
| 6 | -8.191759 | -0.361839 | 0.003856 |
| 7 | -7.030757 | -0.350385 | 0.003315 |

Cartesian coordinates of : PACN6_14

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|-----------|
| 6 | 1.248703 | -5.588759 | -0.003264 |
| 6 | 1.531229 | -4.155752 | -0.002503 |
| 7 | 1.755266 | -3.016563 | -0.001942 |
| 1 | 0.170330 | -5.755810 | 0.054199 |
| 1 | 1.727956 | -6.064302 | 0.855965 |
| 1 | 1.630166 | -6.043956 | -0.920534 |

| | | | |
|---|------------|-----------|-----------|
| 6 | 0.802063 | -0.038152 | -0.000599 |
| 6 | 2.245697 | -0.063674 | -0.000094 |
| 7 | 3.396014 | -0.066748 | 0.000399 |
| 1 | 0.427522 | -0.561674 | 0.882138 |
| 1 | 0.428143 | -0.559115 | -0.885115 |
| 1 | 0.467955 | 1.002057 | 0.000714 |
| 6 | 1.917745 | 5.644078 | -0.003568 |
| 6 | 1.991572 | 4.185299 | -0.002240 |
| 7 | 2.049663 | 3.025692 | -0.001191 |
| 1 | 0.874444 | 5.964104 | -0.060486 |
| 1 | 2.459094 | 6.044802 | -0.864062 |
| 1 | 2.361130 | 6.041408 | 0.912746 |
| 1 | 4.467456 | -0.074924 | 0.000953 |
| 6 | 8.682328 | -0.131221 | 0.004631 |
| 1 | 9.058140 | 0.295224 | -0.928699 |
| 1 | 9.035401 | -1.161206 | 0.097629 |
| 1 | 9.058715 | 0.455613 | 0.846149 |
| 6 | 7.225117 | -0.109592 | 0.003174 |
| 7 | 6.068225 | -0.092623 | 0.002056 |
| 6 | -4.858732 | 0.018732 | 0.000769 |
| 6 | -3.398829 | -0.022417 | -0.000469 |
| 7 | -2.237492 | -0.054980 | -0.001269 |
| 1 | -5.246075 | -0.065728 | 1.018431 |
| 1 | -5.268385 | -0.803150 | -0.590396 |
| 1 | -5.218492 | 0.957869 | -0.425114 |
| 6 | -10.634702 | 0.189340 | 0.001768 |
| 1 | -11.005233 | 0.298177 | -1.020495 |
| 1 | -11.038536 | -0.731893 | 0.428851 |
| 1 | -10.981929 | 1.037635 | 0.596737 |
| 6 | -9.174288 | 0.142609 | 0.002073 |
| 7 | -8.013849 | 0.105497 | 0.002279 |

Cartesian coordinates of : PACN6_15

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.621044 | -0.906531 | -0.000169 |
| 6 | 4.162065 | -0.858587 | 0.000426 |
| 7 | 3.000748 | -0.821232 | 0.000859 |
| 1 | 5.971945 | -1.937836 | 0.077598 |
| 1 | 6.025613 | -0.343231 | 0.843500 |
| 1 | 6.020349 | -0.478112 | -0.922005 |
| 6 | 0.119429 | -1.850984 | 0.003129 |
| 6 | 0.076276 | -0.406304 | 0.002321 |
| 7 | 0.018987 | 0.741742 | 0.001734 |
| 1 | 0.665199 | -2.181600 | 0.890460 |
| 1 | 0.664395 | -2.182611 | -0.884319 |
| 1 | -0.911686 | -2.214706 | 0.003780 |
| 6 | -5.573150 | -0.939013 | 0.000740 |
| 6 | -4.114409 | -0.883699 | 0.001320 |
| 7 | -2.953254 | -0.841117 | 0.001830 |
| 1 | -5.918219 | -1.971685 | -0.084829 |
| 1 | -5.980492 | -0.372119 | -0.839177 |
| 1 | -5.975432 | -0.519904 | 0.925551 |
| 1 | -0.032174 | 1.819855 | 0.001187 |
| 6 | -0.232336 | 6.002823 | -0.000670 |
| 1 | -0.767160 | 6.345055 | -0.890097 |
| 1 | 0.777637 | 6.420144 | -0.004566 |
| 1 | -0.760733 | 6.346122 | 0.892181 |

| | | | |
|---|------------|-----------|-----------|
| 6 | -0.162049 | 4.547455 | -0.000051 |
| 7 | -0.106257 | 3.392037 | 0.000445 |
| 6 | 11.360910 | -1.303435 | -0.001912 |
| 6 | 9.907110 | -1.157678 | -0.001792 |
| 7 | 8.751836 | -1.041896 | -0.001672 |
| 1 | 11.704049 | -1.629622 | 0.982975 |
| 1 | 11.832545 | -0.347638 | -0.243042 |
| 1 | 11.662262 | -2.045046 | -0.745788 |
| 6 | -11.307155 | -1.425054 | -0.003079 |
| 1 | -11.643298 | -1.748148 | -0.991394 |
| 1 | -11.591527 | -2.181266 | 0.732739 |
| 1 | -11.800021 | -0.482755 | 0.248494 |
| 6 | -9.856982 | -1.246726 | -0.001838 |
| 7 | -8.704598 | -1.105033 | -0.000881 |

Cartesian coordinates of : PACN6_16

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.442809 | -6.599192 | 0.001001 |
| 6 | -5.327368 | -5.147170 | 0.000730 |
| 7 | -5.235693 | -3.994260 | 0.000525 |
| 1 | -4.904674 | -7.010381 | 0.858717 |
| 1 | -5.015174 | -7.001946 | -0.920553 |
| 1 | -6.495904 | -6.884237 | 0.065037 |
| 6 | 0.609895 | -0.073723 | -0.001094 |
| 6 | -0.849353 | -0.051068 | -0.001201 |
| 7 | -2.011212 | -0.033026 | -0.001350 |
| 1 | 0.989950 | -0.515474 | -0.924683 |
| 1 | 0.987684 | -0.660842 | 0.838638 |
| 1 | 1.011612 | 0.938315 | 0.082943 |
| 7 | -5.021799 | -1.372672 | 0.000152 |
| 6 | -4.887043 | -0.229571 | -0.000017 |
| 6 | -4.797118 | 1.213408 | -0.000153 |
| 1 | -4.243704 | 1.540862 | 0.883293 |
| 1 | -4.244637 | 1.540762 | -0.884221 |
| 1 | -5.797276 | 1.653104 | 0.000366 |
| 1 | -5.107563 | -2.460018 | 0.000291 |
| 6 | -5.082789 | 6.872349 | 0.000781 |
| 6 | -5.034456 | 5.412435 | 0.000764 |
| 7 | -4.996005 | 4.252019 | 0.000777 |
| 1 | -4.161077 | 7.276411 | -0.424983 |
| 1 | -5.193830 | 7.242154 | 1.023044 |
| 1 | -5.930683 | 7.217741 | -0.595785 |
| 6 | 6.328259 | -0.109314 | -0.001864 |
| 6 | 4.867737 | -0.127766 | -0.001585 |
| 7 | 3.706069 | -0.142357 | -0.001358 |
| 1 | 6.708806 | 0.311294 | 0.931455 |
| 1 | 6.706097 | 0.496025 | -0.828680 |
| 1 | 6.726783 | -1.120546 | -0.108640 |
| 6 | 12.116194 | 0.007080 | 0.002960 |
| 1 | 12.502202 | -0.411112 | -0.929929 |
| 1 | 12.464525 | 1.038320 | 0.099818 |
| 1 | 12.503785 | -0.577934 | 0.840640 |
| 6 | 10.655466 | -0.029393 | 0.000874 |
| 7 | 9.494839 | -0.058413 | -0.000739 |

Cartesian coordinates of : PACN6_17

```

-----
Atomic number (AN) and Cartesian coordinates
AN      X      Y      Z
-----
6      8.094170   -0.013690   0.001537
6      6.635746   -0.054186  -0.005735
7      5.474050   -0.086234  -0.011509
1      8.506438   -1.022867   0.067899
1      8.458951    0.562069   0.854905
1      8.470823    0.450777  -0.912363
6      2.698189   -1.286439  -0.020355
6      2.646890    0.153251  -0.025259
7      2.576131    1.300719  -0.029628
1      3.242495   -1.607571   0.872421
1      3.251005   -1.613475  -0.905715
1      1.666072   -1.650095  -0.023740
6     -2.894326   -0.066461  -0.014167
6     -1.435868   -0.095900  -0.017600
7     -0.273715   -0.118870  -0.020236
1     -3.300533   -1.076898  -0.096465
1     -3.271262    0.521584  -0.853669
1     -3.269928    0.377619   0.910147
1      2.503393    2.306279  -0.033007
6     -8.591179    0.031656   0.001880
6     -7.130703    0.021838  -0.002727
7     -5.968969    0.014020  -0.006358
1     -8.983291   -0.558654  -0.829137
1     -8.970240    1.051398  -0.094249
1     -8.976637   -0.390103   0.932651
6    -14.376325    0.042764   0.027914
6    -12.915175    0.044516   0.020430
7    -11.754202    0.045910   0.014531
1    -14.748642   -0.979814   0.127331
1    -14.755708    0.468933  -0.904080
1    -14.746793    0.637797   0.866284
6     13.825445    0.091670   0.034511
1     14.208213   -0.926743   0.136747
1     14.201030    0.519681  -0.898155
1     14.188332    0.692595   0.871967
6     12.364544    0.077833   0.025415
7     11.203536    0.066792   0.018225
-----

```

Cartesian coordinates of : PACN7_ 1

```

-----
Atomic number (AN) and Cartesian coordinates
AN      X      Y      Z
-----
6      2.587515    4.132084  -0.920476
1      1.538058    4.436115  -0.889638
1      3.047736    4.506201  -1.838403
1      3.115819    4.551705  -0.060776
6      2.653904    2.674555  -0.886600
7      2.704034    1.513877  -0.861620
6     -4.542191   -1.899956  -0.679515
1     -5.133350   -1.948831   0.238319
1     -3.848269   -2.743684  -0.712970
1     -5.215125   -1.947726  -1.539283
6     -3.773998   -0.659709  -0.714765
-----

```

| | | | |
|---|-----------|-----------|-----------|
| 7 | -3.161015 | 0.326941 | -0.744924 |
| 6 | -0.000631 | 0.141333 | 6.030423 |
| 1 | -0.903217 | 0.643021 | 6.387869 |
| 1 | 0.877658 | 0.684712 | 6.387440 |
| 1 | 0.023381 | -0.878055 | 6.423352 |
| 6 | -0.000207 | 0.107603 | 4.572869 |
| 7 | 0.000068 | 0.080806 | 3.415861 |
| 6 | 0.333695 | -4.883607 | -0.918402 |
| 1 | 0.087853 | -5.562215 | -0.097820 |
| 1 | 1.364221 | -4.536006 | -0.810394 |
| 1 | 0.227288 | -5.417530 | -1.866026 |
| 6 | -0.555749 | -3.726890 | -0.894632 |
| 7 | -1.264448 | -2.806215 | -0.876382 |
| 6 | 4.781768 | -1.173923 | -0.745093 |
| 1 | 4.714906 | -0.083292 | -0.769179 |
| 1 | 5.329661 | -1.524877 | -1.623151 |
| 1 | 5.314414 | -1.488247 | 0.155901 |
| 6 | 3.431115 | -1.726271 | -0.745966 |
| 7 | 2.355712 | -2.166207 | -0.747991 |
| 6 | -3.160780 | 3.711749 | -1.013852 |
| 1 | -3.385951 | 4.415555 | -0.208704 |
| 1 | -3.769384 | 2.811865 | -0.895205 |
| 1 | -3.390454 | 4.182654 | -1.972951 |
| 6 | -1.751884 | 3.334445 | -0.968243 |
| 7 | -0.629176 | 3.037232 | -0.931904 |
| 6 | -0.003023 | -0.036183 | -1.879409 |
| 6 | -0.001849 | -0.004178 | -0.436236 |
| 7 | -0.000803 | 0.019859 | 0.712862 |
| 1 | 0.657405 | -0.848490 | -2.196316 |
| 1 | 0.360868 | 0.930125 | -2.237750 |
| 1 | -1.029908 | -0.216923 | -2.209136 |
| 1 | -0.000327 | 0.043557 | 1.772877 |

Cartesian coordinates of : PACN7_ 2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.459510 | -2.767321 | -1.730692 |
| 1 | -3.203228 | -2.242396 | -1.123733 |
| 1 | -2.186876 | -3.694315 | -1.220276 |
| 1 | -2.879629 | -2.998144 | -2.712885 |
| 6 | -1.277658 | -1.922678 | -1.874585 |
| 7 | -0.343277 | -1.242049 | -1.995478 |
| 6 | 1.913173 | 1.295411 | -2.133567 |
| 1 | 2.399449 | 1.997781 | -2.815384 |
| 1 | 1.584677 | 0.411885 | -2.687734 |
| 1 | 2.631623 | 0.989655 | -1.365552 |
| 6 | 0.752369 | 1.925917 | -1.511268 |
| 7 | -0.169935 | 2.430208 | -1.015790 |
| 6 | -2.885849 | 1.415068 | -2.369198 |
| 1 | -3.815577 | 1.253519 | -2.920650 |
| 1 | -2.055466 | 0.930400 | -2.890954 |
| 1 | -2.674098 | 2.485609 | -2.310082 |
| 6 | -2.996590 | 0.859044 | -1.023335 |
| 7 | -3.095956 | 0.402804 | 0.041339 |
| 6 | 6.803571 | 0.400121 | 0.654800 |
| 1 | 7.470579 | -0.203350 | 0.034276 |
| 1 | 7.031109 | 0.214334 | 1.707347 |
| 1 | 6.973328 | 1.457210 | 0.435948 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 5.412956 | 0.051013 | 0.376889 |
| 7 | 4.307185 | -0.227355 | 0.155631 |
| 6 | -2.966946 | -1.481151 | 2.723263 |
| 1 | -3.914125 | -1.419177 | 2.182584 |
| 1 | -2.641619 | -0.463495 | 2.955077 |
| 1 | -3.102810 | -2.046253 | 3.648536 |
| 6 | -1.963750 | -2.129896 | 1.883871 |
| 7 | -1.160957 | -2.652445 | 1.225911 |
| 6 | -2.334624 | 3.416106 | 1.524133 |
| 1 | -2.266944 | 4.247132 | 2.230193 |
| 1 | -3.339869 | 2.987036 | 1.544637 |
| 1 | -2.106751 | 3.767886 | 0.512519 |
| 6 | -1.364462 | 2.386575 | 1.855708 |
| 7 | -0.583481 | 1.563502 | 2.086245 |
| 6 | 1.973779 | -2.339522 | -0.099838 |
| 6 | 1.413120 | -1.174570 | 0.547520 |
| 7 | 0.948997 | -0.268237 | 1.082271 |
| 1 | 1.201480 | -3.115172 | -0.098058 |
| 1 | 2.863109 | -2.659736 | 0.447890 |
| 1 | 2.244670 | -2.073217 | -1.125087 |
| 1 | 0.351471 | 0.523113 | 1.568282 |

Cartesian coordinates of : PACN7_ 3

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.863789 | -2.250458 | 1.106532 |
| 1 | 4.611038 | -2.945125 | 0.714839 |
| 1 | 2.980028 | -2.810553 | 1.426449 |
| 1 | 4.290448 | -1.717796 | 1.960502 |
| 6 | 3.466304 | -1.301195 | 0.071351 |
| 7 | 3.125471 | -0.547166 | -0.745094 |
| 6 | -4.295520 | 0.071165 | -0.615066 |
| 1 | -4.351006 | 0.902487 | -1.322922 |
| 1 | -3.990036 | 0.449796 | 0.364712 |
| 1 | -5.278696 | -0.400193 | -0.540597 |
| 6 | -3.306589 | -0.900993 | -1.072250 |
| 7 | -2.518003 | -1.675779 | -1.430706 |
| 6 | 3.517457 | 2.879642 | -0.992083 |
| 1 | 3.806478 | 1.896246 | -1.372399 |
| 1 | 4.332260 | 3.288005 | -0.388891 |
| 1 | 3.325644 | 3.554341 | -1.830180 |
| 6 | 2.314571 | 2.743625 | -0.175136 |
| 7 | 1.357901 | 2.640043 | 0.476759 |
| 6 | -1.966398 | -3.296071 | 1.349912 |
| 1 | -2.497857 | -2.392135 | 1.663311 |
| 1 | -1.909067 | -3.997526 | 2.186004 |
| 1 | -2.508513 | -3.755521 | 0.519941 |
| 6 | -0.623689 | -2.927946 | 0.912794 |
| 7 | 0.449718 | -2.628977 | 0.581041 |
| 6 | 0.829490 | 0.109598 | 2.339179 |
| 1 | 1.154161 | 1.012461 | 2.861446 |
| 1 | 1.431841 | -0.010234 | 1.434008 |
| 1 | 0.958657 | -0.765378 | 2.982268 |
| 6 | -0.573366 | 0.235528 | 1.955891 |
| 7 | -1.693120 | 0.320039 | 1.654494 |
| 6 | -1.915038 | 3.840127 | 1.161951 |
| 1 | -2.426532 | 4.768579 | 0.897443 |
| 1 | -0.933465 | 4.065621 | 1.590816 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.508285 | 3.279933 | 1.890251 |
| 6 | -1.705395 | 3.014633 | -0.014934 |
| 7 | -1.500719 | 2.330651 | -0.927047 |
| 6 | 0.726381 | -2.047561 | -2.518561 |
| 6 | 0.298140 | -0.754282 | -2.033804 |
| 7 | -0.089206 | 0.274472 | -1.695134 |
| 1 | 1.500491 | -2.435779 | -1.853681 |
| 1 | 1.107171 | -1.943330 | -3.538035 |
| 1 | -0.150840 | -2.703182 | -2.496672 |
| 1 | -0.649042 | 1.171439 | -1.403451 |

Cartesian coordinates of : PACN7_ 4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.345404 | -0.524044 | 2.722187 |
| 1 | -1.362090 | -0.843938 | 3.078108 |
| 1 | -2.810253 | -1.332732 | 2.150839 |
| 1 | -2.979743 | -0.274815 | 3.576697 |
| 6 | -2.184907 | 0.644416 | 1.861999 |
| 7 | -2.058134 | 1.580703 | 1.185031 |
| 6 | 4.431547 | -0.762581 | -2.558476 |
| 1 | 5.462849 | -1.083231 | -2.390933 |
| 1 | 4.334055 | 0.300226 | -2.321347 |
| 1 | 4.175487 | -0.929386 | -3.607729 |
| 6 | 3.526919 | -1.516740 | -1.697133 |
| 7 | 2.805093 | -2.107963 | -1.004848 |
| 6 | -1.796124 | 4.359345 | -0.966802 |
| 1 | -1.099727 | 5.195314 | -0.864416 |
| 1 | -2.282813 | 4.159829 | -0.006738 |
| 1 | -2.551496 | 4.610099 | -1.715490 |
| 6 | -1.083236 | 3.153612 | -1.359621 |
| 7 | -0.528149 | 2.175012 | -1.634185 |
| 6 | 1.344943 | 2.613837 | 1.317181 |
| 1 | 1.263039 | 3.671971 | 1.052790 |
| 1 | 1.803779 | 2.529879 | 2.305951 |
| 1 | 0.345412 | 2.168390 | 1.354163 |
| 6 | 2.159619 | 1.914052 | 0.328211 |
| 7 | 2.800592 | 1.344110 | -0.455519 |
| 6 | -5.646557 | -1.929769 | -1.398594 |
| 1 | -6.162747 | -2.812147 | -1.012420 |
| 1 | -5.608459 | -1.989839 | -2.489062 |
| 1 | -6.205419 | -1.035931 | -1.110839 |
| 6 | -4.292080 | -1.867472 | -0.855619 |
| 7 | -3.215084 | -1.820110 | -0.423183 |
| 6 | 3.661941 | -1.108897 | 2.024323 |
| 1 | 4.095429 | -0.929574 | 3.011369 |
| 1 | 4.084841 | -0.407267 | 1.299067 |
| 1 | 3.892689 | -2.126775 | 1.700578 |
| 6 | 2.214795 | -0.925882 | 2.071293 |
| 7 | 1.063896 | -0.766781 | 2.111641 |
| 6 | -0.217093 | -2.757370 | -0.023003 |
| 6 | -0.183650 | -1.411816 | -0.552423 |
| 7 | -0.157989 | -0.349307 | -0.990807 |
| 1 | 0.810861 | -3.128744 | 0.015320 |
| 1 | -0.841939 | -3.374661 | -0.673158 |
| 1 | -0.654394 | -2.717747 | 0.978362 |
| 1 | -0.225205 | 0.677297 | -1.329168 |

Cartesian coordinates of : PACN7_ 5

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.608726 | -2.003097 | 1.316327 |
| 1 | 3.991489 | -2.434496 | 2.244590 |
| 1 | 3.937764 | -0.963310 | 1.228336 |
| 1 | 3.992163 | -2.567934 | 0.463038 |
| 6 | 2.149953 | -2.039209 | 1.311580 |
| 7 | 0.987815 | -2.059555 | 1.319977 |
| 6 | -1.046954 | 5.146950 | 0.044238 |
| 1 | -0.132216 | 5.602229 | 0.431825 |
| 1 | -1.844146 | 5.251438 | 0.784359 |
| 1 | -1.340660 | 5.659993 | -0.874920 |
| 6 | -0.814435 | 3.735081 | -0.234337 |
| 7 | -0.628817 | 2.615206 | -0.457967 |
| 6 | 0.589391 | 1.189828 | 2.706015 |
| 1 | 0.948940 | 1.699842 | 3.603356 |
| 1 | 0.396119 | 0.137442 | 2.933485 |
| 1 | -0.350374 | 1.639791 | 2.373212 |
| 6 | 1.586110 | 1.278564 | 1.642942 |
| 7 | 2.374807 | 1.344687 | 0.791744 |
| 6 | -5.060447 | -0.047017 | -1.089035 |
| 1 | -5.964595 | -0.598927 | -0.820294 |
| 1 | -5.273546 | 0.577719 | -1.959933 |
| 1 | -4.761204 | 0.587805 | -0.249638 |
| 6 | -3.976574 | -0.976769 | -1.391438 |
| 7 | -3.101676 | -1.709189 | -1.609037 |
| 6 | -2.409402 | -2.396830 | 1.820058 |
| 1 | -3.075540 | -2.607676 | 2.660513 |
| 1 | -1.403595 | -2.759839 | 2.047725 |
| 1 | -2.785109 | -2.906936 | 0.927275 |
| 6 | -2.358328 | -0.959901 | 1.564144 |
| 7 | -2.325057 | 0.180463 | 1.339631 |
| 6 | 4.470203 | 1.022870 | -1.901191 |
| 1 | 5.512005 | 0.701373 | -1.824613 |
| 1 | 4.231692 | 1.696584 | -1.073804 |
| 1 | 4.331668 | 1.545118 | -2.851171 |
| 6 | 3.582813 | -0.133504 | -1.832546 |
| 7 | 2.874439 | -1.051842 | -1.766336 |
| 6 | -0.061794 | -2.476641 | -1.656384 |
| 6 | -0.162729 | -1.076620 | -1.309116 |
| 7 | -0.249546 | 0.039204 | -1.047596 |
| 1 | -0.497797 | -3.060983 | -0.841262 |
| 1 | 0.997916 | -2.715680 | -1.781988 |
| 1 | -0.630187 | -2.651119 | -2.573366 |
| 1 | -0.383742 | 1.072512 | -0.787176 |

Cartesian coordinates of : PACN7_ 6

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|----------|-----------|
| 6 | 4.275333 | 1.247725 | -2.363266 |
| 1 | 3.972340 | 1.498152 | -3.383007 |
| 1 | 5.363276 | 1.147648 | -2.333216 |
| 1 | 3.960048 | 2.043037 | -1.682360 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 3.645751 | -0.001513 | -1.947593 |
| 7 | 3.141803 | -0.990872 | -1.605418 |
| 6 | -5.042892 | -1.328050 | -1.229309 |
| 1 | -5.267949 | -1.060882 | -2.264764 |
| 1 | -5.091930 | -0.431785 | -0.603841 |
| 1 | -5.784090 | -2.051700 | -0.881182 |
| 6 | -3.703392 | -1.901213 | -1.139876 |
| 7 | -2.633422 | -2.344744 | -1.051622 |
| 6 | -2.869855 | 3.922327 | -0.380131 |
| 1 | -3.425540 | 4.211011 | -1.275647 |
| 1 | -2.425832 | 4.813130 | 0.070748 |
| 1 | -3.546948 | 3.444513 | 0.334797 |
| 6 | -1.831474 | 2.963397 | -0.725798 |
| 7 | -1.022853 | 2.173639 | -0.976234 |
| 6 | -1.901010 | -1.497014 | 2.200854 |
| 1 | -0.807301 | -1.428257 | 2.179567 |
| 1 | -2.210774 | -2.377700 | 1.630259 |
| 1 | -2.233472 | -1.603094 | 3.236753 |
| 6 | -2.492713 | -0.302572 | 1.603566 |
| 7 | -2.955802 | 0.650861 | 1.125160 |
| 6 | 4.204849 | -1.003183 | 1.533202 |
| 1 | 4.335332 | 0.026247 | 1.185561 |
| 1 | 4.646666 | -1.682748 | 0.800323 |
| 1 | 4.698754 | -1.132229 | 2.499437 |
| 6 | 2.777928 | -1.279217 | 1.658596 |
| 7 | 1.638867 | -1.483792 | 1.765716 |
| 6 | 0.508794 | 1.763255 | 2.292101 |
| 1 | 0.612162 | 0.826188 | 2.847672 |
| 1 | -0.495664 | 1.810868 | 1.858935 |
| 1 | 0.644209 | 2.604602 | 2.976534 |
| 6 | 1.510521 | 1.807508 | 1.230267 |
| 7 | 2.302719 | 1.825702 | 0.380642 |
| 6 | 0.512348 | -2.807934 | -0.890481 |
| 6 | 0.199947 | -1.396673 | -0.910646 |
| 7 | -0.055185 | -0.275478 | -0.946442 |
| 1 | 1.590132 | -2.914611 | -1.043414 |
| 1 | -0.061805 | -3.300039 | -1.679702 |
| 1 | 0.221345 | -3.211154 | 0.083706 |
| 1 | -0.370662 | 0.760540 | -0.988691 |

Cartesian coordinates of : PACN7_ 7

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.965521 | -0.464202 | -1.471889 |
| 1 | 6.048836 | -0.233671 | -2.536822 |
| 1 | 6.664864 | -1.267647 | -1.227797 |
| 1 | 6.228135 | 0.424933 | -0.893486 |
| 6 | 4.600701 | -0.878573 | -1.157316 |
| 7 | 3.516069 | -1.209955 | -0.907047 |
| 6 | -4.245055 | 0.042523 | -2.506997 |
| 1 | -4.199348 | 0.854406 | -1.775975 |
| 1 | -5.244518 | -0.399783 | -2.503215 |
| 1 | -4.037090 | 0.434996 | -3.505559 |
| 6 | -3.250816 | -0.963592 | -2.148087 |
| 7 | -2.458885 | -1.759875 | -1.850792 |
| 6 | -1.400130 | 1.493283 | 2.595590 |
| 1 | -2.076183 | 1.969700 | 3.310114 |
| 1 | -0.532235 | 2.132948 | 2.414448 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -1.037441 | 0.545383 | 3.003754 |
| 6 | -2.097274 | 1.239932 | 1.338361 |
| 7 | -2.657423 | 1.035435 | 0.340655 |
| 6 | -3.409816 | -2.369762 | 1.248224 |
| 1 | -3.889354 | -1.438530 | 0.932374 |
| 1 | -3.853252 | -2.715052 | 2.185488 |
| 1 | -3.560088 | -3.123131 | 0.471081 |
| 6 | -1.981597 | -2.129442 | 1.428544 |
| 7 | -0.847129 | -1.929454 | 1.583526 |
| 6 | 2.470480 | -1.456155 | 2.445546 |
| 1 | 3.068955 | -1.927744 | 1.660535 |
| 1 | 1.591371 | -2.072370 | 2.652559 |
| 1 | 3.074528 | -1.364981 | 3.351885 |
| 6 | 2.035416 | -0.137259 | 1.994354 |
| 7 | 1.685613 | 0.909572 | 1.630676 |
| 6 | 0.220776 | 5.293225 | -0.328050 |
| 1 | 0.890564 | 5.517956 | 0.505702 |
| 1 | -0.780884 | 5.664336 | -0.097662 |
| 1 | 0.588823 | 5.791240 | -1.228456 |
| 6 | 0.176178 | 3.852681 | -0.546334 |
| 7 | 0.143689 | 2.709880 | -0.720741 |
| 6 | 0.647353 | -2.494249 | -1.156380 |
| 6 | 0.445075 | -1.065382 | -1.057136 |
| 7 | 0.289098 | 0.070891 | -0.990156 |
| 1 | -0.326864 | -2.961392 | -1.324761 |
| 1 | 1.085982 | -2.839665 | -0.216116 |
| 1 | 1.337332 | -2.695702 | -1.979332 |
| 1 | 0.199765 | 1.140140 | -0.872191 |

Cartesian coordinates of : PACN7_8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.644277 | -2.890756 | -2.387324 |
| 1 | -2.772475 | -2.291270 | -3.292738 |
| 1 | -3.590375 | -2.950863 | -1.841518 |
| 1 | -2.308991 | -3.893634 | -2.663280 |
| 6 | -1.658986 | -2.260728 | -1.521460 |
| 7 | -0.881562 | -1.752350 | -0.833259 |
| 6 | -0.855885 | 4.021027 | -0.267341 |
| 1 | -1.670385 | 3.960151 | 0.458889 |
| 1 | -1.144170 | 3.489196 | -1.180071 |
| 1 | -0.656843 | 5.068834 | -0.505394 |
| 6 | 0.340375 | 3.394134 | 0.284378 |
| 7 | 1.298916 | 2.890543 | 0.704807 |
| 6 | -3.210024 | 0.919584 | -1.278399 |
| 1 | -2.474472 | 0.867378 | -2.086682 |
| 1 | -3.824003 | 1.816126 | -1.402213 |
| 1 | -3.860362 | 0.039183 | -1.298056 |
| 6 | -2.504225 | 0.965258 | -0.000973 |
| 7 | -1.942948 | 1.002681 | 1.016891 |
| 6 | 2.656548 | 1.247374 | -1.900316 |
| 1 | 2.912670 | 2.218722 | -1.468803 |
| 1 | 3.149683 | 1.135555 | -2.869241 |
| 1 | 3.009898 | 0.460780 | -1.224648 |
| 6 | 1.207885 | 1.155979 | -2.059354 |
| 7 | 0.053004 | 1.085795 | -2.167381 |
| 6 | 6.391832 | -2.490289 | 0.205796 |
| 1 | 6.384501 | -2.996368 | -0.762673 |

| | | | |
|---|-----------|-----------|----------|
| 1 | 6.467568 | -3.239751 | 0.997464 |
| 1 | 7.261635 | -1.830702 | 0.256307 |
| 6 | 5.166572 | -1.712764 | 0.371523 |
| 7 | 4.192518 | -1.093991 | 0.503910 |
| 6 | -4.171286 | -1.069836 | 2.882056 |
| 1 | -5.162485 | -0.685770 | 3.135671 |
| 1 | -3.436120 | -0.265402 | 2.978538 |
| 1 | -3.918576 | -1.879809 | 3.570770 |
| 6 | -4.162636 | -1.560953 | 1.507341 |
| 7 | -4.145814 | -1.938122 | 0.408891 |
| 6 | 2.367821 | 0.623367 | 2.436448 |
| 6 | 1.481688 | -0.006378 | 1.479723 |
| 7 | 0.767845 | -0.528985 | 0.745099 |
| 1 | 3.129572 | 1.178405 | 1.884134 |
| 1 | 2.836805 | -0.151552 | 3.047905 |
| 1 | 1.787169 | 1.319777 | 3.046549 |
| 1 | 0.053626 | -1.038114 | 0.053799 |

Cartesian coordinates of : PACN7_ 9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.218830 | -0.673665 | 1.497387 |
| 1 | -3.782866 | -1.287347 | 2.289520 |
| 1 | -5.308777 | -0.738843 | 1.541149 |
| 1 | -3.906511 | 0.365069 | 1.643159 |
| 6 | -3.737365 | -1.133915 | 0.199040 |
| 7 | -3.352281 | -1.481263 | -0.840987 |
| 6 | -0.345494 | 1.568680 | 2.592714 |
| 1 | -0.739230 | 1.767591 | 3.592793 |
| 1 | -0.796263 | 2.259841 | 1.874507 |
| 1 | 0.742270 | 1.691307 | 2.602803 |
| 6 | -0.665572 | 0.202622 | 2.190033 |
| 7 | -0.913121 | -0.887738 | 1.871230 |
| 6 | 4.294416 | -0.068215 | -1.767200 |
| 1 | 4.311959 | 0.481927 | -0.821162 |
| 1 | 3.996765 | 0.605009 | -2.575447 |
| 1 | 5.293894 | -0.456686 | -1.977855 |
| 6 | 3.340673 | -1.168380 | -1.658698 |
| 7 | 2.578091 | -2.038899 | -1.557482 |
| 6 | 2.571782 | 3.513668 | 0.466628 |
| 1 | 1.960016 | 4.242549 | 1.004868 |
| 1 | 3.260881 | 4.044982 | -0.194625 |
| 1 | 3.137165 | 2.905884 | 1.180392 |
| 6 | 1.717745 | 2.623236 | -0.305324 |
| 7 | 1.042977 | 1.891889 | -0.897209 |
| 6 | -3.631979 | 1.646413 | -2.404710 |
| 1 | -4.598114 | 2.140108 | -2.272776 |
| 1 | -3.796231 | 0.584081 | -2.607953 |
| 1 | -3.114557 | 2.104504 | -3.251319 |
| 6 | -2.831166 | 1.783220 | -1.191214 |
| 7 | -2.195970 | 1.872037 | -0.222161 |
| 6 | 2.206083 | -2.354322 | 1.842049 |
| 1 | 2.848057 | -2.732124 | 2.641878 |
| 1 | 2.405949 | -2.913312 | 0.922843 |
| 1 | 1.157787 | -2.480242 | 2.129447 |
| 6 | 2.474060 | -0.937768 | 1.610736 |
| 7 | 2.686824 | 0.189881 | 1.424123 |
| 6 | -0.652375 | -2.961867 | -0.948579 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.386742 | -1.549491 | -1.097251 |
| 7 | -0.130208 | -0.434120 | -1.206306 |
| 1 | -0.986560 | -3.127044 | 0.081288 |
| 1 | 0.276627 | -3.501791 | -1.157949 |
| 1 | -1.450044 | -3.254110 | -1.636064 |
| 1 | 0.262193 | 0.574854 | -1.161623 |

Cartesian coordinates of : PACN7_10

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.573880 | -5.010368 | -0.107408 |
| 1 | 4.239740 | -5.044531 | 0.758406 |
| 1 | 4.174793 | -4.923736 | -1.016027 |
| 1 | 2.999022 | -5.938795 | -0.148590 |
| 6 | 2.669438 | -3.868562 | 0.002966 |
| 7 | 1.949989 | -2.960795 | 0.090693 |
| 6 | 0.855830 | 3.087214 | -2.581547 |
| 1 | 1.584950 | 3.749282 | -3.055416 |
| 1 | -0.155641 | 3.452118 | -2.772554 |
| 1 | 0.954181 | 2.080421 | -2.996758 |
| 6 | 1.097130 | 3.035095 | -1.143026 |
| 7 | 1.308283 | 3.001627 | -0.000350 |
| 6 | -4.914136 | -2.919945 | 1.836947 |
| 1 | -5.441569 | -2.281700 | 2.550114 |
| 1 | -4.303227 | -3.638535 | 2.388818 |
| 1 | -5.647199 | -3.464340 | 1.236594 |
| 6 | -4.065163 | -2.105976 | 0.970353 |
| 7 | -3.390428 | -1.458988 | 0.280523 |
| 6 | 3.367907 | 0.224398 | 0.292548 |
| 1 | 3.032293 | 1.166688 | 0.737557 |
| 1 | 4.458624 | 0.224232 | 0.222691 |
| 1 | 3.046002 | -0.614974 | 0.917232 |
| 6 | 2.773911 | 0.088811 | -1.033934 |
| 7 | 2.268347 | -0.014962 | -2.075312 |
| 6 | -4.409800 | 1.537127 | -1.332249 |
| 1 | -4.739419 | 0.650193 | -0.784942 |
| 1 | -4.922702 | 1.579235 | -2.296303 |
| 1 | -4.660539 | 2.431478 | -0.756497 |
| 6 | -2.966323 | 1.462435 | -1.536935 |
| 7 | -1.818107 | 1.402095 | -1.702557 |
| 6 | 1.422686 | 3.675217 | 3.388205 |
| 1 | 1.676874 | 4.206279 | 2.465574 |
| 1 | 2.307158 | 3.593064 | 4.024482 |
| 1 | 0.640752 | 4.219684 | 3.923019 |
| 6 | 0.945425 | 2.352410 | 3.016847 |
| 7 | 0.569076 | 1.308561 | 2.684827 |
| 6 | -0.560330 | -1.472983 | -1.578108 |
| 6 | -0.304616 | -0.778286 | -0.338000 |
| 7 | -0.095099 | -0.238734 | 0.656025 |
| 1 | 0.040074 | -2.386932 | -1.583185 |
| 1 | -0.253926 | -0.817785 | -2.398333 |
| 1 | -1.630898 | -1.689327 | -1.632217 |
| 1 | 0.141202 | 0.336831 | 1.539434 |

Cartesian coordinates of : PACN7_11

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.909252 | -0.100884 | -2.458906 |
| 1 | 6.691052 | 0.654821 | -2.349898 |
| 1 | 5.502116 | -0.046523 | -3.471553 |
| 1 | 6.346878 | -1.090317 | -2.305206 |
| 6 | 4.848579 | 0.134259 | -1.482140 |
| 7 | 4.005159 | 0.322464 | -0.705634 |
| 6 | -4.419787 | 0.511374 | -0.577522 |
| 1 | -5.507368 | 0.408360 | -0.607965 |
| 1 | -4.053665 | 0.825746 | -1.558614 |
| 1 | -4.142296 | 1.266364 | 0.164562 |
| 6 | -3.808893 | -0.762421 | -0.209532 |
| 7 | -3.330891 | -1.777847 | 0.091297 |
| 6 | -1.323635 | -0.856696 | 2.605178 |
| 1 | -2.277452 | -1.305691 | 2.892662 |
| 1 | -0.673976 | -0.747097 | 3.476120 |
| 1 | -0.832030 | -1.509843 | 1.877495 |
| 6 | -1.555787 | 0.450633 | 1.999378 |
| 7 | -1.749039 | 1.486647 | 1.508605 |
| 6 | 4.301902 | -0.286746 | 2.603195 |
| 1 | 4.614516 | -1.169174 | 2.039577 |
| 1 | 4.510341 | -0.440374 | 3.664790 |
| 1 | 4.868296 | 0.575509 | 2.242803 |
| 6 | 2.875054 | -0.055071 | 2.399791 |
| 7 | 1.739867 | 0.131696 | 2.239202 |
| 6 | -2.922419 | 4.043776 | -0.478676 |
| 1 | -2.865905 | 3.762001 | 0.577139 |
| 1 | -3.963954 | 4.013433 | -0.810874 |
| 1 | -2.545872 | 5.061894 | -0.605318 |
| 6 | -2.119064 | 3.105492 | -1.257180 |
| 7 | -1.482009 | 2.341292 | -1.857692 |
| 6 | -2.112967 | -4.774816 | -0.934954 |
| 1 | -1.687548 | -5.597319 | -0.354907 |
| 1 | -2.353793 | -5.126706 | -1.941081 |
| 1 | -3.019434 | -4.404709 | -0.446744 |
| 6 | -1.165960 | -3.673335 | -1.008892 |
| 7 | -0.430900 | -2.780971 | -1.058763 |
| 6 | 1.195957 | 2.084171 | -0.207628 |
| 6 | 0.780325 | 0.737345 | -0.527446 |
| 7 | 0.461774 | -0.338431 | -0.780913 |
| 1 | 0.552869 | 2.444453 | 0.602291 |
| 1 | 1.071266 | 2.708800 | -1.095600 |
| 1 | 2.240531 | 2.047136 | 0.112065 |
| 1 | 0.132369 | -1.367204 | -0.942463 |

Cartesian coordinates of : PACN7_12

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.693994 | -3.530395 | 1.393258 |
| 1 | 1.571744 | -4.132430 | 1.641392 |
| 1 | -0.196391 | -4.163421 | 1.376652 |
| 1 | 0.552252 | -2.748833 | 2.144605 |
| 6 | 0.868365 | -2.903256 | 0.087299 |
| 7 | 1.009211 | -2.409977 | -0.955972 |
| 6 | 3.283529 | 3.816111 | -0.142112 |
| 1 | 4.113871 | 3.112122 | -0.254249 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.340440 | 4.309153 | 0.831879 |
| 1 | 3.335509 | 4.572114 | -0.929523 |
| 6 | 2.039911 | 3.067131 | -0.253056 |
| 7 | 1.064120 | 2.451101 | -0.342173 |
| 6 | 2.980923 | 1.019092 | 2.525907 |
| 1 | 2.808663 | 2.044566 | 2.866171 |
| 1 | 3.641649 | 1.022102 | 1.653717 |
| 1 | 3.454070 | 0.458254 | 3.335985 |
| 6 | 1.709390 | 0.400556 | 2.161431 |
| 7 | 0.692390 | -0.080785 | 1.871723 |
| 6 | 4.002809 | -1.547121 | -2.372465 |
| 1 | 3.071271 | -2.119332 | -2.356520 |
| 1 | 4.826749 | -2.186257 | -2.045093 |
| 1 | 4.205661 | -1.202025 | -3.389479 |
| 6 | 3.877958 | -0.401777 | -1.475831 |
| 7 | 3.787563 | 0.514212 | -0.766804 |
| 6 | -2.520402 | 0.025131 | 2.288438 |
| 1 | -2.161012 | 0.878445 | 1.706180 |
| 1 | -1.952236 | -0.030575 | 3.219824 |
| 1 | -3.582723 | 0.160433 | 2.505771 |
| 6 | -2.321153 | -1.195848 | 1.515292 |
| 7 | -2.158117 | -2.161819 | 0.890260 |
| 6 | -6.360414 | 1.870640 | -0.742853 |
| 1 | -6.583349 | 2.199223 | -1.760934 |
| 1 | -6.401257 | 2.734374 | -0.074700 |
| 1 | -7.114288 | 1.143413 | -0.431395 |
| 6 | -5.032285 | 1.264108 | -0.695157 |
| 7 | -3.976259 | 0.781583 | -0.659141 |
| 6 | -1.948894 | -1.430090 | -2.094518 |
| 6 | -1.187998 | -0.364422 | -1.479803 |
| 7 | -0.577424 | 0.500608 | -1.031400 |
| 1 | -1.485513 | -2.380925 | -1.818228 |
| 1 | -1.936707 | -1.292880 | -3.179349 |
| 1 | -2.970360 | -1.384971 | -1.707646 |
| 1 | 0.057177 | 1.303827 | -0.675489 |

 Cartesian coordinates of : PACN7_13

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 5.222266 | -0.114583 | 1.260326 |
| 1 | 5.013466 | 0.943749 | 1.084535 |
| 1 | 6.167505 | -0.381342 | 0.781102 |
| 1 | 5.305051 | -0.294508 | 2.335047 |
| 6 | 4.136459 | -0.914570 | 0.701769 |
| 7 | 3.273476 | -1.553326 | 0.258000 |
| 6 | -4.422157 | 2.324180 | -1.744560 |
| 1 | -3.537371 | 2.078220 | -2.338716 |
| 1 | -4.411370 | 3.388251 | -1.495676 |
| 1 | -5.319824 | 2.106767 | -2.328855 |
| 6 | -4.417309 | 1.525020 | -0.522205 |
| 7 | -4.406891 | 0.882861 | 0.445991 |
| 6 | -3.712139 | 0.437674 | 3.694665 |
| 1 | -3.818920 | -0.469997 | 4.293747 |
| 1 | -4.544644 | 0.520234 | 2.990200 |
| 1 | -3.699176 | 1.307975 | 4.355413 |
| 6 | -2.476558 | 0.381444 | 2.927860 |
| 7 | -1.497894 | 0.336930 | 2.311924 |
| 6 | -3.200808 | -2.044939 | -1.289199 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.502976 | -2.803152 | -0.924570 |
| 1 | -3.824825 | -2.472800 | -2.077943 |
| 1 | -3.838596 | -1.700499 | -0.469852 |
| 6 | -2.438650 | -0.915636 | -1.811444 |
| 7 | -1.838588 | -0.006056 | -2.216943 |
| 6 | 1.961492 | -4.553042 | 0.160021 |
| 1 | 1.632602 | -5.594936 | 0.143303 |
| 1 | 2.239257 | -4.271356 | 1.178461 |
| 1 | 2.838943 | -4.434861 | -0.480175 |
| 6 | 0.891302 | -3.680733 | -0.313499 |
| 7 | 0.039640 | -2.987693 | -0.693369 |
| 6 | 3.623204 | 4.836945 | -0.411268 |
| 1 | 2.872230 | 5.337984 | -1.027011 |
| 1 | 4.609518 | 5.001725 | -0.851967 |
| 1 | 3.605069 | 5.268638 | 0.592460 |
| 6 | 3.338911 | 3.405447 | -0.344863 |
| 7 | 3.113619 | 2.266906 | -0.291860 |
| 6 | 1.436650 | -0.177038 | -1.919610 |
| 6 | 0.788152 | 0.010367 | -0.642204 |
| 7 | 0.243830 | 0.171614 | 0.358182 |
| 1 | 1.611025 | -1.248503 | -2.050271 |
| 1 | 2.384198 | 0.367478 | -1.913458 |
| 1 | 0.759079 | 0.193998 | -2.694569 |
| 1 | -0.415483 | 0.255075 | 1.220584 |

Cartesian coordinates of : PACN7_14

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.860814 | -2.820847 | -1.621740 |
| 1 | 4.403988 | -2.206885 | -0.897320 |
| 1 | 4.457129 | -2.917243 | -2.532447 |
| 1 | 3.691606 | -3.815281 | -1.201441 |
| 6 | 2.584043 | -2.181517 | -1.925343 |
| 7 | 1.574384 | -1.656151 | -2.158010 |
| 6 | -2.723827 | 4.362730 | -1.015623 |
| 1 | -2.514744 | 5.183811 | -0.325404 |
| 1 | -3.548609 | 3.760479 | -0.624933 |
| 1 | -3.000943 | 4.777243 | -1.988058 |
| 6 | -1.545744 | 3.512579 | -1.151525 |
| 7 | -0.614470 | 2.826202 | -1.257492 |
| 6 | 3.989224 | 0.342534 | 3.527537 |
| 1 | 4.076892 | 1.270530 | 4.097727 |
| 1 | 4.690350 | 0.358394 | 2.687272 |
| 1 | 4.210993 | -0.506637 | 4.178424 |
| 6 | 2.646908 | 0.216955 | 2.981485 |
| 7 | 1.591407 | 0.117759 | 2.514744 |
| 6 | -2.531227 | 0.201242 | 2.651162 |
| 1 | -3.324405 | 0.243626 | 3.401778 |
| 1 | -1.646844 | 0.713337 | 3.041859 |
| 1 | -2.283333 | -0.844480 | 2.445671 |
| 6 | -2.971971 | 0.837353 | 1.412555 |
| 7 | -3.303249 | 1.333994 | 0.415893 |
| 6 | -4.469029 | -4.059634 | 0.011189 |
| 1 | -4.467627 | -4.673303 | 0.915369 |
| 1 | -4.283118 | -4.702084 | -0.853027 |
| 1 | -5.449455 | -3.589855 | -0.099296 |
| 6 | -3.432307 | -3.034566 | 0.102211 |
| 7 | -2.607575 | -2.219781 | 0.174606 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 2.640520 | 1.643109 | -1.893730 |
| 1 | 3.324880 | 2.398556 | -2.288254 |
| 1 | 1.724308 | 2.133436 | -1.548701 |
| 1 | 2.384250 | 0.936620 | -2.689032 |
| 6 | 3.273437 | 0.920295 | -0.794085 |
| 7 | 3.771603 | 0.335722 | 0.078738 |
| 6 | -1.228823 | -0.215396 | -1.875199 |
| 6 | -0.492815 | -0.140403 | -0.635270 |
| 7 | 0.088068 | -0.070889 | 0.355524 |
| 1 | -1.282129 | -1.263630 | -2.177712 |
| 1 | -0.693700 | 0.373415 | -2.625267 |
| 1 | -2.226817 | 0.198332 | -1.696321 |
| 1 | 0.660935 | -0.002986 | 1.269358 |

Cartesian coordinates of : PACN7_15

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.355528 | 2.799637 | -3.231796 |
| 1 | -2.039298 | 2.867004 | -4.081878 |
| 1 | -0.479831 | 3.421200 | -3.434921 |
| 1 | -1.855971 | 3.157139 | -2.327553 |
| 6 | -0.947999 | 1.413351 | -3.024926 |
| 7 | -0.636569 | 0.307899 | -2.850422 |
| 6 | -2.098948 | 0.473540 | 2.179160 |
| 1 | -1.062452 | 0.391424 | 2.521765 |
| 1 | -2.468555 | -0.537310 | 1.986118 |
| 1 | -2.703390 | 0.947700 | 2.956554 |
| 6 | -2.161871 | 1.252040 | 0.945272 |
| 7 | -2.198413 | 1.864268 | -0.041936 |
| 6 | -1.791687 | -4.083640 | 2.369922 |
| 1 | -2.344684 | -4.007153 | 3.309508 |
| 1 | -1.351334 | -5.081530 | 2.301443 |
| 1 | -2.475969 | -3.929981 | 1.530381 |
| 6 | -0.745748 | -3.066381 | 2.316233 |
| 7 | 0.075921 | -2.247226 | 2.253078 |
| 6 | -3.738204 | -0.619231 | -2.111072 |
| 1 | -4.776275 | -0.957933 | -2.065674 |
| 1 | -3.335594 | -0.804193 | -3.109960 |
| 1 | -3.692394 | 0.453582 | -1.900175 |
| 6 | -2.936998 | -1.331774 | -1.120838 |
| 7 | -2.311510 | -1.899340 | -0.322206 |
| 6 | 6.536286 | -1.056485 | -0.958530 |
| 1 | 6.911259 | -0.095257 | -1.318394 |
| 1 | 6.859262 | -1.842386 | -1.645700 |
| 1 | 6.956501 | -1.255237 | 0.030417 |
| 6 | 5.077719 | -1.027935 | -0.884588 |
| 7 | 3.918346 | -1.005945 | -0.826088 |
| 6 | 1.055232 | 4.745817 | 2.855177 |
| 1 | 1.197075 | 4.551292 | 3.921139 |
| 1 | 0.132437 | 5.313212 | 2.711328 |
| 1 | 1.899198 | 5.331607 | 2.482558 |
| 6 | 0.975787 | 3.483780 | 2.129984 |
| 7 | 0.914962 | 2.482418 | 1.552676 |
| 6 | 0.822072 | -2.091454 | -1.098549 |
| 6 | 0.824080 | -0.830242 | -0.397831 |
| 7 | 0.840376 | 0.178343 | 0.152988 |
| 1 | 1.863595 | -2.372482 | -1.277522 |
| 1 | 0.281924 | -1.948236 | -2.039117 |

| | | | |
|---|----------|-----------|-----------|
| 1 | 0.310160 | -2.826445 | -0.472205 |
| 1 | 0.867381 | 1.094913 | 0.689549 |

Cartesian coordinates of : PACN7_16

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.597151 | 1.111646 | -1.683264 |
| 1 | -4.635714 | 0.771758 | -1.660931 |
| 1 | -3.389843 | 1.538658 | -2.669039 |
| 1 | -3.447304 | 1.870832 | -0.909623 |
| 6 | -2.696750 | -0.010839 | -1.434745 |
| 7 | -1.980410 | -0.906430 | -1.247813 |
| 6 | -1.386634 | 4.241548 | -1.878568 |
| 1 | -2.054961 | 4.347930 | -1.018352 |
| 1 | -1.970298 | 4.209629 | -2.802318 |
| 1 | -0.702719 | 5.092966 | -1.917156 |
| 6 | -0.635331 | 3.005024 | -1.714626 |
| 7 | -0.054773 | 2.015475 | -1.558843 |
| 6 | -0.596995 | -3.675957 | -2.789617 |
| 1 | -1.086721 | -4.649367 | -2.873761 |
| 1 | 0.175217 | -3.601268 | -3.559311 |
| 1 | -1.333879 | -2.881700 | -2.935911 |
| 6 | -0.000524 | -3.527520 | -1.466190 |
| 7 | 0.466332 | -3.405152 | -0.409906 |
| 6 | 6.825296 | 1.306896 | -0.370820 |
| 1 | 6.840050 | 1.638405 | -1.411943 |
| 1 | 7.574681 | 0.522769 | -0.237612 |
| 1 | 7.076756 | 2.151485 | 0.275344 |
| 6 | 5.501241 | 0.793664 | -0.028780 |
| 7 | 4.449098 | 0.384978 | 0.243580 |
| 6 | -1.849965 | 1.946209 | 3.565537 |
| 1 | -2.827181 | 1.992459 | 4.052799 |
| 1 | -1.177506 | 2.656281 | 4.053581 |
| 1 | -1.445286 | 0.934669 | 3.656760 |
| 6 | -1.985432 | 2.283082 | 2.151495 |
| 7 | -2.097583 | 2.561918 | 1.029168 |
| 6 | -2.307992 | -3.148405 | 1.385218 |
| 1 | -2.556558 | -2.958345 | 0.337573 |
| 1 | -3.223923 | -3.274194 | 1.968015 |
| 1 | -1.706705 | -4.058813 | 1.447061 |
| 6 | -1.539324 | -2.019726 | 1.899516 |
| 7 | -0.933342 | -1.121803 | 2.320438 |
| 6 | 2.144585 | -1.511450 | 1.625471 |
| 6 | 1.514080 | -0.641328 | 0.659025 |
| 7 | 1.025233 | 0.063005 | -0.106785 |
| 1 | 1.858656 | -2.540120 | 1.386604 |
| 1 | 1.774104 | -1.244027 | 2.618740 |
| 1 | 3.225846 | -1.367078 | 1.553629 |
| 1 | 0.576773 | 0.786066 | -0.760936 |

Cartesian coordinates of : PACN7_17

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|----------|-----------|
| 6 | 5.681645 | 2.734446 | -1.243397 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 5.222885 | 3.426082 | -1.954281 |
| 1 | 6.599062 | 2.333369 | -1.681197 |
| 1 | 5.931459 | 3.278661 | -0.329309 |
| 6 | 4.756133 | 1.645550 | -0.939981 |
| 7 | 4.020606 | 0.778976 | -0.699444 |
| 6 | -3.290400 | 2.988313 | 2.373562 |
| 1 | -3.749557 | 3.833972 | 1.854964 |
| 1 | -3.115501 | 3.260569 | 3.417333 |
| 1 | -3.956773 | 2.120700 | 2.329334 |
| 6 | -2.033748 | 2.627895 | 1.732407 |
| 7 | -1.049982 | 2.305222 | 1.213473 |
| 6 | -3.504758 | -2.287369 | -1.834698 |
| 1 | -4.047136 | -3.234674 | -1.885379 |
| 1 | -3.446271 | -1.847862 | -2.833738 |
| 1 | -4.037065 | -1.600648 | -1.168159 |
| 6 | -2.158589 | -2.501822 | -1.313965 |
| 7 | -1.092059 | -2.659786 | -0.881488 |
| 6 | 4.772640 | -1.733787 | 1.758621 |
| 1 | 5.213665 | -1.016183 | 1.061713 |
| 1 | 5.205238 | -2.721989 | 1.583868 |
| 1 | 4.994375 | -1.425284 | 2.783262 |
| 6 | 3.328390 | -1.776094 | 1.551428 |
| 7 | 2.179651 | -1.810121 | 1.383469 |
| 6 | -3.706933 | 1.869484 | -1.420385 |
| 1 | -4.517877 | 1.861209 | -2.153267 |
| 1 | -3.422734 | 2.907603 | -1.224982 |
| 1 | -4.045664 | 1.398566 | -0.492145 |
| 6 | -2.556946 | 1.130141 | -1.935659 |
| 7 | -1.650591 | 0.533290 | -2.350761 |
| 6 | -1.325907 | -1.986546 | 2.253091 |
| 1 | -1.324249 | -1.868162 | 3.339720 |
| 1 | -0.318700 | -1.809606 | 1.861665 |
| 1 | -1.610271 | -3.010650 | 1.998658 |
| 6 | -2.274778 | -1.052636 | 1.653073 |
| 7 | -3.031195 | -0.306444 | 1.180100 |
| 6 | 1.495459 | -1.197446 | -1.720458 |
| 6 | 0.930511 | -0.238499 | -0.802054 |
| 7 | 0.473698 | 0.554737 | -0.106174 |
| 1 | 1.453295 | -2.183237 | -1.250182 |
| 1 | 2.527542 | -0.903701 | -1.930734 |
| 1 | 0.876955 | -1.191054 | -2.624076 |
| 1 | -0.059893 | 1.291422 | 0.453196 |

Cartesian coordinates of : PACN7_18

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.622943 | 2.568501 | -2.748798 |
| 1 | 2.857275 | 2.306777 | -3.783653 |
| 1 | 3.307189 | 3.354501 | -2.419530 |
| 1 | 1.596217 | 2.940046 | -2.693869 |
| 6 | 2.764490 | 1.393671 | -1.892295 |
| 7 | 2.878615 | 0.456608 | -1.214519 |
| 6 | -1.659020 | -1.206317 | 2.076935 |
| 1 | -1.720345 | -1.256308 | 3.167071 |
| 1 | -0.605273 | -1.249680 | 1.782290 |
| 1 | -2.199532 | -2.055923 | 1.647324 |
| 6 | -2.258552 | 0.035840 | 1.597751 |
| 7 | -2.750535 | 1.010609 | 1.199304 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.172093 | 3.797537 | 0.963580 |
| 1 | -0.729189 | 4.789751 | 0.848592 |
| 1 | -0.838603 | 3.340178 | 1.900628 |
| 1 | -2.262482 | 3.865242 | 0.971034 |
| 6 | -0.753440 | 2.923374 | -0.118242 |
| 7 | -0.410929 | 2.198039 | -0.956286 |
| 6 | 3.296666 | 0.432394 | 2.237336 |
| 1 | 3.761139 | 1.200073 | 2.861378 |
| 1 | 3.829646 | 0.367357 | 1.284016 |
| 1 | 3.352768 | -0.528674 | 2.756343 |
| 6 | 1.900564 | 0.771889 | 1.980246 |
| 7 | 0.790314 | 1.051478 | 1.784649 |
| 6 | 4.209343 | -2.462955 | 0.092996 |
| 1 | 4.810002 | -2.417969 | 1.005789 |
| 1 | 4.445494 | -1.605264 | -0.543521 |
| 1 | 4.449578 | -3.387778 | -0.437447 |
| 6 | 2.788246 | -2.425850 | 0.426021 |
| 7 | 1.657876 | -2.383851 | 0.691905 |
| 6 | -5.453721 | -0.275066 | -0.607287 |
| 1 | -5.842732 | 0.051986 | -1.574706 |
| 1 | -5.144575 | 0.597079 | -0.023668 |
| 1 | -6.240301 | -0.810730 | -0.070072 |
| 6 | -4.298846 | -1.145602 | -0.801000 |
| 7 | -3.368250 | -1.826465 | -0.942227 |
| 6 | -0.548387 | -2.993279 | -1.385618 |
| 6 | -0.434805 | -1.553699 | -1.278270 |
| 7 | -0.339514 | -0.409537 | -1.218965 |
| 1 | 0.406039 | -3.402185 | -1.725504 |
| 1 | -1.362916 | -3.228049 | -2.074644 |
| 1 | -0.782958 | -3.391472 | -0.394437 |
| 1 | -0.309822 | 0.680230 | -1.150574 |

Cartesian coordinates of : PACN7_19

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.854349 | 1.594745 | 2.853785 |
| 1 | 3.543161 | 1.195693 | 2.102642 |
| 1 | 2.685172 | 0.838033 | 3.624106 |
| 1 | 3.290401 | 2.487509 | 3.308733 |
| 6 | 1.587986 | 1.924813 | 2.208018 |
| 7 | 0.583327 | 2.182835 | 1.684441 |
| 6 | 3.544614 | -1.976533 | -2.967832 |
| 1 | 3.881770 | -2.992109 | -2.744473 |
| 1 | 4.202275 | -1.252796 | -2.475428 |
| 1 | 3.575742 | -1.819504 | -4.048857 |
| 6 | 2.189424 | -1.778457 | -2.471605 |
| 7 | 1.124693 | -1.594206 | -2.053782 |
| 6 | -5.359999 | -4.052147 | 0.038523 |
| 1 | -5.426342 | -4.285218 | -1.027009 |
| 1 | -6.338884 | -3.716809 | 0.389913 |
| 1 | -5.078119 | -4.956262 | 0.583695 |
| 6 | -4.365487 | -3.005442 | 0.259967 |
| 7 | -3.575155 | -2.173408 | 0.436376 |
| 6 | 3.390610 | -2.367219 | 0.984507 |
| 1 | 3.924259 | -1.615687 | 0.394713 |
| 1 | 3.098037 | -3.202798 | 0.341862 |
| 1 | 4.045773 | -2.745361 | 1.773397 |
| 6 | 2.201153 | -1.754228 | 1.570431 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 1.259710 | -1.265352 | 2.044062 |
| 6 | 1.234088 | 2.120010 | -1.606179 |
| 1 | 0.525626 | 2.401765 | -0.821130 |
| 1 | 0.705285 | 1.533039 | -2.364186 |
| 1 | 1.641246 | 3.020902 | -2.072390 |
| 6 | 2.313815 | 1.323514 | -1.030382 |
| 7 | 3.166633 | 0.670446 | -0.585132 |
| 6 | -3.521938 | 4.640206 | -1.349186 |
| 1 | -3.143798 | 5.488988 | -0.774092 |
| 1 | -4.579598 | 4.495741 | -1.115470 |
| 1 | -3.421998 | 4.859300 | -2.415080 |
| 6 | -2.768257 | 3.434498 | -1.013740 |
| 7 | -2.170001 | 2.475536 | -0.746530 |
| 6 | -1.908797 | 0.327821 | 1.772076 |
| 6 | -1.221467 | -0.142757 | 0.595642 |
| 7 | -0.664626 | -0.552006 | -0.323324 |
| 1 | -2.011819 | 1.413104 | 1.696932 |
| 1 | -1.284123 | 0.069755 | 2.633843 |
| 1 | -2.877689 | -0.176418 | 1.820647 |
| 1 | -0.048982 | -0.980721 | -1.069293 |

Cartesian coordinates of : PACN7_20

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.258708 | 1.887121 | -1.326558 |
| 1 | -1.665432 | 0.987256 | -1.797158 |
| 1 | -0.236477 | 2.064066 | -1.673711 |
| 1 | -1.881329 | 2.743706 | -1.598659 |
| 6 | -1.251931 | 1.713913 | 0.123117 |
| 7 | -1.247858 | 1.563620 | 1.276141 |
| 6 | -4.893760 | 1.298194 | 1.040040 |
| 1 | -4.093271 | 1.811069 | 1.582590 |
| 1 | -5.519017 | 0.751751 | 1.751398 |
| 1 | -5.512895 | 2.038890 | 0.527691 |
| 6 | -4.308165 | 0.374283 | 0.071065 |
| 7 | -3.823980 | -0.355916 | -0.692123 |
| 6 | -2.778500 | -2.968959 | -2.309747 |
| 1 | -3.608236 | -2.386149 | -2.715388 |
| 1 | -3.010449 | -3.232840 | -1.273583 |
| 1 | -2.621321 | -3.873566 | -2.901881 |
| 6 | -1.570014 | -2.161459 | -2.302543 |
| 7 | -0.596729 | -1.533220 | -2.276502 |
| 6 | 2.985698 | 5.255438 | -0.743758 |
| 1 | 4.056395 | 5.207803 | -0.530488 |
| 1 | 2.523492 | 5.991065 | -0.080944 |
| 1 | 2.844932 | 5.571400 | -1.780338 |
| 6 | 2.377519 | 3.943804 | -0.535150 |
| 7 | 1.895097 | 2.900211 | -0.369797 |
| 6 | -2.675306 | -1.213130 | 2.738955 |
| 1 | -2.550071 | -0.128111 | 2.807417 |
| 1 | -2.433249 | -1.666338 | 3.703578 |
| 1 | -3.713305 | -1.450491 | 2.488550 |
| 6 | -1.787293 | -1.730385 | 1.701553 |
| 7 | -1.079116 | -2.141796 | 0.877578 |
| 6 | 6.128555 | -3.284959 | 0.166588 |
| 1 | 6.932772 | -3.084292 | 0.878670 |
| 1 | 6.521602 | -3.192118 | -0.848786 |
| 1 | 5.768058 | -4.305613 | 0.316328 |

| | | | |
|---|----------|-----------|-----------|
| 6 | 5.036239 | -2.336346 | 0.367271 |
| 7 | 4.167626 | -1.582674 | 0.526759 |
| 6 | 2.089347 | 0.442215 | 1.606090 |
| 6 | 1.575778 | -0.078476 | 0.359733 |
| 7 | 1.119449 | -0.489295 | -0.612854 |
| 1 | 3.051163 | 0.923301 | 1.416778 |
| 1 | 2.226729 | -0.393124 | 2.297333 |
| 1 | 1.362586 | 1.166224 | 1.988282 |
| 1 | 0.499164 | -0.917923 | -1.402031 |

Cartesian coordinates of : PACN7_21

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.277822 | 1.416349 | -2.153838 |
| 1 | 5.290161 | 1.034874 | -2.310007 |
| 1 | 4.209305 | 1.886058 | -1.168670 |
| 1 | 4.058729 | 2.159579 | -2.924564 |
| 6 | 3.313114 | 0.323552 | -2.223338 |
| 7 | 2.548064 | -0.549398 | -2.264497 |
| 6 | -1.284825 | -3.609218 | 2.504092 |
| 1 | -0.202318 | -3.458120 | 2.521507 |
| 1 | -1.503064 | -4.678915 | 2.454363 |
| 1 | -1.727379 | -3.197613 | 3.414576 |
| 6 | -1.833013 | -2.933853 | 1.332419 |
| 7 | -2.267951 | -2.397898 | 0.397637 |
| 6 | -3.009745 | 4.158972 | 0.214724 |
| 1 | -3.461904 | 4.391660 | 1.181889 |
| 1 | -3.725850 | 3.605744 | -0.400353 |
| 1 | -2.730640 | 5.087247 | -0.289520 |
| 6 | -1.838187 | 3.315502 | 0.398199 |
| 7 | -0.915529 | 2.623806 | 0.526885 |
| 6 | 3.980425 | -1.746279 | 0.590695 |
| 1 | 4.314180 | -2.140244 | -0.372697 |
| 1 | 4.553620 | -2.216798 | 1.393485 |
| 1 | 4.136402 | -0.663882 | 0.611445 |
| 6 | 2.557983 | -2.023073 | 0.763559 |
| 7 | 1.428409 | -2.254693 | 0.907799 |
| 6 | 1.664896 | 2.685381 | 2.923086 |
| 1 | 0.620389 | 2.972574 | 2.777073 |
| 1 | 2.267918 | 3.584693 | 3.070982 |
| 1 | 1.744620 | 2.053864 | 3.811337 |
| 6 | 2.133865 | 1.957629 | 1.747305 |
| 7 | 2.505755 | 1.380661 | 0.809921 |
| 6 | -5.051050 | -1.059010 | -1.114578 |
| 1 | -5.940051 | -0.845165 | -0.515879 |
| 1 | -4.550206 | -1.944481 | -0.714544 |
| 1 | -5.357109 | -1.244344 | -2.147302 |
| 6 | -4.131115 | 0.073778 | -1.061044 |
| 7 | -3.402663 | 0.978246 | -1.019484 |
| 6 | -0.241768 | -1.970051 | -1.948949 |
| 6 | -0.247248 | -0.743939 | -1.183198 |
| 7 | -0.273878 | 0.244312 | -0.598583 |
| 1 | -1.277635 | -2.254228 | -2.151192 |
| 1 | 0.242990 | -2.739142 | -1.340202 |
| 1 | 0.331527 | -1.805760 | -2.864204 |
| 1 | -0.396069 | 1.162705 | -0.090082 |

Cartesian coordinates of : PACN7_22

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Atomic number (AN) and Cartesian coordinates
  AN          X          Y          Z
-----
  6    -1.495552    3.928855    -1.348796
  1    -2.314975    4.238497    -2.002169
  1    -0.801297    3.306175    -1.921595
  1    -0.969799    4.818652    -0.993928
  6    -2.018824    3.171711    -0.214289
  7    -2.422822    2.556655     0.684580
  6     2.907554     0.262441    -4.193533
  1     3.483654     1.145116    -4.481377
  1     2.540169    -0.241463    -5.090703
  1     3.539286    -0.420718    -3.617250
  6     1.792947     0.645410    -3.341886
  7     0.916612     0.928124    -2.637337
  6     4.556319     1.950599     2.736305
  1     4.394881     3.020693     2.887933
  1     5.243743     1.809163     1.898690
  1     5.003896     1.529150     3.639785
  6     3.284365     1.289852     2.455074
  7     2.271995     0.765792     2.233724
  6    -2.376605    -4.048695    -0.761175
  1    -2.077671    -4.375921    -1.760045
  1    -3.187555    -3.320277    -0.842644
  1    -2.722011    -4.914810    -0.191289
  6    -1.248566    -3.420741    -0.081320
  7    -0.354435    -2.915967     0.462128
  6     2.766406    -2.461038     1.178726
  1     2.440488    -3.485786     0.987668
  1     2.044500    -1.987844     1.849212
  1     3.752197    -2.467047     1.650995
  6     2.822738    -1.717875    -0.076753
  7     2.885184    -1.127803    -1.075749
  6    -5.349577     0.775497     0.640139
  1    -4.948849     1.730666     0.990293
  1    -6.018159     0.360417     1.398433
  1    -5.915050     0.937332    -0.280987
  6    -4.242157    -0.142812     0.391617
  7    -3.356258    -0.869719     0.198779
  6    -0.925729    -0.180856     2.160746
  6    -0.445788     0.083725     0.824720
  7    -0.059645     0.327868    -0.229809
  1    -1.342105    -1.191508     2.178161
  1    -1.699697     0.558832     2.389821
  1    -0.079031    -0.087970     2.846909
  1     0.303787     0.567547    -1.207565
-----

```

Cartesian coordinates of : PACN7_23

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-----
Atomic number (AN) and Cartesian coordinates
  AN          X          Y          Z
-----
  6     6.027577     5.407541     7.098749
  1     5.507054     4.596620     7.614071
  1     6.052946     5.214641     6.023100
  1     5.513274     6.356951     7.280764
  6     7.391219     5.531002     7.587583
-----

```

| | | | |
|---|-----------|-----------|-----------|
| 7 | 8.478734 | 5.667020 | 7.972243 |
| 6 | 8.199046 | 8.108629 | 10.479211 |
| 1 | 8.413187 | 8.999339 | 11.076067 |
| 1 | 9.149026 | 7.653675 | 10.179212 |
| 1 | 7.632304 | 7.396300 | 11.084633 |
| 6 | 7.424364 | 8.478761 | 9.297646 |
| 7 | 6.798554 | 8.754741 | 8.357705 |
| 6 | 12.518275 | 9.330001 | 11.387352 |
| 1 | 12.624041 | 8.242394 | 11.354020 |
| 1 | 12.160041 | 9.632368 | 12.374630 |
| 1 | 13.489072 | 9.798039 | 11.205968 |
| 6 | 11.564697 | 9.741612 | 10.361891 |
| 7 | 10.802644 | 10.062964 | 9.544866 |
| 6 | 6.362781 | 9.570919 | 4.971247 |
| 1 | 6.961098 | 10.381999 | 4.549553 |
| 1 | 5.994337 | 9.874485 | 5.955539 |
| 1 | 5.518788 | 9.356438 | 4.310845 |
| 6 | 7.192233 | 8.380865 | 5.130251 |
| 7 | 7.841200 | 7.425383 | 5.260002 |
| 6 | 7.988839 | 11.944911 | 8.571259 |
| 1 | 8.558505 | 11.618546 | 9.446673 |
| 1 | 6.945132 | 11.639289 | 8.682791 |
| 1 | 8.044736 | 13.033209 | 8.489502 |
| 6 | 8.558182 | 11.319582 | 7.382553 |
| 7 | 9.011129 | 10.818294 | 6.437361 |
| 6 | 11.079085 | 3.853125 | 9.605969 |
| 1 | 11.950969 | 3.414948 | 9.113974 |
| 1 | 10.189693 | 3.666982 | 8.997698 |
| 1 | 10.951289 | 3.384892 | 10.585072 |
| 6 | 11.261763 | 5.293223 | 9.760044 |
| 7 | 11.398861 | 6.441517 | 9.875487 |
| 6 | 11.730849 | 9.546712 | 6.376136 |
| 6 | 10.837821 | 8.518045 | 6.863503 |
| 7 | 10.170564 | 7.662613 | 7.238891 |
| 1 | 11.703276 | 10.378434 | 7.086016 |
| 1 | 11.367336 | 9.892001 | 5.404958 |
| 1 | 12.740533 | 9.134520 | 6.296663 |
| 1 | 9.542441 | 6.868839 | 7.554113 |

Cartesian coordinates of : PACN7_24

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.342676 | 2.402453 | -0.438263 |
| 1 | -4.894118 | 2.430626 | 0.504678 |
| 1 | -4.742834 | 1.605931 | -1.073181 |
| 1 | -4.443598 | 3.364235 | -0.946946 |
| 6 | -2.938541 | 2.109821 | -0.191477 |
| 7 | -1.820350 | 1.852156 | -0.014018 |
| 6 | 1.901209 | -2.078355 | 2.568390 |
| 1 | 1.858882 | -1.047752 | 2.933456 |
| 1 | 2.755296 | -2.592032 | 3.016926 |
| 1 | 0.980692 | -2.599878 | 2.842780 |
| 6 | 2.034953 | -2.054019 | 1.115878 |
| 7 | 2.155837 | -2.032809 | -0.039082 |
| 6 | -1.119551 | 0.604348 | 3.228306 |
| 1 | -1.251644 | 1.582199 | 2.756536 |
| 1 | -0.141053 | 0.589488 | 3.715698 |
| 1 | -1.903466 | 0.445081 | 3.972865 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.177221 | -0.434018 | 2.203425 |
| 7 | -1.224746 | -1.261192 | 1.388181 |
| 6 | 4.677996 | 0.149101 | -0.172655 |
| 1 | 5.596599 | 0.733338 | -0.267373 |
| 1 | 4.906992 | -0.913576 | -0.285042 |
| 1 | 4.237237 | 0.314028 | 0.815518 |
| 6 | 3.716282 | 0.551844 | -1.193444 |
| 7 | 2.942571 | 0.879593 | -1.996290 |
| 6 | 1.335593 | 3.272076 | -0.131375 |
| 1 | 0.342447 | 3.717475 | -0.031856 |
| 1 | 1.488247 | 2.940075 | -1.163125 |
| 1 | 2.093833 | 4.019988 | 0.114424 |
| 6 | 1.452838 | 2.125092 | 0.765111 |
| 7 | 1.542260 | 1.201168 | 1.464956 |
| 6 | -3.559266 | -3.029544 | -0.384706 |
| 1 | -4.525064 | -3.105659 | 0.121191 |
| 1 | -2.757170 | -3.160724 | 0.346407 |
| 1 | -3.497640 | -3.811999 | -1.145146 |
| 6 | -3.423298 | -1.714405 | -1.004043 |
| 7 | -3.310169 | -0.666846 | -1.494491 |
| 6 | 1.088177 | -1.405108 | -3.006288 |
| 6 | 0.393873 | -0.591301 | -2.033208 |
| 7 | -0.194256 | 0.050607 | -1.284322 |
| 1 | 1.596839 | -0.740856 | -3.710262 |
| 1 | 0.364040 | -2.041762 | -3.522022 |
| 1 | 1.823830 | -2.008228 | -2.465599 |
| 1 | -0.768599 | 0.673351 | -0.658381 |

Cartesian coordinates of : PACN7_25

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.545682 | 3.124412 | 1.786388 |
| 1 | -1.278522 | 2.217624 | 2.337243 |
| 1 | -2.516540 | 3.493045 | 2.127002 |
| 1 | -0.782908 | 3.885305 | 1.969254 |
| 6 | -1.599698 | 2.807191 | 0.362877 |
| 7 | -1.642552 | 2.535814 | -0.766612 |
| 6 | -1.298539 | -3.908450 | 0.598271 |
| 1 | -0.251194 | -4.214044 | 0.533127 |
| 1 | -1.927585 | -4.795940 | 0.701987 |
| 1 | -1.427677 | -3.263722 | 1.473018 |
| 6 | -1.673554 | -3.163630 | -0.600042 |
| 7 | -1.974318 | -2.553038 | -1.541759 |
| 6 | 1.919705 | 3.039591 | -1.117566 |
| 1 | 2.456660 | 2.342002 | -1.766528 |
| 1 | 2.520531 | 3.941632 | -0.976691 |
| 1 | 0.964498 | 3.313696 | -1.577085 |
| 6 | 1.665427 | 2.396533 | 0.167987 |
| 7 | 1.436251 | 1.883082 | 1.185402 |
| 6 | -3.920162 | -0.088481 | -0.183880 |
| 1 | -4.875228 | -0.082659 | 0.347669 |
| 1 | -3.915577 | -0.908196 | -0.908265 |
| 1 | -3.795803 | 0.863959 | -0.708402 |
| 6 | -2.819615 | -0.269033 | 0.759437 |
| 7 | -1.937262 | -0.407216 | 1.503809 |
| 6 | 0.922792 | -0.552282 | 3.470898 |
| 1 | -0.150729 | -0.530798 | 3.680816 |
| 1 | 1.327301 | 0.462034 | 3.535596 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 1.430852 | -1.206707 | 4.183303 |
| 6 | 1.111558 | -1.026826 | 2.110457 |
| 7 | 1.242139 | -1.376395 | 1.010833 |
| 6 | 4.744753 | -1.659752 | -0.193872 |
| 1 | 5.539816 | -1.084319 | 0.286587 |
| 1 | 5.194851 | -2.397233 | -0.862941 |
| 1 | 4.162748 | -2.178469 | 0.573029 |
| 6 | 3.866918 | -0.769263 | -0.947013 |
| 7 | 3.158311 | -0.066391 | -1.541019 |
| 6 | -1.300338 | 0.344781 | -3.219057 |
| 6 | -0.456127 | -0.002294 | -2.097298 |
| 7 | 0.204643 | -0.308170 | -1.209585 |
| 1 | -1.791333 | 1.297155 | -2.997622 |
| 1 | -2.035637 | -0.459411 | -3.333669 |
| 1 | -0.692175 | 0.427608 | -4.123961 |
| 1 | 0.728536 | -0.711359 | -0.366467 |

Cartesian coordinates of : PACN7_26

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.624382 | -2.929971 | 2.038651 |
| 1 | 3.403719 | -3.775309 | 2.694881 |
| 1 | 4.564015 | -2.465960 | 2.348157 |
| 1 | 3.712317 | -3.278520 | 1.005209 |
| 6 | 2.542196 | -1.957524 | 2.093952 |
| 7 | 1.672723 | -1.188767 | 2.114302 |
| 6 | 0.469452 | 3.810480 | -1.362483 |
| 1 | 0.126756 | 3.775081 | -0.324822 |
| 1 | -0.376432 | 4.071849 | -2.002939 |
| 1 | 1.259242 | 4.558351 | -1.468764 |
| 6 | 0.972436 | 2.493906 | -1.739805 |
| 7 | 1.374614 | 1.447692 | -2.047654 |
| 6 | 1.749461 | 1.942894 | 3.767982 |
| 1 | 2.674392 | 2.485866 | 3.558507 |
| 1 | 1.988274 | 0.900816 | 3.996475 |
| 1 | 1.257936 | 2.398018 | 4.631349 |
| 6 | 0.867370 | 1.990953 | 2.605509 |
| 7 | 0.164096 | 2.023164 | 1.681110 |
| 6 | -3.041945 | 1.628846 | 1.168656 |
| 1 | -2.574439 | 0.744546 | 1.611016 |
| 1 | -4.126202 | 1.493085 | 1.155803 |
| 1 | -2.783755 | 2.504453 | 1.768815 |
| 6 | -2.544582 | 1.798577 | -0.192305 |
| 7 | -2.142185 | 1.924391 | -1.275154 |
| 6 | -5.608226 | -2.817925 | 0.308890 |
| 1 | -5.834180 | -2.847789 | 1.377621 |
| 1 | -5.502035 | -3.841188 | -0.059644 |
| 1 | -6.435786 | -2.335318 | -0.216867 |
| 6 | -4.370941 | -2.075697 | 0.080157 |
| 7 | -3.386529 | -1.486773 | -0.102788 |
| 6 | 3.656022 | -0.834115 | -3.144602 |
| 1 | 3.178313 | 0.139352 | -3.282894 |
| 1 | 3.551866 | -1.429555 | -4.055151 |
| 1 | 4.719264 | -0.690671 | -2.936210 |
| 6 | 3.017521 | -1.517933 | -2.023538 |
| 7 | 2.511686 | -2.064739 | -1.130953 |
| 6 | -0.998431 | -0.773002 | -2.321321 |
| 6 | -0.484915 | -0.674256 | -0.975000 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.057885 | -0.634633 | 0.090887 |
| 1 | -0.475031 | -1.591588 | -2.825133 |
| 1 | -0.811471 | 0.178179 | -2.826598 |
| 1 | -2.073175 | -0.966755 | -2.264697 |
| 1 | 0.501967 | -0.680696 | 0.979177 |

Cartesian coordinates of : PACN7_27

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.299769 | 2.270180 | -0.549794 |
| 1 | -5.347138 | 2.173914 | -0.252845 |
| 1 | -4.209950 | 3.098097 | -1.257509 |
| 1 | -3.688061 | 2.477203 | 0.332218 |
| 6 | -3.839009 | 1.029978 | -1.167751 |
| 7 | -3.473677 | 0.041381 | -1.657331 |
| 6 | 0.452564 | 2.789966 | 2.386896 |
| 1 | 1.303418 | 2.134115 | 2.594189 |
| 1 | 0.070241 | 3.205425 | 3.322655 |
| 1 | 0.792936 | 3.597496 | 1.734703 |
| 6 | -0.592487 | 2.022511 | 1.715455 |
| 7 | -1.431591 | 1.401266 | 1.204064 |
| 6 | 4.284715 | 1.062611 | 0.306075 |
| 1 | 4.060772 | 0.171952 | 0.901020 |
| 1 | 4.894257 | 1.753840 | 0.893563 |
| 1 | 4.834830 | 0.771296 | -0.592424 |
| 6 | 3.027350 | 1.698169 | -0.073793 |
| 7 | 2.025426 | 2.208721 | -0.366599 |
| 6 | 3.691036 | -2.889878 | -0.448269 |
| 1 | 4.781070 | -2.945935 | -0.507629 |
| 1 | 3.272508 | -3.853820 | -0.748354 |
| 1 | 3.389985 | -2.671055 | 0.580285 |
| 6 | 3.194811 | -1.833373 | -1.324753 |
| 7 | 2.804948 | -0.981716 | -2.011386 |
| 6 | -4.127030 | -2.918923 | -0.016060 |
| 1 | -4.601000 | -2.369270 | -0.835100 |
| 1 | -4.719283 | -2.798069 | 0.894233 |
| 1 | -4.066829 | -3.979327 | -0.272533 |
| 6 | -2.792006 | -2.371439 | 0.176183 |
| 7 | -1.732744 | -1.915951 | 0.302650 |
| 6 | -0.300176 | -1.368037 | 3.178465 |
| 1 | 0.017314 | -1.153951 | 4.202257 |
| 1 | -0.572698 | -2.423452 | 3.099802 |
| 1 | -1.171639 | -0.757561 | 2.925084 |
| 6 | 0.782830 | -1.068957 | 2.245237 |
| 7 | 1.647750 | -0.823281 | 1.508449 |
| 6 | 0.722542 | 1.327330 | -3.025723 |
| 6 | 0.175340 | 0.498562 | -1.973731 |
| 7 | -0.288299 | -0.170806 | -1.164838 |
| 1 | 0.120079 | 1.199318 | -3.929220 |
| 1 | 1.752498 | 1.000777 | -3.198358 |
| 1 | 0.715659 | 2.367541 | -2.691224 |
| 1 | -0.775933 | -0.808024 | -0.470504 |

Cartesian coordinates of : PACN7_28

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.053175 | -2.865372 | 0.733648 |
| 1 | -4.961464 | -2.913463 | 0.126558 |
| 1 | -4.070065 | -1.961898 | 1.350465 |
| 1 | -4.020032 | -3.745015 | 1.381351 |
| 6 | -2.873627 | -2.826421 | -0.125851 |
| 7 | -1.934551 | -2.778579 | -0.808430 |
| 6 | -4.127378 | 0.083787 | -1.756781 |
| 1 | -4.293649 | -0.025259 | -0.680386 |
| 1 | -4.253581 | -0.883943 | -2.250001 |
| 1 | -4.843107 | 0.798465 | -2.170509 |
| 6 | -2.765510 | 0.557414 | -1.959549 |
| 7 | -1.675565 | 0.930194 | -2.105147 |
| 6 | -0.552632 | 4.205567 | -1.824427 |
| 1 | 0.264017 | 4.762841 | -2.289880 |
| 1 | -1.271489 | 4.913609 | -1.404716 |
| 1 | -1.049492 | 3.592626 | -2.581481 |
| 6 | -0.032551 | 3.337127 | -0.772459 |
| 7 | 0.378314 | 2.635177 | 0.057607 |
| 6 | -1.237660 | 1.658431 | 3.001943 |
| 1 | -2.030828 | 2.252161 | 3.463445 |
| 1 | -0.514612 | 2.317716 | 2.514184 |
| 1 | -0.718925 | 1.074627 | 3.765908 |
| 6 | -1.808955 | 0.759706 | 2.003670 |
| 7 | -2.288388 | 0.050944 | 1.216339 |
| 6 | 3.190814 | 1.638055 | 1.383590 |
| 1 | 2.951054 | 2.660058 | 1.686795 |
| 1 | 3.127799 | 1.567534 | 0.294643 |
| 1 | 4.203298 | 1.383201 | 1.706298 |
| 6 | 2.231444 | 0.710655 | 1.973111 |
| 7 | 1.463084 | -0.028390 | 2.435794 |
| 6 | 5.968855 | -1.660455 | -1.683082 |
| 1 | 6.401294 | -0.748689 | -2.102355 |
| 1 | 5.831800 | -2.389489 | -2.485504 |
| 1 | 6.657859 | -2.073043 | -0.941989 |
| 6 | 4.683244 | -1.361869 | -1.056973 |
| 7 | 3.660525 | -1.125782 | -0.559240 |
| 6 | 0.917952 | -2.486308 | 0.677794 |
| 6 | 0.572353 | -1.329000 | -0.112848 |
| 7 | 0.278734 | -0.419148 | -0.750791 |
| 1 | 0.325531 | -2.446147 | 1.597058 |
| 1 | 1.982420 | -2.436933 | 0.920566 |
| 1 | 0.672558 | -3.381095 | 0.099096 |
| 1 | -0.244503 | 0.303318 | -1.293178 |

Cartesian coordinates of : PACN7_29

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.291011 | 3.307013 | -0.253973 |
| 1 | 2.506058 | 4.264157 | -0.735240 |
| 1 | 2.905153 | 3.200893 | 0.643850 |
| 1 | 1.238416 | 3.273247 | 0.043856 |
| 6 | 2.569563 | 2.207281 | -1.172748 |
| 7 | 2.778278 | 1.330487 | -1.905647 |
| 6 | -4.126360 | -2.457389 | -0.668255 |
| 1 | -5.172702 | -2.410959 | -0.356133 |
| 1 | -3.500608 | -2.716160 | 0.190004 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.023168 | -3.225418 | -1.438874 |
| 6 | -3.702465 | -1.161850 | -1.191537 |
| 7 | -3.365416 | -0.129450 | -1.605118 |
| 6 | -0.400659 | 0.997311 | 3.313928 |
| 1 | -1.248032 | 0.401124 | 2.963034 |
| 1 | -0.699503 | 2.047384 | 3.365467 |
| 1 | -0.101153 | 0.661321 | 4.310000 |
| 6 | 0.709206 | 0.845272 | 2.377057 |
| 7 | 1.588814 | 0.715790 | 1.628322 |
| 6 | 0.730447 | -3.006924 | 2.120309 |
| 1 | 0.388933 | -3.557473 | 3.000450 |
| 1 | 1.528263 | -2.313686 | 2.402853 |
| 1 | 1.130453 | -3.702119 | 1.378701 |
| 6 | -0.376459 | -2.251002 | 1.541439 |
| 7 | -1.262790 | -1.638900 | 1.103624 |
| 6 | 4.442701 | -0.625640 | 0.203446 |
| 1 | 5.169611 | -1.267278 | 0.707675 |
| 1 | 4.122541 | 0.172979 | 0.878917 |
| 1 | 4.900028 | -0.182410 | -0.684686 |
| 6 | 3.270811 | -1.401709 | -0.186959 |
| 7 | 2.335459 | -2.020930 | -0.491304 |
| 6 | -4.064734 | 2.752965 | 0.098422 |
| 1 | -4.646330 | 2.591548 | 1.009299 |
| 1 | -4.527792 | 2.209921 | -0.731214 |
| 1 | -4.037680 | 3.820911 | -0.131152 |
| 6 | -2.712936 | 2.240353 | 0.267636 |
| 7 | -1.639322 | 1.813253 | 0.376397 |
| 6 | 0.975693 | -1.171723 | -3.096232 |
| 6 | 0.336687 | -0.470925 | -2.003961 |
| 7 | -0.192788 | 0.106103 | -1.164741 |
| 1 | 1.971259 | -0.734510 | -3.225828 |
| 1 | 0.376919 | -1.044038 | -4.002210 |
| 1 | 1.070998 | -2.227029 | -2.829375 |
| 1 | -0.702339 | 0.684920 | -0.441552 |

Cartesian coordinates of : PACN7_30

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.036602 | 0.383082 | 0.122931 |
| 1 | -5.789795 | 0.496602 | -0.660870 |
| 1 | -5.452877 | 0.740627 | 1.068109 |
| 1 | -4.763917 | -0.670735 | 0.223714 |
| 6 | -3.841847 | 1.150944 | -0.216135 |
| 7 | -2.893031 | 1.765757 | -0.486277 |
| 6 | 3.227341 | -2.847620 | 0.069917 |
| 1 | 3.193133 | -2.235978 | 0.975531 |
| 1 | 3.921637 | -2.385450 | -0.635194 |
| 1 | 3.569088 | -3.855189 | 0.319306 |
| 6 | 1.894208 | -2.902066 | -0.520243 |
| 7 | 0.832171 | -2.960931 | -0.986748 |
| 6 | 2.723915 | 0.901355 | 2.426641 |
| 1 | 3.666099 | 0.497902 | 2.045317 |
| 1 | 2.787635 | 1.013245 | 3.511784 |
| 1 | 2.549862 | 1.878989 | 1.967811 |
| 6 | 1.626781 | 0.005502 | 2.072682 |
| 7 | 0.756697 | -0.708750 | 1.784878 |
| 6 | 3.489088 | 2.749447 | -1.664925 |
| 1 | 2.729721 | 3.429158 | -1.268041 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.477707 | 2.796602 | -2.756670 |
| 1 | 4.473838 | 3.062283 | -1.308889 |
| 6 | 3.201585 | 1.389266 | -1.217423 |
| 7 | 2.962360 | 0.311821 | -0.853859 |
| 6 | -1.273735 | 4.402930 | 0.932441 |
| 1 | -1.396068 | 4.453142 | 2.017147 |
| 1 | -2.233017 | 4.156250 | 0.468160 |
| 1 | -0.922050 | 5.368779 | 0.561639 |
| 6 | -0.324100 | 3.354934 | 0.585811 |
| 7 | 0.420726 | 2.510845 | 0.299749 |
| 6 | -1.138537 | -3.548787 | 1.690712 |
| 1 | -1.761834 | -3.933151 | 2.501971 |
| 1 | -0.281761 | -3.009205 | 2.103013 |
| 1 | -0.780880 | -4.380473 | 1.078460 |
| 6 | -1.909925 | -2.631127 | 0.860055 |
| 7 | -2.532193 | -1.905768 | 0.198734 |
| 6 | -1.465939 | -1.461524 | -2.636777 |
| 6 | -0.769761 | -0.562976 | -1.742719 |
| 7 | -0.216782 | 0.185635 | -1.071267 |
| 1 | -1.153928 | -1.258282 | -3.664830 |
| 1 | -2.540244 | -1.299483 | -2.513133 |
| 1 | -1.205024 | -2.484082 | -2.349899 |
| 1 | 0.188184 | 0.928024 | -0.458705 |

Cartesian coordinates of : PACN7_31

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.001303 | -3.232687 | 2.814085 |
| 1 | 0.922082 | -3.229730 | 2.988410 |
| 1 | 2.515186 | -2.882543 | 3.712694 |
| 1 | 2.330073 | -4.250068 | 2.588159 |
| 6 | 2.303189 | -2.350175 | 1.691280 |
| 7 | 2.539455 | -1.647606 | 0.795673 |
| 6 | 4.129590 | -1.539451 | -2.355675 |
| 1 | 3.996336 | -2.325825 | -3.102817 |
| 1 | 4.091399 | -1.980341 | -1.355479 |
| 1 | 5.104052 | -1.068625 | -2.510990 |
| 6 | 3.067788 | -0.545047 | -2.479117 |
| 7 | 2.227994 | 0.252868 | -2.564860 |
| 6 | -0.886659 | 4.004188 | 2.075007 |
| 1 | 0.137161 | 4.097342 | 1.703566 |
| 1 | -0.872674 | 3.945344 | 3.166199 |
| 1 | -1.467799 | 4.879411 | 1.774025 |
| 6 | -1.481276 | 2.792959 | 1.518089 |
| 7 | -1.955403 | 1.829980 | 1.072159 |
| 6 | -3.490440 | -1.064754 | 2.129343 |
| 1 | -4.168709 | -1.811955 | 1.710107 |
| 1 | -3.618807 | -0.113078 | 1.604788 |
| 1 | -3.705840 | -0.931719 | 3.192447 |
| 6 | -2.110800 | -1.495792 | 1.949956 |
| 7 | -1.007742 | -1.826870 | 1.793693 |
| 6 | 4.046829 | 1.514630 | 0.153302 |
| 1 | 4.451599 | 1.738075 | -0.837544 |
| 1 | 4.025838 | 0.431253 | 0.305141 |
| 1 | 4.681509 | 1.977595 | 0.913096 |
| 6 | 2.687482 | 2.037045 | 0.252246 |
| 7 | 1.608579 | 2.460232 | 0.333494 |
| 6 | -5.376624 | -1.233147 | -2.621483 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -6.215518 | -0.659655 | -2.219593 |
| 1 | -5.582395 | -2.299454 | -2.499785 |
| 1 | -5.275657 | -1.012865 | -3.687086 |
| 6 | -4.144638 | -0.877716 | -1.920497 |
| 7 | -3.164192 | -0.594457 | -1.365251 |
| 6 | -0.598595 | 1.552722 | -2.001762 |
| 6 | -0.280059 | 0.488924 | -1.082020 |
| 7 | -0.038753 | -0.357388 | -0.345088 |
| 1 | 0.064724 | 2.393902 | -1.778133 |
| 1 | -1.646928 | 1.821122 | -1.839640 |
| 1 | -0.424601 | 1.203855 | -3.022516 |
| 1 | -0.013118 | -1.049557 | 0.419680 |

Cartesian coordinates of : PACN7_32

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.903800 | 1.942634 | -1.636014 |
| 1 | -3.979285 | 2.134240 | -1.671033 |
| 1 | -2.483771 | 2.030555 | -2.640955 |
| 1 | -2.419624 | 2.671685 | -0.980272 |
| 6 | -2.657432 | 0.600486 | -1.117165 |
| 7 | -2.491252 | -0.473923 | -0.706166 |
| 6 | -2.511845 | -3.769641 | -1.687606 |
| 1 | -3.159866 | -2.888535 | -1.664024 |
| 1 | -2.957245 | -4.569737 | -1.089889 |
| 1 | -2.413501 | -4.118234 | -2.718729 |
| 6 | -1.203067 | -3.407992 | -1.150734 |
| 7 | -0.167552 | -3.109696 | -0.716561 |
| 6 | 0.530187 | 4.412586 | -1.511648 |
| 1 | 1.569870 | 4.736909 | -1.420684 |
| 1 | 0.044665 | 4.481381 | -0.534193 |
| 1 | 0.018337 | 5.064566 | -2.224067 |
| 6 | 0.476022 | 3.028052 | -1.970293 |
| 7 | 0.418177 | 1.925369 | -2.331160 |
| 6 | -2.729786 | -2.604473 | 2.004426 |
| 1 | -3.288618 | -2.382620 | 1.089922 |
| 1 | -3.415896 | -2.657461 | 2.853320 |
| 1 | -2.210124 | -3.560545 | 1.896527 |
| 6 | -1.754375 | -1.542802 | 2.208018 |
| 7 | -0.977459 | -0.692004 | 2.351723 |
| 6 | -1.199830 | 2.476305 | 3.680478 |
| 1 | -2.205673 | 2.821309 | 3.932524 |
| 1 | -0.468814 | 3.113122 | 4.184727 |
| 1 | -1.076685 | 1.444177 | 4.019540 |
| 6 | -1.000023 | 2.531762 | 2.235346 |
| 7 | -0.836807 | 2.568114 | 1.085254 |
| 6 | 6.429727 | -1.101677 | 1.109667 |
| 1 | 6.819964 | -0.177454 | 1.542789 |
| 1 | 7.123775 | -1.455180 | 0.343216 |
| 1 | 6.352818 | -1.857871 | 1.894753 |
| 6 | 5.115612 | -0.860428 | 0.519373 |
| 7 | 4.071064 | -0.668629 | 0.050170 |
| 6 | 1.773912 | -0.846837 | -2.027696 |
| 6 | 1.184732 | -0.459715 | -0.768098 |
| 7 | 0.695217 | -0.164929 | 0.228467 |
| 1 | 2.196733 | -1.847326 | -1.905145 |
| 1 | 2.554612 | -0.128520 | -2.287044 |
| 1 | 0.984582 | -0.837461 | -2.783981 |

1 0.133825 -0.096675 1.102288

Cartesian coordinates of : PACN7_33

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 9.243235 | 7.738847 | 4.175115 |
| 1 | 9.507578 | 8.173455 | 3.207903 |
| 1 | 9.241854 | 6.648234 | 4.096086 |
| 1 | 9.972223 | 8.050360 | 4.929181 |
| 6 | 7.922934 | 8.201982 | 4.587844 |
| 7 | 6.873060 | 8.575177 | 4.919692 |
| 6 | 3.627264 | 7.400612 | 4.098977 |
| 1 | 3.441922 | 6.452485 | 3.587964 |
| 1 | 4.538724 | 7.853764 | 3.698458 |
| 1 | 2.778799 | 8.066649 | 3.919959 |
| 6 | 3.792382 | 7.172720 | 5.531933 |
| 7 | 3.924922 | 6.998475 | 6.672880 |
| 6 | 9.326077 | 10.578848 | 9.431320 |
| 1 | 10.154038 | 11.289645 | 9.371952 |
| 1 | 9.386332 | 10.028031 | 10.373974 |
| 1 | 8.375263 | 11.117752 | 9.381872 |
| 6 | 9.387837 | 9.644463 | 8.312809 |
| 7 | 9.435021 | 8.903335 | 7.418327 |
| 6 | 5.995244 | 10.459373 | 11.467291 |
| 1 | 6.733566 | 10.945490 | 12.110824 |
| 1 | 5.051272 | 10.383626 | 12.012825 |
| 1 | 5.843518 | 11.060312 | 10.565974 |
| 6 | 6.460879 | 9.128913 | 11.085700 |
| 7 | 6.836781 | 8.073469 | 10.778416 |
| 6 | 11.268100 | 5.903973 | 6.966645 |
| 1 | 11.351717 | 6.984350 | 7.116045 |
| 1 | 11.735907 | 5.628915 | 6.017403 |
| 1 | 11.789159 | 5.387058 | 7.776410 |
| 6 | 9.857251 | 5.527078 | 6.958419 |
| 7 | 8.733616 | 5.232079 | 6.946286 |
| 6 | 4.391281 | 10.692923 | 6.069308 |
| 1 | 4.171216 | 11.748317 | 5.890466 |
| 1 | 3.478468 | 10.178932 | 6.382656 |
| 1 | 4.771502 | 10.236552 | 5.150569 |
| 6 | 5.407984 | 10.562876 | 7.107380 |
| 7 | 6.221679 | 10.460016 | 7.931314 |
| 6 | 5.931379 | 5.370374 | 8.905555 |
| 6 | 6.409640 | 6.561481 | 8.250882 |
| 7 | 6.790397 | 7.507800 | 7.729486 |
| 1 | 6.521853 | 4.524019 | 8.540799 |
| 1 | 4.873876 | 5.246292 | 8.652157 |
| 1 | 6.061968 | 5.501331 | 9.984294 |
| 1 | 7.132967 | 8.345818 | 7.262351 |

Cartesian coordinates of : PACN7_34

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|----------|
| 6 | -0.585364 | -4.421091 | 3.528973 |
| 6 | -0.357005 | -3.259564 | 2.672356 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.175717 | -2.336094 | 1.992856 |
| 1 | -1.602943 | -4.794246 | 3.389552 |
| 1 | -0.450349 | -4.144889 | 4.577615 |
| 1 | 0.121009 | -5.216279 | 3.278311 |
| 6 | -1.077139 | 0.001731 | 0.009980 |
| 6 | 0.361611 | -0.000531 | 0.100125 |
| 7 | 1.509568 | -0.002326 | 0.159278 |
| 1 | -1.492424 | 0.002260 | 1.019457 |
| 1 | -1.388966 | -0.897456 | -0.526682 |
| 1 | -1.386118 | 0.902044 | -0.526447 |
| 6 | 0.337604 | 4.270792 | -3.775833 |
| 6 | 0.290341 | 3.207924 | -2.774130 |
| 7 | 0.252727 | 2.362875 | -1.979098 |
| 1 | -0.668119 | 4.657173 | -3.958641 |
| 1 | 0.743392 | 3.883499 | -4.713645 |
| 1 | 0.972650 | 5.088213 | -3.425582 |
| 1 | 2.555865 | -0.003939 | 0.219611 |
| 6 | 6.861598 | -0.010249 | 0.523289 |
| 1 | 7.304934 | -0.245272 | -0.447395 |
| 1 | 7.176788 | -0.760442 | 1.252599 |
| 1 | 7.209632 | 0.973421 | 0.847764 |
| 6 | 5.407197 | -0.008143 | 0.414587 |
| 7 | 4.252784 | -0.006460 | 0.328698 |
| 6 | -6.867702 | 0.008316 | -0.341914 |
| 6 | -5.409439 | 0.006578 | -0.245641 |
| 7 | -4.250895 | 0.005214 | -0.169403 |
| 1 | -7.307488 | 0.221273 | 0.635545 |
| 1 | -7.221698 | -0.967255 | -0.684148 |
| 1 | -7.195345 | 0.772192 | -1.051363 |
| 6 | -0.569443 | 4.424640 | 3.527122 |
| 1 | 0.139452 | 5.217111 | 3.274978 |
| 1 | -1.585845 | 4.801156 | 3.388150 |
| 1 | -0.434478 | 4.149134 | 4.575953 |
| 6 | -0.345827 | 3.261388 | 2.671594 |
| 7 | -0.168309 | 2.336548 | 1.992963 |
| 6 | 0.319528 | -4.271593 | -3.776110 |
| 1 | 0.727441 | -3.886938 | -4.714086 |
| 1 | 0.950077 | -5.092330 | -3.425487 |
| 1 | -0.688297 | -4.652529 | -3.958769 |
| 6 | 0.278072 | -3.208044 | -2.774872 |
| 7 | 0.245075 | -2.362448 | -1.980215 |

Cartesian coordinates of : PACN8_1

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.688428 | -1.487659 | -0.685735 |
| 1 | -4.561755 | -1.118552 | -1.229024 |
| 1 | -3.575963 | -0.922869 | 0.243732 |
| 1 | -3.812519 | -2.545077 | -0.440555 |
| 6 | -2.487535 | -1.306383 | -1.494623 |
| 7 | -1.532685 | -1.156094 | -2.140684 |
| 6 | 4.780087 | -1.716885 | 0.859583 |
| 1 | 4.162745 | -2.536625 | 0.481125 |
| 1 | 5.019304 | -1.891265 | 1.911733 |
| 1 | 5.710948 | -1.672528 | 0.288628 |
| 6 | 4.042752 | -0.465419 | 0.712946 |
| 7 | 3.444979 | 0.524264 | 0.592488 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.090739 | -4.121251 | -1.540610 |
| 1 | -0.939212 | -4.108438 | -0.849682 |
| 1 | 0.313171 | -5.134351 | -1.609606 |
| 1 | -0.429500 | -3.791298 | -2.525829 |
| 6 | 0.932693 | -3.208170 | -1.042675 |
| 7 | 1.748921 | -2.486702 | -0.636097 |
| 6 | -1.729512 | 2.405441 | -2.512868 |
| 1 | -2.248130 | 3.075957 | -3.202795 |
| 1 | -1.476350 | 1.478709 | -3.039289 |
| 1 | -0.814787 | 2.892616 | -2.158084 |
| 6 | -2.592517 | 2.087833 | -1.378625 |
| 7 | -3.271583 | 1.822222 | -0.473683 |
| 6 | 0.745618 | -1.773848 | 2.611825 |
| 1 | 0.497471 | -0.887341 | 3.202965 |
| 1 | 1.543017 | -1.525420 | 1.902756 |
| 1 | 1.090277 | -2.565252 | 3.282183 |
| 6 | -0.431420 | -2.217004 | 1.869676 |
| 7 | -1.364007 | -2.546359 | 1.259917 |
| 6 | 3.446350 | 4.048998 | 0.483749 |
| 1 | 3.894147 | 3.152240 | 0.920326 |
| 1 | 3.124718 | 4.722710 | 1.281804 |
| 1 | 4.186648 | 4.560647 | -0.136269 |
| 6 | 2.300413 | 3.656674 | -0.329960 |
| 7 | 1.388509 | 3.340561 | -0.976487 |
| 6 | -3.982301 | 1.594166 | 2.872185 |
| 1 | -4.524226 | 1.878888 | 1.964721 |
| 1 | -3.917651 | 2.452662 | 3.545143 |
| 1 | -4.503005 | 0.775858 | 3.375558 |
| 6 | -2.648929 | 1.170516 | 2.474418 |
| 7 | -1.595004 | 0.840792 | 2.123805 |
| 6 | 1.448022 | 0.304501 | -2.083482 |
| 6 | 0.712759 | 0.411391 | -0.843644 |
| 7 | 0.094848 | 0.511005 | 0.121158 |
| 1 | 1.510668 | 1.302921 | -2.526648 |
| 1 | 0.906222 | -0.390791 | -2.732129 |
| 1 | 2.447566 | -0.076480 | -1.859849 |
| 1 | -0.545534 | 0.627825 | 0.983199 |

Cartesian coordinates of : PACN8_2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.832789 | 1.824134 | 2.396242 |
| 1 | -0.771850 | 2.095329 | 2.417480 |
| 1 | -1.943420 | 0.752820 | 2.594921 |
| 1 | -2.365224 | 2.390494 | 3.164338 |
| 6 | -2.377081 | 2.123167 | 1.075376 |
| 7 | -2.796868 | 2.327441 | 0.010447 |
| 6 | 2.364541 | -2.492213 | -2.391803 |
| 1 | 1.626473 | -1.777435 | -2.766956 |
| 1 | 1.905508 | -3.482303 | -2.356862 |
| 1 | 3.227471 | -2.503392 | -3.062466 |
| 6 | 2.785279 | -2.092054 | -1.052434 |
| 7 | 3.139545 | -1.760592 | 0.003871 |
| 6 | -5.498109 | 0.100087 | 0.039883 |
| 1 | -6.045823 | -0.379462 | -0.775185 |
| 1 | -5.271375 | 1.134851 | -0.233303 |
| 1 | -6.121278 | 0.092980 | 0.937697 |
| 6 | -4.248330 | -0.611696 | 0.292966 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -3.243796 | -1.161752 | 0.492961 |
| 6 | 3.727806 | 1.592238 | -0.530228 |
| 1 | 4.185822 | 0.668623 | -0.163664 |
| 1 | 3.256747 | 2.125203 | 0.302003 |
| 1 | 4.493101 | 2.227571 | -0.983203 |
| 6 | 2.702716 | 1.259375 | -1.514484 |
| 7 | 1.872078 | 0.995921 | -2.284018 |
| 6 | -0.222636 | 3.854603 | -1.728323 |
| 1 | -1.313495 | 3.782767 | -1.684269 |
| 1 | 0.157811 | 3.219743 | -2.535147 |
| 1 | 0.063187 | 4.891147 | -1.924067 |
| 6 | 0.341829 | 3.404917 | -0.459246 |
| 7 | 0.788155 | 3.018216 | 0.542136 |
| 6 | -2.049941 | -4.431908 | 0.628057 |
| 1 | -1.437648 | -4.936910 | 1.379235 |
| 1 | -2.620008 | -5.180655 | 0.072477 |
| 1 | -2.740546 | -3.743504 | 1.122576 |
| 6 | -1.199667 | -3.673334 | -0.283621 |
| 7 | -0.527133 | -3.062631 | -1.007779 |
| 6 | 4.015902 | -0.688778 | 3.185636 |
| 1 | 4.646416 | 0.183065 | 3.376937 |
| 1 | 4.469735 | -1.315900 | 2.411498 |
| 1 | 3.907006 | -1.265758 | 4.107207 |
| 6 | 2.710841 | -0.268759 | 2.700721 |
| 7 | 1.678661 | 0.045542 | 2.280378 |
| 6 | -1.311485 | -0.055420 | -1.961596 |
| 6 | -0.579518 | -0.071633 | -0.715386 |
| 7 | 0.017837 | -0.043093 | 0.266132 |
| 1 | -2.063853 | 0.739047 | -1.904800 |
| 1 | -1.786073 | -1.031188 | -2.095470 |
| 1 | -0.595196 | 0.143517 | -2.765911 |
| 1 | 0.661024 | 0.019623 | 1.145481 |

Cartesian coordinates of : PACN8_3

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.851176 | -3.204590 | -1.442296 |
| 1 | -1.084650 | -4.250820 | -1.655908 |
| 1 | 0.183667 | -3.134651 | -1.090486 |
| 1 | -0.958861 | -2.607846 | -2.351820 |
| 6 | -1.759510 | -2.689929 | -0.421546 |
| 7 | -2.481965 | -2.286022 | 0.394212 |
| 6 | -2.135375 | 2.408517 | -2.927127 |
| 1 | -2.960106 | 2.369617 | -3.643496 |
| 1 | -1.334262 | 3.040096 | -3.317715 |
| 1 | -2.478423 | 2.840093 | -1.982165 |
| 6 | -1.622832 | 1.064828 | -2.677951 |
| 7 | -1.236458 | -0.011692 | -2.471068 |
| 6 | -4.494604 | -0.091698 | -0.735203 |
| 1 | -4.910901 | -0.884426 | -0.108435 |
| 1 | -3.982538 | -0.560032 | -1.580878 |
| 1 | -5.300420 | 0.551463 | -1.098403 |
| 6 | -3.530740 | 0.692032 | 0.032616 |
| 7 | -2.762673 | 1.328605 | 0.628953 |
| 6 | -3.424788 | -0.879298 | 3.414102 |
| 1 | -3.856523 | -1.584323 | 2.696319 |
| 1 | -3.961743 | 0.071940 | 3.364840 |
| 1 | -3.493040 | -1.290157 | 4.424143 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -2.036284 | -0.666869 | 3.040347 |
| 7 | -0.941577 | -0.501350 | 2.700508 |
| 6 | 4.379372 | -4.715410 | 0.112967 |
| 1 | 5.042726 | -4.906929 | -0.734020 |
| 1 | 3.867041 | -5.643054 | 0.379721 |
| 1 | 4.976553 | -4.382090 | 0.965233 |
| 6 | 3.401297 | -3.690206 | -0.241458 |
| 7 | 2.623516 | -2.875185 | -0.523534 |
| 6 | 0.098799 | 2.951134 | 1.595541 |
| 1 | -0.828556 | 2.445421 | 1.879897 |
| 1 | 0.087916 | 3.973743 | 1.981373 |
| 1 | 0.957822 | 2.417546 | 2.014905 |
| 6 | 0.207072 | 2.961788 | 0.140098 |
| 7 | 0.307662 | 2.945940 | -1.017714 |
| 6 | 5.164060 | 3.532061 | 0.847705 |
| 1 | 5.305805 | 3.771727 | 1.904413 |
| 1 | 4.898316 | 4.444082 | 0.307553 |
| 1 | 6.101641 | 3.141272 | 0.444761 |
| 6 | 4.104310 | 2.537650 | 0.698730 |
| 7 | 3.261904 | 1.746875 | 0.580302 |
| 6 | 1.838324 | -0.003600 | -1.680864 |
| 6 | 1.107693 | -0.176855 | -0.446547 |
| 7 | 0.524307 | -0.308423 | 0.535931 |
| 1 | 2.899317 | -0.159502 | -1.473503 |
| 1 | 1.654460 | 1.017555 | -2.031760 |
| 1 | 1.471711 | -0.733655 | -2.407395 |
| 1 | -0.033670 | -0.395657 | 1.465010 |

Cartesian coordinates of : PACN8_4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.649909 | 1.038170 | -2.197966 |
| 1 | 4.271647 | 1.424000 | -1.386963 |
| 1 | 4.045188 | 1.370060 | -3.161323 |
| 1 | 3.653111 | -0.054064 | -2.152718 |
| 6 | 2.278585 | 1.508246 | -2.033611 |
| 7 | 1.185649 | 1.887044 | -1.919154 |
| 6 | -3.109905 | -3.691123 | 1.652075 |
| 1 | -3.593256 | -4.570155 | 1.218470 |
| 1 | -3.786403 | -2.834570 | 1.593521 |
| 1 | -2.869467 | -3.896463 | 2.698189 |
| 6 | -1.891734 | -3.376660 | 0.912909 |
| 7 | -0.921639 | -3.128554 | 0.322580 |
| 6 | 2.458214 | -2.239661 | 1.313531 |
| 1 | 2.541770 | -2.505077 | 2.370682 |
| 1 | 3.028416 | -2.958834 | 0.719614 |
| 1 | 1.409170 | -2.288994 | 1.004313 |
| 6 | 2.985664 | -0.894888 | 1.096601 |
| 7 | 3.403749 | 0.179890 | 0.952288 |
| 6 | 3.189825 | 2.305701 | 3.809432 |
| 1 | 4.013299 | 1.960719 | 3.176441 |
| 1 | 3.313865 | 1.911887 | 4.821062 |
| 1 | 3.188066 | 3.397780 | 3.844108 |
| 6 | 1.944358 | 1.822484 | 3.231805 |
| 7 | 0.975228 | 1.419248 | 2.742850 |
| 6 | -5.101498 | 1.610473 | 0.797934 |
| 1 | -5.293525 | 1.828707 | 1.851406 |
| 1 | -6.053643 | 1.437708 | 0.290096 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.589858 | 2.458806 | 0.336086 |
| 6 | -4.251653 | 0.430048 | 0.679359 |
| 7 | -3.575163 | -0.510038 | 0.582960 |
| 6 | 1.024711 | -4.254692 | -2.299965 |
| 1 | 0.343383 | -4.594484 | -1.514948 |
| 1 | 1.926508 | -4.872148 | -2.294531 |
| 1 | 0.535608 | -4.354299 | -3.272273 |
| 6 | 1.369726 | -2.857981 | -2.052233 |
| 7 | 1.637403 | -1.747148 | -1.840374 |
| 6 | -0.925288 | 4.551551 | -2.054297 |
| 1 | 0.056339 | 4.143206 | -2.308195 |
| 1 | -0.804076 | 5.404720 | -1.382193 |
| 1 | -1.430251 | 4.884242 | -2.964610 |
| 6 | -1.710578 | 3.509580 | -1.400969 |
| 7 | -2.337383 | 2.680050 | -0.882055 |
| 6 | -1.285269 | -0.336184 | -1.641159 |
| 6 | -0.714796 | 0.056016 | -0.373710 |
| 7 | -0.265599 | 0.378902 | 0.634501 |
| 1 | -0.545094 | -0.126954 | -2.418670 |
| 1 | -2.192030 | 0.255612 | -1.792736 |
| 1 | -1.521752 | -1.402802 | -1.595039 |
| 1 | 0.175635 | 0.779160 | 1.526625 |

Cartesian coordinates of : PACN8_ 5

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.391040 | 4.188562 | 2.230266 |
| 1 | 0.761950 | 4.569799 | 1.421025 |
| 1 | 2.351014 | 4.711057 | 2.226308 |
| 1 | 0.896332 | 4.368435 | 3.188105 |
| 6 | 1.596653 | 2.756863 | 2.032476 |
| 7 | 1.754825 | 1.618691 | 1.858881 |
| 6 | 3.522527 | -1.324771 | 2.244955 |
| 1 | 4.124683 | -1.753196 | 1.440614 |
| 1 | 3.874912 | -1.693395 | 3.211595 |
| 1 | 3.612599 | -0.235936 | 2.208525 |
| 6 | 2.121181 | -1.683768 | 2.055833 |
| 7 | 1.003624 | -1.973933 | 1.921651 |
| 6 | -2.859210 | 3.769679 | -1.669641 |
| 1 | -2.779434 | 4.777205 | -2.085129 |
| 1 | -3.719491 | 3.711663 | -0.998900 |
| 1 | -3.007063 | 3.046933 | -2.475373 |
| 6 | -1.645176 | 3.435131 | -0.932228 |
| 7 | -0.674071 | 3.180905 | -0.346222 |
| 6 | -5.116733 | -1.245888 | -0.767433 |
| 1 | -4.606808 | -2.064479 | -1.280502 |
| 1 | -6.023009 | -0.973138 | -1.313617 |
| 1 | -5.379750 | -1.585057 | 0.237204 |
| 6 | -4.221708 | -0.096582 | -0.675238 |
| 7 | -3.514574 | 0.822905 | -0.604441 |
| 6 | 2.640220 | 2.053774 | -1.299726 |
| 1 | 1.594571 | 2.188680 | -1.004456 |
| 1 | 2.756613 | 2.301845 | -2.357986 |
| 1 | 3.258913 | 2.731618 | -0.705604 |
| 6 | 3.057302 | 0.673676 | -1.064714 |
| 7 | 3.386654 | -0.429544 | -0.905956 |
| 6 | -1.343553 | -4.444826 | 1.999049 |
| 1 | -1.873703 | -4.740727 | 2.907752 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.329703 | -4.125552 | 2.254205 |
| 1 | -1.298393 | -5.299281 | 1.319209 |
| 6 | -2.036799 | -3.332589 | 1.357267 |
| 7 | -2.589671 | -2.446623 | 0.847630 |
| 6 | 3.036157 | -2.525202 | -3.776677 |
| 1 | 3.200451 | -2.137002 | -4.784741 |
| 1 | 2.949498 | -3.613610 | -3.817882 |
| 1 | 3.877886 | -2.248972 | -3.134022 |
| 6 | 1.826652 | -1.949118 | -3.207876 |
| 7 | 0.887278 | -1.473743 | -2.725658 |
| 6 | -1.257215 | 0.454382 | 1.643935 |
| 6 | -0.711826 | 0.016679 | 0.380300 |
| 7 | -0.284575 | -0.341514 | -0.625544 |
| 1 | -1.398458 | 1.537840 | 1.599022 |
| 1 | -0.544802 | 0.180127 | 2.427106 |
| 1 | -2.213501 | -0.056009 | 1.786447 |
| 1 | 0.131192 | -0.774872 | -1.514581 |

Cartesian coordinates of : PACN8_ 6

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.585948 | 2.129586 | -0.959100 |
| 1 | 2.494071 | 2.776915 | -1.835185 |
| 1 | 2.484248 | 1.082968 | -1.263358 |
| 1 | 3.576354 | 2.260697 | -0.514125 |
| 6 | 1.557289 | 2.468369 | 0.020573 |
| 7 | 0.725457 | 2.740271 | 0.785599 |
| 6 | -3.535981 | -2.468000 | 1.771238 |
| 1 | -2.954034 | -2.417276 | 2.695051 |
| 1 | -4.322528 | -3.219227 | 1.876893 |
| 1 | -3.989093 | -1.490653 | 1.577555 |
| 6 | -2.656725 | -2.811621 | 0.658446 |
| 7 | -1.959452 | -3.073841 | -0.233316 |
| 6 | 1.938799 | 0.749582 | 3.459847 |
| 1 | 2.754811 | 1.030013 | 4.130521 |
| 1 | 1.285767 | 0.029292 | 3.958670 |
| 1 | 1.357195 | 1.639376 | 3.198971 |
| 6 | 2.475232 | 0.159823 | 2.237440 |
| 7 | 2.908730 | -0.298101 | 1.260803 |
| 6 | 5.617700 | -0.958969 | -0.919977 |
| 1 | 6.179008 | -0.208497 | -1.482369 |
| 1 | 6.201582 | -1.882164 | -0.886067 |
| 1 | 5.447320 | -0.602228 | 0.100159 |
| 6 | 4.325953 | -1.203315 | -1.553901 |
| 7 | 3.285062 | -1.388227 | -2.035882 |
| 6 | -2.173075 | 1.687820 | 2.223499 |
| 1 | -3.029644 | 1.663012 | 1.543788 |
| 1 | -1.546145 | 2.558049 | 2.007680 |
| 1 | -2.529880 | 1.744049 | 3.255372 |
| 6 | -1.380682 | 0.476559 | 2.033661 |
| 7 | -0.747368 | -0.489765 | 1.903357 |
| 6 | -3.162520 | -1.073522 | -2.722591 |
| 1 | -4.099967 | -1.290461 | -3.240817 |
| 1 | -2.658714 | -2.013568 | -2.478274 |
| 1 | -2.523364 | -0.475161 | -3.379271 |
| 6 | -3.426008 | -0.334201 | -1.491332 |
| 7 | -3.615514 | 0.266875 | -0.514598 |
| 6 | -2.295814 | 3.663529 | -1.123579 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.479612 | 4.391486 | -1.917542 |
| 1 | -1.743606 | 4.141616 | -0.308240 |
| 1 | -3.250574 | 3.280160 | -0.749831 |
| 6 | -1.510310 | 2.548604 | -1.628683 |
| 7 | -0.884832 | 1.647006 | -2.002146 |
| 6 | 1.115433 | -2.724870 | 0.071685 |
| 6 | 0.607792 | -1.568824 | -0.626665 |
| 7 | 0.197665 | -0.648347 | -1.181063 |
| 1 | 0.750208 | -2.663626 | 1.102078 |
| 1 | 2.207210 | -2.688804 | 0.041361 |
| 1 | 0.725406 | -3.624329 | -0.411658 |
| 1 | -0.202432 | 0.243960 | -1.604009 |

Cartesian coordinates of : PACN8_7

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.600080 | -0.209494 | -3.240392 |
| 1 | -3.926426 | 0.781666 | -2.910946 |
| 1 | -4.187454 | -0.977154 | -2.728164 |
| 1 | -3.722289 | -0.300953 | -4.322201 |
| 6 | -2.208318 | -0.380029 | -2.863640 |
| 7 | -1.109390 | -0.507047 | -2.518911 |
| 6 | 1.135938 | 2.257549 | -2.143802 |
| 1 | 1.475326 | 3.055050 | -2.809469 |
| 1 | 0.066906 | 2.082525 | -2.303564 |
| 1 | 1.691327 | 1.340219 | -2.367165 |
| 6 | 1.363425 | 2.627548 | -0.750462 |
| 7 | 1.545115 | 2.886433 | 0.368522 |
| 6 | 4.988542 | 2.160157 | 0.499110 |
| 1 | 4.285292 | 2.933956 | 0.821119 |
| 1 | 5.614019 | 2.554382 | -0.305757 |
| 1 | 5.628539 | 1.878985 | 1.339157 |
| 6 | 4.238705 | 0.999097 | 0.027313 |
| 7 | 3.623833 | 0.085664 | -0.345858 |
| 6 | 4.150664 | -3.351035 | -0.832442 |
| 1 | 4.495363 | -2.372348 | -1.177155 |
| 1 | 3.923307 | -3.981480 | -1.695631 |
| 1 | 4.937843 | -3.827012 | -0.242523 |
| 6 | 2.954534 | -3.170227 | -0.016549 |
| 7 | 2.003102 | -3.017179 | 0.632129 |
| 6 | -1.489570 | 3.274328 | 1.520924 |
| 1 | -0.842558 | 2.639205 | 2.132811 |
| 1 | -2.394055 | 3.513444 | 2.086951 |
| 1 | -0.953467 | 4.195435 | 1.280611 |
| 6 | -1.843346 | 2.565287 | 0.293598 |
| 7 | -2.134504 | 1.989523 | -0.673773 |
| 6 | -4.349561 | 0.226151 | 1.567461 |
| 1 | -4.288314 | 0.461197 | 0.500730 |
| 1 | -4.880139 | 1.023193 | 2.094891 |
| 1 | -4.894195 | -0.713631 | 1.687448 |
| 6 | -2.995722 | 0.086749 | 2.095126 |
| 7 | -1.910267 | -0.014244 | 2.498238 |
| 6 | -1.477161 | -3.320374 | 1.278485 |
| 1 | -1.442978 | -2.768762 | 2.223588 |
| 1 | -0.461310 | -3.393523 | 0.877552 |
| 1 | -1.863127 | -4.325957 | 1.463862 |
| 6 | -2.346889 | -2.612336 | 0.343262 |
| 7 | -3.036985 | -2.028591 | -0.387648 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 1.336232 | -0.147326 | 2.043732 |
| 6 | 0.702100 | -0.307355 | 0.754616 |
| 7 | 0.194327 | -0.420457 | -0.271489 |
| 1 | 2.201988 | -0.814065 | 2.080694 |
| 1 | 0.606463 | -0.399282 | 2.818679 |
| 1 | 1.646478 | 0.899398 | 2.138465 |
| 1 | -0.300119 | -0.495336 | -1.250476 |

Cartesian coordinates of : PACN8_ 8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.543342 | 3.176293 | -1.100633 |
| 1 | 1.887233 | 4.208705 | -1.203162 |
| 1 | 0.522997 | 3.175283 | -0.704477 |
| 1 | 1.539197 | 2.698301 | -2.085352 |
| 6 | 2.432954 | 2.437090 | -0.209008 |
| 7 | 3.138648 | 1.837030 | 0.493021 |
| 6 | 3.839654 | -0.003064 | 3.279406 |
| 1 | 4.326344 | 0.871795 | 2.838558 |
| 1 | 4.300873 | -0.910235 | 2.878571 |
| 1 | 3.926709 | 0.020462 | 4.368159 |
| 6 | 2.445922 | 0.009602 | 2.875590 |
| 7 | 1.343995 | 0.019652 | 2.516655 |
| 6 | 1.412858 | -3.187483 | -0.997693 |
| 1 | 0.410521 | -3.171874 | -0.558994 |
| 1 | 1.736094 | -4.224573 | -1.118617 |
| 1 | 1.375554 | -2.704556 | -1.979432 |
| 6 | 2.350554 | -2.465653 | -0.141784 |
| 7 | 3.094844 | -1.879645 | 0.531582 |
| 6 | -4.576795 | -3.157672 | -0.654590 |
| 1 | -4.784791 | -3.512644 | -1.666990 |
| 1 | -5.131983 | -2.232626 | -0.472884 |
| 1 | -4.897792 | -3.918819 | 0.060898 |
| 6 | -3.149842 | -2.893461 | -0.498159 |
| 7 | -2.019755 | -2.657885 | -0.365176 |
| 6 | 4.448480 | -0.076555 | -2.011297 |
| 1 | 4.933726 | 0.783620 | -2.479654 |
| 1 | 4.895029 | -0.996009 | -2.398502 |
| 1 | 4.590498 | -0.031356 | -0.927853 |
| 6 | 3.017137 | -0.058871 | -2.295754 |
| 7 | 1.873511 | -0.044516 | -2.505053 |
| 6 | -2.407601 | -0.526835 | 2.579876 |
| 1 | -3.025688 | -0.777435 | 3.445597 |
| 1 | -1.739365 | 0.296973 | 2.847283 |
| 1 | -1.807605 | -1.399674 | 2.301620 |
| 6 | -3.251160 | -0.145443 | 1.449930 |
| 7 | -3.910922 | 0.138480 | 0.536071 |
| 6 | -4.389018 | 3.506145 | -0.100901 |
| 1 | -4.457345 | 4.171588 | 0.763272 |
| 1 | -4.990014 | 2.610897 | 0.081858 |
| 1 | -4.771285 | 4.027634 | -0.981890 |
| 6 | -3.001874 | 3.107817 | -0.317345 |
| 7 | -1.902525 | 2.773545 | -0.488122 |
| 6 | -1.248490 | 0.064631 | -1.958945 |
| 6 | -0.545909 | 0.061298 | -0.695100 |
| 7 | 0.001845 | 0.053675 | 0.317332 |
| 1 | -0.921970 | 0.936311 | -2.532350 |
| 1 | -2.321600 | 0.120174 | -1.748815 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.997524 | -0.853990 | -2.496186 |
| 1 | 0.543431 | 0.042657 | 1.293631 |

Cartesian coordinates of : PACN8_9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.953881 | 4.621449 | -0.479567 |
| 1 | -2.897935 | 5.263898 | 0.402746 |
| 1 | -3.794113 | 4.941866 | -1.100560 |
| 1 | -2.024381 | 4.705617 | -1.048863 |
| 6 | -3.132131 | 3.230621 | -0.074527 |
| 7 | -3.269240 | 2.120580 | 0.240905 |
| 6 | -2.967785 | -4.510096 | -0.960294 |
| 1 | -3.280503 | -4.835548 | -1.955582 |
| 1 | -3.779435 | -3.953190 | -0.484850 |
| 1 | -2.727460 | -5.389542 | -0.357723 |
| 6 | -1.801236 | -3.639522 | -1.062404 |
| 7 | -0.875222 | -2.942535 | -1.144421 |
| 6 | 3.650556 | -0.329328 | 3.692913 |
| 1 | 4.267351 | 0.553676 | 3.510591 |
| 1 | 4.215173 | -1.208599 | 3.374202 |
| 1 | 3.402764 | -0.404144 | 4.754481 |
| 6 | 2.428908 | -0.231908 | 2.906383 |
| 7 | 1.446484 | -0.154897 | 2.297356 |
| 6 | 2.166681 | -2.552614 | -0.263289 |
| 1 | 2.141172 | -3.442642 | -0.896505 |
| 1 | 1.348498 | -2.625452 | 0.458538 |
| 1 | 3.123123 | -2.490092 | 0.264239 |
| 6 | 1.985080 | -1.357093 | -1.080782 |
| 7 | 1.851409 | -0.392264 | -1.715854 |
| 6 | 5.376285 | 0.248185 | -1.816799 |
| 1 | 5.865272 | 1.219512 | -1.928467 |
| 1 | 4.487693 | 0.209738 | -2.455060 |
| 1 | 6.074027 | -0.533864 | -2.126808 |
| 6 | 4.977747 | 0.043279 | -0.426801 |
| 7 | 4.637039 | -0.119464 | 0.672059 |
| 6 | -5.322996 | -0.004509 | 1.937354 |
| 1 | -6.364486 | -0.078708 | 1.614651 |
| 1 | -4.988277 | 1.032053 | 1.847024 |
| 1 | -5.249470 | -0.324689 | 2.979634 |
| 6 | -4.479131 | -0.845125 | 1.094464 |
| 7 | -3.807055 | -1.513820 | 0.422811 |
| 6 | 2.388671 | 2.556595 | -0.532817 |
| 1 | 2.792833 | 3.475988 | -0.101755 |
| 1 | 2.973781 | 2.270892 | -1.411109 |
| 1 | 2.455815 | 1.745073 | 0.198952 |
| 6 | 0.997374 | 2.756253 | -0.926376 |
| 7 | -0.112582 | 2.917424 | -1.228607 |
| 6 | -1.797575 | 0.068173 | -1.742664 |
| 6 | -1.126607 | 0.017338 | -0.466695 |
| 7 | -0.543259 | -0.019269 | 0.524611 |
| 1 | -1.188536 | -0.503598 | -2.450643 |
| 1 | -1.870345 | 1.117139 | -2.043130 |
| 1 | -2.788468 | -0.381093 | -1.630342 |
| 1 | 0.173144 | -0.064775 | 1.315712 |

Cartesian coordinates of : PACN8_10

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Atomic number (AN) and Cartesian coordinates
  AN          X          Y          Z
-----
  6    -3.425908      0.941075      2.785491
  1    -3.787439     -0.085419      2.893400
  1    -3.981889      1.436370      1.983215
  1    -3.552320      1.486164      3.723916
  6    -2.024840      0.890451      2.403146
  7    -0.918532      0.842737      2.059859
  6     5.040638     -2.216562      1.292729
  1     5.324802     -1.288589      0.789383
  1     5.699537     -3.024915      0.966233
  1     5.141759     -2.089021      2.373339
  6     3.656888     -2.532310      0.955021
  7     2.555925     -2.779949      0.680252
  6     4.132162      3.041256     -0.476371
  1     5.189012      3.256156     -0.652434
  1     3.838333      3.428952      0.502004
  1     3.523564      3.533848     -1.238030
  6     3.900012      1.600902     -0.523447
  7     3.727884      0.452496     -0.562486
  6    -0.953692      4.131980      1.202904
  1    -1.933964      3.714699      0.951551
  1    -0.949323      5.203128      0.986376
  1    -0.757088      3.978472      2.267196
  6     0.068453      3.454193      0.410585
  7     0.874422      2.911194     -0.227014
  6    -4.187807     -1.481708     -1.389453
  1    -4.821751     -1.208765     -2.236758
  1    -4.236498     -0.701191     -0.624663
  1    -4.540432     -2.422223     -0.958756
  6    -2.802176     -1.624883     -1.824426
  7    -1.693590     -1.729179     -2.158637
  6    -0.818166     -3.793234      0.596577
  1    -0.910107     -3.896494     -0.489669
  1    -1.039163     -4.754646      1.067215
  1     0.208438     -3.502410      0.842286
  6    -1.759663     -2.778532      1.060684
  7    -2.512052     -1.963621      1.407886
  6    -1.100379      1.624082     -2.726312
  1    -1.450209      2.377361     -3.436884
  1    -1.116143      0.640965     -3.206628
  1    -0.080703      1.874146     -2.415492
  6    -1.967268      1.601037     -1.550893
  7    -2.652471      1.579859     -0.611898
  6     1.468743     -1.499670     -1.936532
  6     0.896047     -0.806569     -0.802620
  7     0.435991     -0.243098      0.087801
  1     1.018198     -1.110798     -2.853446
  1     1.237573     -2.564156     -1.840831
  1     2.550204     -1.339278     -1.915625
  1    -0.035694      0.255524      0.930275
-----

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Cartesian coordinates of : PACN8_11

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-----
Atomic number (AN) and Cartesian coordinates
  AN          X          Y          Z
-----

```

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.116944 | 4.886950 | -0.199328 |
| 1 | -0.711412 | 5.507073 | 0.476406 |
| 1 | -0.759559 | 4.510667 | -0.999441 |
| 1 | 0.682828 | 5.496316 | -0.627590 |
| 6 | 0.451339 | 3.758213 | 0.532401 |
| 7 | 0.910021 | 2.863184 | 1.114565 |
| 6 | -0.633758 | 0.087383 | 1.786521 |
| 1 | -0.909842 | 0.806429 | 1.007892 |
| 1 | -0.709596 | 0.590703 | 2.753857 |
| 1 | -1.320241 | -0.763083 | 1.750105 |
| 6 | 0.735734 | -0.373928 | 1.578051 |
| 7 | 1.820876 | -0.756299 | 1.408156 |
| 6 | -4.663210 | 2.497596 | -0.169273 |
| 1 | -4.745544 | 3.266481 | 0.602964 |
| 1 | -5.007381 | 1.540111 | 0.230142 |
| 1 | -5.283238 | 2.781891 | -1.023153 |
| 6 | -3.272878 | 2.354441 | -0.588308 |
| 7 | -2.166164 | 2.238703 | -0.924485 |
| 6 | -4.386398 | -3.249713 | 0.794442 |
| 1 | -3.484138 | -3.842059 | 0.620573 |
| 1 | -5.176144 | -3.577994 | 0.114146 |
| 1 | -4.722020 | -3.392704 | 1.824618 |
| 6 | -4.076526 | -1.843196 | 0.560292 |
| 7 | -3.823359 | -0.724906 | 0.370786 |
| 6 | 4.121168 | 1.683117 | 1.775251 |
| 1 | 4.303393 | 0.681674 | 2.174794 |
| 1 | 3.325235 | 2.158647 | 2.357388 |
| 1 | 5.032897 | 2.282808 | 1.827539 |
| 6 | 3.655939 | 1.574224 | 0.402592 |
| 7 | 3.242619 | 1.481922 | -0.677264 |
| 6 | 4.194338 | -1.906756 | -0.866279 |
| 1 | 4.734338 | -2.854160 | -0.941744 |
| 1 | 4.069951 | -1.633815 | 0.186592 |
| 1 | 4.768403 | -1.127710 | -1.374738 |
| 6 | 2.873123 | -2.029699 | -1.476040 |
| 7 | 1.814298 | -2.137466 | -1.942255 |
| 6 | 1.252567 | -4.181299 | 0.698753 |
| 1 | 1.971012 | -3.450579 | 1.083662 |
| 1 | 1.635636 | -4.614929 | -0.228482 |
| 1 | 1.108449 | -4.972975 | 1.438249 |
| 6 | -0.014102 | -3.505680 | 0.435629 |
| 7 | -1.025668 | -2.969048 | 0.237518 |
| 6 | -1.270412 | -0.590350 | -2.054943 |
| 6 | -0.093171 | 0.202936 | -1.796989 |
| 7 | 0.866528 | 0.805533 | -1.598190 |
| 1 | -1.886672 | -0.625000 | -1.148189 |
| 1 | -0.934106 | -1.600147 | -2.313478 |
| 1 | -1.841105 | -0.134251 | -2.868324 |
| 1 | 1.843960 | 1.169807 | -1.322234 |

Cartesian coordinates of : PACN8_12

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|----------|
| 6 | 2.186347 | 0.037555 | 3.037500 |
| 1 | 1.375310 | 0.769770 | 3.086628 |
| 1 | 3.054233 | 0.404685 | 3.591460 |
| 1 | 1.829015 | -0.894901 | 3.479004 |
| 6 | 2.543317 | -0.179793 | 1.638303 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 2.848263 | -0.328194 | 0.526390 |
| 6 | -5.439172 | 0.166795 | -1.616873 |
| 1 | -5.357458 | 0.677475 | -0.653103 |
| 1 | -6.095601 | -0.701445 | -1.517699 |
| 1 | -5.868193 | 0.849612 | -2.354529 |
| 6 | -4.106811 | -0.255288 | -2.038011 |
| 7 | -3.039611 | -0.586692 | -2.356603 |
| 6 | -2.512424 | -2.292145 | 0.671068 |
| 1 | -2.831401 | -3.263897 | 1.056266 |
| 1 | -2.156058 | -2.405256 | -0.358159 |
| 1 | -3.359579 | -1.600458 | 0.661557 |
| 6 | -1.450919 | -1.739887 | 1.507311 |
| 7 | -0.593428 | -1.292080 | 2.151294 |
| 6 | 2.103797 | -5.090424 | 0.144322 |
| 1 | 1.671514 | -5.478767 | 1.069800 |
| 1 | 3.178341 | -4.947855 | 0.283200 |
| 1 | 1.937552 | -5.810711 | -0.660446 |
| 6 | 1.480939 | -3.816656 | -0.194540 |
| 7 | 0.990643 | -2.803583 | -0.463227 |
| 6 | -2.009982 | 1.781645 | 3.063413 |
| 1 | -1.581322 | 2.782143 | 2.972519 |
| 1 | -1.210494 | 1.070671 | 3.292035 |
| 1 | -2.754951 | 1.767225 | 3.862882 |
| 6 | -2.626987 | 1.398307 | 1.798449 |
| 7 | -3.126052 | 1.081536 | 0.797403 |
| 6 | 2.775636 | 3.416668 | 0.512198 |
| 1 | 3.494926 | 2.593957 | 0.457348 |
| 1 | 3.058468 | 4.103060 | 1.314237 |
| 1 | 2.780455 | 3.945668 | -0.443824 |
| 6 | 1.445568 | 2.870106 | 0.763887 |
| 7 | 0.392550 | 2.427697 | 0.979846 |
| 6 | 4.206824 | 0.229825 | -2.587322 |
| 1 | 5.137132 | 0.794931 | -2.685776 |
| 1 | 4.065240 | -0.375227 | -3.486402 |
| 1 | 4.264566 | -0.420064 | -1.709897 |
| 6 | 3.081365 | 1.143402 | -2.417860 |
| 7 | 2.183518 | 1.866385 | -2.273655 |
| 6 | -1.064826 | 1.863187 | -1.801310 |
| 6 | -0.470339 | 0.627147 | -1.346441 |
| 7 | 0.014939 | -0.360908 | -1.015754 |
| 1 | -1.543495 | 1.672838 | -2.765789 |
| 1 | -0.267399 | 2.604753 | -1.897114 |
| 1 | -1.810359 | 2.174669 | -1.063465 |
| 1 | 0.439819 | -1.304660 | -0.755156 |

Cartesian coordinates of : PACN8_13

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.540804 | 0.797834 | -2.696625 |
| 1 | -4.048748 | 1.411926 | -1.946187 |
| 1 | -3.937101 | -0.221555 | -2.666457 |
| 1 | -3.685928 | 1.226156 | -3.691275 |
| 6 | -2.127892 | 0.739920 | -2.362089 |
| 7 | -1.010944 | 0.686657 | -2.056757 |
| 6 | 4.391508 | 2.854058 | 0.496367 |
| 1 | 4.955017 | 3.041778 | -0.421014 |
| 1 | 5.015755 | 3.111016 | 1.355779 |
| 1 | 3.490225 | 3.472292 | 0.498429 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 4.001924 | 1.449002 | 0.563687 |
| 7 | 3.694430 | 0.329787 | 0.621189 |
| 6 | 4.948537 | -2.275188 | -1.412800 |
| 1 | 5.276845 | -1.390373 | -0.860860 |
| 1 | 4.994874 | -2.071261 | -2.485395 |
| 1 | 5.608925 | -3.114422 | -1.181036 |
| 6 | 3.579035 | -2.594007 | -1.023755 |
| 7 | 2.490241 | -2.842966 | -0.705280 |
| 6 | -0.865121 | -3.822626 | -0.294324 |
| 1 | 0.150463 | -3.600324 | -0.636964 |
| 1 | -1.127467 | -4.842611 | -0.586614 |
| 1 | -0.900365 | -3.743409 | 0.797495 |
| 6 | -1.815000 | -2.875284 | -0.869807 |
| 7 | -2.573665 | -2.110231 | -1.305533 |
| 6 | -0.794392 | 4.031774 | -1.484717 |
| 1 | -0.724918 | 5.117780 | -1.384482 |
| 1 | -1.793032 | 3.701991 | -1.181596 |
| 1 | -0.621992 | 3.753587 | -2.527631 |
| 6 | 0.197990 | 3.384521 | -0.631614 |
| 7 | 0.981355 | 2.869441 | 0.055454 |
| 6 | -0.964993 | 1.791949 | 2.663816 |
| 1 | -1.294896 | 2.527899 | 3.401503 |
| 1 | 0.044661 | 2.049595 | 2.327274 |
| 1 | -0.967025 | 0.797748 | 3.122046 |
| 6 | -1.866009 | 1.793144 | 1.514271 |
| 7 | -2.577756 | 1.788966 | 0.594997 |
| 6 | -4.277908 | -1.151590 | 1.316280 |
| 1 | -4.673065 | -2.093592 | 0.928205 |
| 1 | -4.236684 | -0.421219 | 0.502895 |
| 1 | -4.929448 | -0.779028 | 2.110600 |
| 6 | -2.927416 | -1.356284 | 1.829707 |
| 7 | -1.846796 | -1.511782 | 2.228751 |
| 6 | 1.462339 | -1.354246 | 2.040410 |
| 6 | 0.890278 | -0.759538 | 0.852197 |
| 7 | 0.404498 | -0.285490 | -0.075699 |
| 1 | 2.229151 | -2.067088 | 1.725042 |
| 1 | 0.657152 | -1.845996 | 2.594780 |
| 1 | 1.927310 | -0.565551 | 2.638449 |
| 1 | -0.091695 | 0.153339 | -0.938882 |

Cartesian coordinates of : PACN8_14

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.355418 | -0.785110 | -2.922666 |
| 1 | -2.781571 | -1.635869 | -3.460489 |
| 1 | -1.272392 | -0.776957 | -3.071629 |
| 1 | -2.768334 | 0.149683 | -3.307978 |
| 6 | -2.647258 | -0.905607 | -1.497189 |
| 7 | -2.891193 | -1.021069 | -0.366054 |
| 6 | 6.445021 | -1.344029 | 0.479641 |
| 1 | 6.624926 | -1.699254 | 1.497282 |
| 1 | 7.097967 | -0.490904 | 0.279716 |
| 1 | 6.682680 | -2.146368 | -0.223151 |
| 6 | 5.047021 | -0.948201 | 0.329152 |
| 7 | 3.935151 | -0.634259 | 0.209204 |
| 6 | -0.353800 | 4.345192 | -1.018848 |
| 1 | -0.355656 | 4.306162 | 0.074664 |
| 1 | -1.064478 | 5.099375 | -1.366148 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 0.654760 | 4.603313 | -1.349715 |
| 6 | -0.717247 | 3.032270 | -1.541755 |
| 7 | -1.025091 | 1.985645 | -1.943313 |
| 6 | -1.349681 | -4.313562 | -0.152529 |
| 1 | -1.657714 | -5.276075 | -0.568253 |
| 1 | -2.235822 | -3.738604 | 0.133514 |
| 1 | -0.734701 | -4.485511 | 0.734736 |
| 6 | -0.590196 | -3.556519 | -1.143865 |
| 7 | 0.005564 | -2.938092 | -1.926460 |
| 6 | -3.241434 | -1.243549 | 3.110043 |
| 1 | -3.484339 | -2.033513 | 3.824800 |
| 1 | -3.928974 | -1.288452 | 2.259316 |
| 1 | -3.327686 | -0.270875 | 3.602985 |
| 6 | -1.888037 | -1.406815 | 2.603075 |
| 7 | -0.820720 | -1.508911 | 2.162939 |
| 6 | 2.192745 | 1.624499 | 2.267592 |
| 1 | 1.165927 | 1.487694 | 2.620116 |
| 1 | 2.721064 | 2.305152 | 2.939945 |
| 1 | 2.710562 | 0.660668 | 2.249158 |
| 6 | 2.161064 | 2.170222 | 0.914557 |
| 7 | 2.121409 | 2.570956 | -0.175914 |
| 6 | -3.599074 | 2.032890 | 0.562002 |
| 1 | -4.044993 | 2.967632 | 0.911354 |
| 1 | -4.250581 | 1.195013 | 0.824100 |
| 1 | -3.494544 | 2.058244 | -0.526718 |
| 6 | -2.280827 | 1.846805 | 1.163008 |
| 7 | -1.227062 | 1.714104 | 1.634908 |
| 6 | 1.716195 | 0.057386 | -2.152742 |
| 6 | 1.063239 | -0.254694 | -0.903401 |
| 7 | 0.541116 | -0.538622 | 0.080068 |
| 1 | 2.741310 | 0.366615 | -1.930164 |
| 1 | 1.170513 | 0.873893 | -2.634460 |
| 1 | 1.700889 | -0.847631 | -2.769200 |
| 1 | 0.043093 | -0.898763 | 0.952120 |

Cartesian coordinates of : PACN8_15

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.217706 | -1.139486 | 2.694574 |
| 1 | 2.574280 | -1.481263 | 3.509323 |
| 1 | 4.211178 | -0.914487 | 3.090664 |
| 1 | 3.291628 | -1.925442 | 1.936990 |
| 6 | 2.639240 | 0.051481 | 2.080310 |
| 7 | 2.184711 | 0.998898 | 1.583753 |
| 6 | -4.397574 | -2.388841 | -0.393652 |
| 1 | -4.843396 | -3.370881 | -0.569489 |
| 1 | -4.900124 | -1.638124 | -1.007697 |
| 1 | -4.522483 | -2.107102 | 0.654493 |
| 6 | -2.976148 | -2.420118 | -0.725370 |
| 7 | -1.845077 | -2.461806 | -0.991361 |
| 6 | 0.989456 | -1.761427 | -2.858106 |
| 1 | -0.061413 | -2.026823 | -2.707335 |
| 1 | 1.424829 | -2.423188 | -3.611282 |
| 1 | 1.069592 | -0.725783 | -3.203709 |
| 6 | 1.704474 | -1.902017 | -1.592612 |
| 7 | 2.276625 | -2.003163 | -0.585543 |
| 6 | 4.216200 | 1.050368 | -0.992904 |
| 1 | 4.425876 | 1.732455 | -0.164499 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 4.966009 | 1.184219 | -1.776541 |
| 1 | 4.251905 | 0.021500 | -0.621736 |
| 6 | 2.882575 | 1.317563 | -1.521451 |
| 7 | 1.822168 | 1.525825 | -1.948231 |
| 6 | 0.422437 | -4.349722 | 1.155625 |
| 1 | 0.146846 | -5.055274 | 1.943070 |
| 1 | 1.470642 | -4.492108 | 0.878194 |
| 1 | -0.205865 | -4.515920 | 0.275105 |
| 6 | 0.229223 | -2.978922 | 1.605467 |
| 7 | 0.084281 | -1.873740 | 1.929194 |
| 6 | -4.107139 | 2.930193 | 1.540251 |
| 1 | -4.219569 | 2.688396 | 2.600045 |
| 1 | -5.012096 | 3.433557 | 1.191024 |
| 1 | -3.245743 | 3.590446 | 1.406745 |
| 6 | -3.887165 | 1.709491 | 0.770880 |
| 7 | -3.706672 | 0.741385 | 0.153283 |
| 6 | 1.548956 | 4.195385 | 0.334744 |
| 1 | 1.601769 | 5.129914 | 0.898885 |
| 1 | 1.930372 | 4.360484 | -0.676349 |
| 1 | 2.150270 | 3.428764 | 0.831784 |
| 6 | 0.166338 | 3.734012 | 0.265202 |
| 7 | -0.937755 | 3.374710 | 0.213918 |
| 6 | -1.418773 | 1.151866 | -2.005352 |
| 6 | -0.868200 | 0.598495 | -0.788580 |
| 7 | -0.432542 | 0.117033 | 0.158591 |
| 1 | -0.589909 | 1.491070 | -2.633214 |
| 1 | -2.062519 | 1.992957 | -1.736454 |
| 1 | -2.006454 | 0.368559 | -2.495435 |
| 1 | -0.135444 | -0.469858 | 0.978022 |

Cartesian coordinates of : PACN8_16

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.294646 | 0.429984 | 0.881802 |
| 1 | 5.112328 | 0.960730 | 0.387522 |
| 1 | 4.130445 | -0.529619 | 0.381755 |
| 1 | 4.566506 | 0.262951 | 1.928329 |
| 6 | 3.070801 | 1.223064 | 0.814089 |
| 7 | 2.099593 | 1.859310 | 0.769696 |
| 6 | -3.692085 | -3.894358 | 0.383527 |
| 1 | -4.126967 | -3.043976 | 0.915476 |
| 1 | -3.320019 | -4.625590 | 1.105353 |
| 1 | -4.457942 | -4.365689 | -0.237428 |
| 6 | -2.596551 | -3.416019 | -0.453493 |
| 7 | -1.726857 | -3.029201 | -1.119551 |
| 6 | 1.268695 | -2.339507 | -2.879491 |
| 1 | 1.749632 | -3.058227 | -3.548006 |
| 1 | 1.218243 | -1.362413 | -3.368145 |
| 1 | 0.259348 | -2.689358 | -2.639926 |
| 6 | 2.040304 | -2.216039 | -1.646946 |
| 7 | 2.656096 | -2.126242 | -0.665413 |
| 6 | 3.324486 | -2.895217 | 2.653160 |
| 1 | 3.785511 | -3.126915 | 1.687489 |
| 1 | 2.962988 | -3.817694 | 3.113942 |
| 1 | 4.059337 | -2.428444 | 3.314139 |
| 6 | 2.213038 | -1.986855 | 2.409638 |
| 7 | 1.339856 | -1.263041 | 2.172844 |
| 6 | -4.680030 | 1.914462 | 1.413109 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.662015 | 2.037184 | 2.498934 |
| 1 | -5.713336 | 1.987602 | 1.064908 |
| 1 | -4.083718 | 2.705106 | 0.949865 |
| 6 | -4.122082 | 0.615092 | 1.049635 |
| 7 | -3.682220 | -0.419750 | 0.756907 |
| 6 | 1.351726 | 3.662511 | -2.041766 |
| 1 | 1.749394 | 3.785657 | -1.029918 |
| 1 | 0.386697 | 4.171135 | -2.116837 |
| 1 | 2.045976 | 4.101088 | -2.762896 |
| 6 | 1.180591 | 2.238363 | -2.312093 |
| 7 | 1.050567 | 1.105109 | -2.530960 |
| 6 | -0.068061 | 4.320755 | 1.600025 |
| 1 | -0.573267 | 4.468661 | 2.557828 |
| 1 | 0.077367 | 5.294764 | 1.124693 |
| 1 | 0.901970 | 3.845516 | 1.768616 |
| 6 | -0.870629 | 3.459608 | 0.736464 |
| 7 | -1.509610 | 2.780625 | 0.042578 |
| 6 | -1.791758 | 0.051789 | -1.832337 |
| 6 | -0.944250 | -0.179460 | -0.683118 |
| 7 | -0.273437 | -0.363863 | 0.231413 |
| 1 | -1.277053 | -0.319412 | -2.722311 |
| 1 | -1.964027 | 1.128891 | -1.910870 |
| 1 | -2.729734 | -0.485492 | -1.673315 |
| 1 | 0.351368 | -0.626115 | 1.054966 |

Cartesian coordinates of : PACN8_17

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.000593 | -3.471109 | 1.575738 |
| 1 | 1.701503 | -3.823716 | 2.336632 |
| 1 | 0.591968 | -4.332750 | 1.041280 |
| 1 | 0.190756 | -2.915928 | 2.056926 |
| 6 | 1.686966 | -2.590461 | 0.635361 |
| 7 | 2.231774 | -1.897350 | -0.122082 |
| 6 | -0.044673 | 1.780372 | 3.485278 |
| 1 | -0.175232 | 2.522098 | 2.691130 |
| 1 | 0.986293 | 1.827536 | 3.841520 |
| 1 | -0.735403 | 2.005717 | 4.301763 |
| 6 | -0.321525 | 0.451698 | 2.948690 |
| 7 | -0.566387 | -0.596921 | 2.511252 |
| 6 | 4.014337 | -0.942443 | -2.906373 |
| 1 | 3.778147 | -1.155897 | -3.951838 |
| 1 | 3.711416 | -1.788391 | -2.282938 |
| 1 | 5.092938 | -0.787232 | -2.814944 |
| 6 | 3.297987 | 0.249230 | -2.462300 |
| 7 | 2.731433 | 1.195327 | -2.097245 |
| 6 | -2.703381 | 2.328373 | -2.660313 |
| 1 | -2.541923 | 2.930185 | -1.760264 |
| 1 | -3.443952 | 2.823719 | -3.293234 |
| 1 | -1.767302 | 2.239472 | -3.219499 |
| 6 | -3.180312 | 1.003992 | -2.270954 |
| 7 | -3.557750 | -0.046571 | -1.950017 |
| 6 | 4.746475 | 0.253259 | 0.716549 |
| 1 | 5.198037 | 0.912760 | -0.029810 |
| 1 | 4.529354 | -0.718626 | 0.263384 |
| 1 | 5.444184 | 0.121611 | 1.547342 |
| 6 | 3.499310 | 0.839766 | 1.195872 |
| 7 | 2.509502 | 1.310894 | 1.580012 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -3.827492 | 0.093323 | 1.485527 |
| 1 | -4.310265 | -0.309251 | 0.589727 |
| 1 | -4.590038 | 0.376555 | 2.215426 |
| 1 | -3.165914 | -0.662462 | 1.920951 |
| 6 | -3.030380 | 1.257886 | 1.113230 |
| 7 | -2.385072 | 2.177613 | 0.814893 |
| 6 | -3.489392 | -3.308957 | -0.979679 |
| 1 | -3.949937 | -3.681863 | -0.061269 |
| 1 | -3.257257 | -4.151981 | -1.635119 |
| 1 | -4.176519 | -2.627372 | -1.490637 |
| 6 | -2.275736 | -2.567601 | -0.668049 |
| 7 | -1.323920 | -1.950613 | -0.432405 |
| 6 | 0.637641 | 2.873392 | -0.543868 |
| 6 | 0.299776 | 1.466596 | -0.506257 |
| 7 | -0.026974 | 0.365580 | -0.470337 |
| 1 | -0.196782 | 3.428852 | -0.103123 |
| 1 | 0.816556 | 3.167793 | -1.581117 |
| 1 | 1.554836 | 3.017146 | 0.033942 |
| 1 | -0.434866 | -0.627594 | -0.405435 |

Cartesian coordinates of : PACN8_18

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.834436 | 1.241851 | 3.260758 |
| 1 | -0.863850 | 2.177342 | 2.695939 |
| 1 | 0.140337 | 1.167174 | 3.750245 |
| 1 | -1.624893 | 1.238971 | 4.015442 |
| 6 | -1.013650 | 0.120558 | 2.342483 |
| 7 | -1.159726 | -0.780793 | 1.622598 |
| 6 | -3.839818 | 3.461488 | -0.441687 |
| 1 | -4.407182 | 3.622527 | 0.478216 |
| 1 | -4.350447 | 2.718105 | -1.061460 |
| 1 | -3.759196 | 4.404470 | -0.987769 |
| 6 | -2.514885 | 2.944323 | -0.131527 |
| 7 | -1.463626 | 2.506704 | 0.097865 |
| 6 | -0.447576 | -4.097917 | 0.781590 |
| 1 | 0.607496 | -4.383914 | 0.766904 |
| 1 | -1.060511 | -4.995669 | 0.895781 |
| 1 | -0.630330 | -3.420114 | 1.621283 |
| 6 | -0.787603 | -3.408900 | -0.458734 |
| 7 | -1.075997 | -2.860255 | -1.441067 |
| 6 | 1.681486 | 3.549163 | -0.343849 |
| 1 | 2.649637 | 4.049556 | -0.427704 |
| 1 | 0.922437 | 4.269873 | -0.030329 |
| 1 | 1.416858 | 3.139422 | -1.323216 |
| 6 | 1.763088 | 2.462736 | 0.628097 |
| 7 | 1.823897 | 1.589418 | 1.392653 |
| 6 | 2.085379 | -1.538848 | 2.666038 |
| 1 | 1.183834 | -1.987351 | 3.093774 |
| 1 | 2.113768 | -0.474590 | 2.917442 |
| 1 | 2.965878 | -2.038030 | 3.078712 |
| 6 | 2.062576 | -1.675567 | 1.212861 |
| 7 | 2.056243 | -1.795170 | 0.057068 |
| 6 | -4.015207 | -2.025910 | -0.196394 |
| 1 | -3.901585 | -2.832890 | -0.924158 |
| 1 | -5.056803 | -1.972567 | 0.130301 |
| 1 | -3.369821 | -2.225704 | 0.664114 |
| 6 | -3.617561 | -0.759644 | -0.803664 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -3.320465 | 0.256295 | -1.282820 |
| 6 | 4.759733 | 0.192057 | -0.337786 |
| 1 | 4.402376 | 0.445510 | 0.665449 |
| 1 | 5.724698 | 0.673473 | -0.514495 |
| 1 | 4.874224 | -0.892356 | -0.410951 |
| 6 | 3.780630 | 0.648626 | -1.318950 |
| 7 | 2.994858 | 1.022712 | -2.088895 |
| 6 | 0.914263 | -1.146879 | -2.999479 |
| 6 | 0.310660 | -0.303384 | -1.993504 |
| 7 | -0.175505 | 0.393463 | -1.220289 |
| 1 | 1.496882 | -0.513875 | -3.674091 |
| 1 | 0.120375 | -1.688117 | -3.520049 |
| 1 | 1.570570 | -1.853354 | -2.481829 |
| 1 | -0.644988 | 1.062979 | -0.574871 |

Cartesian coordinates of : PACN8_19

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.682861 | 1.271344 | 1.763273 |
| 1 | 4.011385 | 1.635086 | 2.740009 |
| 1 | 4.193636 | 1.827965 | 0.973172 |
| 1 | 3.923981 | 0.208187 | 1.664121 |
| 6 | 2.240958 | 1.436779 | 1.624225 |
| 7 | 1.090015 | 1.556551 | 1.516073 |
| 6 | -3.797602 | -2.673935 | 0.402946 |
| 1 | -3.987705 | -1.679583 | 0.817733 |
| 1 | -4.257279 | -3.431719 | 1.042239 |
| 1 | -4.224783 | -2.737145 | -0.601169 |
| 6 | -2.355585 | -2.882192 | 0.332530 |
| 7 | -1.206758 | -3.048255 | 0.279411 |
| 6 | 0.444668 | -1.893255 | 2.753665 |
| 1 | -0.346339 | -1.225207 | 2.394117 |
| 1 | 0.837940 | -1.518265 | 3.702219 |
| 1 | 0.016222 | -2.887806 | 2.898445 |
| 6 | 1.513698 | -1.961174 | 1.762531 |
| 7 | 2.362269 | -1.985669 | 0.968219 |
| 6 | 4.737323 | -1.615305 | -1.417846 |
| 1 | 5.747221 | -1.254823 | -1.205732 |
| 1 | 4.747995 | -2.138504 | -2.377547 |
| 1 | 4.418849 | -2.301233 | -0.627638 |
| 6 | 3.804565 | -0.493302 | -1.466311 |
| 7 | 3.054405 | 0.394548 | -1.490473 |
| 6 | -2.159228 | 2.844120 | 2.155144 |
| 1 | -2.670633 | 3.461831 | 1.412226 |
| 1 | -1.105680 | 3.136255 | 2.186664 |
| 1 | -2.614113 | 2.993093 | 3.137423 |
| 6 | -2.245447 | 1.440598 | 1.766331 |
| 7 | -2.307164 | 0.322589 | 1.452015 |
| 6 | -4.157651 | 1.207781 | -1.365701 |
| 1 | -4.691369 | 0.909142 | -0.458689 |
| 1 | -4.881299 | 1.449238 | -2.148165 |
| 1 | -3.543569 | 2.086584 | -1.148906 |
| 6 | -3.289422 | 0.118984 | -1.803673 |
| 7 | -2.605717 | -0.753882 | -2.150997 |
| 6 | 1.368903 | 3.575204 | -1.496976 |
| 1 | 1.378720 | 4.101360 | -2.454836 |
| 1 | 2.021281 | 2.697561 | -1.559616 |
| 1 | 1.736122 | 4.247812 | -0.717096 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.011933 | 3.144485 | -1.175495 |
| 7 | -1.057639 | 2.777222 | -0.907295 |
| 6 | 0.436165 | -2.075613 | -2.128911 |
| 6 | 0.183989 | -0.988254 | -1.215064 |
| 7 | 0.007658 | -0.112880 | -0.495146 |
| 1 | 1.065828 | -1.710481 | -2.945451 |
| 1 | -0.529389 | -2.427421 | -2.504824 |
| 1 | 0.936774 | -2.870390 | -1.566034 |
| 1 | -0.064052 | 0.639314 | 0.200686 |

Cartesian coordinates of : PACN8_20

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.073747 | -1.027687 | 2.301279 |
| 1 | -2.445208 | -1.252925 | 3.167542 |
| 1 | -4.062973 | -1.469085 | 2.448284 |
| 1 | -3.163850 | 0.057691 | 2.195796 |
| 6 | -2.456422 | -1.566984 | 1.093524 |
| 7 | -1.979240 | -2.006587 | 0.129542 |
| 6 | -1.495777 | 3.157247 | -1.643727 |
| 1 | -0.552694 | 3.641370 | -1.376378 |
| 1 | -2.226007 | 3.919825 | -1.926322 |
| 1 | -1.336826 | 2.483757 | -2.491765 |
| 6 | -1.990468 | 2.384298 | -0.507964 |
| 7 | -2.377132 | 1.751868 | 0.387428 |
| 6 | -0.648291 | 2.322266 | 3.114457 |
| 1 | -0.224934 | 2.554026 | 4.094895 |
| 1 | -1.739853 | 2.355775 | 3.168017 |
| 1 | -0.315150 | 3.065670 | 2.384902 |
| 6 | -0.217411 | 0.997741 | 2.677474 |
| 7 | 0.120830 | -0.057525 | 2.327360 |
| 6 | -4.500917 | -0.440799 | -1.578480 |
| 1 | -4.564841 | -1.509788 | -1.359883 |
| 1 | -5.366163 | -0.138439 | -2.173534 |
| 1 | -4.492305 | 0.118951 | -0.637543 |
| 6 | -3.266838 | -0.162262 | -2.305896 |
| 7 | -2.283090 | 0.073661 | -2.877378 |
| 6 | 3.814110 | 3.415713 | 0.276207 |
| 1 | 4.193478 | 3.488155 | 1.298354 |
| 1 | 3.845804 | 4.401440 | -0.194260 |
| 1 | 4.430500 | 2.714337 | -0.293872 |
| 6 | 2.450707 | 2.906028 | 0.283762 |
| 7 | 1.369328 | 2.483105 | 0.277741 |
| 6 | 4.859229 | -2.026290 | -1.001341 |
| 1 | 5.279367 | -2.235854 | -1.988314 |
| 1 | 4.150062 | -2.812092 | -0.728358 |
| 1 | 5.670555 | -2.001773 | -0.269481 |
| 6 | 4.164413 | -0.742093 | -1.016292 |
| 7 | 3.615989 | 0.282412 | -1.030132 |
| 6 | 0.377759 | -3.476579 | 2.238135 |
| 1 | 0.120192 | -2.567528 | 2.788724 |
| 1 | 0.989875 | -4.127589 | 2.867337 |
| 1 | -0.536295 | -4.004028 | 1.952891 |
| 6 | 1.118567 | -3.101164 | 1.038690 |
| 7 | 1.716231 | -2.813772 | 0.084713 |
| 6 | 0.105529 | -1.901928 | -2.413419 |
| 6 | 0.279377 | -0.766814 | -1.536235 |
| 7 | 0.441233 | 0.147833 | -0.860579 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 1.066264 | -2.415880 | -2.501694 |
| 1 | -0.260912 | -1.541931 | -3.378210 |
| 1 | -0.633111 | -2.564056 | -1.951075 |
| 1 | 0.687041 | 0.988845 | -0.287955 |

Cartesian coordinates of : PACN8_21

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.500152 | -0.516279 | 1.628650 |
| 1 | 5.362331 | -0.225507 | 2.233847 |
| 1 | 4.511853 | 0.041022 | 0.686286 |
| 1 | 4.550658 | -1.586652 | 1.413341 |
| 6 | 3.261398 | -0.217369 | 2.339867 |
| 7 | 2.274316 | 0.034781 | 2.898539 |
| 6 | 3.131498 | -1.091001 | -2.269778 |
| 1 | 3.249218 | -0.008532 | -2.161540 |
| 1 | 2.507730 | -1.298723 | -3.143896 |
| 1 | 4.110346 | -1.558357 | -2.405318 |
| 6 | 2.484040 | -1.614879 | -1.070984 |
| 7 | 1.978481 | -2.041428 | -0.115683 |
| 6 | 0.750722 | 2.198319 | -3.145456 |
| 1 | 0.342137 | 2.429442 | -4.132309 |
| 1 | 1.843168 | 2.197553 | -3.191049 |
| 1 | 0.436308 | 2.961930 | -2.428659 |
| 6 | 0.274974 | 0.893935 | -2.694068 |
| 7 | -0.100233 | -0.145757 | -2.334881 |
| 6 | 1.552404 | 3.123334 | 1.636977 |
| 1 | 2.297232 | 3.869407 | 1.925469 |
| 1 | 1.368039 | 2.456714 | 2.485290 |
| 1 | 0.624175 | 3.628827 | 1.357472 |
| 6 | 2.041132 | 2.335232 | 0.509123 |
| 7 | 2.421372 | 1.690650 | -0.380300 |
| 6 | -0.705864 | -3.346578 | -2.372164 |
| 1 | -1.063813 | -2.670016 | -3.151120 |
| 1 | -0.946035 | -4.380159 | -2.633323 |
| 1 | 0.377778 | -3.233556 | -2.283061 |
| 6 | -1.326791 | -2.996323 | -1.099360 |
| 7 | -1.831634 | -2.737146 | -0.085579 |
| 6 | -3.699402 | 3.493241 | -0.348583 |
| 1 | -4.076923 | 3.551640 | -1.372311 |
| 1 | -3.696874 | 4.491597 | 0.095579 |
| 1 | -4.338886 | 2.828771 | 0.239973 |
| 6 | -2.354384 | 2.936908 | -0.342483 |
| 7 | -1.288423 | 2.476952 | -0.325066 |
| 6 | -4.888484 | -1.880392 | 1.181169 |
| 1 | -5.744084 | -1.858967 | 0.501471 |
| 1 | -5.249520 | -2.052542 | 2.198313 |
| 1 | -4.214361 | -2.689287 | 0.887409 |
| 6 | -4.168396 | -0.611807 | 1.114035 |
| 7 | -3.599275 | 0.400072 | 1.062130 |
| 6 | -0.133543 | -1.924106 | 2.392877 |
| 6 | -0.280756 | -0.781983 | 1.520004 |
| 7 | -0.420545 | 0.138239 | 0.846999 |
| 1 | 0.257744 | -1.578460 | 3.353205 |
| 1 | 0.576062 | -2.609571 | 1.919241 |
| 1 | -1.109672 | -2.405733 | 2.493176 |
| 1 | -0.645229 | 0.983105 | 0.270445 |

Cartesian coordinates of : PACN8_22

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.277242 | -3.845895 | 0.770829 |
| 1 | 2.215627 | -4.347092 | 1.021216 |
| 1 | 1.200893 | -3.726763 | -0.313360 |
| 1 | 0.434313 | -4.446831 | 1.119825 |
| 6 | 1.233463 | -2.528872 | 1.397848 |
| 7 | 1.201389 | -1.478814 | 1.896240 |
| 6 | -3.253906 | 3.047447 | -0.411345 |
| 1 | -2.464598 | 3.418318 | 0.249909 |
| 1 | -4.228351 | 3.374983 | -0.040468 |
| 1 | -3.088983 | 3.443742 | -1.416123 |
| 6 | -3.197124 | 1.589693 | -0.446485 |
| 7 | -3.157744 | 0.427786 | -0.458250 |
| 6 | -4.255331 | -2.832623 | 0.162584 |
| 1 | -4.627019 | -1.808902 | 0.060606 |
| 1 | -4.505434 | -3.215455 | 1.155241 |
| 1 | -4.728648 | -3.467959 | -0.590237 |
| 6 | -2.807767 | -2.825667 | -0.023960 |
| 7 | -1.655776 | -2.796268 | -0.176102 |
| 6 | 4.632074 | -0.913928 | -1.736668 |
| 1 | 4.562092 | -0.027043 | -1.101138 |
| 1 | 5.022115 | -0.627583 | -2.716557 |
| 1 | 5.316463 | -1.633145 | -1.279985 |
| 6 | 3.306706 | -1.509436 | -1.884458 |
| 7 | 2.250629 | -1.978443 | -2.007524 |
| 6 | -1.680650 | -0.127226 | 2.495189 |
| 1 | -2.729459 | 0.097701 | 2.706351 |
| 1 | -1.195118 | -0.526484 | 3.388971 |
| 1 | -1.622785 | -0.875191 | 1.697794 |
| 6 | -0.994118 | 1.083290 | 2.056274 |
| 7 | -0.450923 | 2.042971 | 1.686651 |
| 6 | 1.120063 | 4.111796 | -0.675972 |
| 1 | 0.885834 | 3.980192 | 0.384430 |
| 1 | 0.977813 | 5.157066 | -0.961459 |
| 1 | 2.161769 | 3.828329 | -0.846593 |
| 6 | 0.240823 | 3.252241 | -1.463630 |
| 7 | -0.464489 | 2.567369 | -2.083699 |
| 6 | 2.600359 | 1.421992 | 3.118584 |
| 1 | 1.965264 | 2.267517 | 3.395949 |
| 1 | 3.608441 | 1.569688 | 3.513614 |
| 1 | 2.175891 | 0.498464 | 3.524803 |
| 6 | 2.635612 | 1.299192 | 1.668652 |
| 7 | 2.634622 | 1.182237 | 0.511466 |
| 6 | -1.098533 | -0.814077 | -2.674779 |
| 6 | -0.327032 | -0.401785 | -1.528357 |
| 7 | 0.335393 | -0.047934 | -0.660758 |
| 1 | -2.105143 | -1.081183 | -2.346110 |
| 1 | -0.592982 | -1.672761 | -3.128222 |
| 1 | -1.137484 | 0.035230 | -3.365111 |
| 1 | 1.056498 | 0.315986 | -0.015357 |

Cartesian coordinates of : PACN8_23

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.460640 | 2.794450 | -0.678552 |
| 1 | -3.656470 | 2.546202 | -1.724784 |
| 1 | -4.031715 | 3.684076 | -0.401451 |
| 1 | -3.758438 | 1.952592 | -0.047267 |
| 6 | -2.034121 | 3.040638 | -0.493620 |
| 7 | -0.900037 | 3.248021 | -0.346067 |
| 6 | 1.993369 | 4.628107 | 1.009137 |
| 1 | 2.161215 | 4.684394 | 2.087516 |
| 1 | 0.926085 | 4.738728 | 0.798894 |
| 1 | 2.547400 | 5.433317 | 0.520231 |
| 6 | 2.441165 | 3.335146 | 0.500909 |
| 7 | 2.792354 | 2.306005 | 0.090207 |
| 6 | 1.354701 | -4.019276 | 1.651743 |
| 1 | 2.041106 | -3.946964 | 0.802288 |
| 1 | 0.526144 | -4.677978 | 1.380161 |
| 1 | 1.882442 | -4.414375 | 2.523143 |
| 6 | 0.834934 | -2.689229 | 1.931549 |
| 7 | 0.422904 | -1.621261 | 2.128170 |
| 6 | -2.185236 | -0.358359 | 4.043115 |
| 1 | -1.191133 | -0.794831 | 4.171972 |
| 1 | -2.939802 | -1.078735 | 4.368546 |
| 1 | -2.267449 | 0.543527 | 4.654676 |
| 6 | -2.383982 | -0.027990 | 2.634939 |
| 7 | -2.535174 | 0.233829 | 1.512881 |
| 6 | 0.357706 | -2.363329 | -3.002246 |
| 1 | -0.261334 | -1.567159 | -3.428372 |
| 1 | 0.378509 | -3.207360 | -3.696380 |
| 1 | 1.378677 | -2.003857 | -2.842411 |
| 6 | -0.205733 | -2.777801 | -1.721079 |
| 7 | -0.663691 | -3.094578 | -0.700911 |
| 6 | 4.920051 | -0.175777 | 0.114112 |
| 1 | 5.777232 | -0.852730 | 0.146222 |
| 1 | 4.735508 | 0.235854 | 1.109118 |
| 1 | 5.130667 | 0.655447 | -0.562655 |
| 6 | 3.734632 | -0.892726 | -0.346891 |
| 7 | 2.798380 | -1.475627 | -0.714942 |
| 6 | -3.781312 | -1.572102 | -0.889552 |
| 1 | -4.445604 | -0.976836 | -0.257983 |
| 1 | -3.176342 | -2.225158 | -0.253885 |
| 1 | -4.372747 | -2.178683 | -1.579939 |
| 6 | -2.892664 | -0.688490 | -1.636528 |
| 7 | -2.181349 | 0.008287 | -2.236367 |
| 6 | 0.826677 | 1.295079 | -2.180852 |
| 6 | 0.483905 | 0.678777 | -0.918915 |
| 7 | 0.228754 | 0.151979 | 0.068575 |
| 1 | 1.773824 | 0.863013 | -2.520266 |
| 1 | 0.938768 | 2.369724 | -2.018452 |
| 1 | 0.014170 | 1.099271 | -2.886763 |
| 1 | 0.133594 | -0.420772 | 0.943411 |

Cartesian coordinates of : PACN8_24

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.508318 | -1.638931 | -1.616696 |
| 1 | -5.532213 | -1.367134 | -1.346830 |
| 1 | -4.145048 | -2.415931 | -0.938117 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.507148 | -2.015770 | -2.642788 |
| 6 | -3.635499 | -0.473030 | -1.507347 |
| 7 | -2.936749 | 0.451124 | -1.408062 |
| 6 | 4.093886 | -2.334714 | 0.264682 |
| 1 | 4.168738 | -1.350295 | 0.735841 |
| 1 | 4.520246 | -2.288886 | -0.740664 |
| 1 | 4.641379 | -3.069549 | 0.860084 |
| 6 | 2.685571 | -2.704918 | 0.179619 |
| 7 | 1.563572 | -3.000245 | 0.114520 |
| 6 | 1.838897 | 2.857305 | 2.286983 |
| 1 | 0.758913 | 3.018695 | 2.346936 |
| 1 | 2.255879 | 3.556673 | 1.557276 |
| 1 | 2.294474 | 3.029150 | 3.265196 |
| 6 | 2.084808 | 1.487491 | 1.848868 |
| 7 | 2.274936 | 0.396318 | 1.494639 |
| 6 | 3.899840 | 1.790476 | -1.263105 |
| 1 | 3.133941 | 2.526193 | -1.000517 |
| 1 | 4.555850 | 2.203141 | -2.033547 |
| 1 | 4.491244 | 1.551476 | -0.374528 |
| 6 | 3.245727 | 0.581913 | -1.755501 |
| 7 | 2.730769 | -0.383018 | -2.147300 |
| 6 | -1.854855 | 3.632656 | -1.321492 |
| 1 | -1.865254 | 4.721915 | -1.407619 |
| 1 | -2.541497 | 3.318492 | -0.530380 |
| 1 | -2.189228 | 3.182925 | -2.259013 |
| 6 | -0.508483 | 3.169074 | -1.001758 |
| 7 | 0.561763 | 2.802433 | -0.735522 |
| 6 | -3.762503 | 0.712738 | 1.918179 |
| 1 | -4.332673 | 1.329487 | 1.218283 |
| 1 | -4.094234 | 0.916261 | 2.939323 |
| 1 | -3.926849 | -0.343478 | 1.681098 |
| 6 | -2.340424 | 1.004175 | 1.781634 |
| 7 | -1.204549 | 1.221097 | 1.668314 |
| 6 | -0.286250 | -2.208744 | 2.585776 |
| 1 | 0.224789 | -3.171864 | 2.654498 |
| 1 | -0.723084 | -1.950830 | 3.554160 |
| 1 | 0.448630 | -1.447175 | 2.300113 |
| 6 | -1.332294 | -2.279970 | 1.570370 |
| 7 | -2.163847 | -2.301141 | 0.757987 |
| 6 | -0.120171 | -2.045501 | -2.265430 |
| 6 | -0.021745 | -1.005023 | -1.270236 |
| 7 | 0.022712 | -0.167654 | -0.488160 |
| 1 | -0.810232 | -1.718997 | -3.049041 |
| 1 | -0.484152 | -2.949572 | -1.767130 |
| 1 | 0.880933 | -2.215171 | -2.673501 |
| 1 | -0.032768 | 0.547869 | 0.248682 |

Cartesian coordinates of : PACN8_25

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.068999 | -1.756170 | -2.338619 |
| 1 | 5.159784 | -1.750512 | -2.268857 |
| 1 | 3.786912 | -1.928545 | -3.380777 |
| 1 | 3.669048 | -2.556432 | -1.709439 |
| 6 | 3.533303 | -0.477614 | -1.878460 |
| 7 | 3.109949 | 0.539625 | -1.508338 |
| 6 | -4.302819 | -1.350441 | 0.770151 |
| 1 | -4.799940 | -1.736155 | -0.123974 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.329833 | -0.256991 | 0.758542 |
| 1 | -4.820300 | -1.720689 | 1.658704 |
| 6 | -2.911256 | -1.790245 | 0.780893 |
| 7 | -1.807931 | -2.153847 | 0.791547 |
| 6 | 3.327726 | 0.320170 | 1.830891 |
| 1 | 3.860431 | 0.406757 | 2.781224 |
| 1 | 3.565924 | 1.177128 | 1.194391 |
| 1 | 3.642953 | -0.589116 | 1.311111 |
| 6 | 1.887587 | 0.265642 | 2.063943 |
| 7 | 0.741679 | 0.215521 | 2.251884 |
| 6 | -4.608676 | 1.540753 | -2.021494 |
| 1 | -4.331631 | 2.089743 | -1.117303 |
| 1 | -5.631682 | 1.167187 | -1.925191 |
| 1 | -4.558468 | 2.209824 | -2.884165 |
| 6 | -3.682919 | 0.426200 | -2.195933 |
| 7 | -2.947876 | -0.464376 | -2.321290 |
| 6 | -1.340236 | 2.573378 | 2.803981 |
| 1 | -0.347566 | 2.937230 | 2.525789 |
| 1 | -1.221909 | 1.801916 | 3.568045 |
| 1 | -1.940788 | 3.398265 | 3.195358 |
| 6 | -1.984182 | 2.001374 | 1.626119 |
| 7 | -2.505655 | 1.561581 | 0.685226 |
| 6 | 2.992704 | 3.981476 | -0.755075 |
| 1 | 2.732881 | 4.765598 | -1.470407 |
| 1 | 3.674628 | 3.268481 | -1.228686 |
| 1 | 3.477231 | 4.434555 | 0.113445 |
| 6 | 1.795105 | 3.259430 | -0.347165 |
| 7 | 0.852760 | 2.658077 | -0.036562 |
| 6 | 0.678760 | -3.307729 | 2.394912 |
| 1 | 0.190763 | -2.430127 | 2.827703 |
| 1 | 1.397032 | -3.728831 | 3.102976 |
| 1 | -0.087880 | -4.049692 | 2.160451 |
| 6 | 1.362796 | -2.905525 | 1.170728 |
| 7 | 1.922576 | -2.575582 | 0.206466 |
| 6 | -0.251135 | -2.074785 | -2.055023 |
| 6 | -0.157068 | -0.821152 | -1.339924 |
| 7 | -0.055024 | 0.188881 | -0.804372 |
| 1 | 0.759840 | -2.408449 | -2.305194 |
| 1 | -0.869518 | -1.920365 | -2.942392 |
| 1 | -0.728279 | -2.801537 | -1.391103 |
| 1 | 0.124887 | 1.123008 | -0.361736 |

Cartesian coordinates of : PACN8_26

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|----------|-----------|
| 6 | 3.560561 | 1.605655 | -2.093660 |
| 1 | 3.811325 | 1.957862 | -3.097193 |
| 1 | 4.201131 | 0.757995 | -1.831041 |
| 1 | 3.700158 | 2.415814 | -1.371177 |
| 6 | 2.176447 | 1.165226 | -2.035754 |
| 7 | 1.076170 | 0.807782 | -1.951812 |
| 6 | -0.376951 | 1.894134 | 2.425280 |
| 1 | -0.630078 | 2.737289 | 3.072967 |
| 1 | -0.011371 | 1.065100 | 3.039805 |
| 1 | -1.270075 | 1.574562 | 1.877806 |
| 6 | 0.665321 | 2.282070 | 1.478625 |
| 7 | 1.495265 | 2.578861 | 0.720141 |
| 6 | 4.194533 | 0.481255 | 1.638287 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 4.605432 | -0.137718 | 0.836148 |
| 1 | 4.924920 | 0.570733 | 2.446206 |
| 1 | 3.959886 | 1.477315 | 1.249819 |
| 6 | 2.967713 | -0.133315 | 2.132939 |
| 7 | 1.984213 | -0.612647 | 2.523889 |
| 6 | 1.820598 | -3.934470 | -1.012850 |
| 1 | 2.099026 | -4.586360 | -0.180431 |
| 1 | 2.114995 | -4.416963 | -1.948428 |
| 1 | 0.733708 | -3.794087 | -1.018380 |
| 6 | 2.497863 | -2.645942 | -0.884558 |
| 7 | 3.025245 | -1.615775 | -0.780015 |
| 6 | -0.596002 | 3.703975 | -1.903511 |
| 1 | -0.348198 | 3.407872 | -2.926166 |
| 1 | 0.327219 | 3.823131 | -1.328434 |
| 1 | -1.139328 | 4.651963 | -1.923668 |
| 6 | -1.416189 | 2.668775 | -1.281820 |
| 7 | -2.067858 | 1.842642 | -0.787393 |
| 6 | -5.028661 | 1.005467 | 0.818552 |
| 1 | -4.672009 | 1.640279 | 0.002018 |
| 1 | -5.357069 | 1.636079 | 1.648529 |
| 1 | -5.877144 | 0.407028 | 0.476034 |
| 6 | -3.938866 | 0.135049 | 1.247200 |
| 7 | -3.060869 | -0.555392 | 1.565617 |
| 6 | -3.535014 | -1.430762 | -1.886711 |
| 1 | -4.494000 | -1.622100 | -1.397064 |
| 1 | -3.665865 | -1.510527 | -2.968769 |
| 1 | -3.193686 | -0.420389 | -1.633521 |
| 6 | -2.546076 | -2.402549 | -1.429197 |
| 7 | -1.739981 | -3.154281 | -1.061923 |
| 6 | -0.548271 | -2.275277 | 1.902937 |
| 6 | -0.311229 | -1.313222 | 0.850173 |
| 7 | -0.105055 | -0.577314 | -0.009523 |
| 1 | 0.361800 | -2.868215 | 2.033238 |
| 1 | -1.400771 | -2.894680 | 1.611984 |
| 1 | -0.768368 | -1.735306 | 2.827277 |
| 1 | 0.223764 | 0.029779 | -0.826017 |

 Cartesian coordinates of : PACN8_27

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|----------|-----------|
| 6 | -0.725644 | 3.811139 | 1.982751 |
| 1 | -0.403905 | 4.853849 | 2.043360 |
| 1 | -1.072276 | 3.483509 | 2.966545 |
| 1 | -1.538804 | 3.716862 | 1.257394 |
| 6 | 0.387345 | 2.969529 | 1.554921 |
| 7 | 1.278478 | 2.301253 | 1.222670 |
| 6 | 3.342452 | 2.636195 | -1.475767 |
| 1 | 4.168446 | 1.932719 | -1.614337 |
| 1 | 3.226793 | 2.864045 | -0.412169 |
| 1 | 3.561986 | 3.555895 | -2.023832 |
| 6 | 2.103854 | 2.043188 | -1.969290 |
| 7 | 1.118940 | 1.576684 | -2.370423 |
| 6 | -2.230194 | 1.112609 | -2.999625 |
| 1 | -1.254636 | 1.266464 | -3.469033 |
| 1 | -3.010079 | 1.543187 | -3.632951 |
| 1 | -2.425441 | 0.043305 | -2.871088 |
| 6 | -2.237419 | 1.755820 | -1.690027 |
| 7 | -2.247067 | 2.266520 | -0.646564 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -4.260048 | 1.095533 | 1.640754 |
| 1 | -4.892374 | 0.851750 | 2.497753 |
| 1 | -4.567260 | 0.506813 | 0.770730 |
| 1 | -4.352224 | 2.156651 | 1.394640 |
| 6 | -2.866535 | 0.789884 | 1.928597 |
| 7 | -1.748262 | 0.546949 | 2.123902 |
| 6 | 4.284620 | 0.739874 | 1.694014 |
| 1 | 3.559859 | 1.500018 | 1.997892 |
| 1 | 5.154397 | 1.222723 | 1.239798 |
| 1 | 4.613313 | 0.177647 | 2.571693 |
| 6 | 3.653099 | -0.158161 | 0.731260 |
| 7 | 3.156539 | -0.874920 | -0.037189 |
| 6 | 2.891074 | -4.275520 | 0.927056 |
| 1 | 3.571591 | -3.487294 | 0.593619 |
| 1 | 3.171651 | -5.221333 | 0.456955 |
| 1 | 2.965598 | -4.382145 | 2.012167 |
| 6 | 1.525102 | -3.919358 | 0.554836 |
| 7 | 0.438669 | -3.637466 | 0.254290 |
| 6 | -3.042529 | -3.952717 | 0.212844 |
| 1 | -2.038968 | -4.337095 | 0.413466 |
| 1 | -3.543026 | -4.597321 | -0.514050 |
| 1 | -3.621076 | -3.947061 | 1.139996 |
| 6 | -2.935847 | -2.595839 | -0.316233 |
| 7 | -2.853462 | -1.516123 | -0.739786 |
| 6 | 0.565117 | -1.480484 | -2.052362 |
| 6 | 0.208091 | -0.812312 | -0.821024 |
| 7 | -0.097016 | -0.298761 | 0.159384 |
| 1 | -0.004106 | -2.412618 | -2.107952 |
| 1 | 1.639019 | -1.689150 | -2.020155 |
| 1 | 0.340410 | -0.814857 | -2.889214 |
| 1 | -0.551851 | 0.108205 | 1.018568 |

Cartesian coordinates of : PACN8_28

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.550460 | -0.396031 | 2.748139 |
| 1 | 3.252695 | -0.752575 | 3.737167 |
| 1 | 4.379347 | 0.308411 | 2.850930 |
| 1 | 3.864587 | -1.246337 | 2.134935 |
| 6 | 2.423085 | 0.242531 | 2.084651 |
| 7 | 1.524881 | 0.724845 | 1.531990 |
| 6 | -3.508376 | -2.950349 | 0.105089 |
| 1 | -3.148671 | -3.380341 | 1.043569 |
| 1 | -4.265664 | -3.603948 | -0.334818 |
| 1 | -3.942379 | -1.967481 | 0.308793 |
| 6 | -2.388376 | -2.785917 | -0.814975 |
| 7 | -1.493115 | -2.659704 | -1.545372 |
| 6 | 0.775160 | -4.148288 | 0.351270 |
| 1 | -0.060044 | -3.876034 | 1.002478 |
| 1 | 1.381625 | -4.923284 | 0.826929 |
| 1 | 0.381389 | -4.519759 | -0.597757 |
| 6 | 1.589076 | -2.960791 | 0.111135 |
| 7 | 2.259514 | -2.028226 | -0.070739 |
| 6 | 4.450986 | -0.339130 | -2.139841 |
| 1 | 5.454630 | -0.029677 | -1.837405 |
| 1 | 4.439787 | -0.485006 | -3.222917 |
| 1 | 4.190850 | -1.277819 | -1.643362 |
| 6 | 3.477220 | 0.681641 | -1.762907 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 2.700577 | 1.493061 | -1.464873 |
| 6 | -1.694818 | 0.824014 | 2.551294 |
| 1 | -2.768994 | 0.899385 | 2.740929 |
| 1 | -1.420231 | 1.522787 | 1.753145 |
| 1 | -1.148315 | 1.089413 | 3.460043 |
| 6 | -1.355638 | -0.538638 | 2.150726 |
| 7 | -1.059066 | -1.615171 | 1.829446 |
| 6 | -4.113882 | 2.982321 | -0.054987 |
| 1 | -4.704650 | 3.034214 | 0.863347 |
| 1 | -4.728802 | 3.329417 | -0.889169 |
| 1 | -3.231097 | 3.620769 | 0.038831 |
| 6 | -3.677580 | 1.609685 | -0.291963 |
| 7 | -3.322083 | 0.517691 | -0.472393 |
| 6 | 1.735884 | 4.140155 | 0.142106 |
| 1 | 1.708260 | 5.100873 | 0.662113 |
| 1 | 2.157157 | 4.268854 | -0.857322 |
| 1 | 2.368804 | 3.436207 | 0.688709 |
| 6 | 0.388423 | 3.589564 | 0.040076 |
| 7 | -0.688680 | 3.158077 | -0.029224 |
| 6 | -1.206790 | -0.004465 | -2.961869 |
| 6 | -0.520694 | 0.105964 | -1.692676 |
| 7 | 0.051943 | 0.240086 | -0.708100 |
| 1 | -1.047014 | 0.917098 | -3.528446 |
| 1 | -2.270611 | -0.154986 | -2.758876 |
| 1 | -0.815572 | -0.872147 | -3.498518 |
| 1 | 0.610284 | 0.433753 | 0.169923 |

Cartesian coordinates of : PACN8_29

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.219102 | -2.596815 | 2.565246 |
| 1 | 1.153081 | -2.825325 | 2.650459 |
| 1 | 2.686797 | -2.644521 | 3.551650 |
| 1 | 2.683343 | -3.330685 | 1.900976 |
| 6 | 2.371095 | -1.260812 | 1.998264 |
| 7 | 2.488419 | -0.199323 | 1.539057 |
| 6 | -4.730944 | 0.418235 | -1.651057 |
| 1 | -5.614334 | -0.095498 | -1.262245 |
| 1 | -4.912879 | 0.681998 | -2.696003 |
| 1 | -4.551299 | 1.327737 | -1.070872 |
| 6 | -3.560317 | -0.448522 | -1.546043 |
| 7 | -2.628228 | -1.136374 | -1.448913 |
| 6 | -1.203321 | -4.076523 | -0.871461 |
| 1 | -1.045572 | -5.155694 | -0.803555 |
| 1 | -1.625600 | -3.823485 | -1.846362 |
| 1 | -1.909243 | -3.758156 | -0.099219 |
| 6 | 0.061549 | -3.373553 | -0.682885 |
| 7 | 1.070899 | -2.820963 | -0.520864 |
| 6 | 4.229339 | -1.404464 | -1.136743 |
| 1 | 4.805959 | -1.068280 | -0.270616 |
| 1 | 4.912213 | -1.764085 | -1.910436 |
| 1 | 3.558736 | -2.212845 | -0.831188 |
| 6 | 3.429079 | -0.297105 | -1.649974 |
| 7 | 2.797390 | 0.587808 | -2.059654 |
| 6 | -3.588046 | -0.998377 | 1.976577 |
| 1 | -3.818755 | -0.008866 | 1.569153 |
| 1 | -3.910746 | -1.050071 | 3.019359 |
| 1 | -4.113606 | -1.761603 | 1.395951 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -2.148943 | -1.214624 | 1.883626 |
| 7 | -1.001923 | -1.379925 | 1.804250 |
| 6 | -1.455451 | 3.988667 | 1.758003 |
| 1 | -0.622111 | 3.630576 | 2.367134 |
| 1 | -2.223225 | 4.427185 | 2.400207 |
| 1 | -1.071533 | 4.743357 | 1.067867 |
| 6 | -2.016769 | 2.876255 | 0.997854 |
| 7 | -2.478287 | 1.993108 | 0.398550 |
| 6 | 3.637089 | 2.850217 | 0.266592 |
| 1 | 4.050628 | 3.666767 | 0.863750 |
| 1 | 4.118278 | 2.833366 | -0.714506 |
| 1 | 3.811398 | 1.896010 | 0.771713 |
| 6 | 2.199608 | 3.032882 | 0.098116 |
| 7 | 1.054815 | 3.185652 | -0.033355 |
| 6 | -0.282068 | 1.621503 | -2.390077 |
| 6 | -0.055009 | 0.764177 | -1.251041 |
| 7 | 0.104963 | 0.067165 | -0.355539 |
| 1 | -0.836821 | 2.498825 | -2.045235 |
| 1 | -0.853862 | 1.064090 | -3.137807 |
| 1 | 0.693715 | 1.917895 | -2.786515 |
| 1 | 0.143142 | -0.555564 | 0.461646 |

Cartesian coordinates of : PACN8_30

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.477958 | -2.050666 | -0.016104 |
| 1 | -4.481817 | -1.135809 | 0.585391 |
| 1 | -5.109865 | -2.803827 | 0.460929 |
| 1 | -4.867537 | -1.825077 | -1.012028 |
| 6 | -3.106257 | -2.536113 | -0.125580 |
| 7 | -2.007567 | -2.907203 | -0.199781 |
| 6 | 3.891863 | 0.253677 | 2.150648 |
| 1 | 4.408737 | 0.346136 | 1.189866 |
| 1 | 4.014171 | -0.761509 | 2.537886 |
| 1 | 4.312447 | 0.968719 | 2.861933 |
| 6 | 2.478055 | 0.525996 | 1.932794 |
| 7 | 1.353849 | 0.738023 | 1.734605 |
| 6 | -3.807521 | 2.156346 | -0.741345 |
| 1 | -3.282097 | 3.071162 | -1.027127 |
| 1 | -3.703564 | 1.999505 | 0.336785 |
| 1 | -4.865281 | 2.251295 | -0.999726 |
| 6 | -3.220875 | 1.016505 | -1.438834 |
| 7 | -2.769454 | 0.100041 | -1.991866 |
| 6 | -1.054900 | 3.218678 | 2.140808 |
| 1 | -0.810138 | 4.250727 | 2.403588 |
| 1 | -0.495560 | 2.530140 | 2.780612 |
| 1 | -2.122635 | 3.041025 | 2.294227 |
| 6 | -0.704738 | 2.954955 | 0.749075 |
| 7 | -0.419726 | 2.738278 | -0.357004 |
| 6 | 4.591606 | -2.263620 | -0.810364 |
| 1 | 4.675643 | -3.024729 | -1.590183 |
| 1 | 5.371766 | -2.441730 | -0.065170 |
| 1 | 4.726448 | -1.272411 | -1.252946 |
| 6 | 3.274551 | -2.327376 | -0.182466 |
| 7 | 2.228792 | -2.363408 | 0.323307 |
| 6 | -0.722649 | -1.739170 | 2.584415 |
| 1 | -0.000241 | -2.016892 | 1.808426 |
| 1 | -1.335061 | -2.614764 | 2.814179 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.185114 | -1.420680 | 3.481340 |
| 6 | -1.572696 | -0.651811 | 2.106180 |
| 7 | -2.238613 | 0.212722 | 1.704332 |
| 6 | 2.342023 | 3.068239 | -2.385504 |
| 1 | 2.968606 | 3.899996 | -2.053652 |
| 1 | 1.299299 | 3.278163 | -2.132217 |
| 1 | 2.444542 | 2.957979 | -3.468009 |
| 6 | 2.759222 | 1.838070 | -1.718376 |
| 7 | 3.094866 | 0.857128 | -1.192216 |
| 6 | -0.269075 | -1.935186 | -2.509190 |
| 6 | -0.070055 | -1.009278 | -1.418230 |
| 7 | 0.131221 | -0.266292 | -0.567185 |
| 1 | -0.091569 | -2.945244 | -2.128511 |
| 1 | 0.426054 | -1.689322 | -3.316663 |
| 1 | -1.305705 | -1.838418 | -2.844844 |
| 1 | 0.411310 | 0.315072 | 0.249002 |

Cartesian coordinates of : PACN8_31

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.332943 | 1.451510 | -0.580285 |
| 1 | -5.797333 | 2.279035 | -1.122313 |
| 1 | -5.870869 | 1.295533 | 0.358169 |
| 1 | -5.389827 | 0.541848 | -1.184301 |
| 6 | -3.931077 | 1.754148 | -0.308423 |
| 7 | -2.812735 | 1.990468 | -0.100132 |
| 6 | 1.235107 | -1.486371 | 3.912276 |
| 1 | 1.447021 | -2.373629 | 4.513783 |
| 1 | 0.738008 | -0.726070 | 4.519131 |
| 1 | 2.167864 | -1.070572 | 3.517784 |
| 6 | 0.384746 | -1.828444 | 2.783419 |
| 7 | -0.270965 | -2.082808 | 1.858196 |
| 6 | 3.399267 | 2.100734 | 1.065301 |
| 1 | 3.658577 | 3.120813 | 1.359960 |
| 1 | 4.301152 | 1.570248 | 0.748892 |
| 1 | 2.965580 | 1.562525 | 1.912381 |
| 6 | 2.427140 | 2.124125 | -0.023678 |
| 7 | 1.646767 | 2.154393 | -0.884751 |
| 6 | 4.036117 | 0.367309 | -2.605329 |
| 1 | 4.766903 | -0.017918 | -3.320609 |
| 1 | 4.390291 | 0.177194 | -1.586919 |
| 1 | 3.918596 | 1.444451 | -2.749635 |
| 6 | 2.748831 | -0.294459 | -2.791047 |
| 7 | 1.725445 | -0.828183 | -2.924590 |
| 6 | -3.422419 | -3.438612 | 0.123135 |
| 1 | -3.316966 | -4.325687 | -0.506357 |
| 1 | -4.363822 | -3.506466 | 0.674016 |
| 1 | -2.593425 | -3.399236 | 0.835996 |
| 6 | -3.414237 | -2.235551 | -0.705881 |
| 7 | -3.395715 | -1.276557 | -1.361601 |
| 6 | 2.003063 | -3.232604 | -0.540622 |
| 1 | 1.523435 | -2.971193 | -1.488960 |
| 1 | 1.276921 | -3.718760 | 0.117278 |
| 1 | 2.829056 | -3.921278 | -0.735713 |
| 6 | 2.499254 | -2.015728 | 0.096537 |
| 7 | 2.868967 | -1.038909 | 0.607222 |
| 6 | -0.584303 | 3.550149 | 1.634395 |
| 1 | -0.440336 | 3.648998 | 0.554791 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.011810 | 4.322165 | 2.155250 |
| 1 | -1.647591 | 3.669107 | 1.852655 |
| 6 | -0.134539 | 2.227515 | 2.057802 |
| 7 | 0.255945 | 1.184881 | 2.391316 |
| 6 | -0.940766 | 1.023939 | -2.443867 |
| 6 | -0.654352 | 0.244965 | -1.263580 |
| 7 | -0.456279 | -0.402592 | -0.335524 |
| 1 | -1.949593 | 0.757200 | -2.775266 |
| 1 | -0.193271 | 0.779535 | -3.203510 |
| 1 | -0.886637 | 2.082106 | -2.176557 |
| 1 | -0.365268 | -1.000538 | 0.518190 |

Cartesian coordinates of : PACN8_32

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.422616 | -3.438555 | 0.123211 |
| 1 | -4.364147 | -3.506422 | 0.673874 |
| 1 | -2.593790 | -3.399131 | 0.836264 |
| 1 | -3.316989 | -4.325649 | -0.506225 |
| 6 | -3.414279 | -2.235525 | -0.705847 |
| 7 | -3.395641 | -1.276558 | -1.361604 |
| 6 | 2.002683 | -3.232625 | -0.540418 |
| 1 | 2.828638 | -3.921237 | -0.735892 |
| 1 | 1.522718 | -2.971121 | -1.488561 |
| 1 | 1.276797 | -3.718897 | 0.117676 |
| 6 | 2.499054 | -2.015805 | 0.096711 |
| 7 | 2.868910 | -1.039027 | 0.607371 |
| 6 | -5.332864 | 1.451624 | -0.580391 |
| 1 | -5.870846 | 1.295983 | 0.358087 |
| 1 | -5.389756 | 0.541771 | -1.184117 |
| 1 | -5.797183 | 2.278994 | -1.122715 |
| 6 | -3.930994 | 1.754274 | -0.308562 |
| 7 | -2.812646 | 1.990593 | -0.100301 |
| 6 | 4.036279 | 0.366896 | -2.605234 |
| 1 | 3.918853 | 1.444042 | -2.749591 |
| 1 | 4.767062 | -0.018421 | -3.320468 |
| 1 | 4.390396 | 0.176797 | -1.586801 |
| 6 | 2.748946 | -0.294774 | -2.790976 |
| 7 | 1.725522 | -0.828422 | -2.924534 |
| 6 | -0.584146 | 3.550335 | 1.634106 |
| 1 | -0.011649 | 4.322359 | 2.154946 |
| 1 | -1.647441 | 3.669353 | 1.852298 |
| 1 | -0.440109 | 3.649113 | 0.554506 |
| 6 | -0.134460 | 2.227710 | 2.057623 |
| 7 | 0.255965 | 1.185082 | 2.391225 |
| 6 | 1.234882 | -1.486162 | 3.912429 |
| 1 | 0.737870 | -0.725708 | 4.519166 |
| 1 | 2.167728 | -1.070558 | 3.517941 |
| 1 | 1.446622 | -2.373381 | 4.514055 |
| 6 | 0.384524 | -1.828233 | 2.783569 |
| 7 | -0.271182 | -2.082596 | 1.858343 |
| 6 | 3.399362 | 2.100591 | 1.065250 |
| 1 | 3.658750 | 3.120672 | 1.359834 |
| 1 | 4.301212 | 1.569991 | 0.748933 |
| 1 | 2.965577 | 1.562495 | 1.912353 |
| 6 | 2.427290 | 2.123973 | -0.023779 |
| 7 | 1.646961 | 2.154232 | -0.884891 |
| 6 | -0.940605 | 1.023908 | -2.443923 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.654270 | 0.244966 | -1.263597 |
| 7 | -0.456272 | -0.402571 | -0.335510 |
| 1 | -1.949361 | 0.757063 | -2.775457 |
| 1 | -0.192982 | 0.779584 | -3.203465 |
| 1 | -0.886634 | 2.082083 | -2.176607 |
| 1 | -0.365359 | -1.000486 | 0.518241 |

Cartesian coordinates of : PACN8_33

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.830959 | -1.284667 | -3.427274 |
| 1 | -1.434690 | -2.302212 | -3.471626 |
| 1 | -1.012225 | -0.570527 | -3.560388 |
| 1 | -2.564974 | -1.147239 | -4.225178 |
| 6 | -2.450973 | -1.052510 | -2.126285 |
| 7 | -2.932769 | -0.858033 | -1.086789 |
| 6 | 4.130762 | -0.893189 | 2.519311 |
| 1 | 4.965074 | -1.571301 | 2.322776 |
| 1 | 4.185994 | -0.560438 | 3.558872 |
| 1 | 4.200510 | -0.032237 | 1.849337 |
| 6 | 2.864307 | -1.578055 | 2.276210 |
| 7 | 1.855052 | -2.119920 | 2.079084 |
| 6 | 1.262034 | -4.451939 | -0.326879 |
| 1 | 0.496996 | -5.215085 | -0.488949 |
| 1 | 1.515389 | -4.403837 | 0.736386 |
| 1 | 2.155490 | -4.705625 | -0.902634 |
| 6 | 0.760335 | -3.145176 | -0.729116 |
| 7 | 0.358590 | -2.097432 | -1.028532 |
| 6 | -5.294702 | -0.851772 | 1.418864 |
| 1 | -5.106453 | -1.233386 | 0.411777 |
| 1 | -6.172525 | -0.200996 | 1.405672 |
| 1 | -5.482585 | -1.687691 | 2.097241 |
| 6 | -4.123245 | -0.103220 | 1.860655 |
| 7 | -3.186306 | 0.492153 | 2.202255 |
| 6 | 2.469461 | -0.048643 | -2.896804 |
| 1 | 3.373743 | -0.500349 | -3.312128 |
| 1 | 2.256930 | 0.893386 | -3.408531 |
| 1 | 1.617284 | -0.717897 | -3.045896 |
| 6 | 2.637927 | 0.193569 | -1.466739 |
| 7 | 2.779050 | 0.385207 | -0.329016 |
| 6 | 2.410061 | 3.691360 | -0.968849 |
| 1 | 1.993758 | 3.257194 | -1.883600 |
| 1 | 3.400286 | 3.265932 | -0.787788 |
| 1 | 2.493561 | 4.774579 | -1.086386 |
| 6 | 1.527944 | 3.371871 | 0.148456 |
| 7 | 0.813621 | 3.116043 | 1.027796 |
| 6 | -2.154692 | 2.487148 | -0.615052 |
| 1 | -2.795262 | 3.164431 | -1.185537 |
| 1 | -1.709099 | 3.030125 | 0.224573 |
| 1 | -2.753492 | 1.655340 | -0.230296 |
| 6 | -1.092570 | 1.959013 | -1.464932 |
| 7 | -0.238724 | 1.515582 | -2.118332 |
| 6 | -0.328527 | 1.129263 | 3.061667 |
| 6 | -0.290084 | 0.459340 | 1.781183 |
| 7 | -0.233289 | -0.099637 | 0.779438 |
| 1 | -0.762904 | 0.446094 | 3.795916 |
| 1 | -0.955963 | 2.018606 | 2.968585 |
| 1 | 0.690590 | 1.421880 | 3.327327 |

1 -0.084474 -0.710853 -0.057344

Cartesian coordinates of : PACN8_34

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.736168 | 2.788604 | 2.451890 |
| 1 | 2.518996 | 2.935675 | 3.200365 |
| 1 | 0.865219 | 2.311413 | 2.910356 |
| 1 | 1.431926 | 3.758270 | 2.050551 |
| 6 | 2.230150 | 1.938697 | 1.371941 |
| 7 | 2.628634 | 1.246053 | 0.527520 |
| 6 | 2.128983 | -1.459532 | 2.980718 |
| 1 | 2.936390 | -1.003064 | 2.399262 |
| 1 | 2.080149 | -2.523961 | 2.734648 |
| 1 | 2.337619 | -1.343213 | 4.047222 |
| 6 | 0.865494 | -0.811798 | 2.637466 |
| 7 | -0.135113 | -0.285076 | 2.369119 |
| 6 | 3.885760 | -1.732697 | -0.872348 |
| 1 | 4.064608 | -0.700879 | -0.555247 |
| 1 | 3.976908 | -1.793382 | -1.959679 |
| 1 | 4.619025 | -2.397924 | -0.408959 |
| 6 | 2.536865 | -2.121405 | -0.472065 |
| 7 | 1.472569 | -2.444766 | -0.134104 |
| 6 | 3.650495 | 2.222966 | -2.487562 |
| 1 | 4.176673 | 2.496758 | -3.405251 |
| 1 | 4.374887 | 1.962612 | -1.711118 |
| 1 | 3.063436 | 3.076126 | -2.138572 |
| 6 | 2.768847 | 1.085768 | -2.731993 |
| 7 | 2.075404 | 0.173886 | -2.922573 |
| 6 | -3.243112 | 3.884150 | 0.850705 |
| 1 | -3.675473 | 3.813862 | 1.851714 |
| 1 | -3.924376 | 3.429704 | 0.125414 |
| 1 | -3.083387 | 4.934638 | 0.595967 |
| 6 | -1.982906 | 3.156983 | 0.798691 |
| 7 | -0.986535 | 2.565237 | 0.741657 |
| 6 | -1.188328 | -3.566099 | 1.905155 |
| 1 | -0.121705 | -3.640166 | 1.673340 |
| 1 | -1.602134 | -4.567985 | 2.044300 |
| 1 | -1.324039 | -2.984395 | 2.820392 |
| 6 | -1.860717 | -2.898325 | 0.795827 |
| 7 | -2.402099 | -2.383440 | -0.093750 |
| 6 | -5.231421 | -0.917226 | -1.300647 |
| 1 | -4.728464 | -1.856277 | -1.055529 |
| 1 | -5.623700 | -0.963068 | -2.319749 |
| 1 | -6.063232 | -0.762900 | -0.608686 |
| 6 | -4.274984 | 0.179816 | -1.180595 |
| 7 | -3.516890 | 1.055673 | -1.085701 |
| 6 | -0.642331 | -1.524319 | -2.486784 |
| 6 | -0.510758 | -0.511085 | -1.463839 |
| 7 | -0.421848 | 0.317793 | -0.674538 |
| 1 | -1.694066 | -1.574318 | -2.782736 |
| 1 | -0.334954 | -2.482457 | -2.059590 |
| 1 | 0.006120 | -1.251174 | -3.323366 |
| 1 | -0.484511 | 1.121603 | 0.002187 |

Cartesian coordinates of : PACN8_35

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.662725 | 1.286756 | 2.931407 |
| 1 | 2.714031 | 1.232265 | 4.021609 |
| 1 | 1.996175 | 2.100280 | 2.632341 |
| 1 | 3.660584 | 1.481506 | 2.530841 |
| 6 | 2.145798 | 0.033615 | 2.390376 |
| 7 | 1.722037 | -0.957766 | 1.955638 |
| 6 | 2.274080 | -3.872915 | 0.139407 |
| 1 | 2.121445 | -3.454940 | 1.138505 |
| 1 | 3.233409 | -4.394917 | 0.100361 |
| 1 | 1.466187 | -4.573987 | -0.084796 |
| 6 | 2.257684 | -2.783862 | -0.831370 |
| 7 | 2.248340 | -1.916229 | -1.605125 |
| 6 | 4.248163 | 0.908670 | -1.747089 |
| 1 | 3.973641 | -0.099819 | -2.068574 |
| 1 | 5.158121 | 0.860981 | -1.143657 |
| 1 | 4.437371 | 1.533856 | -2.623340 |
| 6 | 3.155843 | 1.473221 | -0.959089 |
| 7 | 2.285679 | 1.925909 | -0.334941 |
| 6 | -0.045395 | 4.255794 | -1.125088 |
| 1 | -0.670166 | 5.149979 | -1.055767 |
| 1 | 0.780602 | 4.449841 | -1.813863 |
| 1 | 0.374915 | 4.013046 | -0.145001 |
| 6 | -0.836485 | 3.125669 | -1.606296 |
| 7 | -1.468910 | 2.223188 | -1.976145 |
| 6 | -1.298457 | -2.088131 | 2.382313 |
| 1 | -1.263256 | -0.997894 | 2.281346 |
| 1 | -0.482324 | -2.406056 | 3.035071 |
| 1 | -2.259156 | -2.377257 | 2.816151 |
| 6 | -1.147222 | -2.694909 | 1.063775 |
| 7 | -1.045547 | -3.156067 | 0.001191 |
| 6 | -4.198367 | -2.048152 | -1.293285 |
| 1 | -5.176178 | -2.351972 | -0.911137 |
| 1 | -3.526365 | -2.912334 | -1.281764 |
| 1 | -4.318699 | -1.690594 | -2.319531 |
| 6 | -3.637683 | -0.991619 | -0.454583 |
| 7 | -3.172719 | -0.164908 | 0.216826 |
| 6 | -3.010321 | 2.763791 | 1.563622 |
| 1 | -3.704853 | 2.114878 | 2.102316 |
| 1 | -3.300206 | 2.778733 | 0.508464 |
| 1 | -3.045470 | 3.773501 | 1.980093 |
| 6 | -1.661764 | 2.222187 | 1.663296 |
| 7 | -0.583574 | 1.791906 | 1.718985 |
| 6 | -0.649457 | -1.082778 | -2.589626 |
| 6 | -0.266169 | -0.462658 | -1.343729 |
| 7 | 0.007614 | 0.050429 | -0.355801 |
| 1 | -1.463018 | -0.487607 | -3.018385 |
| 1 | -0.964830 | -2.109276 | -2.373560 |
| 1 | 0.217577 | -1.098792 | -3.255452 |
| 1 | 0.132185 | 0.623278 | 0.499076 |

Cartesian coordinates of : PACN8_36

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|----------|
| 6 | 2.927830 | -2.813902 | 2.696052 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.616241 | -2.838455 | 1.846135 |
| 1 | 2.664182 | -3.834060 | 2.985479 |
| 1 | 3.404445 | -2.309447 | 3.540040 |
| 6 | 1.737620 | -2.084145 | 2.283974 |
| 7 | 0.799112 | -1.498310 | 1.933487 |
| 6 | -2.485194 | 3.130731 | 1.243592 |
| 1 | -2.716746 | 3.824978 | 2.055288 |
| 1 | -3.246145 | 2.345994 | 1.197346 |
| 1 | -2.485705 | 3.660235 | 0.288231 |
| 6 | -1.179065 | 2.517683 | 1.467096 |
| 7 | -0.146565 | 2.024369 | 1.672817 |
| 6 | -4.403840 | -0.053325 | -1.844057 |
| 1 | -4.281113 | -0.632457 | -2.762589 |
| 1 | -5.345204 | 0.500526 | -1.882344 |
| 1 | -4.410917 | -0.735363 | -0.988995 |
| 6 | -3.282955 | 0.868521 | -1.695091 |
| 7 | -2.393243 | 1.605781 | -1.569839 |
| 6 | -1.792865 | -3.510760 | -0.452860 |
| 1 | -1.554679 | -4.528357 | -0.771932 |
| 1 | -2.780019 | -3.493137 | 0.015602 |
| 1 | -1.057315 | -3.175318 | 0.285617 |
| 6 | -1.775369 | -2.607046 | -1.599263 |
| 7 | -1.745779 | -1.882458 | -2.506881 |
| 6 | -1.853587 | -0.430940 | 3.563741 |
| 1 | -1.603256 | -1.401599 | 3.999258 |
| 1 | -2.646918 | 0.032795 | 4.155729 |
| 1 | -0.964343 | 0.205690 | 3.576104 |
| 6 | -2.294784 | -0.607998 | 2.182785 |
| 7 | -2.640166 | -0.741857 | 1.080924 |
| 6 | 2.896294 | 3.483003 | 1.102981 |
| 1 | 2.161311 | 3.165082 | 1.847314 |
| 1 | 2.756121 | 4.545038 | 0.886470 |
| 1 | 3.905638 | 3.330887 | 1.493423 |
| 6 | 2.709901 | 2.699321 | -0.114286 |
| 7 | 2.565168 | 2.076081 | -1.083992 |
| 6 | 4.502802 | -0.412219 | -2.460554 |
| 1 | 5.579423 | -0.455373 | -2.277131 |
| 1 | 4.195860 | 0.633625 | -2.551725 |
| 1 | 4.284681 | -0.943805 | -3.390605 |
| 6 | 3.782675 | -1.029101 | -1.349336 |
| 7 | 3.209644 | -1.519121 | -0.465251 |
| 6 | 0.279765 | 0.746415 | -2.810889 |
| 6 | 0.247851 | 0.249064 | -1.454380 |
| 7 | 0.242496 | -0.176721 | -0.388332 |
| 1 | 1.285158 | 0.587841 | -3.211052 |
| 1 | 0.048094 | 1.814120 | -2.791869 |
| 1 | -0.475359 | 0.202001 | -3.386287 |
| 1 | 0.329416 | -0.587602 | 0.574937 |

Cartesian coordinates of : PACN8_37

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.379076 | -1.069069 | -0.919329 |
| 1 | -5.184370 | -1.663323 | -1.358028 |
| 1 | -4.671406 | -0.016566 | -0.897399 |
| 1 | -4.193715 | -1.398900 | 0.107447 |
| 6 | -3.155203 | -1.226317 | -1.699929 |
| 7 | -2.174882 | -1.363961 | -2.308580 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -2.249356 | 0.517272 | 3.462005 |
| 1 | -2.230871 | -0.571463 | 3.566136 |
| 1 | -3.063175 | 0.933382 | 4.060903 |
| 1 | -1.294913 | 0.937178 | 3.793597 |
| 6 | -2.432313 | 0.849008 | 2.056449 |
| 7 | -2.545832 | 1.100284 | 0.925846 |
| 6 | 2.240097 | 3.473491 | 0.792398 |
| 1 | 2.206191 | 3.333287 | -0.291132 |
| 1 | 3.253859 | 3.266214 | 1.143563 |
| 1 | 1.970937 | 4.502654 | 1.043156 |
| 6 | 1.304028 | 2.545815 | 1.418998 |
| 7 | 0.557337 | 1.809183 | 1.920434 |
| 6 | -1.005349 | -3.998761 | -0.438368 |
| 1 | -1.900543 | -4.576642 | -0.682063 |
| 1 | -0.229393 | -4.664503 | -0.053033 |
| 1 | -0.637141 | -3.512140 | -1.346691 |
| 6 | -1.323415 | -2.977597 | 0.555283 |
| 7 | -1.570507 | -2.150905 | 1.334838 |
| 6 | 5.220021 | -1.086041 | -0.676799 |
| 1 | 5.740889 | -0.914651 | -1.622121 |
| 1 | 4.807595 | -2.099595 | -0.668170 |
| 1 | 5.934296 | -0.981875 | 0.143774 |
| 6 | 4.131370 | -0.125251 | -0.520457 |
| 7 | 3.245246 | 0.616721 | -0.396249 |
| 6 | 1.723468 | -1.384791 | 2.260214 |
| 1 | 0.656421 | -1.232632 | 2.455946 |
| 1 | 2.202183 | -0.405010 | 2.171495 |
| 1 | 2.168080 | -1.943687 | 3.087518 |
| 6 | 1.886002 | -2.116000 | 1.008113 |
| 7 | 2.008566 | -2.665350 | -0.009707 |
| 6 | -2.154335 | 3.938233 | -1.320789 |
| 1 | -1.962138 | 4.943210 | -0.936900 |
| 1 | -2.700645 | 3.361431 | -0.569336 |
| 1 | -2.758012 | 4.016509 | -2.228459 |
| 6 | -0.891869 | 3.267931 | -1.621113 |
| 7 | 0.110499 | 2.730918 | -1.860968 |
| 6 | 1.125797 | -0.537226 | -2.549802 |
| 6 | 0.414953 | -0.202169 | -1.341381 |
| 7 | -0.183755 | 0.057493 | -0.397414 |
| 1 | 0.381297 | -0.842000 | -3.292916 |
| 1 | 1.814635 | -1.359581 | -2.330719 |
| 1 | 1.670454 | 0.353638 | -2.877548 |
| 1 | -0.836147 | 0.383222 | 0.330616 |

Cartesian coordinates of : PACN8_38

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 13.974475 | 9.777218 | 8.370072 |
| 1 | 14.880005 | 10.384629 | 8.442075 |
| 1 | 13.559661 | 9.846416 | 7.361470 |
| 1 | 14.210478 | 8.731043 | 8.587952 |
| 6 | 12.982301 | 10.234629 | 9.333045 |
| 7 | 12.187422 | 10.583912 | 10.104776 |
| 6 | 9.703942 | 8.505749 | 15.375116 |
| 1 | 9.314366 | 9.409855 | 14.898914 |
| 1 | 10.199869 | 8.762971 | 16.314419 |
| 1 | 8.871450 | 7.825462 | 15.570167 |
| 6 | 10.649888 | 7.862753 | 14.469138 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 11.406593 | 7.348441 | 13.752063 |
| 6 | 14.375052 | 6.622304 | 12.846313 |
| 1 | 13.857444 | 5.862397 | 13.435972 |
| 1 | 14.306005 | 7.570267 | 13.384631 |
| 1 | 15.423362 | 6.342888 | 12.715442 |
| 6 | 13.727090 | 6.751804 | 11.544846 |
| 7 | 13.226922 | 6.848736 | 10.499629 |
| 6 | 12.075153 | 5.521600 | 7.576721 |
| 1 | 12.738527 | 5.327320 | 8.424266 |
| 1 | 12.623486 | 5.365769 | 6.644159 |
| 1 | 11.229890 | 4.828447 | 7.605325 |
| 6 | 11.598430 | 6.899998 | 7.655061 |
| 7 | 11.224505 | 7.998691 | 7.719774 |
| 6 | 11.115143 | 13.047760 | 12.372287 |
| 1 | 10.480334 | 13.907387 | 12.143750 |
| 1 | 11.808393 | 12.878458 | 11.544017 |
| 1 | 11.682934 | 13.257183 | 13.282192 |
| 6 | 10.293855 | 11.855212 | 12.558530 |
| 7 | 9.641693 | 10.903700 | 12.700923 |
| 6 | 6.495694 | 9.509667 | 11.835189 |
| 1 | 7.082675 | 10.430354 | 11.893784 |
| 1 | 5.549519 | 9.645690 | 12.364952 |
| 1 | 6.296131 | 9.269048 | 10.787773 |
| 6 | 7.257783 | 8.422659 | 12.439299 |
| 7 | 7.871783 | 7.559874 | 12.917856 |
| 6 | 8.035132 | 8.768476 | 6.647395 |
| 1 | 7.635691 | 8.049272 | 5.927983 |
| 1 | 9.087321 | 8.961948 | 6.421836 |
| 1 | 7.468394 | 9.699561 | 6.568536 |
| 6 | 7.930797 | 8.231608 | 8.000983 |
| 7 | 7.854261 | 7.805263 | 9.079104 |
| 6 | 9.833200 | 6.071123 | 11.081185 |
| 6 | 10.172716 | 7.471000 | 10.989620 |
| 7 | 10.470437 | 8.575131 | 10.894331 |
| 1 | 10.577187 | 5.507746 | 10.508114 |
| 1 | 8.826246 | 5.936912 | 10.675565 |
| 1 | 9.859657 | 5.785155 | 12.136604 |
| 1 | 10.902717 | 9.508043 | 10.755488 |

Cartesian coordinates of : PACN8_39

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.788499 | -0.801226 | -0.002553 |
| 6 | -4.333191 | -0.919933 | -0.000375 |
| 7 | -3.175376 | -1.014376 | 0.001376 |
| 1 | -6.255151 | -1.788613 | 0.003963 |
| 1 | -6.130239 | -0.267219 | -0.891837 |
| 1 | -6.131871 | -0.254764 | 0.878497 |
| 6 | -0.404837 | -2.434303 | 0.005635 |
| 6 | -0.203198 | -1.003868 | 0.005320 |
| 7 | -0.022556 | 0.132066 | 0.005165 |
| 1 | -0.980236 | -2.718860 | -0.878264 |
| 1 | -0.981605 | -2.718331 | 0.888810 |
| 1 | 0.572126 | -2.923546 | 0.006474 |
| 6 | 5.398900 | -1.979197 | -0.002681 |
| 6 | 3.948088 | -1.814030 | -0.000120 |
| 7 | 2.793816 | -1.682930 | 0.001871 |
| 1 | 5.665431 | -3.037034 | 0.049308 |

| | | | |
|---|------------|-----------|-----------|
| 1 | 5.846441 | -1.471542 | 0.854507 |
| 1 | 5.832910 | -1.561799 | -0.913834 |
| 1 | 0.144580 | 1.200557 | 0.004922 |
| 6 | 0.785926 | 5.327914 | 0.003762 |
| 1 | 1.360544 | 5.624672 | 0.883840 |
| 1 | -0.166947 | 5.861441 | 0.015952 |
| 1 | 1.339405 | 5.627391 | -0.888854 |
| 6 | 0.562580 | 3.888950 | 0.004213 |
| 7 | 0.385009 | 2.745170 | 0.004551 |
| 6 | -1.200849 | -8.094582 | 0.006080 |
| 6 | -1.012226 | -6.645771 | 0.006297 |
| 7 | -0.862144 | -5.494559 | 0.006409 |
| 1 | -1.216306 | -8.469362 | -1.020298 |
| 1 | -2.146801 | -8.348558 | 0.490639 |
| 1 | -0.384183 | -8.577984 | 0.547842 |
| 6 | 11.113625 | -2.814828 | -0.008568 |
| 1 | 11.442042 | -3.117272 | 0.988844 |
| 1 | 11.356462 | -3.609882 | -0.717848 |
| 1 | 11.648408 | -1.906735 | -0.297577 |
| 6 | 9.673426 | -2.568251 | -0.007514 |
| 7 | 8.529050 | -2.372333 | -0.006642 |
| 6 | -11.550112 | -0.403291 | -0.008633 |
| 1 | -11.935359 | -0.576669 | 0.999181 |
| 1 | -11.868162 | 0.586885 | -0.344117 |
| 1 | -11.967117 | -1.156316 | -0.681844 |
| 6 | -10.091320 | -0.486312 | -0.007538 |
| 7 | -8.932171 | -0.552293 | -0.006623 |
| 6 | 1.658724 | 10.975882 | -0.000211 |
| 1 | 1.040221 | 11.447860 | -0.767552 |
| 1 | 1.396358 | 11.394963 | 0.974292 |
| 1 | 2.709304 | 11.192782 | -0.208445 |
| 6 | 1.437570 | 9.531796 | 0.001127 |
| 7 | 1.261814 | 8.384147 | 0.002170 |

Cartesian coordinates of : PACN8_40

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.732965 | -4.528900 | -3.448329 |
| 6 | 1.597261 | -3.335987 | -2.615465 |
| 7 | 1.489576 | -2.387525 | -1.955079 |
| 1 | 2.728918 | -4.960931 | -3.323492 |
| 1 | 1.589223 | -4.269126 | -4.500010 |
| 1 | 0.985534 | -5.272859 | -3.161961 |
| 6 | 2.507954 | 0.000150 | -0.096810 |
| 6 | 1.065853 | -0.000564 | -0.088902 |
| 7 | -0.083623 | -0.001090 | -0.072735 |
| 1 | 2.853965 | 0.000519 | -1.132051 |
| 1 | 2.854853 | -0.899537 | 0.416744 |
| 1 | 2.853920 | 0.900003 | 0.417088 |
| 6 | 1.220421 | 4.194429 | 3.864608 |
| 6 | 1.277947 | 3.154899 | 2.839198 |
| 7 | 1.323810 | 2.328494 | 2.025315 |
| 1 | 2.189790 | 4.692063 | 3.947528 |
| 1 | 0.965858 | 3.752932 | 4.831272 |
| 1 | 0.462369 | 4.936996 | 3.603630 |
| 1 | -1.139867 | -0.001512 | -0.065582 |
| 6 | -5.412715 | -0.002498 | -0.108535 |
| 1 | -5.811162 | -0.110899 | 0.902470 |

| | | | |
|---|------------|-----------|-----------|
| 1 | -5.785138 | -0.829284 | -0.717133 |
| 1 | -5.788487 | 0.932489 | -0.529538 |
| 6 | -3.955422 | -0.002233 | -0.085743 |
| 7 | -2.797388 | -0.002011 | -0.068248 |
| 6 | 8.316287 | 0.006887 | -0.123287 |
| 6 | 6.854859 | 0.003948 | -0.130670 |
| 7 | 5.693858 | 0.001669 | -0.136353 |
| 1 | 8.695944 | 0.097944 | -1.143956 |
| 1 | 8.690642 | -0.923042 | 0.311768 |
| 1 | 8.686225 | 0.848026 | 0.468171 |
| 6 | 1.726115 | 4.529958 | -3.446679 |
| 1 | 0.975894 | 5.271459 | -3.161234 |
| 1 | 2.720503 | 4.965075 | -3.320096 |
| 1 | 1.584861 | 4.270120 | -4.498681 |
| 6 | 1.592831 | 3.336320 | -2.614462 |
| 7 | 1.487073 | 2.387284 | -1.954590 |
| 6 | 1.227303 | -4.198101 | 3.861964 |
| 1 | 0.972131 | -3.758255 | 4.829220 |
| 1 | 0.470709 | -4.941933 | 3.600355 |
| 1 | 2.197727 | -4.693821 | 3.944006 |
| 6 | 1.282359 | -3.157264 | 2.837744 |
| 7 | 1.326253 | -2.329817 | 2.024810 |
| 6 | -11.146472 | 0.001785 | -0.246307 |
| 1 | -11.537081 | 0.840681 | 0.334910 |
| 1 | -11.488883 | 0.096429 | -1.279716 |
| 1 | -11.534306 | -0.930369 | 0.171786 |
| 6 | -9.686141 | 0.000024 | -0.201881 |
| 7 | -8.525640 | -0.001328 | -0.166572 |

Cartesian coordinates of : PACN8_41

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.733799 | 0.166568 | -0.659583 |
| 6 | -4.277047 | 0.251367 | -0.594025 |
| 7 | -3.118664 | 0.320406 | -0.543188 |
| 1 | -6.050599 | -0.317707 | -1.585813 |
| 1 | -6.179366 | 1.163183 | -0.625786 |
| 1 | -6.125979 | -0.411845 | 0.179685 |
| 6 | -0.205298 | 0.285819 | -1.654610 |
| 6 | -0.113772 | 0.336653 | -0.216468 |
| 7 | -0.033579 | 0.370932 | 0.929184 |
| 1 | -0.822160 | 1.124713 | -1.983403 |
| 1 | -0.672003 | -0.665874 | -1.920596 |
| 1 | 0.810276 | 0.367147 | -2.050263 |
| 6 | 5.543591 | -0.413870 | -0.756179 |
| 6 | 4.101701 | -0.180532 | -0.734543 |
| 7 | 2.955091 | 0.004763 | -0.717962 |
| 1 | 5.956969 | -0.180946 | -1.739916 |
| 1 | 5.768485 | -1.458536 | -0.530336 |
| 1 | 6.048389 | 0.211912 | -0.017061 |
| 1 | 0.034496 | 0.408577 | 1.977098 |
| 6 | 0.256526 | 0.639412 | 6.266563 |
| 1 | 0.682736 | -0.281649 | 6.671522 |
| 1 | -0.746359 | 0.781529 | 6.676516 |
| 1 | 0.885768 | 1.484128 | 6.557291 |
| 6 | 0.187092 | 0.553597 | 4.812441 |
| 7 | 0.131630 | 0.485919 | 3.658306 |
| 6 | 11.245818 | -1.342798 | -1.041763 |

| | | | |
|---|------------|-----------|-----------|
| 6 | 9.813213 | -1.081868 | -0.920583 |
| 7 | 8.674873 | -0.874596 | -0.824326 |
| 1 | 11.740289 | -0.497811 | -1.527204 |
| 1 | 11.412988 | -2.242098 | -1.639654 |
| 1 | 11.684571 | -1.488968 | -0.051670 |
| 6 | 2.211839 | 5.346426 | -1.327892 |
| 1 | 3.086093 | 5.399556 | -0.674489 |
| 1 | 2.543816 | 5.389440 | -2.368139 |
| 1 | 1.565626 | 6.204422 | -1.126874 |
| 6 | 1.481994 | 4.103815 | -1.087288 |
| 7 | 0.900114 | 3.117759 | -0.896429 |
| 6 | -1.617154 | -5.211921 | -0.196142 |
| 1 | -0.754745 | -5.839260 | 0.042284 |
| 1 | -2.369078 | -5.328993 | 0.588095 |
| 1 | -2.042717 | -5.542343 | -1.146885 |
| 6 | -1.206685 | -3.812890 | -0.291901 |
| 7 | -0.879189 | -2.701868 | -0.368358 |
| 6 | -11.492364 | -0.062373 | -1.130964 |
| 1 | -11.837650 | 0.917387 | -1.470093 |
| 1 | -11.779627 | -0.814419 | -1.869928 |
| 1 | -11.974958 | -0.298189 | -0.179311 |
| 6 | -10.040495 | -0.051630 | -0.966451 |
| 7 | -8.886879 | -0.043031 | -0.835619 |

Cartesian coordinates of : PACN8_42

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.514799 | -5.567507 | 0.007456 |
| 6 | -1.796372 | -4.134274 | 0.006428 |
| 7 | -2.019601 | -2.994992 | 0.005650 |
| 1 | -0.436480 | -5.735327 | -0.048846 |
| 1 | -1.993523 | -6.042723 | -0.852249 |
| 1 | -1.897609 | -6.022491 | 0.924270 |
| 6 | -1.062557 | -0.014384 | 0.004517 |
| 6 | -2.507045 | -0.026809 | 0.003115 |
| 7 | -3.657501 | -0.020223 | 0.001900 |
| 1 | -0.691621 | -0.541062 | -0.877703 |
| 1 | -0.693318 | -0.538625 | 0.888902 |
| 1 | -0.718279 | 1.022398 | 0.003489 |
| 6 | -2.135218 | 5.691009 | 0.007820 |
| 6 | -2.207134 | 4.232104 | 0.006104 |
| 7 | -2.263734 | 3.072499 | 0.004756 |
| 1 | -1.092493 | 6.012463 | 0.067249 |
| 1 | -2.679230 | 6.090873 | 0.867035 |
| 1 | -2.577045 | 6.087882 | -0.909444 |
| 1 | -4.742670 | -0.019527 | 0.000694 |
| 6 | -8.908468 | -0.037742 | -0.004887 |
| 1 | -9.293515 | 0.395744 | 0.920670 |
| 1 | -9.283340 | -1.059932 | -0.090950 |
| 1 | -9.291909 | 0.543850 | -0.846048 |
| 6 | -7.452472 | -0.029155 | -0.002844 |
| 7 | -6.295013 | -0.022576 | -0.001216 |
| 6 | 4.599650 | -0.043676 | 0.005026 |
| 6 | 3.139400 | -0.061409 | 0.006116 |
| 7 | 1.977607 | -0.075641 | 0.006768 |
| 1 | 4.987181 | -0.146048 | -1.010843 |
| 1 | 4.997293 | -0.864659 | 0.605433 |
| 1 | 4.975675 | 0.893913 | 0.419974 |

| | | | |
|---|------------|-----------|-----------|
| 6 | 10.348124 | 0.018407 | -0.000270 |
| 1 | 10.733398 | 0.141494 | 1.014256 |
| 1 | 10.745955 | -0.914212 | -0.406211 |
| 1 | 10.721862 | 0.843615 | -0.610357 |
| 6 | 8.887478 | -0.001372 | 0.001551 |
| 7 | 7.725898 | -0.017118 | 0.002969 |
| 6 | -14.617459 | -0.089075 | -0.010935 |
| 1 | -14.990405 | -0.216296 | 1.008304 |
| 1 | -15.001846 | 0.850795 | -0.414676 |
| 1 | -14.980838 | -0.914951 | -0.627385 |
| 6 | -13.156657 | -0.071870 | -0.009729 |
| 7 | -11.995689 | -0.058231 | -0.008736 |
| 6 | 16.145345 | 0.096501 | -0.013810 |
| 1 | 16.528340 | -0.338955 | 0.912403 |
| 1 | 16.525002 | -0.480982 | -0.860308 |
| 1 | 16.504942 | 1.125077 | -0.096896 |
| 6 | 14.684285 | 0.076172 | -0.009473 |
| 7 | 13.523441 | 0.060019 | -0.006075 |

 Cartesian coordinates of : PACN8_43

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.344088 | -0.251339 | -0.311848 |
| 6 | 2.890011 | -0.250402 | -0.170351 |
| 7 | 1.733809 | -0.249726 | -0.058997 |
| 1 | 4.783499 | 0.602050 | 0.209194 |
| 1 | 4.628431 | -0.191481 | -1.364700 |
| 1 | 4.773138 | -1.164719 | 0.105792 |
| 6 | -1.123118 | 1.107678 | 0.076331 |
| 6 | -1.296437 | -0.317895 | -0.049950 |
| 7 | -1.444793 | -1.453610 | -0.146509 |
| 1 | -0.495528 | 1.459431 | -0.744763 |
| 1 | -0.637433 | 1.310278 | 1.033637 |
| 1 | -2.107285 | 1.579424 | 0.028255 |
| 6 | -6.751026 | 0.488592 | 1.527325 |
| 6 | -5.406269 | 0.354838 | 0.971376 |
| 7 | -4.337713 | 0.248588 | 0.530422 |
| 1 | -7.063272 | 1.535536 | 1.503080 |
| 1 | -6.763904 | 0.139691 | 2.562827 |
| 1 | -7.458849 | -0.105537 | 0.944102 |
| 1 | -1.573865 | -2.488332 | -0.238123 |
| 6 | -2.060995 | -6.758731 | -0.696431 |
| 1 | -2.458234 | -7.193268 | 0.224095 |
| 1 | -1.093530 | -7.214840 | -0.920011 |
| 1 | -2.752252 | -6.964193 | -1.517380 |
| 6 | -1.901662 | -5.318079 | -0.534074 |
| 7 | -1.775057 | -4.174625 | -0.405590 |
| 6 | -0.430706 | 6.847311 | 0.570440 |
| 6 | -0.634211 | 5.407452 | 0.424898 |
| 7 | -0.796052 | 4.263594 | 0.309451 |
| 1 | -0.007961 | 7.260698 | -0.348573 |
| 1 | 0.255989 | 7.046910 | 1.396752 |
| 1 | -1.383593 | 7.341506 | 0.775287 |
| 6 | -3.370054 | 1.192380 | -5.088158 |
| 1 | -4.300215 | 0.636607 | -5.229695 |
| 1 | -3.595742 | 2.261401 | -5.067884 |
| 1 | -2.703017 | 0.987312 | -5.929097 |
| 6 | -2.733201 | 0.792284 | -3.835464 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -2.225601 | 0.474545 | -2.841166 |
| 6 | 0.908602 | -0.847910 | 5.154776 |
| 1 | 0.276012 | -1.303451 | 5.920603 |
| 1 | 1.759086 | -1.505747 | 4.959687 |
| 1 | 1.280109 | 0.109948 | 5.527206 |
| 6 | 0.141663 | -0.643609 | 3.927896 |
| 7 | -0.469412 | -0.481182 | 2.954450 |
| 6 | 10.095530 | -0.226517 | -0.991851 |
| 1 | 10.349317 | 0.502464 | -1.765381 |
| 1 | 10.606620 | 0.047405 | -0.065612 |
| 1 | 10.441023 | -1.213701 | -1.308495 |
| 6 | 8.650105 | -0.246982 | -0.778553 |
| 7 | 7.501610 | -0.263274 | -0.609058 |

Cartesian coordinates of : PACN8_44

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.773524 | 4.506343 | -3.443017 |
| 6 | 1.094183 | 3.331759 | -2.635235 |
| 7 | 1.348573 | 2.397772 | -1.994678 |
| 1 | -0.256726 | 4.818755 | -3.255546 |
| 1 | 0.884629 | 4.271860 | -4.504546 |
| 1 | 1.445498 | 5.330072 | -3.189956 |
| 6 | 0.389807 | -0.000210 | -0.131462 |
| 6 | 1.830917 | -0.000140 | -0.168041 |
| 7 | 2.980182 | -0.000107 | -0.189683 |
| 1 | 0.010145 | -0.000501 | -1.154883 |
| 1 | 0.057589 | 0.899006 | 0.392388 |
| 1 | 0.057696 | -0.899199 | 0.392844 |
| 6 | 1.574970 | -4.113671 | 3.863230 |
| 6 | 1.614831 | -3.091224 | 2.819984 |
| 7 | 1.646464 | -2.278490 | 1.991744 |
| 1 | 0.542082 | -4.418905 | 4.048083 |
| 1 | 1.998403 | -3.719385 | 4.790266 |
| 1 | 2.152609 | -4.988068 | 3.553539 |
| 1 | 4.026991 | -0.000175 | -0.216978 |
| 6 | 8.342134 | -0.001493 | -0.428097 |
| 1 | 8.767893 | 0.226747 | 0.552017 |
| 1 | 8.672428 | 0.752296 | -1.146934 |
| 1 | 8.693977 | -0.983997 | -0.751980 |
| 6 | 6.885928 | -0.000923 | -0.346558 |
| 7 | 5.730125 | -0.000493 | -0.282459 |
| 6 | -5.376295 | -0.000989 | -0.023476 |
| 6 | -3.916099 | -0.001085 | -0.074930 |
| 7 | -2.755072 | -0.001106 | -0.115578 |
| 1 | -5.798187 | 0.095593 | -1.026246 |
| 1 | -5.741403 | 0.831453 | 0.582001 |
| 1 | -5.747465 | -0.929952 | 0.414835 |
| 6 | 0.773984 | -4.506604 | -3.443112 |
| 1 | 1.444809 | -5.330936 | -3.188968 |
| 1 | -0.256831 | -4.818006 | -3.257074 |
| 1 | 0.886838 | -4.272379 | -4.504513 |
| 6 | 1.094601 | -3.332210 | -2.635037 |
| 7 | 1.348956 | -2.398377 | -1.994243 |
| 6 | 1.573909 | 4.118368 | 3.858418 |
| 1 | 1.995937 | 3.725467 | 4.786682 |
| 1 | 2.152628 | 4.991708 | 3.547765 |
| 1 | 0.541060 | 4.424802 | 4.041505 |

| | | | |
|---|------------|-----------|-----------|
| 6 | 1.614132 | 3.093938 | 2.817132 |
| 7 | 1.646056 | 2.279625 | 1.990456 |
| 6 | -11.170688 | 0.000002 | 0.181636 |
| 1 | -11.572443 | -0.667394 | -0.584746 |
| 1 | -11.510545 | -0.341641 | 1.162428 |
| 1 | -11.550901 | 1.009493 | 0.006886 |
| 6 | -9.710371 | -0.000525 | 0.130029 |
| 7 | -8.550072 | -0.000928 | 0.089063 |

Cartesian coordinates of : PACN8_45

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|------------|-----------|-----------|
| 6 | 5.339253 | -1.968344 | 0.000259 |
| 6 | 3.880034 | -1.918495 | -0.000440 |
| 7 | 2.719001 | -1.879785 | -0.000994 |
| 1 | 5.758299 | -0.961618 | 0.061320 |
| 1 | 5.709185 | -2.438336 | -0.913523 |
| 1 | 5.704804 | -2.543661 | 0.853551 |
| 6 | -0.029152 | -0.418883 | -0.000738 |
| 6 | -0.237870 | -1.847202 | -0.000967 |
| 7 | -0.424413 | -2.982130 | -0.001182 |
| 1 | 0.549141 | -0.135861 | -0.883354 |
| 1 | 0.547124 | -0.135823 | 0.883189 |
| 1 | -1.002862 | 0.076978 | -0.001771 |
| 6 | -5.808392 | -0.744367 | 0.000232 |
| 6 | -4.369466 | -0.992325 | -0.000242 |
| 7 | -3.224680 | -1.190068 | -0.000668 |
| 1 | -6.013878 | 0.325264 | 0.080920 |
| 1 | -6.286523 | -1.248837 | 0.842627 |
| 1 | -6.263233 | -1.111354 | -0.922364 |
| 1 | -0.595178 | -4.034066 | -0.001397 |
| 6 | -1.269461 | -8.215939 | -0.002642 |
| 1 | -1.573274 | -8.540583 | 0.995573 |
| 1 | -0.352101 | -8.737231 | -0.286918 |
| 1 | -2.059069 | -8.461728 | -0.716939 |
| 6 | -1.037333 | -6.776965 | -0.002188 |
| 7 | -0.852949 | -5.634701 | -0.001791 |
| 6 | 0.847035 | 5.184837 | -0.001315 |
| 6 | 0.634097 | 3.739888 | -0.000473 |
| 7 | 0.464552 | 2.590660 | 0.000092 |
| 1 | 0.856537 | 5.572474 | -1.022330 |
| 1 | 1.801081 | 5.434289 | 0.468104 |
| 1 | 0.052087 | 5.691945 | 0.549787 |
| 6 | -11.482512 | 0.323402 | 0.003346 |
| 1 | -11.800394 | 0.624193 | 1.004663 |
| 1 | -11.692008 | 1.137776 | -0.694554 |
| 1 | -12.052656 | -0.558256 | -0.299578 |
| 6 | -10.053342 | 0.019380 | 0.002600 |
| 7 | -8.917729 | -0.222211 | 0.002021 |
| 6 | 11.109293 | -2.181981 | 0.003684 |
| 1 | 11.487141 | -2.001060 | 1.012972 |
| 1 | 11.459390 | -3.159918 | -0.335766 |
| 1 | 11.503070 | -1.412892 | -0.665340 |
| 6 | 9.648598 | -2.145660 | 0.002566 |
| 7 | 8.487933 | -2.116821 | 0.001713 |
| 6 | 1.691183 | 10.911404 | -0.000151 |
| 1 | 0.875269 | 11.408143 | -0.530906 |
| 1 | 1.724382 | 11.283684 | 1.026727 |

| | | | |
|---|----------|-----------|-----------|
| 1 | 2.634874 | 11.153075 | -0.495336 |
| 6 | 1.481587 | 9.465327 | -0.001403 |
| 7 | 1.315068 | 8.316333 | -0.002351 |

Cartesian coordinates of : PACN8_46

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|------------|-----------|-----------|
| 6 | -3.597491 | 0.127915 | 0.000130 |
| 6 | -2.137754 | 0.146039 | 0.000387 |
| 7 | -0.976007 | 0.160972 | 0.000643 |
| 1 | -3.970950 | -0.896647 | -0.058455 |
| 1 | -3.991147 | 0.683180 | -0.853861 |
| 1 | -3.990135 | 0.581906 | 0.912447 |
| 6 | 1.882587 | -1.041369 | 0.000064 |
| 6 | 1.960144 | 0.400327 | 0.000174 |
| 7 | 2.042986 | 1.547365 | 0.000261 |
| 1 | 1.332039 | -1.373211 | -0.883319 |
| 1 | 1.332595 | -1.373385 | 0.883726 |
| 1 | 2.897829 | -1.445267 | -0.000302 |
| 6 | 7.615064 | -0.117950 | -0.001585 |
| 6 | 6.156527 | -0.049710 | -0.001386 |
| 7 | 4.996060 | 0.004916 | -0.001257 |
| 1 | 7.951485 | -1.152832 | 0.091400 |
| 1 | 8.028066 | 0.451888 | 0.833557 |
| 1 | 8.020170 | 0.291067 | -0.929675 |
| 1 | 2.109027 | 2.612584 | 0.000332 |
| 6 | 2.323573 | 6.836129 | 0.000484 |
| 1 | 2.666209 | 7.188735 | 0.976400 |
| 1 | 1.334222 | 7.251974 | -0.205407 |
| 1 | 3.022482 | 7.171948 | -0.769498 |
| 6 | 2.254369 | 5.380262 | 0.000431 |
| 7 | 2.199150 | 4.224588 | 0.000420 |
| 6 | 1.475569 | -6.732802 | 0.000738 |
| 6 | 1.587607 | -5.276111 | 0.000392 |
| 7 | 1.676877 | -4.118585 | 0.000093 |
| 1 | 1.370253 | -7.099784 | -1.023163 |
| 1 | 0.601114 | -7.040315 | 0.579431 |
| 1 | 2.369377 | -7.176314 | 0.446302 |
| 6 | 13.373517 | -0.506547 | 0.001191 |
| 1 | 13.760652 | -0.368161 | 1.013679 |
| 1 | 13.659515 | -1.499300 | -0.354895 |
| 1 | 13.817885 | 0.246516 | -0.654231 |
| 6 | 11.918325 | -0.374781 | -0.000145 |
| 7 | 10.762026 | -0.270007 | -0.001153 |
| 6 | -9.332564 | 0.041215 | 0.000719 |
| 1 | -9.714723 | -0.084032 | 1.016150 |
| 1 | -9.743788 | 0.966960 | -0.407590 |
| 1 | -9.695737 | -0.790964 | -0.606252 |
| 6 | -7.872387 | 0.081079 | 0.000421 |
| 7 | -6.711104 | 0.112750 | 0.000208 |
| 6 | -15.123746 | -0.144968 | -0.001388 |
| 1 | -15.493680 | -0.249173 | -1.024359 |
| 1 | -15.468073 | -0.998008 | 0.588476 |
| 1 | -15.531101 | 0.772264 | 0.430956 |
| 6 | -13.663477 | -0.092897 | -0.000413 |
| 7 | -12.503240 | -0.051515 | 0.000336 |

Cartesian coordinates of : PACN8_47

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-----  
Atomic number (AN) and Cartesian coordinates  
AN      X      Y      Z  
-----  
6      -5.603553   -0.558606   -0.013689  
6      -4.144140   -0.539982   -0.018265  
7      -2.982224   -0.525264   -0.021851  
1      -5.976577   -1.583984   -0.059877  
1      -6.000102   -0.012930   -0.872507  
1      -5.993446   -0.094939    0.894930  
6      -0.108206   -1.561162   -0.036019  
6      -0.069804   -0.116480   -0.026958  
7      -0.015748    1.031657   -0.020027  
1      -0.655156   -1.888190   -0.923944  
1      -0.650619   -1.899349    0.850513  
1      0.924252   -1.921034   -0.040677  
6      5.571319   -0.537836   -0.012967  
6      4.111780   -0.529278   -0.018196  
7      2.949776   -0.522989   -0.022410  
1      5.950322   -1.556067    0.097862  
1      5.959193    0.061330    0.813548  
1      5.964172   -0.128006   -0.945863  
1      0.032953    2.108008   -0.013426  
6      0.227739    6.296874    0.011854  
1      0.559144    6.643730    0.993731  
1     -0.759441    6.713297   -0.203233  
1      0.935610    6.636481   -0.748274  
6      0.159050    4.841404    0.003082  
7      0.104517    3.685943   -0.003856  
6     17.048351   -1.366510    0.029080  
6     15.596757   -1.199399    0.024395  
7     14.443413   -1.066546    0.020661  
1     17.414609   -1.484668   -0.993696  
1     17.321058   -2.252565    0.607624  
1     17.524290   -0.490669    0.476921  
6     11.287234   -0.775351    0.008799  
1     11.682201   -0.634696    1.017285  
1     11.593236   -1.762866   -0.343310  
1     11.739088   -0.024815   -0.643392  
6      9.831595   -0.654372    0.003480  
7      8.673852   -0.558276   -0.000724  
6     -11.319709   -0.772490    0.007300  
1     -11.694133   -0.889680    1.026558  
1     -11.770665    0.124973   -0.421678  
1     -11.648291   -1.633643   -0.578582  
6     -9.862609   -0.670816    0.001703  
7     -8.703699   -0.590052   -0.002703  
6     -17.089754   -1.265988    0.031533  
1     -17.397176   -2.005544   -0.711924  
1     -17.429838   -1.592260    1.017467  
1     -17.559285   -0.308289   -0.206216  
6     -15.635372   -1.125243    0.025377  
7     -14.479809   -1.013361    0.020499  
-----
```

Cartesian coordinates of : PACN9_1

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-----  
Atomic number (AN) and Cartesian coordinates
```

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.154563 | -3.522637 | 1.180611 |
| 1 | 1.235019 | -3.388842 | 1.291932 |
| 1 | -0.101054 | -4.569784 | 1.362409 |
| 1 | -0.370828 | -2.886639 | 1.899825 |
| 6 | -0.234173 | -3.138816 | -0.172986 |
| 7 | -0.537601 | -2.824668 | -1.250269 |
| 6 | 0.493669 | 4.202691 | -1.123748 |
| 1 | -0.481721 | 4.673380 | -0.984714 |
| 1 | 0.427180 | 3.490783 | -1.952763 |
| 1 | 1.245302 | 4.958970 | -1.363462 |
| 6 | 0.871742 | 3.486144 | 0.089768 |
| 7 | 1.186884 | 2.899301 | 1.042614 |
| 6 | 2.347196 | -1.994972 | -2.849851 |
| 1 | 3.047412 | -2.623063 | -3.406492 |
| 1 | 2.372411 | -0.979252 | -3.256634 |
| 1 | 1.337995 | -2.407617 | -2.943528 |
| 6 | 2.721246 | -1.956878 | -1.438954 |
| 7 | 3.016984 | -1.920213 | -0.315047 |
| 6 | 4.094299 | 1.430747 | -0.070647 |
| 1 | 4.979675 | 2.020451 | -0.321282 |
| 1 | 4.394650 | 0.405537 | 0.167748 |
| 1 | 3.587119 | 1.879488 | 0.789849 |
| 6 | 3.169721 | 1.406465 | -1.200016 |
| 7 | 2.423135 | 1.385518 | -2.090711 |
| 6 | 3.643708 | -1.116171 | 3.027101 |
| 1 | 3.457041 | -1.722954 | 3.916596 |
| 1 | 4.284096 | -0.272344 | 3.297422 |
| 1 | 4.137025 | -1.725708 | 2.262899 |
| 6 | 2.388563 | -0.631883 | 2.471510 |
| 7 | 1.402632 | -0.260012 | 1.990264 |
| 6 | -4.577178 | 1.755615 | 0.366732 |
| 1 | -5.089486 | 2.556043 | 0.906553 |
| 1 | -4.475458 | 0.876359 | 1.010378 |
| 1 | -5.162252 | 1.470656 | -0.511033 |
| 6 | -3.252912 | 2.199764 | -0.057051 |
| 7 | -2.196147 | 2.555998 | -0.383854 |
| 6 | -1.453165 | 1.419695 | 2.929739 |
| 1 | -2.338293 | 2.056211 | 3.017178 |
| 1 | -0.723625 | 1.913668 | 2.277883 |
| 1 | -1.010246 | 1.284715 | 3.919864 |
| 6 | -1.820868 | 0.122020 | 2.369973 |
| 7 | -2.090878 | -0.910993 | 1.909879 |
| 6 | -3.778621 | -3.010712 | -0.282712 |
| 1 | -4.849252 | -3.212095 | -0.195617 |
| 1 | -3.323024 | -3.025413 | 0.712020 |
| 1 | -3.315406 | -3.777194 | -0.909195 |
| 6 | -3.559923 | -1.696392 | -0.877036 |
| 7 | -3.385883 | -0.647297 | -1.344999 |
| 6 | -0.832642 | 0.437985 | -2.680770 |
| 6 | -0.372882 | 0.306203 | -1.317983 |
| 7 | 0.044865 | 0.201272 | -0.253321 |
| 1 | -1.131801 | -0.553915 | -3.035139 |
| 1 | -0.007555 | 0.845588 | -3.274532 |
| 1 | -1.701764 | 1.102031 | -2.689786 |
| 1 | 0.514841 | 0.065385 | 0.697651 |

Cartesian coordinates of : PACN9_2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.683255 | 0.456094 | -2.598843 |
| 1 | -3.580366 | 0.455631 | -3.223082 |
| 1 | -1.900524 | 1.037592 | -3.094230 |
| 1 | -2.916475 | 0.911793 | -1.630136 |
| 6 | -2.218732 | -0.910772 | -2.381239 |
| 7 | -1.836156 | -1.989257 | -2.180792 |
| 6 | 0.805176 | -3.373653 | -1.094943 |
| 1 | 1.784229 | -3.822172 | -0.909747 |
| 1 | 0.930903 | -2.513362 | -1.757582 |
| 1 | 0.136493 | -4.093120 | -1.573030 |
| 6 | 0.221676 | -2.922694 | 0.164389 |
| 7 | -0.244111 | -2.567157 | 1.169169 |
| 6 | 1.099554 | 3.515719 | 1.367102 |
| 1 | 1.302788 | 2.937737 | 2.273784 |
| 1 | 0.031016 | 3.467627 | 1.129904 |
| 1 | 1.378913 | 4.559452 | 1.532138 |
| 6 | 1.880185 | 2.957954 | 0.266271 |
| 7 | 2.497916 | 2.510217 | -0.610406 |
| 6 | 2.568768 | -2.171493 | 2.908540 |
| 1 | 1.692351 | -2.738231 | 3.232380 |
| 1 | 3.364394 | -2.267113 | 3.651681 |
| 1 | 2.909282 | -2.573095 | 1.949196 |
| 6 | 2.211091 | -0.766935 | 2.733849 |
| 7 | 1.941979 | 0.354205 | 2.585980 |
| 6 | -5.014643 | 2.648459 | 0.366151 |
| 1 | -5.536660 | 3.103993 | 1.211362 |
| 1 | -5.270900 | 1.586283 | 0.312497 |
| 1 | -5.326730 | 3.150086 | -0.553413 |
| 6 | -3.571325 | 2.774978 | 0.542143 |
| 7 | -2.420458 | 2.857499 | 0.679625 |
| 6 | 3.167488 | 0.768685 | -3.529233 |
| 1 | 3.646912 | 1.575414 | -2.965114 |
| 1 | 3.083912 | 1.051783 | -4.581232 |
| 1 | 3.757485 | -0.147358 | -3.438333 |
| 6 | 1.851264 | 0.551957 | -2.952325 |
| 7 | 0.816617 | 0.392085 | -2.455584 |
| 6 | 4.844782 | 0.624000 | 0.423084 |
| 1 | 5.769611 | 0.111747 | 0.700276 |
| 1 | 4.418698 | 1.120271 | 1.300024 |
| 1 | 5.056392 | 1.385479 | -0.331777 |
| 6 | 3.874098 | -0.334418 | -0.097847 |
| 7 | 3.101369 | -1.107592 | -0.493674 |
| 6 | -3.513070 | -3.186437 | 0.541811 |
| 1 | -2.929958 | -3.540368 | 1.395555 |
| 1 | -3.012352 | -3.493129 | -0.381445 |
| 1 | -4.517889 | -3.614685 | 0.577033 |
| 6 | -3.590739 | -1.729685 | 0.569660 |
| 7 | -3.660703 | -0.569016 | 0.580715 |
| 6 | -1.195916 | 0.427404 | 2.371097 |
| 6 | -0.699499 | 0.430814 | 1.012898 |
| 7 | -0.293811 | 0.424448 | -0.062914 |
| 1 | -2.263562 | 0.656710 | 2.347111 |
| 1 | -0.643385 | 1.173439 | 2.948650 |
| 1 | -1.022484 | -0.573643 | 2.779190 |
| 1 | 0.117991 | 0.393360 | -1.061886 |

Cartesian coordinates of : PACN9_3

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.870410 | 0.450256 | -0.486909 |
| 1 | -5.216136 | -0.538887 | -0.796794 |
| 1 | -5.695765 | 1.164435 | -0.541746 |
| 1 | -4.503414 | 0.393122 | 0.542551 |
| 6 | -3.774069 | 0.880633 | -1.348121 |
| 7 | -2.891167 | 1.225273 | -2.020722 |
| 6 | 4.296801 | 2.497245 | 0.140156 |
| 1 | 4.647767 | 2.479802 | -0.894567 |
| 1 | 4.503143 | 1.524834 | 0.597870 |
| 1 | 4.816058 | 3.284493 | 0.692305 |
| 6 | 2.857288 | 2.733648 | 0.161212 |
| 7 | 1.709857 | 2.916861 | 0.189789 |
| 6 | -1.674684 | 3.756570 | 0.108443 |
| 1 | -2.065879 | 3.597305 | -0.901481 |
| 1 | -0.586388 | 3.863762 | 0.069193 |
| 1 | -2.114463 | 4.666847 | 0.523974 |
| 6 | -2.019183 | 2.607492 | 0.940836 |
| 7 | -2.295597 | 1.682178 | 1.588573 |
| 6 | 1.191504 | 1.136449 | 3.004091 |
| 1 | 1.744921 | 2.030638 | 3.302198 |
| 1 | 0.837791 | 0.611964 | 3.895395 |
| 1 | 0.326893 | 1.439769 | 2.404703 |
| 6 | 2.051151 | 0.254886 | 2.218662 |
| 7 | 2.727036 | -0.446110 | 1.583739 |
| 6 | -1.677630 | -2.018273 | -2.876351 |
| 1 | -1.847165 | -1.021453 | -3.297937 |
| 1 | -2.107617 | -2.765435 | -3.548205 |
| 1 | -0.605015 | -2.205166 | -2.766636 |
| 6 | -2.315014 | -2.093355 | -1.564900 |
| 7 | -2.828450 | -2.124321 | -0.522620 |
| 6 | -3.128485 | -1.497296 | 2.820208 |
| 1 | -3.521745 | -0.497887 | 3.030175 |
| 1 | -3.107324 | -2.086919 | 3.739938 |
| 1 | -3.752615 | -1.996034 | 2.072319 |
| 6 | -1.791216 | -1.355958 | 2.269061 |
| 7 | -0.738531 | -1.223253 | 1.798956 |
| 6 | 4.290103 | -1.904886 | -1.139202 |
| 1 | 3.856601 | -2.773722 | -1.640713 |
| 1 | 4.172598 | -2.013500 | -0.056868 |
| 1 | 5.351646 | -1.832902 | -1.389200 |
| 6 | 3.591361 | -0.696958 | -1.564541 |
| 7 | 3.046824 | 0.273084 | -1.900062 |
| 6 | 1.466154 | -3.711499 | 1.454593 |
| 1 | 0.518934 | -3.990063 | 1.923149 |
| 1 | 1.966737 | -2.962976 | 2.075520 |
| 1 | 2.098333 | -4.598808 | 1.366785 |
| 6 | 1.212000 | -3.142106 | 0.135001 |
| 7 | 1.019937 | -2.684893 | -0.916001 |
| 6 | 0.338613 | 1.557082 | -2.560021 |
| 6 | 0.159057 | 0.757933 | -1.367967 |
| 7 | -0.021971 | 0.121976 | -0.428307 |
| 1 | 0.817992 | 0.939400 | -3.324296 |
| 1 | 1.002851 | 2.389609 | -2.310537 |
| 1 | -0.646010 | 1.905681 | -2.885830 |
| 1 | -0.208341 | -0.464637 | 0.439818 |

 Cartesian coordinates of : PACN9_4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.485918 | 2.632827 | 1.943467 |
| 1 | 3.672354 | 3.142765 | 2.891685 |
| 1 | 3.797785 | 3.269283 | 1.110552 |
| 1 | 4.044538 | 1.692148 | 1.910307 |
| 6 | 2.074123 | 2.311725 | 1.805213 |
| 7 | 0.955515 | 2.030148 | 1.670077 |
| 6 | 1.213416 | -4.782725 | -1.310874 |
| 1 | 1.984952 | -5.231197 | -0.679270 |
| 1 | 1.183780 | -5.316868 | -2.263909 |
| 1 | 0.239041 | -4.865215 | -0.820661 |
| 6 | 1.506461 | -3.370567 | -1.536581 |
| 7 | 1.732705 | -2.243341 | -1.706869 |
| 6 | -4.657513 | 2.089714 | -1.682217 |
| 1 | -3.897708 | 2.818986 | -1.976505 |
| 1 | -5.372288 | 2.563294 | -1.004458 |
| 1 | -5.191547 | 1.738270 | -2.568625 |
| 6 | -3.999853 | 0.970068 | -1.015318 |
| 7 | -3.464215 | 0.083656 | -0.487628 |
| 6 | -3.526919 | -2.772751 | 1.428889 |
| 1 | -4.249082 | -3.578551 | 1.275653 |
| 1 | -4.006905 | -1.806646 | 1.251366 |
| 1 | -3.150700 | -2.800517 | 2.454491 |
| 6 | -2.412710 | -2.915533 | 0.499220 |
| 7 | -1.526265 | -3.038762 | -0.242812 |
| 6 | 0.617682 | 4.482979 | -0.865988 |
| 1 | 1.575306 | 3.973126 | -1.004971 |
| 1 | 0.533723 | 4.829457 | 0.167608 |
| 1 | 0.553816 | 5.340645 | -1.540286 |
| 6 | -0.457694 | 3.539779 | -1.155974 |
| 7 | -1.317321 | 2.793796 | -1.392560 |
| 6 | 1.307374 | -2.686774 | 1.914796 |
| 1 | 0.893857 | -2.608213 | 2.922981 |
| 1 | 1.870336 | -3.619874 | 1.818418 |
| 1 | 0.473912 | -2.679129 | 1.204585 |
| 6 | 2.184050 | -1.551118 | 1.648766 |
| 7 | 2.882958 | -0.648945 | 1.429340 |
| 6 | -2.287217 | 1.687205 | 2.241832 |
| 1 | -2.037231 | 2.032480 | 1.232360 |
| 1 | -1.862804 | 2.380574 | 2.972092 |
| 1 | -3.374620 | 1.657777 | 2.348724 |
| 6 | -1.729607 | 0.353452 | 2.447307 |
| 7 | -1.262102 | -0.700629 | 2.592097 |
| 6 | 4.316955 | -0.214519 | -1.650898 |
| 1 | 4.324646 | -0.866933 | -0.773729 |
| 1 | 5.304984 | 0.231221 | -1.791324 |
| 1 | 4.052431 | -0.808060 | -2.528814 |
| 6 | 3.322331 | 0.833645 | -1.447941 |
| 7 | 2.543180 | 1.680959 | -1.285688 |
| 6 | -0.943233 | -0.634178 | -2.424730 |
| 6 | -0.416485 | -0.188462 | -1.156621 |
| 7 | 0.009652 | 0.218692 | -0.171210 |
| 1 | -1.544540 | 0.184237 | -2.833134 |
| 1 | -1.559289 | -1.521392 | -2.252377 |
| 1 | -0.101844 | -0.873369 | -3.080444 |
| 1 | 0.381882 | 0.784089 | 0.630365 |

Cartesian coordinates of : PACN9_ 5

| ----- | | | |
|--|-----------|-----------|-----------|
| Atomic number (AN) and Cartesian coordinates | | | |
| AN | X | Y | Z |
| ----- | | | |
| 6 | 1.146159 | 4.381783 | -0.432018 |
| 1 | 1.319857 | 4.556523 | 0.633171 |
| 1 | 0.079118 | 4.208100 | -0.598806 |
| 1 | 1.474629 | 5.254916 | -1.001285 |
| 6 | 1.887699 | 3.200052 | -0.860562 |
| 7 | 2.476604 | 2.257302 | -1.201781 |
| 6 | -3.367889 | -2.928542 | -1.446497 |
| 1 | -3.955579 | -3.466982 | -2.194181 |
| 1 | -4.024089 | -2.624506 | -0.625458 |
| 1 | -2.578526 | -3.580660 | -1.062236 |
| 6 | -2.750008 | -1.749418 | -2.043513 |
| 7 | -2.266061 | -0.807164 | -2.520518 |
| 6 | 1.882175 | -4.008586 | 0.902545 |
| 1 | 2.753392 | -3.361894 | 0.768832 |
| 1 | 2.118419 | -5.023230 | 0.572416 |
| 1 | 1.608750 | -4.016753 | 1.960895 |
| 6 | 0.776431 | -3.470138 | 0.117954 |
| 7 | -0.109721 | -3.049327 | -0.506156 |
| 6 | 2.816502 | 0.670882 | 2.213456 |
| 1 | 3.831125 | 0.278566 | 2.322206 |
| 1 | 2.624662 | 1.416673 | 2.988790 |
| 1 | 2.715407 | 1.144793 | 1.231019 |
| 6 | 1.847855 | -0.414749 | 2.327168 |
| 7 | 1.059748 | -1.264422 | 2.406650 |
| 6 | -2.025465 | -2.644543 | 2.288009 |
| 1 | -2.704481 | -2.769167 | 3.135383 |
| 1 | -0.989873 | -2.640851 | 2.639277 |
| 1 | -2.162012 | -3.471481 | 1.585554 |
| 6 | -2.296959 | -1.376898 | 1.616124 |
| 7 | -2.537373 | -0.366715 | 1.092432 |
| 6 | 5.295171 | 0.304745 | -1.276492 |
| 1 | 6.005846 | 0.377672 | -0.449128 |
| 1 | 4.911011 | 1.300261 | -1.515590 |
| 1 | 5.809830 | -0.108304 | -2.147672 |
| 6 | 4.175183 | -0.553322 | -0.901923 |
| 7 | 3.274983 | -1.225957 | -0.604606 |
| 6 | -2.580929 | 2.876203 | 2.387847 |
| 1 | -2.781899 | 3.775977 | 1.800496 |
| 1 | -2.698537 | 3.095112 | 3.451900 |
| 1 | -3.281134 | 2.086999 | 2.095332 |
| 6 | -1.231515 | 2.405244 | 2.111304 |
| 7 | -0.165665 | 2.013865 | 1.864764 |
| 6 | -4.148278 | 1.565274 | -1.379465 |
| 1 | -4.278466 | 0.729231 | -0.685763 |
| 1 | -4.213138 | 1.190227 | -2.403535 |
| 1 | -4.928541 | 2.312429 | -1.212472 |
| 6 | -2.833032 | 2.157001 | -1.158273 |
| 7 | -1.795571 | 2.644878 | -0.968673 |
| 6 | 0.898049 | -0.665364 | -2.654487 |
| 6 | 0.472425 | -0.162223 | -1.369909 |
| 7 | 0.154858 | 0.280772 | -0.360461 |
| 1 | 1.127495 | -1.729168 | -2.547334 |
| 1 | 1.792501 | -0.107276 | -2.948193 |
| 1 | 0.080958 | -0.519604 | -3.365979 |
| 1 | -0.080768 | 0.785359 | 0.513209 |
| ----- | | | |

Cartesian coordinates of : PACN9_ 6

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.796286 | -1.879746 | 2.368888 |
| 1 | -0.273699 | -1.104700 | 2.938040 |
| 1 | -1.236951 | -2.602563 | 3.060362 |
| 1 | -1.592126 | -1.426469 | 1.764859 |
| 6 | 0.159202 | -2.543714 | 1.486977 |
| 7 | 0.898899 | -3.056621 | 0.750700 |
| 6 | 3.643080 | 2.017477 | -2.996847 |
| 1 | 4.373120 | 2.824685 | -2.896478 |
| 1 | 3.387618 | 1.904363 | -4.053662 |
| 1 | 4.076893 | 1.085812 | -2.622053 |
| 6 | 2.444580 | 2.327643 | -2.222118 |
| 7 | 1.492858 | 2.566049 | -1.598982 |
| 6 | -4.513693 | -0.327011 | -1.345874 |
| 1 | -3.843897 | -0.382540 | -2.208306 |
| 1 | -5.390090 | 0.276103 | -1.596620 |
| 1 | -4.828910 | -1.337928 | -1.077325 |
| 6 | -3.798025 | 0.276478 | -0.226343 |
| 7 | -3.238129 | 0.771377 | 0.664467 |
| 6 | 4.050246 | -2.415345 | 1.026750 |
| 1 | 3.554883 | -2.214351 | 1.981220 |
| 1 | 5.134768 | -2.404196 | 1.161306 |
| 1 | 3.730284 | -3.395806 | 0.666763 |
| 6 | 3.656261 | -1.388804 | 0.067488 |
| 7 | 3.348610 | -0.559960 | -0.688015 |
| 6 | -1.515753 | -4.948915 | -0.993556 |
| 1 | -2.235792 | -5.528296 | -0.410272 |
| 1 | -0.517257 | -5.079364 | -0.565562 |
| 1 | -1.520558 | -5.312311 | -2.024188 |
| 6 | -1.864470 | -3.531523 | -0.957689 |
| 7 | -2.115269 | -2.397369 | -0.917115 |
| 6 | -2.673602 | 2.689103 | 3.571924 |
| 1 | -2.742832 | 3.779404 | 3.592985 |
| 1 | -2.582836 | 2.312331 | 4.593518 |
| 1 | -3.570553 | 2.272606 | 3.102821 |
| 6 | -1.527246 | 2.273683 | 2.779051 |
| 7 | -0.641092 | 1.923019 | 2.119636 |
| 6 | 2.884815 | 2.097457 | 1.580981 |
| 1 | 3.464493 | 2.700195 | 2.284524 |
| 1 | 2.020891 | 2.673087 | 1.233793 |
| 1 | 3.501262 | 1.844636 | 0.713446 |
| 6 | 2.430097 | 0.867508 | 2.221457 |
| 7 | 2.049217 | -0.117638 | 2.706389 |
| 6 | -1.719933 | 3.266346 | -1.433241 |
| 1 | -1.014543 | 3.989883 | -1.847683 |
| 1 | -1.408574 | 3.018493 | -0.413115 |
| 1 | -2.725021 | 3.695057 | -1.406874 |
| 6 | -1.716536 | 2.051308 | -2.241460 |
| 7 | -1.716275 | 1.068680 | -2.862231 |
| 6 | 0.565051 | -1.029927 | -2.063590 |
| 6 | 0.258286 | -0.265683 | -0.877225 |
| 7 | 0.022346 | 0.350692 | 0.064071 |
| 1 | -0.349324 | -1.118328 | -2.656243 |
| 1 | 0.940857 | -2.008547 | -1.747360 |
| 1 | 1.339795 | -0.491774 | -2.617696 |
| 1 | -0.196520 | 0.974908 | 0.903911 |

Cartesian coordinates of : PACN9_7

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.901248 | 0.247956 | 2.392901 |
| 1 | -2.338926 | 1.170741 | 2.211890 |
| 1 | -2.215026 | -0.537590 | 2.726362 |
| 1 | -3.650791 | 0.427352 | 3.167697 |
| 6 | -3.544616 | -0.172701 | 1.152074 |
| 7 | -4.028792 | -0.493590 | 0.144678 |
| 6 | 0.590196 | 3.790101 | -1.221100 |
| 1 | -0.309166 | 4.353681 | -0.964591 |
| 1 | 0.336211 | 3.025035 | -1.959484 |
| 1 | 1.339851 | 4.463588 | -1.645030 |
| 6 | 1.126629 | 3.144207 | -0.026916 |
| 7 | 1.575775 | 2.641606 | 0.920082 |
| 6 | 1.607936 | -3.428843 | 0.874108 |
| 1 | 1.317755 | -2.649910 | 1.585609 |
| 1 | 2.698131 | -3.483275 | 0.836942 |
| 1 | 1.190000 | -4.383914 | 1.202019 |
| 6 | 1.083266 | -3.086860 | -0.443984 |
| 7 | 0.643336 | -2.813478 | -1.485375 |
| 6 | 3.014260 | -1.374605 | -3.170776 |
| 1 | 2.379329 | -2.155942 | -3.595157 |
| 1 | 3.482617 | -1.765985 | -2.262643 |
| 1 | 3.784168 | -1.091182 | -3.892811 |
| 6 | 2.199939 | -0.214027 | -2.823040 |
| 7 | 1.567833 | 0.718517 | -2.536463 |
| 6 | -2.773528 | -3.657471 | -0.592127 |
| 1 | -3.161157 | -4.662041 | -0.405179 |
| 1 | -2.071534 | -3.695089 | -1.431678 |
| 1 | -3.606101 | -2.989670 | -0.833886 |
| 6 | -2.081317 | -3.152807 | 0.590019 |
| 7 | -1.517398 | -2.727953 | 1.513418 |
| 6 | 2.866353 | 1.096252 | 3.778110 |
| 1 | 2.722986 | 1.255283 | 4.849521 |
| 1 | 3.016009 | 2.058538 | 3.277780 |
| 1 | 3.737476 | 0.455630 | 3.615692 |
| 6 | 1.692209 | 0.473443 | 3.190206 |
| 7 | 0.768153 | -0.002517 | 2.678469 |
| 6 | 4.363741 | 1.561841 | -0.316602 |
| 1 | 5.402185 | 1.339783 | -0.575283 |
| 1 | 4.334676 | 2.308438 | 0.481107 |
| 1 | 3.845820 | 1.968651 | -1.190726 |
| 6 | 3.680382 | 0.346233 | 0.116848 |
| 7 | 3.140001 | -0.630854 | 0.439482 |
| 6 | -4.950984 | 2.730694 | -0.911127 |
| 1 | -5.180212 | 3.131204 | -1.901722 |
| 1 | -5.364663 | 3.400913 | -0.153448 |
| 1 | -5.405342 | 1.741113 | -0.805180 |
| 6 | -3.506019 | 2.610881 | -0.738963 |
| 7 | -2.358762 | 2.491615 | -0.595702 |
| 6 | -1.406840 | -0.224730 | -2.066339 |
| 6 | -0.769560 | -0.119848 | -0.772432 |
| 7 | -0.288771 | -0.079523 | 0.270175 |
| 1 | -1.233123 | 0.701642 | -2.619842 |
| 1 | -2.479119 | -0.380049 | -1.902276 |
| 1 | -0.955579 | -1.073015 | -2.591325 |

1 0.129107 -0.079001 1.269135

Cartesian coordinates of : PACN9_ 8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.587926 | -0.587080 | 2.954580 |
| 1 | -4.169115 | -0.795640 | 2.050735 |
| 1 | -3.858438 | 0.402310 | 3.330607 |
| 1 | -3.784350 | -1.347911 | 3.714118 |
| 6 | -2.183652 | -0.589611 | 2.579208 |
| 7 | -1.072356 | -0.594884 | 2.243569 |
| 6 | 3.639623 | -2.924538 | -1.556302 |
| 1 | 3.220087 | -3.332354 | -0.631817 |
| 1 | 4.540907 | -2.352197 | -1.322772 |
| 1 | 3.892574 | -3.743943 | -2.233634 |
| 6 | 2.650138 | -2.047814 | -2.172390 |
| 7 | 1.858239 | -1.350980 | -2.658735 |
| 6 | 2.694021 | -1.226227 | 2.383593 |
| 1 | 2.813887 | -2.309316 | 2.298400 |
| 1 | 1.628928 | -1.007208 | 2.508642 |
| 1 | 3.244680 | -0.865331 | 3.255907 |
| 6 | 3.194752 | -0.579500 | 1.173657 |
| 7 | 3.594251 | -0.055511 | 0.216073 |
| 6 | 4.736582 | 3.136507 | 0.981645 |
| 1 | 5.159869 | 3.947929 | 0.384418 |
| 1 | 5.151424 | 2.182308 | 0.644579 |
| 1 | 4.997918 | 3.295469 | 2.030835 |
| 6 | 3.285715 | 3.103972 | 0.826481 |
| 7 | 2.132302 | 3.062336 | 0.695820 |
| 6 | -1.372026 | -3.965491 | 1.541493 |
| 1 | -2.289117 | -3.464327 | 1.216456 |
| 1 | -1.269328 | -3.866390 | 2.625586 |
| 1 | -1.427427 | -5.026052 | 1.283544 |
| 6 | -0.225769 | -3.346012 | 0.881738 |
| 7 | 0.685835 | -2.846270 | 0.361617 |
| 6 | -4.427215 | 1.310926 | -1.770998 |
| 1 | -4.995587 | 2.221051 | -1.978351 |
| 1 | -4.511126 | 1.058572 | -0.709852 |
| 1 | -4.830509 | 0.490174 | -2.369756 |
| 6 | -3.017985 | 1.515892 | -2.090477 |
| 7 | -1.890431 | 1.672037 | -2.326157 |
| 6 | -1.259395 | 3.891553 | 0.302115 |
| 1 | -0.228059 | 3.693408 | 0.611555 |
| 1 | -1.570118 | 4.863957 | 0.692744 |
| 1 | -1.309033 | 3.910341 | -0.791307 |
| 6 | -2.144229 | 2.843925 | 0.802796 |
| 7 | -2.848016 | 2.002242 | 1.186364 |
| 6 | -1.411401 | -1.825979 | -2.449821 |
| 1 | -1.175078 | -0.867086 | -2.922175 |
| 1 | -1.919694 | -2.468260 | -3.173601 |
| 1 | -0.472826 | -2.293088 | -2.138560 |
| 6 | -2.263206 | -1.604981 | -1.285642 |
| 7 | -2.932317 | -1.427347 | -0.350931 |
| 6 | 1.279510 | 1.553671 | -1.963324 |
| 6 | 0.648120 | 0.860134 | -0.864312 |
| 7 | 0.150587 | 0.326394 | 0.025231 |
| 1 | 1.048776 | 2.618642 | -1.870642 |
| 1 | 0.891286 | 1.149411 | -2.900901 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 2.357469 | 1.377009 | -1.888975 |
| 1 | -0.298597 | -0.103693 | 0.890022 |

Cartesian coordinates of : PACN9_ 9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.080007 | -4.527109 | 0.110291 |
| 1 | -1.144388 | -4.469953 | -0.138350 |
| 1 | 0.122019 | -5.479093 | 0.607601 |
| 1 | 0.514251 | -4.454113 | -0.804410 |
| 6 | 0.264470 | -3.415323 | 0.991018 |
| 7 | 0.521817 | -2.521901 | 1.688962 |
| 6 | 2.690189 | 2.788175 | -0.967742 |
| 1 | 3.732602 | 2.460720 | -0.958395 |
| 1 | 2.274089 | 2.656998 | 0.035620 |
| 1 | 2.629315 | 3.841590 | -1.252744 |
| 6 | 1.924573 | 1.972183 | -1.904756 |
| 7 | 1.302739 | 1.328031 | -2.646381 |
| 6 | 3.301159 | -1.326717 | 2.685191 |
| 1 | 3.318252 | -2.404957 | 2.510837 |
| 1 | 2.419888 | -1.094356 | 3.289037 |
| 1 | 4.209161 | -1.024093 | 3.212724 |
| 6 | 3.203539 | -0.621654 | 1.411125 |
| 7 | 3.127792 | -0.041419 | 0.407161 |
| 6 | -1.582769 | 3.231164 | -2.101490 |
| 1 | -1.173206 | 4.008766 | -2.751370 |
| 1 | -2.663855 | 3.354503 | -2.008574 |
| 1 | -1.372785 | 2.253479 | -2.545566 |
| 6 | -0.962545 | 3.308819 | -0.782223 |
| 7 | -0.452634 | 3.380437 | 0.259618 |
| 6 | 0.654997 | 3.492228 | 3.511593 |
| 1 | 0.010148 | 3.494828 | 4.393692 |
| 1 | 0.272936 | 4.204688 | 2.773894 |
| 1 | 1.669758 | 3.772309 | 3.804490 |
| 6 | 0.654977 | 2.174985 | 2.892803 |
| 7 | 0.641773 | 1.140050 | 2.369692 |
| 6 | -2.382438 | -0.864969 | 2.326745 |
| 1 | -3.108820 | -1.030480 | 3.126428 |
| 1 | -2.433676 | 0.179747 | 1.999175 |
| 1 | -1.375393 | -1.080945 | 2.698558 |
| 6 | -2.669566 | -1.735203 | 1.190277 |
| 7 | -2.882212 | -2.399169 | 0.259556 |
| 6 | 3.739788 | -1.056462 | -2.775629 |
| 1 | 3.436226 | -0.460851 | -3.640355 |
| 1 | 4.516310 | -1.764920 | -3.074634 |
| 1 | 4.127622 | -0.391924 | -1.998187 |
| 6 | 2.584924 | -1.773189 | -2.245080 |
| 7 | 1.667873 | -2.348649 | -1.823445 |
| 6 | -5.679223 | -0.346810 | -0.659932 |
| 1 | -6.320359 | -0.003414 | 0.155793 |
| 1 | -5.461140 | -1.410605 | -0.526052 |
| 1 | -6.203781 | -0.201649 | -1.607546 |
| 6 | -4.424011 | 0.399156 | -0.660084 |
| 7 | -3.409932 | 0.967272 | -0.653962 |
| 6 | -1.053149 | -0.984838 | -2.149051 |
| 6 | -0.496542 | -0.446630 | -0.928279 |
| 7 | -0.070867 | -0.015916 | 0.047861 |
| 1 | -1.071365 | -2.075495 | -2.064897 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.406261 | -0.679779 | -2.977156 |
| 1 | -2.067779 | -0.593172 | -2.263994 |
| 1 | 0.295580 | 0.364198 | 0.972286 |

Cartesian coordinates of : PACN9_10

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.009445 | 0.603148 | -0.966972 |
| 1 | -4.222748 | 0.705805 | -1.720741 |
| 1 | -5.093312 | 1.543475 | -0.417181 |
| 1 | -5.959202 | 0.368685 | -1.453938 |
| 6 | -4.639162 | -0.465552 | -0.044837 |
| 7 | -4.344969 | -1.328361 | 0.675657 |
| 6 | 5.175278 | -0.243568 | 2.073360 |
| 1 | 5.810591 | 0.481680 | 1.559118 |
| 1 | 5.796037 | -0.894669 | 2.693710 |
| 1 | 4.467879 | 0.303283 | 2.700725 |
| 6 | 4.442799 | -1.036928 | 1.091198 |
| 7 | 3.864511 | -1.675908 | 0.312064 |
| 6 | 3.216971 | 4.381441 | -0.251984 |
| 1 | 3.240771 | 5.119276 | 0.553883 |
| 1 | 2.317656 | 4.528490 | -0.856557 |
| 1 | 4.102302 | 4.513429 | -0.879048 |
| 6 | 3.191696 | 3.031622 | 0.303361 |
| 7 | 3.157408 | 1.954341 | 0.738738 |
| 6 | -3.361395 | -1.609621 | 3.606486 |
| 1 | -3.092755 | -1.793582 | 4.649556 |
| 1 | -3.850333 | -2.486707 | 3.176587 |
| 1 | -4.053859 | -0.766966 | 3.536778 |
| 6 | -2.167235 | -1.304976 | 2.832408 |
| 7 | -1.207086 | -1.059673 | 2.233545 |
| 6 | -1.984956 | 2.910278 | -2.476647 |
| 1 | -2.119971 | 3.882329 | -2.957449 |
| 1 | -2.750949 | 2.765735 | -1.708855 |
| 1 | -2.068797 | 2.109286 | -3.214718 |
| 6 | -0.674420 | 2.844978 | -1.840240 |
| 7 | 0.367801 | 2.811974 | -1.326193 |
| 6 | -0.350504 | 2.420381 | 2.048696 |
| 1 | -0.451673 | 3.376845 | 2.568023 |
| 1 | 0.479956 | 2.479344 | 1.337877 |
| 1 | -0.137121 | 1.638435 | 2.783954 |
| 6 | -1.583596 | 2.105984 | 1.331795 |
| 7 | -2.561097 | 1.848554 | 0.759003 |
| 6 | 3.092565 | -4.667463 | -1.176414 |
| 1 | 2.759115 | -5.529138 | -0.592828 |
| 1 | 3.871959 | -4.134353 | -0.625561 |
| 1 | 3.493577 | -5.017828 | -2.130723 |
| 6 | 1.976165 | -3.756451 | -1.407267 |
| 7 | 1.092674 | -3.024653 | -1.591344 |
| 6 | -2.112782 | -2.782870 | -1.299245 |
| 1 | -3.186359 | -2.982523 | -1.326316 |
| 1 | -1.759859 | -2.913201 | -0.271681 |
| 1 | -1.575135 | -3.477005 | -1.948247 |
| 6 | -1.849126 | -1.412418 | -1.727993 |
| 7 | -1.635650 | -0.320875 | -2.067165 |
| 6 | 1.920348 | 0.022358 | -1.772180 |
| 6 | 1.178254 | -0.205516 | -0.554851 |
| 7 | 0.562503 | -0.402256 | 0.396828 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 1.238612 | -0.169740 | -2.607557 |
| 1 | 2.761820 | -0.675424 | -1.790645 |
| 1 | 2.261148 | 1.060026 | -1.782894 |
| 1 | -0.120758 | -0.665941 | 1.194745 |

Cartesian coordinates of : PACN9_11

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.024469 | 3.292370 | 1.010686 |
| 1 | 2.679717 | 3.523361 | 0.166046 |
| 1 | 2.183518 | 4.025944 | 1.805350 |
| 1 | 0.982387 | 3.348625 | 0.673978 |
| 6 | 2.317327 | 1.946501 | 1.497634 |
| 7 | 2.531158 | 0.865031 | 1.867289 |
| 6 | 0.188553 | -2.069673 | -3.106754 |
| 1 | 0.318879 | -2.795663 | -3.913250 |
| 1 | 1.170736 | -1.705042 | -2.788758 |
| 1 | -0.428141 | -1.241060 | -3.471465 |
| 6 | -0.478605 | -2.696649 | -1.969487 |
| 7 | -1.023787 | -3.183462 | -1.066393 |
| 6 | -4.084110 | -1.692790 | -0.759074 |
| 1 | -4.380759 | -1.320005 | 0.225189 |
| 1 | -3.519577 | -2.623651 | -0.646562 |
| 1 | -4.971542 | -1.880785 | -1.368737 |
| 6 | -3.231330 | -0.701704 | -1.406876 |
| 7 | -2.554486 | 0.085220 | -1.930252 |
| 6 | -1.920902 | -3.275006 | 2.180751 |
| 1 | -2.876028 | -2.760935 | 2.328881 |
| 1 | -1.654130 | -3.816140 | 3.091829 |
| 1 | -1.998960 | -3.971983 | 1.341080 |
| 6 | -0.903814 | -2.286941 | 1.858368 |
| 7 | -0.112113 | -1.485158 | 1.584123 |
| 6 | -4.023306 | 2.793978 | -0.537026 |
| 1 | -4.565912 | 3.707924 | -0.283078 |
| 1 | -4.374040 | 1.971056 | 0.093249 |
| 1 | -4.201570 | 2.541173 | -1.585268 |
| 6 | -2.593431 | 2.982406 | -0.315711 |
| 7 | -1.455542 | 3.131235 | -0.131071 |
| 6 | 3.205735 | -2.369189 | 1.868742 |
| 1 | 4.166591 | -1.893992 | 2.085193 |
| 1 | 3.290393 | -3.446957 | 2.027897 |
| 1 | 2.456898 | -1.945652 | 2.542686 |
| 6 | 2.813976 | -2.092553 | 0.490180 |
| 7 | 2.503543 | -1.866219 | -0.606654 |
| 6 | -1.046856 | 1.582406 | 2.921857 |
| 1 | -0.836712 | 2.500769 | 2.364866 |
| 1 | -0.154281 | 0.947758 | 2.922552 |
| 1 | -1.308549 | 1.836064 | 3.952307 |
| 6 | -2.151105 | 0.875176 | 2.279989 |
| 7 | -3.018278 | 0.300126 | 1.762063 |
| 6 | 5.158389 | 0.214250 | -0.678966 |
| 1 | 5.199182 | -0.784333 | -1.121154 |
| 1 | 5.007782 | 0.123241 | 0.401772 |
| 1 | 6.097448 | 0.738851 | -0.871553 |
| 6 | 4.039728 | 0.956925 | -1.249267 |
| 7 | 3.147334 | 1.559597 | -1.684780 |
| 6 | 0.200461 | 1.817921 | -2.467476 |
| 6 | 0.262811 | 0.969633 | -1.297450 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 0.298104 | 0.276383 | -0.381315 |
| 1 | 0.891611 | 1.426985 | -3.218986 |
| 1 | 0.513600 | 2.826393 | -2.183911 |
| 1 | -0.834436 | 1.815276 | -2.821734 |
| 1 | 0.266438 | -0.408847 | 0.439782 |

Cartesian coordinates of : PACN9_12

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.272195 | -3.652944 | 1.214278 |
| 1 | 0.613895 | -3.816682 | 0.188108 |
| 1 | -0.011675 | -4.605771 | 1.668322 |
| 1 | 1.098015 | -3.205237 | 1.773294 |
| 6 | -0.868984 | -2.743827 | 1.205344 |
| 7 | -1.778814 | -2.019718 | 1.186341 |
| 6 | 3.215078 | -1.611878 | -2.473748 |
| 1 | 4.122242 | -2.071465 | -2.874341 |
| 1 | 3.285714 | -0.525691 | -2.588881 |
| 1 | 2.346347 | -1.996876 | -3.015639 |
| 6 | 3.076816 | -1.928994 | -1.056457 |
| 7 | 2.971037 | -2.180135 | 0.072816 |
| 6 | -1.728699 | -0.095187 | 3.908367 |
| 1 | -1.899361 | 0.453362 | 4.837946 |
| 1 | -0.760734 | -0.601704 | 3.953548 |
| 1 | -2.512543 | -0.845820 | 3.775207 |
| 6 | -1.731608 | 0.821801 | 2.772984 |
| 7 | -1.739930 | 1.547122 | 1.864994 |
| 6 | 2.934411 | 4.005070 | -0.253607 |
| 1 | 2.554365 | 4.504036 | -1.148068 |
| 1 | 3.917146 | 4.407145 | 0.004551 |
| 1 | 2.231256 | 4.189565 | 0.562051 |
| 6 | 3.029682 | 2.569361 | -0.501122 |
| 7 | 3.116257 | 1.426786 | -0.698294 |
| 6 | -2.800772 | -2.909782 | -2.128264 |
| 1 | -3.151015 | -2.802547 | -1.097023 |
| 1 | -3.010669 | -3.921682 | -2.483681 |
| 1 | -3.322485 | -2.185522 | -2.758878 |
| 6 | -1.364659 | -2.652113 | -2.172127 |
| 7 | -0.219099 | -2.457859 | -2.202472 |
| 6 | -4.392173 | 0.125262 | 0.491450 |
| 1 | -3.990329 | -0.647988 | 1.152842 |
| 1 | -5.371456 | -0.179518 | 0.113418 |
| 1 | -4.493687 | 1.057568 | 1.053847 |
| 6 | -3.464002 | 0.320623 | -0.617747 |
| 7 | -2.739481 | 0.471581 | -1.513820 |
| 6 | 3.936392 | -0.394280 | 2.499142 |
| 1 | 4.346097 | 0.050389 | 1.586807 |
| 1 | 4.261454 | -1.436014 | 2.553294 |
| 1 | 4.284730 | 0.157501 | 3.375532 |
| 6 | 2.483973 | -0.347020 | 2.413919 |
| 7 | 1.326242 | -0.306251 | 2.324479 |
| 6 | -2.623218 | 3.862495 | -0.486036 |
| 1 | -2.760822 | 4.943899 | -0.408847 |
| 1 | -2.877234 | 3.388761 | 0.466072 |
| 1 | -3.272208 | 3.470161 | -1.273512 |
| 6 | -1.232067 | 3.556271 | -0.801779 |
| 7 | -0.122923 | 3.323325 | -1.058591 |
| 6 | 0.277007 | 0.723089 | -2.696242 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.253683 | 0.396323 | -1.288242 |
| 7 | 0.257604 | 0.136479 | -0.170341 |
| 1 | 1.044317 | 1.487614 | -2.849945 |
| 1 | -0.708835 | 1.110754 | -2.967338 |
| 1 | 0.493105 | -0.187813 | -3.260850 |
| 1 | 0.409793 | -0.045359 | 0.845716 |

Cartesian coordinates of : PACN9_13

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.965604 | 3.677387 | 0.345635 |
| 1 | -1.280342 | 2.861130 | -0.312410 |
| 1 | -0.464342 | 4.446672 | -0.247341 |
| 1 | -1.850918 | 4.096577 | 0.829769 |
| 6 | -0.053301 | 3.154003 | 1.356443 |
| 7 | 0.672413 | 2.721243 | 2.154469 |
| 6 | -1.159762 | -4.033572 | -0.977244 |
| 1 | -1.208834 | -3.817880 | -2.047100 |
| 1 | -1.636776 | -4.994169 | -0.767006 |
| 1 | -0.110652 | -4.065971 | -0.671993 |
| 6 | -1.832599 | -2.972909 | -0.234787 |
| 7 | -2.383537 | -2.140603 | 0.361882 |
| 6 | 0.215888 | 1.738552 | -3.992861 |
| 1 | 0.906704 | 1.982934 | -4.803595 |
| 1 | -0.664534 | 2.382573 | -4.059460 |
| 1 | -0.106074 | 0.696211 | -4.077971 |
| 6 | 0.867376 | 1.930319 | -2.700145 |
| 7 | 1.382719 | 2.067656 | -1.666598 |
| 6 | -4.463963 | 0.093329 | -1.315766 |
| 1 | -4.998510 | -0.117206 | -2.245304 |
| 1 | -4.957619 | 0.914913 | -0.789521 |
| 1 | -4.462997 | -0.800380 | -0.683505 |
| 6 | -3.081275 | 0.454304 | -1.598616 |
| 7 | -1.975418 | 0.736617 | -1.811977 |
| 6 | 3.625405 | 2.960911 | 0.904994 |
| 1 | 4.679639 | 3.162357 | 0.698971 |
| 1 | 3.317643 | 3.483210 | 1.814004 |
| 1 | 3.011406 | 3.305371 | 0.068196 |
| 6 | 3.415317 | 1.528482 | 1.077902 |
| 7 | 3.259113 | 0.384363 | 1.213302 |
| 6 | -4.437218 | -0.546946 | 2.582465 |
| 1 | -4.197873 | -1.530995 | 2.169302 |
| 1 | -5.447584 | -0.258085 | 2.279873 |
| 1 | -4.399161 | -0.589366 | 3.673897 |
| 6 | -3.467006 | 0.422059 | 2.080672 |
| 7 | -2.694897 | 1.186779 | 1.668552 |
| 6 | 4.066062 | -2.924322 | 1.450621 |
| 1 | 4.462696 | -1.905816 | 1.491827 |
| 1 | 4.593420 | -3.494609 | 0.681197 |
| 1 | 4.217993 | -3.412858 | 2.416401 |
| 6 | 2.641550 | -2.859112 | 1.139059 |
| 7 | 1.509770 | -2.793150 | 0.882365 |
| 6 | 2.835817 | -1.159563 | -1.929687 |
| 1 | 3.302280 | -0.531074 | -2.693038 |
| 1 | 3.367441 | -2.113725 | -1.874776 |
| 1 | 2.898880 | -0.649344 | -0.962100 |
| 6 | 1.433296 | -1.388728 | -2.261293 |
| 7 | 0.308913 | -1.541858 | -2.514702 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.342502 | -0.401949 | 2.649130 |
| 6 | 0.113609 | -0.138079 | 1.249188 |
| 7 | -0.110971 | 0.071229 | 0.142886 |
| 1 | -0.222237 | 0.339941 | 3.222186 |
| 1 | 1.412487 | -0.293972 | 2.850245 |
| 1 | 0.007375 | -1.421769 | 2.860547 |
| 1 | -0.522812 | 0.274400 | -0.786816 |

Cartesian coordinates of : PACN9_14

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.954453 | -0.268760 | 2.428836 |
| 1 | 4.298380 | -1.304633 | 2.478198 |
| 1 | 4.314196 | 0.291180 | 3.295412 |
| 1 | 4.335419 | 0.180148 | 1.506216 |
| 6 | 2.499588 | -0.246089 | 2.377858 |
| 7 | 1.339486 | -0.224212 | 2.316085 |
| 6 | -2.732600 | -3.043289 | -2.013527 |
| 1 | -3.296074 | -2.355180 | -2.648713 |
| 1 | -3.058382 | -2.919117 | -0.976152 |
| 1 | -2.916716 | -4.071347 | -2.335278 |
| 6 | -1.307986 | -2.738195 | -2.104672 |
| 7 | -0.171084 | -2.506439 | -2.173102 |
| 6 | 3.210312 | -1.544557 | -2.516849 |
| 1 | 2.356456 | -1.965165 | -3.055816 |
| 1 | 4.133264 | -1.981106 | -2.907008 |
| 1 | 3.247128 | -0.458555 | -2.648360 |
| 6 | 3.075878 | -1.844678 | -1.095612 |
| 7 | 2.972745 | -2.081783 | 0.036893 |
| 6 | -2.792761 | 3.744446 | -0.538486 |
| 1 | -2.970948 | 4.819732 | -0.458873 |
| 1 | -3.034802 | 3.258055 | 0.410462 |
| 1 | -3.421753 | 3.330402 | -1.331010 |
| 6 | -1.389109 | 3.491440 | -0.846376 |
| 7 | -0.270460 | 3.300350 | -1.096813 |
| 6 | -1.424972 | 0.115341 | 4.042306 |
| 1 | -2.252596 | 0.262447 | 4.740692 |
| 1 | -0.489906 | 0.424521 | 4.515304 |
| 1 | -1.353422 | -0.942585 | 3.775284 |
| 6 | -1.644697 | 0.897335 | 2.829713 |
| 7 | -1.824472 | 1.515131 | 1.862023 |
| 6 | -4.372821 | -0.055528 | 0.548755 |
| 1 | -3.899685 | -0.774086 | 1.224048 |
| 1 | -5.333409 | -0.444210 | 0.200736 |
| 1 | -4.532919 | 0.882923 | 1.086565 |
| 6 | -3.484502 | 0.175852 | -0.585599 |
| 7 | -2.791561 | 0.352839 | -1.501759 |
| 6 | 0.421983 | -3.688481 | 1.277638 |
| 1 | 0.139511 | -4.639188 | 1.736918 |
| 1 | 1.246512 | -3.235373 | 1.834147 |
| 1 | 0.764319 | -3.855927 | 0.252404 |
| 6 | -0.720153 | -2.780699 | 1.265296 |
| 7 | -1.631280 | -2.058062 | 1.248110 |
| 6 | 2.784957 | 4.093439 | -0.383354 |
| 1 | 2.371765 | 4.559899 | -1.280656 |
| 1 | 3.759930 | 4.530854 | -0.154942 |
| 1 | 2.092901 | 4.275663 | 0.442201 |
| 6 | 2.919185 | 2.655899 | -0.600351 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 3.036868 | 1.512268 | -0.773845 |
| 6 | 0.197664 | 0.690035 | -2.713330 |
| 6 | 0.198907 | 0.382892 | -1.300719 |
| 7 | 0.222804 | 0.139132 | -0.179587 |
| 1 | 0.938430 | 1.476307 | -2.886173 |
| 1 | -0.803016 | 1.041125 | -2.979793 |
| 1 | 0.437414 | -0.221759 | -3.266909 |
| 1 | 0.386739 | -0.028006 | 0.835894 |

Cartesian coordinates of : PACN9_15

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.054296 | -1.312008 | -3.706535 |
| 1 | 2.187292 | -0.247479 | -3.922601 |
| 1 | 1.002783 | -1.589176 | -3.836141 |
| 1 | 2.665766 | -1.898455 | -4.396935 |
| 6 | 2.452584 | -1.577251 | -2.327146 |
| 7 | 2.746383 | -1.777369 | -1.220247 |
| 6 | -3.341621 | -3.172445 | 0.600687 |
| 1 | -3.200116 | -3.039535 | -0.475671 |
| 1 | -4.285503 | -2.702308 | 0.887008 |
| 1 | -3.379628 | -4.237217 | 0.845657 |
| 6 | -2.236280 | -2.531932 | 1.307568 |
| 7 | -1.340595 | -2.037023 | 1.859148 |
| 6 | -5.177699 | 1.691055 | -0.813558 |
| 1 | -5.607147 | 1.627619 | -1.816462 |
| 1 | -4.689190 | 2.661816 | -0.686619 |
| 1 | -5.979718 | 1.593134 | -0.077701 |
| 6 | -4.187442 | 0.635127 | -0.622181 |
| 7 | -3.377061 | -0.183601 | -0.467464 |
| 6 | 0.846329 | 4.526025 | -0.415222 |
| 1 | -0.235314 | 4.681587 | -0.458958 |
| 1 | 1.204301 | 4.179455 | -1.389642 |
| 1 | 1.341071 | 5.467272 | -0.162898 |
| 6 | 1.146227 | 3.513071 | 0.592292 |
| 7 | 1.382154 | 2.691336 | 1.380406 |
| 6 | -1.659860 | 1.474988 | 2.382157 |
| 1 | -2.260485 | 1.813046 | 3.230326 |
| 1 | -0.597476 | 1.537543 | 2.641062 |
| 1 | -1.910499 | 0.434770 | 2.146087 |
| 6 | -1.914436 | 2.313436 | 1.215574 |
| 7 | -2.108350 | 2.955400 | 0.265288 |
| 6 | 2.836157 | -1.371886 | 4.378922 |
| 1 | 3.718801 | -1.975924 | 4.154785 |
| 1 | 2.149740 | -1.953245 | 4.999548 |
| 1 | 3.141939 | -0.474540 | 4.922502 |
| 6 | 2.169854 | -0.992637 | 3.139877 |
| 7 | 1.634890 | -0.692935 | 2.160013 |
| 6 | 4.038860 | 1.147815 | -0.118344 |
| 1 | 5.025382 | 1.577451 | -0.310098 |
| 1 | 4.117803 | 0.058359 | -0.053353 |
| 1 | 3.641895 | 1.541774 | 0.822263 |
| 6 | 3.121185 | 1.490903 | -1.199813 |
| 7 | 2.372396 | 1.751684 | -2.050402 |
| 6 | 0.556464 | -3.905973 | -0.209775 |
| 1 | 0.918968 | -3.213457 | 0.556605 |
| 1 | 1.413322 | -4.395161 | -0.679133 |
| 1 | -0.086094 | -4.655581 | 0.260186 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.196865 | -3.154231 | -1.209728 |
| 7 | -0.792355 | -2.537299 | -1.994965 |
| 6 | -0.850224 | 0.804082 | -2.163670 |
| 6 | -0.253783 | 0.348350 | -0.928008 |
| 7 | 0.258928 | 0.001536 | 0.040410 |
| 1 | -1.485334 | 1.667558 | -1.938410 |
| 1 | -1.445946 | -0.015118 | -2.577612 |
| 1 | -0.038752 | 1.096682 | -2.838362 |
| 1 | 0.814937 | -0.301903 | 0.930680 |

Cartesian coordinates of : PACN9_16

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.493417 | -1.745347 | -2.248906 |
| 1 | 1.941964 | -0.837690 | -1.828539 |
| 1 | 0.533476 | -1.494671 | -2.712854 |
| 1 | 2.163192 | -2.166142 | -3.003111 |
| 6 | 1.263364 | -2.712358 | -1.180494 |
| 7 | 1.073271 | -3.455655 | -0.306458 |
| 6 | -4.151972 | 0.193817 | -0.788311 |
| 1 | -3.662749 | -0.221762 | -1.674761 |
| 1 | -3.886352 | 1.250637 | -0.688720 |
| 1 | -5.235919 | 0.095200 | -0.887639 |
| 6 | -3.686330 | -0.525672 | 0.392856 |
| 7 | -3.285987 | -1.090730 | 1.327281 |
| 6 | 4.085822 | 2.030911 | 0.341918 |
| 1 | 3.636300 | 1.846881 | 1.321642 |
| 1 | 4.510141 | 3.037860 | 0.305295 |
| 1 | 4.880687 | 1.298197 | 0.183129 |
| 6 | 3.064998 | 1.881511 | -0.691478 |
| 7 | 2.249693 | 1.789383 | -1.515261 |
| 6 | -2.400149 | 1.523480 | 3.479350 |
| 1 | -2.885756 | 0.542831 | 3.493169 |
| 1 | -2.946142 | 2.204343 | 4.137171 |
| 1 | -1.368489 | 1.433141 | 3.835655 |
| 6 | -2.390917 | 2.037392 | 2.112902 |
| 7 | -2.359497 | 2.428744 | 1.018737 |
| 6 | -2.311616 | -4.093011 | -0.325899 |
| 1 | -2.780997 | -3.718679 | 0.589177 |
| 1 | -1.357267 | -4.567655 | -0.079991 |
| 1 | -2.972072 | -4.825657 | -0.796392 |
| 6 | -2.070946 | -2.974576 | -1.232420 |
| 7 | -1.869989 | -2.071122 | -1.936042 |
| 6 | 0.504257 | 3.814435 | 0.660907 |
| 1 | 1.420472 | 4.362846 | 0.425220 |
| 1 | -0.246669 | 4.501956 | 1.057372 |
| 1 | 0.112816 | 3.355101 | -0.252354 |
| 6 | 0.782516 | 2.765709 | 1.638386 |
| 7 | 0.996383 | 1.917731 | 2.404415 |
| 6 | 0.004108 | 2.705337 | -4.333375 |
| 1 | 1.073599 | 2.879283 | -4.179578 |
| 1 | -0.518154 | 3.663204 | -4.393886 |
| 1 | -0.146856 | 2.151443 | -5.263049 |
| 6 | -0.493185 | 1.933842 | -3.204836 |
| 7 | -0.851345 | 1.320734 | -2.291038 |
| 6 | 4.045735 | -3.200082 | 1.494849 |
| 1 | 4.230545 | -3.301825 | 2.567122 |
| 1 | 4.991136 | -3.318286 | 0.959515 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.348336 | -3.977667 | 1.168768 |
| 6 | 3.463710 | -1.892594 | 1.205198 |
| 7 | 2.972836 | -0.867003 | 0.963705 |
| 6 | -0.016137 | -1.260806 | 2.150518 |
| 6 | -0.197140 | -0.545291 | 0.907813 |
| 7 | -0.385292 | 0.018397 | -0.076009 |
| 1 | -1.000422 | -1.367869 | 2.619176 |
| 1 | 0.670014 | -0.683919 | 2.778575 |
| 1 | 0.403829 | -2.245943 | 1.920363 |
| 1 | -0.626396 | 0.551317 | -0.999653 |

Cartesian coordinates of : PACN9_17

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.995804 | 0.330935 | 3.751116 |
| 1 | -0.214848 | -0.294402 | 4.190742 |
| 1 | -1.796888 | 0.475266 | 4.480792 |
| 1 | -0.567610 | 1.297015 | 3.470593 |
| 6 | -1.524066 | -0.312304 | 2.551774 |
| 7 | -1.956495 | -0.819200 | 1.598447 |
| 6 | 2.295777 | -2.613625 | -2.309511 |
| 1 | 2.592686 | -3.553796 | -1.837713 |
| 1 | 2.610070 | -2.619668 | -3.356545 |
| 1 | 1.204764 | -2.531983 | -2.246057 |
| 6 | 2.918920 | -1.496970 | -1.604113 |
| 7 | 3.403481 | -0.600254 | -1.046095 |
| 6 | -3.825803 | -2.008765 | -1.122041 |
| 1 | -4.401957 | -1.290559 | -1.711061 |
| 1 | -3.796939 | -1.680098 | -0.078438 |
| 1 | -4.299230 | -2.992008 | -1.188735 |
| 6 | -2.459009 | -2.076299 | -1.629358 |
| 7 | -1.369488 | -2.152738 | -2.026342 |
| 6 | -1.167062 | -4.103992 | 0.859181 |
| 1 | -1.962677 | -3.403900 | 1.131101 |
| 1 | -1.088877 | -4.880122 | 1.624737 |
| 1 | -1.402461 | -4.569375 | -0.101664 |
| 6 | 0.093805 | -3.375309 | 0.755746 |
| 7 | 1.105449 | -2.808968 | 0.680415 |
| 6 | -4.110903 | 1.660511 | 0.964725 |
| 1 | -3.394661 | 2.079356 | 1.678331 |
| 1 | -4.483857 | 0.709910 | 1.355997 |
| 1 | -4.945921 | 2.353013 | 0.832325 |
| 6 | -3.434735 | 1.436896 | -0.309323 |
| 7 | -2.897868 | 1.264365 | -1.325307 |
| 6 | 3.927160 | 2.541939 | 0.180935 |
| 1 | 3.567000 | 2.633345 | 1.209373 |
| 1 | 4.653035 | 3.333690 | -0.020129 |
| 1 | 4.399822 | 1.565239 | 0.043372 |
| 6 | 2.802152 | 2.646292 | -0.742637 |
| 7 | 1.908812 | 2.729558 | -1.480789 |
| 6 | 3.804772 | -1.245937 | 2.155454 |
| 1 | 4.075333 | -1.340987 | 3.209786 |
| 1 | 4.628644 | -0.794827 | 1.595893 |
| 1 | 3.587467 | -2.232125 | 1.733408 |
| 6 | 2.610242 | -0.429151 | 2.005444 |
| 7 | 1.646127 | 0.202215 | 1.863091 |
| 6 | -0.901173 | 4.174905 | -0.842039 |
| 1 | -1.753099 | 4.856195 | -0.771678 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -1.043564 | 3.510926 | -1.700489 |
| 1 | 0.018329 | 4.744593 | -0.992091 |
| 6 | -0.801795 | 3.372345 | 0.373701 |
| 7 | -0.747734 | 2.716517 | 1.331721 |
| 6 | -0.158357 | 0.577448 | -2.993354 |
| 6 | 0.032977 | 0.394715 | -1.571889 |
| 7 | 0.223391 | 0.277506 | -0.445944 |
| 1 | -1.222917 | 0.750026 | -3.176478 |
| 1 | 0.165265 | -0.328119 | -3.514158 |
| 1 | 0.442768 | 1.441960 | -3.294604 |
| 1 | 0.578006 | 0.256639 | 0.546125 |

Cartesian coordinates of : PACN9_18

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.233053 | 2.748522 | 1.487839 |
| 1 | -1.401011 | 2.745709 | 0.776216 |
| 1 | -1.888808 | 3.160579 | 2.439938 |
| 1 | -3.034978 | 3.377744 | 1.092597 |
| 6 | -2.718783 | 1.385471 | 1.682894 |
| 7 | -3.100922 | 0.296926 | 1.822244 |
| 6 | -4.906999 | 0.582434 | -1.294396 |
| 1 | -5.614459 | 1.359872 | -1.593339 |
| 1 | -5.029795 | 0.358471 | -0.230321 |
| 1 | -5.096734 | -0.327658 | -1.868817 |
| 6 | -3.538118 | 1.031058 | -1.528743 |
| 7 | -2.448928 | 1.396376 | -1.705933 |
| 6 | 1.421224 | -2.403164 | 2.518152 |
| 1 | 0.678484 | -1.773924 | 3.018300 |
| 1 | 1.833418 | -3.112975 | 3.239812 |
| 1 | 0.946084 | -2.953678 | 1.700310 |
| 6 | 2.484280 | -1.562237 | 1.975203 |
| 7 | 3.315962 | -0.876382 | 1.540519 |
| 6 | 4.119656 | 1.542778 | -0.627386 |
| 1 | 4.933594 | 1.866202 | -1.281224 |
| 1 | 4.519672 | 0.957812 | 0.205102 |
| 1 | 3.598720 | 2.423619 | -0.238598 |
| 6 | 3.168159 | 0.726187 | -1.374294 |
| 7 | 2.406424 | 0.090029 | -1.979297 |
| 6 | 0.290954 | 2.699963 | -2.849715 |
| 1 | 0.275448 | 1.631574 | -3.084126 |
| 1 | 1.036226 | 3.194289 | -3.478148 |
| 1 | -0.699638 | 3.115551 | -3.044962 |
| 6 | 0.634763 | 2.877454 | -1.442320 |
| 7 | 0.935135 | 3.019954 | -0.328111 |
| 6 | 2.467362 | 2.575479 | 2.796775 |
| 1 | 3.405901 | 2.019955 | 2.702602 |
| 1 | 2.375898 | 2.964839 | 3.813654 |
| 1 | 2.449534 | 3.402480 | 2.080215 |
| 6 | 1.361849 | 1.681803 | 2.491127 |
| 7 | 0.494593 | 0.961651 | 2.219373 |
| 6 | -4.296063 | -2.868506 | 1.528222 |
| 1 | -4.193150 | -2.059683 | 2.256840 |
| 1 | -3.830300 | -3.776987 | 1.918240 |
| 1 | -5.355684 | -3.066336 | 1.347373 |
| 6 | -3.643089 | -2.463825 | 0.287408 |
| 7 | -3.124760 | -2.127831 | -0.696647 |
| 6 | 4.011389 | -2.827170 | -1.395830 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 4.525847 | -3.791113 | -1.411897 |
| 1 | 4.468594 | -2.182104 | -0.639009 |
| 1 | 4.101067 | -2.349191 | -2.374628 |
| 6 | 2.601057 | -3.013772 | -1.070334 |
| 7 | 1.479709 | -3.156221 | -0.800807 |
| 6 | -0.593309 | -1.408122 | -2.337113 |
| 6 | -0.425275 | -0.848734 | -1.016171 |
| 7 | -0.279596 | -0.376595 | 0.022189 |
| 1 | 0.345678 | -1.260541 | -2.879513 |
| 1 | -1.430276 | -0.893265 | -2.817472 |
| 1 | -0.816338 | -2.472732 | -2.234156 |
| 1 | -0.082339 | 0.112423 | 0.942376 |

Cartesian coordinates of : PACN9_19

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.687376 | -4.266012 | 0.941433 |
| 1 | 1.213625 | -5.080768 | 1.445024 |
| 1 | 0.148306 | -4.650947 | 0.072767 |
| 1 | -0.025982 | -3.808360 | 1.633497 |
| 6 | 1.638536 | -3.249136 | 0.506851 |
| 7 | 2.404004 | -2.441370 | 0.171074 |
| 6 | -2.998441 | 2.903577 | 2.755857 |
| 1 | -3.045796 | 2.690859 | 3.826674 |
| 1 | -3.792803 | 2.353255 | 2.241679 |
| 1 | -3.129544 | 3.976251 | 2.593864 |
| 6 | -1.720407 | 2.463808 | 2.215217 |
| 7 | -0.718542 | 2.090795 | 1.765132 |
| 6 | 2.439907 | 3.930616 | 0.183605 |
| 1 | 3.491873 | 3.751210 | -0.049010 |
| 1 | 2.197841 | 3.407274 | 1.113571 |
| 1 | 2.266252 | 5.001804 | 0.311871 |
| 6 | 1.605171 | 3.408767 | -0.894155 |
| 7 | 0.934208 | 2.985947 | -1.743537 |
| 6 | 2.006384 | -0.089285 | 2.758944 |
| 1 | 2.696305 | -0.549044 | 2.045337 |
| 1 | 2.426370 | -0.137405 | 3.766674 |
| 1 | 1.864281 | 0.959457 | 2.476663 |
| 6 | 0.726693 | -0.789708 | 2.706899 |
| 7 | -0.295914 | -1.336213 | 2.627123 |
| 6 | -3.282363 | -2.179159 | -2.534262 |
| 1 | -3.866720 | -3.102826 | -2.532084 |
| 1 | -3.093272 | -1.861956 | -3.562376 |
| 1 | -3.837935 | -1.383194 | -2.029375 |
| 6 | -2.011885 | -2.386080 | -1.845822 |
| 7 | -1.010463 | -2.557029 | -1.280402 |
| 6 | -3.167405 | -2.266650 | 1.579779 |
| 1 | -2.373051 | -2.873097 | 1.136106 |
| 1 | -4.141740 | -2.712970 | 1.363603 |
| 1 | -3.007334 | -2.226635 | 2.659386 |
| 6 | -3.101543 | -0.918726 | 1.022446 |
| 7 | -3.071356 | 0.149763 | 0.565210 |
| 6 | 5.361556 | -0.929042 | -0.679763 |
| 1 | 6.193060 | -0.807296 | 0.018970 |
| 1 | 5.743683 | -0.848809 | -1.700584 |
| 1 | 4.905173 | -1.912159 | -0.534718 |
| 6 | 4.351143 | 0.096484 | -0.439019 |
| 7 | 3.537421 | 0.902889 | -0.242883 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -2.488846 | 2.720234 | -1.692826 |
| 1 | -3.090161 | 2.440021 | -0.823259 |
| 1 | -3.069450 | 3.370578 | -2.352001 |
| 1 | -1.587497 | 3.249817 | -1.369811 |
| 6 | -2.093946 | 1.509196 | -2.403825 |
| 7 | -1.774536 | 0.539764 | -2.959063 |
| 6 | 1.266582 | -0.504135 | -2.346755 |
| 6 | 0.675480 | -0.032407 | -1.118820 |
| 7 | 0.211508 | 0.391090 | -0.156699 |
| 1 | 1.884594 | 0.310897 | -2.738935 |
| 1 | 0.455748 | -0.736430 | -3.043402 |
| 1 | 1.868138 | -1.390804 | -2.126612 |
| 1 | -0.172217 | 0.957781 | 0.640079 |

Cartesian coordinates of : PACN9_20

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.412804 | 0.637053 | 3.536641 |
| 1 | -0.362545 | 1.378684 | 3.326109 |
| 1 | 1.394224 | 1.086431 | 3.359557 |
| 1 | 0.338732 | 0.313221 | 4.577883 |
| 6 | 0.243226 | -0.507108 | 2.646489 |
| 7 | 0.123672 | -1.428362 | 1.947645 |
| 6 | -5.114779 | 0.108651 | -0.821792 |
| 1 | -4.899625 | 0.157893 | 0.250814 |
| 1 | -5.187456 | -0.938785 | -1.125608 |
| 1 | -6.063170 | 0.612046 | -1.025163 |
| 6 | -4.031665 | 0.757198 | -1.554452 |
| 7 | -3.165968 | 1.282251 | -2.124374 |
| 6 | 3.425363 | -2.378380 | 1.370337 |
| 1 | 4.169102 | -2.621547 | 2.133357 |
| 1 | 3.709785 | -2.847388 | 0.424234 |
| 1 | 2.447061 | -2.759807 | 1.678316 |
| 6 | 3.339329 | -0.930914 | 1.198899 |
| 7 | 3.284921 | 0.223158 | 1.075313 |
| 6 | 4.228646 | -0.274767 | -2.211194 |
| 1 | 4.965003 | -0.065405 | -1.430675 |
| 1 | 4.725858 | -0.281965 | -3.184381 |
| 1 | 3.771454 | -1.251406 | -2.027272 |
| 6 | 3.185852 | 0.746855 | -2.186501 |
| 7 | 2.359966 | 1.564614 | -2.171350 |
| 6 | 0.132257 | -4.138712 | -0.187542 |
| 1 | -0.790685 | -4.376942 | -0.722107 |
| 1 | -0.117722 | -3.799528 | 0.822297 |
| 1 | 0.763147 | -5.030144 | -0.137390 |
| 6 | 0.838911 | -3.064600 | -0.878282 |
| 7 | 1.426119 | -2.219826 | -1.419396 |
| 6 | -2.308334 | 3.494796 | 0.294892 |
| 1 | -3.288806 | 3.963365 | 0.177570 |
| 1 | -1.890516 | 3.304793 | -0.698713 |
| 1 | -1.645201 | 4.165031 | 0.847140 |
| 6 | -2.439346 | 2.229284 | 1.011276 |
| 7 | -2.528022 | 1.210152 | 1.563669 |
| 6 | 3.193756 | 3.559863 | 0.443222 |
| 1 | 3.940735 | 2.789784 | 0.656821 |
| 1 | 3.362964 | 4.433277 | 1.077780 |
| 1 | 3.258238 | 3.844921 | -0.610233 |
| 6 | 1.879618 | 2.992550 | 0.700245 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 0.836889 | 2.521477 | 0.900275 |
| 6 | -3.060640 | -2.152155 | 1.907857 |
| 1 | -3.022546 | -1.161025 | 2.368384 |
| 1 | -2.363015 | -2.812442 | 2.430410 |
| 1 | -4.072248 | -2.560280 | 1.981950 |
| 6 | -2.667350 | -2.036024 | 0.507166 |
| 7 | -2.366726 | -1.955636 | -0.612711 |
| 6 | -0.690030 | -0.463896 | -3.043465 |
| 6 | -0.439402 | 0.134038 | -1.753571 |
| 7 | -0.220543 | 0.627825 | -0.739973 |
| 1 | -1.193963 | 0.276700 | -3.670345 |
| 1 | -1.337739 | -1.332550 | -2.892035 |
| 1 | 0.270903 | -0.766335 | -3.469267 |
| 1 | 0.096567 | 1.217447 | 0.065516 |

Cartesian coordinates of : PACN9_21

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.946151 | 0.555324 | 3.898409 |
| 1 | -2.739105 | -0.192987 | 3.816582 |
| 1 | -2.169919 | 1.240199 | 4.719989 |
| 1 | -0.997985 | 0.046564 | 4.092874 |
| 6 | -1.839058 | 1.291206 | 2.642701 |
| 7 | -1.757863 | 1.869451 | 1.637746 |
| 6 | 3.042900 | -3.261203 | -2.223099 |
| 1 | 3.580099 | -4.199319 | -2.062149 |
| 1 | 3.624535 | -2.637735 | -2.907463 |
| 1 | 2.064505 | -3.476902 | -2.662124 |
| 6 | 2.851886 | -2.568770 | -0.951267 |
| 7 | 2.691404 | -2.020554 | 0.060532 |
| 6 | -2.981821 | -2.949544 | -1.811440 |
| 1 | -3.274333 | -3.979443 | -2.030884 |
| 1 | -3.414525 | -2.279430 | -2.558436 |
| 1 | -3.350033 | -2.667822 | -0.819992 |
| 6 | -1.527372 | -2.828885 | -1.830872 |
| 7 | -0.368028 | -2.748035 | -1.841050 |
| 6 | 3.805788 | -0.057813 | 2.642028 |
| 1 | 4.149461 | -0.494090 | 1.700035 |
| 1 | 4.166646 | -0.650737 | 3.486110 |
| 1 | 4.180180 | 0.965579 | 2.720675 |
| 6 | 2.350633 | -0.047413 | 2.622671 |
| 7 | 1.188560 | -0.047113 | 2.592912 |
| 6 | -4.343780 | 0.501338 | 0.142797 |
| 1 | -5.308943 | 0.210926 | -0.280452 |
| 1 | -4.413911 | 1.515498 | 0.545763 |
| 1 | -4.069062 | -0.182373 | 0.951388 |
| 6 | -3.309091 | 0.450938 | -0.885743 |
| 7 | -2.500208 | 0.401797 | -1.718934 |
| 6 | 3.339136 | 4.003935 | -1.018631 |
| 1 | 3.497104 | 4.670427 | -0.167009 |
| 1 | 2.412878 | 4.283139 | -1.527552 |
| 1 | 4.181821 | 4.102527 | -1.707487 |
| 6 | 3.228276 | 2.623118 | -0.556765 |
| 7 | 3.142326 | 1.523007 | -0.191321 |
| 6 | 0.049401 | -3.311469 | 1.688712 |
| 1 | -0.207774 | -4.154673 | 2.334816 |
| 1 | 0.889798 | -2.758176 | 2.116517 |
| 1 | 0.348730 | -3.675854 | 0.701879 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.098872 | -2.422480 | 1.544369 |
| 7 | -2.011634 | -1.713617 | 1.415676 |
| 6 | -2.342299 | 3.868694 | -1.094879 |
| 1 | -2.407666 | 4.958920 | -1.134521 |
| 1 | -2.609424 | 3.520019 | -0.093261 |
| 1 | -3.028178 | 3.439135 | -1.830023 |
| 6 | -0.979664 | 3.439177 | -1.390825 |
| 7 | 0.107755 | 3.108955 | -1.632500 |
| 6 | 0.714540 | 0.199806 | -2.572480 |
| 6 | 0.465043 | 0.173797 | -1.150861 |
| 7 | 0.280968 | 0.150370 | -0.018905 |
| 1 | 1.419642 | 1.010866 | -2.773928 |
| 1 | -0.238128 | 0.389752 | -3.076541 |
| 1 | 1.115363 | -0.773141 | -2.870206 |
| 1 | 0.308288 | 0.140777 | 1.017362 |

Cartesian coordinates of : PACN9_22

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.966939 | -0.017844 | 2.700229 |
| 1 | -2.374144 | 0.020036 | 1.685187 |
| 1 | -2.378705 | 0.809300 | 3.284535 |
| 1 | -2.246669 | -0.971856 | 3.154412 |
| 6 | -0.513579 | 0.094752 | 2.641327 |
| 7 | 0.644271 | 0.192618 | 2.590125 |
| 6 | 3.401380 | 3.439487 | -2.461807 |
| 1 | 3.700055 | 3.194811 | -3.484181 |
| 1 | 4.007858 | 2.865191 | -1.756386 |
| 1 | 3.557729 | 4.508013 | -2.293959 |
| 6 | 1.996755 | 3.100272 | -2.257480 |
| 7 | 0.880474 | 2.825833 | -2.089325 |
| 6 | -3.045050 | -3.074856 | -1.229825 |
| 1 | -3.920522 | -2.423913 | -1.164511 |
| 1 | -3.349489 | -4.115982 | -1.095544 |
| 1 | -2.573646 | -2.959789 | -2.210370 |
| 6 | -2.090668 | -2.695423 | -0.192784 |
| 7 | -1.326969 | -2.395989 | 0.631074 |
| 6 | 2.041899 | -3.699172 | -2.630007 |
| 1 | 2.670996 | -3.551504 | -3.511301 |
| 1 | 1.762511 | -4.753824 | -2.566929 |
| 1 | 2.601493 | -3.419571 | -1.733121 |
| 6 | 0.843132 | -2.871280 | -2.730138 |
| 7 | -0.106436 | -2.206838 | -2.811376 |
| 6 | -5.190521 | 2.309235 | 0.342271 |
| 1 | -4.395875 | 3.010048 | 0.612576 |
| 1 | -5.868611 | 2.178317 | 1.189281 |
| 1 | -5.755094 | 2.707148 | -0.504695 |
| 6 | -4.584416 | 1.031362 | -0.016664 |
| 7 | -4.089721 | 0.018567 | -0.299154 |
| 6 | 4.103951 | 0.039997 | 2.380463 |
| 1 | 3.238505 | -0.103072 | 3.034498 |
| 1 | 4.851488 | 0.652744 | 2.890354 |
| 1 | 4.541065 | -0.930925 | 2.132936 |
| 6 | 3.658584 | 0.701530 | 1.158725 |
| 7 | 3.296935 | 1.226947 | 0.187147 |
| 6 | 1.201772 | -3.182140 | 2.761932 |
| 1 | 1.458453 | -2.555990 | 3.621222 |
| 1 | 1.618134 | -4.183266 | 2.897948 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 0.113137 | -3.242364 | 2.668543 |
| 6 | 1.725251 | -2.572803 | 1.547663 |
| 7 | 2.128008 | -2.062516 | 0.584074 |
| 6 | 0.652223 | 3.378008 | 1.218081 |
| 1 | 0.856368 | 4.342910 | 0.747011 |
| 1 | 1.366951 | 2.638304 | 0.843217 |
| 1 | 0.762934 | 3.464273 | 2.302204 |
| 6 | -0.702902 | 2.948787 | 0.892522 |
| 7 | -1.780725 | 2.592964 | 0.640866 |
| 6 | -1.423028 | 0.724512 | -2.138281 |
| 6 | -0.351912 | 0.317489 | -1.262107 |
| 7 | 0.499364 | -0.038399 | -0.576924 |
| 1 | -2.228454 | -0.012312 | -2.053612 |
| 1 | -1.029554 | 0.757979 | -3.157831 |
| 1 | -1.770907 | 1.712855 | -1.825593 |
| 1 | 1.231994 | -0.541362 | -0.046153 |

Cartesian coordinates of : PACN9_23

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.741076 | -1.967664 | -3.107244 |
| 1 | 4.502898 | -2.746347 | -3.194717 |
| 1 | 4.225161 | -1.022481 | -2.841700 |
| 1 | 3.231625 | -1.861870 | -4.068537 |
| 6 | 2.780509 | -2.320440 | -2.065723 |
| 7 | 2.022008 | -2.575911 | -1.223218 |
| 6 | -1.973058 | -2.117254 | 4.384191 |
| 1 | -2.031545 | -1.466579 | 5.260004 |
| 1 | -1.727438 | -3.132963 | 4.703498 |
| 1 | -2.933959 | -2.118674 | 3.860131 |
| 6 | -0.964471 | -1.624311 | 3.459685 |
| 7 | -0.191216 | -1.227866 | 2.694450 |
| 6 | -2.595639 | 3.686558 | -2.670617 |
| 1 | -1.809361 | 4.312943 | -2.238068 |
| 1 | -3.567554 | 4.147803 | -2.478389 |
| 1 | -2.448070 | 3.608636 | -3.750633 |
| 6 | -2.536084 | 2.363699 | -2.055406 |
| 7 | -2.458621 | 1.322265 | -1.545277 |
| 6 | 3.033632 | 3.547099 | 1.064975 |
| 1 | 2.316325 | 4.175581 | 0.529318 |
| 1 | 3.705648 | 3.071091 | 0.344735 |
| 1 | 3.615857 | 4.162779 | 1.754979 |
| 6 | 2.308928 | 2.514669 | 1.798983 |
| 7 | 1.724547 | 1.684765 | 2.366073 |
| 6 | -1.585499 | 2.195962 | 1.751855 |
| 1 | -0.881747 | 1.790483 | 2.486623 |
| 1 | -2.124593 | 1.372879 | 1.267951 |
| 1 | -2.300429 | 2.851393 | 2.255656 |
| 6 | -0.839179 | 2.941987 | 0.743385 |
| 7 | -0.238725 | 3.505779 | -0.077698 |
| 6 | -4.413075 | -1.135050 | -1.131269 |
| 1 | -3.753589 | -1.140744 | -2.003542 |
| 1 | -4.989475 | -0.206792 | -1.133825 |
| 1 | -5.096094 | -1.987499 | -1.171546 |
| 6 | -3.600329 | -1.204054 | 0.079281 |
| 7 | -2.959505 | -1.277347 | 1.046840 |
| 6 | -0.939534 | -3.626551 | -0.524252 |
| 1 | -0.183230 | -4.364733 | -0.799930 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -1.894189 | -4.121601 | -0.328200 |
| 1 | -0.613970 | -3.111360 | 0.385446 |
| 6 | -1.091600 | -2.650535 | -1.599264 |
| 7 | -1.212932 | -1.859638 | -2.442265 |
| 6 | 3.407639 | -1.153530 | 1.591897 |
| 1 | 2.849937 | -2.035521 | 1.259805 |
| 1 | 2.835100 | -0.623737 | 2.360048 |
| 1 | 4.369090 | -1.467861 | 2.005800 |
| 6 | 3.612567 | -0.268362 | 0.449582 |
| 7 | 3.740557 | 0.429742 | -0.471836 |
| 6 | 0.738319 | 0.776464 | -2.031934 |
| 6 | 0.460887 | 0.232246 | -0.723051 |
| 7 | 0.272136 | -0.194966 | 0.327707 |
| 1 | 0.081304 | 0.275859 | -2.751091 |
| 1 | 1.795738 | 0.595972 | -2.252748 |
| 1 | 0.540102 | 1.853222 | -1.999782 |
| 1 | 0.128186 | -0.603253 | 1.324853 |

Cartesian coordinates of : PACN9_24

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.649833 | -0.947569 | 3.355834 |
| 1 | 4.295022 | -1.342139 | 2.565177 |
| 1 | 3.449415 | -1.731640 | 4.090088 |
| 1 | 4.142014 | -0.106201 | 3.849682 |
| 6 | 2.405691 | -0.512100 | 2.737323 |
| 7 | 1.422622 | -0.173290 | 2.221827 |
| 6 | -4.396470 | 1.973605 | -0.440162 |
| 1 | -5.419436 | 2.086338 | -0.072504 |
| 1 | -4.356659 | 2.227646 | -1.502178 |
| 1 | -3.730444 | 2.644862 | 0.110910 |
| 6 | -3.944403 | 0.599219 | -0.251344 |
| 7 | -3.587047 | -0.494811 | -0.087809 |
| 6 | 4.026199 | 0.734248 | -2.279307 |
| 1 | 4.294931 | 0.429603 | -1.263750 |
| 1 | 3.836672 | 1.809735 | -2.286338 |
| 1 | 4.843880 | 0.495576 | -2.963895 |
| 6 | 2.817694 | 0.021070 | -2.676840 |
| 7 | 1.864615 | -0.566102 | -2.988151 |
| 6 | -0.660324 | 4.180772 | -1.225140 |
| 1 | -1.230953 | 4.972163 | -1.717715 |
| 1 | 0.399055 | 4.291765 | -1.468938 |
| 1 | -0.792853 | 4.253257 | -0.141114 |
| 6 | -1.132033 | 2.872429 | -1.666149 |
| 7 | -1.533989 | 1.839236 | -2.012609 |
| 6 | 1.970054 | -3.501182 | -1.274096 |
| 1 | 1.855655 | -3.101482 | -2.286659 |
| 1 | 0.983636 | -3.627295 | -0.814654 |
| 1 | 2.470023 | -4.471919 | -1.322469 |
| 6 | 2.765367 | -2.566264 | -0.483441 |
| 7 | 3.390043 | -1.812763 | 0.143569 |
| 6 | -1.882329 | -0.184630 | 2.701977 |
| 1 | -1.240592 | -0.308458 | 3.577718 |
| 1 | -1.686648 | -0.994010 | 1.989911 |
| 1 | -2.931760 | -0.235253 | 3.003582 |
| 6 | -1.611293 | 1.103638 | 2.067819 |
| 7 | -1.388954 | 2.123340 | 1.555757 |
| 6 | 1.569740 | 3.364509 | 2.070651 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 1.311738 | 2.627677 | 2.836482 |
| 1 | 0.746220 | 4.079994 | 1.998432 |
| 1 | 2.486110 | 3.888369 | 2.353754 |
| 6 | 1.750114 | 2.684362 | 0.791120 |
| 7 | 1.894627 | 2.142121 | -0.226664 |
| 6 | -3.882383 | -3.844359 | 0.603050 |
| 1 | -4.454020 | -2.915952 | 0.519933 |
| 1 | -3.990032 | -4.253775 | 1.610620 |
| 1 | -4.264369 | -4.572378 | -0.117008 |
| 6 | -2.478753 | -3.557233 | 0.325785 |
| 7 | -1.362876 | -3.321703 | 0.103228 |
| 6 | -1.114767 | -1.197059 | -2.352013 |
| 6 | -0.433265 | -0.749423 | -1.159230 |
| 7 | 0.111925 | -0.431954 | -0.198428 |
| 1 | -0.793337 | -2.221755 | -2.560420 |
| 1 | -0.840326 | -0.531915 | -3.173074 |
| 1 | -2.190452 | -1.158417 | -2.157527 |
| 1 | 0.618707 | -0.207103 | 0.691881 |

Cartesian coordinates of : PACN9_25

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.692616 | -1.679517 | 2.730432 |
| 1 | -0.764517 | -1.125059 | 2.900165 |
| 1 | -1.447253 | -2.595217 | 2.185233 |
| 1 | -2.152062 | -1.933142 | 3.689216 |
| 6 | -2.608673 | -0.869111 | 1.934129 |
| 7 | -3.330329 | -0.210334 | 1.303943 |
| 6 | -3.920665 | 1.987406 | -1.223398 |
| 1 | -4.383896 | 1.647702 | -0.292889 |
| 1 | -4.694770 | 2.298448 | -1.929456 |
| 1 | -3.253475 | 2.829440 | -1.019182 |
| 6 | -3.136992 | 0.894161 | -1.787763 |
| 7 | -2.521966 | 0.019578 | -2.242483 |
| 6 | 5.426145 | -0.138070 | -1.133086 |
| 1 | 5.169627 | 0.890746 | -0.867038 |
| 1 | 6.005026 | -0.144180 | -2.059976 |
| 1 | 6.031846 | -0.574774 | -0.334927 |
| 6 | 4.197956 | -0.908028 | -1.304374 |
| 7 | 3.220382 | -1.519203 | -1.444985 |
| 6 | 1.606754 | 3.987762 | -1.909787 |
| 1 | 2.417873 | 3.386692 | -1.490225 |
| 1 | 1.753404 | 5.036023 | -1.637406 |
| 1 | 1.608167 | 3.902371 | -2.999390 |
| 6 | 0.334844 | 3.510413 | -1.374741 |
| 7 | -0.680021 | 3.135590 | -0.950757 |
| 6 | 1.783649 | -3.948130 | 0.502918 |
| 1 | 2.173050 | -4.734222 | 1.154835 |
| 1 | 2.457659 | -3.813933 | -0.348026 |
| 1 | 0.791432 | -4.232008 | 0.140410 |
| 6 | 1.684045 | -2.689031 | 1.235225 |
| 7 | 1.599870 | -1.681939 | 1.809434 |
| 6 | -2.271626 | 3.113016 | 2.137501 |
| 1 | -2.244937 | 3.835567 | 1.316400 |
| 1 | -2.190594 | 3.637299 | 3.092825 |
| 1 | -3.210775 | 2.551809 | 2.104756 |
| 6 | -1.165319 | 2.183001 | 1.970470 |
| 7 | -0.297289 | 1.429341 | 1.811080 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 2.969763 | 1.047749 | 2.849353 |
| 1 | 3.566840 | 0.145070 | 2.997919 |
| 1 | 1.959998 | 0.852007 | 3.218706 |
| 1 | 3.415141 | 1.882324 | 3.396561 |
| 6 | 2.897819 | 1.364691 | 1.426400 |
| 7 | 2.839514 | 1.631192 | 0.296164 |
| 6 | -3.970230 | -2.698229 | -1.150717 |
| 1 | -4.039482 | -2.439712 | -2.210194 |
| 1 | -4.394326 | -1.880536 | -0.560436 |
| 1 | -4.525220 | -3.619818 | -0.958437 |
| 6 | -2.569060 | -2.871598 | -0.781427 |
| 7 | -1.455775 | -3.013227 | -0.477942 |
| 6 | 0.348353 | -1.484950 | -2.590978 |
| 6 | 0.299386 | -0.696858 | -1.379443 |
| 7 | 0.254922 | -0.061984 | -0.424259 |
| 1 | 1.105263 | -1.063716 | -3.256850 |
| 1 | -0.647412 | -1.457983 | -3.042354 |
| 1 | 0.629660 | -2.506380 | -2.321127 |
| 1 | 0.177366 | 0.494021 | 0.465237 |

Cartesian coordinates of : PACN9_26

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.936194 | -0.531615 | 3.649553 |
| 1 | 2.346101 | -1.367161 | 3.073707 |
| 1 | 1.667441 | -0.864012 | 4.655501 |
| 1 | 2.682164 | 0.264594 | 3.700598 |
| 6 | 0.758775 | -0.045813 | 2.945758 |
| 7 | -0.183411 | 0.322089 | 2.370812 |
| 6 | 4.254094 | -2.026203 | -0.541702 |
| 1 | 4.012797 | -1.658510 | 0.460148 |
| 1 | 5.297455 | -1.801246 | -0.776887 |
| 1 | 4.105330 | -3.108709 | -0.569422 |
| 6 | 3.369594 | -1.374654 | -1.503121 |
| 7 | 2.656340 | -0.843369 | -2.251436 |
| 6 | -3.661435 | 1.248085 | 1.613618 |
| 1 | -2.861016 | 0.931223 | 2.289410 |
| 1 | -4.372181 | 0.424323 | 1.504258 |
| 1 | -4.177376 | 2.116772 | 2.031319 |
| 6 | -3.087689 | 1.580661 | 0.311773 |
| 7 | -2.627757 | 1.859576 | -0.718576 |
| 6 | -4.425757 | -0.719784 | -2.103412 |
| 1 | -5.092880 | -1.359310 | -2.686625 |
| 1 | -4.730336 | 0.323678 | -2.218428 |
| 1 | -4.480863 | -1.000558 | -1.047397 |
| 6 | -3.048993 | -0.880168 | -2.558080 |
| 7 | -1.952179 | -1.011865 | -2.917262 |
| 6 | -0.808913 | 3.948658 | 1.485015 |
| 1 | -0.345432 | 4.733192 | 2.088334 |
| 1 | -0.930355 | 3.048886 | 2.096790 |
| 1 | -1.788708 | 4.291067 | 1.141236 |
| 6 | 0.031550 | 3.639285 | 0.332260 |
| 7 | 0.697950 | 3.389157 | -0.585235 |
| 6 | 0.104081 | -3.170147 | -1.378542 |
| 1 | 0.252725 | -4.231048 | -1.595315 |
| 1 | 0.541835 | -2.568995 | -2.182091 |
| 1 | -0.965983 | -2.947620 | -1.330292 |
| 6 | 0.729988 | -2.820288 | -0.107636 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 1.215716 | -2.514197 | 0.904238 |
| 6 | -1.655699 | -2.751966 | 2.877739 |
| 1 | -1.839175 | -2.064028 | 3.707735 |
| 1 | -0.583800 | -2.964126 | 2.813952 |
| 1 | -2.199914 | -3.682821 | 3.055662 |
| 6 | -2.096042 | -2.141088 | 1.626730 |
| 7 | -2.438105 | -1.647068 | 0.631603 |
| 6 | 3.821098 | 2.334516 | -1.028132 |
| 1 | 4.857676 | 2.621777 | -0.834211 |
| 1 | 3.204326 | 3.230256 | -1.136357 |
| 1 | 3.777405 | 1.752094 | -1.954210 |
| 6 | 3.308143 | 1.523710 | 0.072530 |
| 7 | 2.902158 | 0.859113 | 0.935365 |
| 6 | 0.213732 | 1.149567 | -2.888690 |
| 6 | 0.102187 | 0.615545 | -1.553500 |
| 7 | 0.007992 | 0.229138 | -0.475678 |
| 1 | -0.704611 | 1.712439 | -3.087855 |
| 1 | 0.321445 | 0.322464 | -3.593859 |
| 1 | 1.083476 | 1.812280 | -2.915698 |
| 1 | -0.097911 | 0.065295 | 0.540210 |

Cartesian coordinates of : PACN9_27

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.194224 | -1.798075 | -3.498087 |
| 1 | 4.159177 | -2.235877 | -3.228920 |
| 1 | 3.311902 | -0.721945 | -3.655980 |
| 1 | 2.841202 | -2.266357 | -4.420364 |
| 6 | 2.229027 | -2.009333 | -2.423371 |
| 7 | 1.461769 | -2.154021 | -1.562361 |
| 6 | -2.578563 | -1.500221 | 2.048776 |
| 1 | -1.659218 | -1.505696 | 2.642119 |
| 1 | -3.367384 | -2.027087 | 2.591752 |
| 1 | -2.885455 | -0.461848 | 1.882601 |
| 6 | -2.336868 | -2.139634 | 0.758510 |
| 7 | -2.138501 | -2.616523 | -0.283435 |
| 6 | -5.074443 | -1.210678 | -1.785008 |
| 1 | -6.024343 | -1.350660 | -1.262990 |
| 1 | -4.518952 | -2.153502 | -1.780861 |
| 1 | -5.278738 | -0.912554 | -2.816376 |
| 6 | -4.279892 | -0.186638 | -1.112663 |
| 7 | -3.627772 | 0.608948 | -0.571662 |
| 6 | 3.850042 | -0.431519 | 0.367793 |
| 1 | 3.981836 | -0.234408 | -0.700519 |
| 1 | 3.306195 | -1.371696 | 0.492122 |
| 1 | 4.827059 | -0.501562 | 0.852674 |
| 6 | 3.074273 | 0.653517 | 0.958710 |
| 7 | 2.464670 | 1.527351 | 1.423291 |
| 6 | 1.505289 | 0.785471 | 4.522695 |
| 1 | 1.948294 | -0.191388 | 4.304491 |
| 1 | 1.159368 | 0.812787 | 5.558807 |
| 1 | 2.251430 | 1.566499 | 4.355477 |
| 6 | 0.393969 | 0.985279 | 3.607340 |
| 7 | -0.472218 | 1.123494 | 2.846021 |
| 6 | 0.826410 | -4.138014 | 0.868922 |
| 1 | 0.090866 | -4.073099 | 0.062814 |
| 1 | 0.527136 | -4.905633 | 1.587108 |
| 1 | 1.795411 | -4.401786 | 0.437685 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.921044 | -2.841810 | 1.534551 |
| 7 | 0.993653 | -1.814296 | 2.074672 |
| 6 | 2.139664 | 3.682211 | -1.307470 |
| 1 | 1.377378 | 4.258511 | -1.836509 |
| 1 | 3.114701 | 4.164084 | -1.415442 |
| 1 | 1.878274 | 3.626817 | -0.246480 |
| 6 | 2.191786 | 2.329886 | -1.851680 |
| 7 | 2.246405 | 1.248072 | -2.274354 |
| 6 | -2.628428 | 3.494533 | 0.630406 |
| 1 | -2.481549 | 4.499267 | 1.034119 |
| 1 | -2.380155 | 2.755012 | 1.398857 |
| 1 | -3.673497 | 3.360209 | 0.342580 |
| 6 | -1.770412 | 3.288210 | -0.532468 |
| 7 | -1.075864 | 3.101630 | -1.445564 |
| 6 | -0.819100 | -0.088292 | -2.292829 |
| 6 | -0.518623 | 0.163605 | -0.903684 |
| 7 | -0.321145 | 0.379376 | 0.207723 |
| 1 | -1.603637 | 0.615478 | -2.587725 |
| 1 | -1.151246 | -1.128133 | -2.381759 |
| 1 | 0.088430 | 0.086170 | -2.877580 |
| 1 | -0.267865 | 0.639201 | 1.225336 |

Cartesian coordinates of : PACN9_28

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.305127 | 1.794811 | 1.746081 |
| 1 | 2.826216 | 1.359326 | 2.602179 |
| 1 | 2.716220 | 2.783248 | 1.523274 |
| 1 | 2.443592 | 1.139935 | 0.880891 |
| 6 | 0.880698 | 1.907217 | 2.038705 |
| 7 | -0.256307 | 2.007409 | 2.260578 |
| 6 | -4.471019 | -0.138961 | -2.881243 |
| 1 | -4.323475 | 0.867967 | -2.482062 |
| 1 | -5.355336 | -0.584432 | -2.418652 |
| 1 | -4.625592 | -0.086209 | -3.961807 |
| 6 | -3.291807 | -0.946176 | -2.583617 |
| 7 | -2.350050 | -1.585610 | -2.351349 |
| 6 | -0.729141 | 4.243940 | -0.540973 |
| 1 | -1.626814 | 4.134967 | -1.154014 |
| 1 | -0.356968 | 5.269250 | -0.609311 |
| 1 | -0.982819 | 4.010562 | 0.497372 |
| 6 | 0.293836 | 3.311311 | -1.003868 |
| 7 | 1.122046 | 2.581797 | -1.369073 |
| 6 | -3.639919 | 1.656517 | 1.922298 |
| 1 | -4.429980 | 2.410129 | 1.971188 |
| 1 | -2.838385 | 1.915170 | 2.620170 |
| 1 | -4.051491 | 0.680634 | 2.192097 |
| 6 | -3.083495 | 1.599214 | 0.573581 |
| 7 | -2.643474 | 1.566356 | -0.502180 |
| 6 | 4.457299 | 1.987086 | -2.228787 |
| 1 | 3.653150 | 2.724313 | -2.309094 |
| 1 | 4.817156 | 1.729028 | -3.228005 |
| 1 | 5.284900 | 2.412116 | -1.655296 |
| 6 | 3.939963 | 0.798090 | -1.558398 |
| 7 | 3.508692 | -0.139681 | -1.024209 |
| 6 | -1.558282 | -4.055784 | -0.338371 |
| 1 | -2.218096 | -4.240920 | -1.189066 |
| 1 | -1.969391 | -3.228929 | 0.249504 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -1.497524 | -4.951601 | 0.284552 |
| 6 | -0.230758 | -3.689951 | -0.822057 |
| 7 | 0.823861 | -3.380221 | -1.199170 |
| 6 | -0.671803 | -0.689625 | 4.424666 |
| 1 | -1.157328 | -1.360830 | 5.137160 |
| 1 | -0.820225 | 0.349608 | 4.731375 |
| 1 | 0.400191 | -0.905340 | 4.381217 |
| 6 | -1.217302 | -0.878083 | 3.089601 |
| 7 | -1.623882 | -1.004444 | 2.008733 |
| 6 | 3.487503 | -2.841518 | 0.843169 |
| 1 | 4.422087 | -2.283206 | 0.752492 |
| 1 | 3.125952 | -3.095018 | -0.156766 |
| 1 | 3.658018 | -3.757062 | 1.415224 |
| 6 | 2.488370 | -2.016089 | 1.514183 |
| 7 | 1.697048 | -1.361572 | 2.059554 |
| 6 | 0.799190 | -0.510755 | -2.677906 |
| 6 | 0.273653 | -0.423681 | -1.336026 |
| 7 | -0.183309 | -0.373609 | -0.283408 |
| 1 | 1.116550 | 0.486482 | -2.994936 |
| 1 | -0.003832 | -0.900375 | -3.311866 |
| 1 | 1.642428 | -1.206586 | -2.666098 |
| 1 | -0.704263 | -0.490581 | 0.615717 |

Cartesian coordinates of : PACN9_29

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.297021 | -3.031691 | 1.493005 |
| 1 | -3.167682 | -2.528465 | 1.920544 |
| 1 | -1.410774 | -2.744344 | 2.065885 |
| 1 | -2.433657 | -4.115017 | 1.541418 |
| 6 | -2.112824 | -2.610048 | 0.108031 |
| 7 | -1.958091 | -2.288256 | -0.998068 |
| 6 | 0.089325 | 3.508473 | -2.167013 |
| 1 | 1.002237 | 2.973970 | -2.452159 |
| 1 | 0.206301 | 4.564916 | -2.421586 |
| 1 | -0.772945 | 3.099262 | -2.701050 |
| 6 | -0.120162 | 3.353930 | -0.730830 |
| 7 | -0.266778 | 3.206283 | 0.412825 |
| 6 | 0.441414 | -0.994029 | 4.007886 |
| 1 | 0.752993 | -2.024003 | 3.809760 |
| 1 | -0.649230 | -0.945753 | 4.085846 |
| 1 | 0.890641 | -0.643222 | 4.940145 |
| 6 | 0.862000 | -0.163735 | 2.890819 |
| 7 | 1.174010 | 0.477553 | 1.975632 |
| 6 | 3.020141 | 3.204045 | 1.465607 |
| 1 | 1.996965 | 3.395622 | 1.802397 |
| 1 | 3.558220 | 4.149637 | 1.363006 |
| 1 | 3.527748 | 2.577903 | 2.204073 |
| 6 | 2.967507 | 2.511424 | 0.181690 |
| 7 | 2.905712 | 1.956294 | -0.838004 |
| 6 | 0.989903 | -4.101344 | -1.151925 |
| 1 | 0.480370 | -3.489449 | -1.902037 |
| 1 | 0.416978 | -5.017831 | -0.988151 |
| 1 | 1.986755 | -4.349944 | -1.523387 |
| 6 | 1.093826 | -3.348555 | 0.095451 |
| 7 | 1.159956 | -2.749009 | 1.089509 |
| 6 | -3.087238 | 2.572565 | 1.618289 |
| 1 | -4.077054 | 2.589575 | 2.081797 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -3.158564 | 2.882336 | 0.571703 |
| 1 | -2.422983 | 3.270779 | 2.132208 |
| 6 | -2.527474 | 1.225603 | 1.684222 |
| 7 | -2.109209 | 0.142105 | 1.738778 |
| 6 | 4.129652 | -0.998240 | -0.033412 |
| 1 | 4.697121 | -1.862105 | 0.322071 |
| 1 | 3.414594 | -0.695030 | 0.739310 |
| 1 | 4.809328 | -0.167934 | -0.238968 |
| 6 | 3.398487 | -1.347023 | -1.246922 |
| 7 | 2.794398 | -1.639309 | -2.195503 |
| 6 | -4.541387 | -0.219090 | -1.150496 |
| 1 | -5.478712 | 0.316114 | -1.321801 |
| 1 | -4.444942 | -0.461776 | -0.087530 |
| 1 | -4.542337 | -1.150219 | -1.722597 |
| 6 | -3.408836 | 0.606283 | -1.559275 |
| 7 | -2.511961 | 1.273872 | -1.875510 |
| 6 | -0.120500 | -0.441758 | -3.063610 |
| 6 | 0.154719 | -0.104446 | -1.684469 |
| 7 | 0.399470 | 0.165473 | -0.595515 |
| 1 | -0.955644 | -1.149039 | -3.075097 |
| 1 | 0.784996 | -0.890533 | -3.485218 |
| 1 | -0.400697 | 0.468344 | -3.601227 |
| 1 | 0.688233 | 0.396981 | 0.399351 |

Cartesian coordinates of : PACN9_30

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.768720 | 3.606909 | 1.324989 |
| 1 | -1.394909 | 4.504632 | 1.824142 |
| 1 | -2.792240 | 3.401430 | 1.648653 |
| 1 | -1.756329 | 3.753156 | 0.239445 |
| 6 | -0.920457 | 2.463578 | 1.627405 |
| 7 | -0.235203 | 1.549652 | 1.833772 |
| 6 | 4.982230 | -0.769192 | -1.265834 |
| 1 | 5.274718 | -1.749749 | -0.882312 |
| 1 | 4.983983 | -0.051370 | -0.440759 |
| 1 | 5.686877 | -0.449549 | -2.037572 |
| 6 | 3.633666 | -0.844349 | -1.816965 |
| 7 | 2.559841 | -0.901154 | -2.257790 |
| 6 | -2.498451 | -0.666672 | 3.516886 |
| 1 | -3.090276 | -1.181091 | 4.278086 |
| 1 | -3.110677 | 0.089653 | 3.018323 |
| 1 | -1.645109 | -0.177965 | 3.994464 |
| 6 | -2.025920 | -1.622442 | 2.519066 |
| 7 | -1.652374 | -2.386359 | 1.726969 |
| 6 | 3.059681 | -0.514483 | 3.036676 |
| 1 | 3.061261 | -1.019835 | 4.005549 |
| 1 | 2.125449 | 0.042633 | 2.910398 |
| 1 | 3.887110 | 0.197759 | 2.992090 |
| 6 | 3.193825 | -1.490956 | 1.959763 |
| 7 | 3.282847 | -2.268005 | 1.100713 |
| 6 | -3.995130 | -2.740985 | -0.466743 |
| 1 | -4.369952 | -1.984684 | 0.229501 |
| 1 | -3.620811 | -3.589307 | 0.111292 |
| 1 | -4.802477 | -3.070141 | -1.125647 |
| 6 | -2.908283 | -2.164963 | -1.252239 |
| 7 | -2.054100 | -1.690445 | -1.881740 |
| 6 | -3.702423 | 1.411412 | -2.020365 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.770169 | 1.456069 | -2.249506 |
| 1 | -3.226035 | 0.652254 | -2.648536 |
| 1 | -3.245029 | 2.382449 | -2.228059 |
| 6 | -3.504190 | 1.061498 | -0.616386 |
| 7 | -3.359486 | 0.776625 | 0.501082 |
| 6 | 2.006608 | 3.834684 | 0.097727 |
| 1 | 1.806377 | 4.292310 | 1.070924 |
| 1 | 1.084055 | 3.795482 | -0.489138 |
| 1 | 2.745843 | 4.441474 | -0.431251 |
| 6 | 2.511633 | 2.477698 | 0.286873 |
| 7 | 2.911749 | 1.399204 | 0.449246 |
| 6 | -0.015414 | 0.515077 | -3.631157 |
| 1 | -0.672820 | 0.865471 | -4.432018 |
| 1 | -0.248564 | -0.527664 | -3.399702 |
| 1 | 1.027100 | 0.578754 | -3.949120 |
| 6 | -0.222035 | 1.328018 | -2.436842 |
| 7 | -0.417510 | 1.986925 | -1.498555 |
| 6 | 0.691332 | -2.946861 | -0.838651 |
| 6 | 0.549782 | -1.632251 | -0.259371 |
| 7 | 0.425269 | -0.607637 | 0.244172 |
| 1 | -0.062859 | -3.590954 | -0.374810 |
| 1 | 1.703686 | -3.300899 | -0.619974 |
| 1 | 0.532910 | -2.874765 | -1.917504 |
| 1 | 0.255260 | 0.268482 | 0.788962 |

Cartesian coordinates of : PACN9_31

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.284429 | 2.740101 | 2.833415 |
| 1 | -2.962159 | 2.860581 | 1.982706 |
| 1 | -1.643484 | 3.622487 | 2.900699 |
| 1 | -2.859413 | 2.619390 | 3.754710 |
| 6 | -1.458379 | 1.567201 | 2.590590 |
| 7 | -0.803566 | 0.633769 | 2.370597 |
| 6 | 3.156622 | 3.114320 | -0.102806 |
| 1 | 4.017145 | 2.587230 | 0.317027 |
| 1 | 2.413324 | 3.253774 | 0.687118 |
| 1 | 3.469715 | 4.086425 | -0.491858 |
| 6 | 2.563322 | 2.315900 | -1.170252 |
| 7 | 2.084972 | 1.690148 | -2.025417 |
| 6 | 4.610137 | -0.553047 | -1.227497 |
| 1 | 4.733039 | 0.152549 | -2.053474 |
| 1 | 5.467787 | -1.229751 | -1.198840 |
| 1 | 4.544070 | -0.003456 | -0.283966 |
| 6 | 3.378342 | -1.312006 | -1.414621 |
| 7 | 2.401092 | -1.920766 | -1.569304 |
| 6 | 0.642971 | -4.502940 | -0.512274 |
| 1 | -0.184569 | -4.333122 | -1.208684 |
| 1 | 0.566785 | -5.514233 | -0.105012 |
| 1 | 1.588247 | -4.385641 | -1.046811 |
| 6 | 0.569118 | -3.520207 | 0.564454 |
| 7 | 0.487794 | -2.734161 | 1.416682 |
| 6 | -2.833087 | -2.108115 | 1.539807 |
| 1 | -3.253791 | -1.105605 | 1.664146 |
| 1 | -1.891037 | -2.167234 | 2.093864 |
| 1 | -3.534011 | -2.852588 | 1.925858 |
| 6 | -2.570097 | -2.347027 | 0.124172 |
| 7 | -2.349863 | -2.506899 | -1.006548 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.026581 | 3.154597 | -2.121414 |
| 1 | -0.205124 | 2.728139 | -2.706124 |
| 1 | -1.270230 | 4.143970 | -2.516963 |
| 1 | -1.909873 | 2.513392 | -2.193439 |
| 6 | -0.619428 | 3.255956 | -0.722999 |
| 7 | -0.282642 | 3.328582 | 0.386754 |
| 6 | 1.971035 | -0.719212 | 3.711251 |
| 1 | 1.518463 | 0.044909 | 4.348202 |
| 1 | 2.860682 | -1.120380 | 4.203136 |
| 1 | 1.250893 | -1.523737 | 3.541266 |
| 6 | 2.331435 | -0.134517 | 2.423704 |
| 7 | 2.611931 | 0.335917 | 1.398496 |
| 6 | -4.831553 | -0.224031 | -1.948314 |
| 1 | -5.774812 | -0.407478 | -1.427364 |
| 1 | -4.398474 | -1.182046 | -2.250896 |
| 1 | -5.032709 | 0.384113 | -2.833901 |
| 6 | -3.899375 | 0.468099 | -1.060963 |
| 7 | -3.151866 | 1.005593 | -0.350338 |
| 6 | -0.163247 | -0.678082 | -2.660506 |
| 6 | -0.084862 | -0.365581 | -1.250745 |
| 7 | -0.070088 | -0.106304 | -0.133080 |
| 1 | -1.135954 | -0.342756 | -3.035064 |
| 1 | -0.070166 | -1.761266 | -2.776307 |
| 1 | 0.661440 | -0.169225 | -3.168559 |
| 1 | -0.171803 | 0.111947 | 0.893624 |

Cartesian coordinates of : PACN9_32

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.146450 | 0.194802 | 1.618312 |
| 1 | 5.134746 | 0.578670 | 1.353235 |
| 1 | 3.996419 | -0.780478 | 1.145328 |
| 1 | 4.083298 | 0.086438 | 2.704654 |
| 6 | 3.108266 | 1.110765 | 1.157579 |
| 7 | 2.268067 | 1.833794 | 0.808945 |
| 6 | -3.026488 | -4.135585 | -0.768311 |
| 1 | -3.547784 | -4.791516 | -0.066484 |
| 1 | -2.730586 | -4.720336 | -1.642996 |
| 1 | -3.702072 | -3.331454 | -1.076187 |
| 6 | -1.849950 | -3.551572 | -0.129590 |
| 7 | -0.923192 | -3.061058 | 0.372305 |
| 6 | 0.886089 | 3.431856 | -1.688510 |
| 1 | 1.747654 | 4.017930 | -1.359671 |
| 1 | 0.274530 | 3.176961 | -0.816712 |
| 1 | 0.281657 | 4.009042 | -2.392270 |
| 6 | 1.339925 | 2.200869 | -2.326400 |
| 7 | 1.690612 | 1.209504 | -2.821275 |
| 6 | -3.978743 | 2.607444 | -0.764410 |
| 1 | -4.769496 | 1.861821 | -0.879897 |
| 1 | -4.345845 | 3.583079 | -1.092448 |
| 1 | -3.683216 | 2.663187 | 0.287414 |
| 6 | -2.819918 | 2.212355 | -1.557622 |
| 7 | -1.896387 | 1.893591 | -2.186457 |
| 6 | 3.702046 | -1.427231 | -3.109319 |
| 1 | 3.305150 | -0.539402 | -3.608948 |
| 1 | 3.530617 | -2.310834 | -3.729377 |
| 1 | 4.777515 | -1.308193 | -2.954986 |
| 6 | 3.028857 | -1.580373 | -1.822733 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 2.493628 | -1.703566 | -0.797610 |
| 6 | -2.842347 | -0.587824 | 2.192607 |
| 1 | -3.355306 | -1.380561 | 2.743441 |
| 1 | -3.105814 | 0.384468 | 2.615782 |
| 1 | -1.759548 | -0.727840 | 2.283264 |
| 6 | -3.221103 | -0.636985 | 0.784180 |
| 7 | -3.507519 | -0.703254 | -0.340744 |
| 6 | 0.489563 | 2.877712 | 3.360640 |
| 1 | 1.249552 | 3.534855 | 2.930925 |
| 1 | 0.967701 | 1.953447 | 3.698199 |
| 1 | 0.007201 | 3.374696 | 4.205887 |
| 6 | -0.499878 | 2.545702 | 2.341065 |
| 7 | -1.287398 | 2.269789 | 1.530929 |
| 6 | 1.678004 | -3.063154 | 2.307981 |
| 1 | 0.889092 | -3.761162 | 2.597583 |
| 1 | 2.559210 | -3.222869 | 2.935083 |
| 1 | 1.927918 | -3.228007 | 1.256270 |
| 6 | 1.199662 | -1.694025 | 2.456925 |
| 7 | 0.830189 | -0.597383 | 2.574117 |
| 6 | -0.765092 | -0.974251 | -2.385230 |
| 6 | -0.371641 | -0.361769 | -1.139679 |
| 7 | -0.049727 | 0.104702 | -0.142519 |
| 1 | -0.270004 | -1.948049 | -2.452858 |
| 1 | -0.451770 | -0.310744 | -3.197036 |
| 1 | -1.855729 | -1.077789 | -2.379369 |
| 1 | 0.294790 | 0.479383 | 0.743438 |

Cartesian coordinates of : PACN9_33

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.297707 | -3.918577 | 2.204244 |
| 1 | 0.574015 | -4.364233 | 3.162916 |
| 1 | 0.932070 | -4.325798 | 1.411189 |
| 1 | -0.752247 | -4.137387 | 1.985013 |
| 6 | 0.475120 | -2.475705 | 2.241534 |
| 7 | 0.596261 | -1.321107 | 2.233812 |
| 6 | -4.598975 | -0.934049 | -1.629876 |
| 1 | -4.275034 | -1.109049 | -2.658732 |
| 1 | -5.685378 | -0.819668 | -1.599033 |
| 1 | -4.300511 | -1.787165 | -1.012806 |
| 6 | -3.953721 | 0.269157 | -1.115720 |
| 7 | -3.444364 | 1.227291 | -0.698314 |
| 6 | 4.282465 | -1.624970 | -1.012348 |
| 1 | 4.959851 | -2.478053 | -0.922980 |
| 1 | 4.553222 | -0.860021 | -0.278608 |
| 1 | 4.355894 | -1.208959 | -2.020605 |
| 6 | 2.910347 | -2.054546 | -0.760301 |
| 7 | 1.825999 | -2.419492 | -0.556555 |
| 6 | 5.081204 | 2.179712 | -1.219242 |
| 1 | 5.226217 | 1.866041 | -0.181217 |
| 1 | 5.173744 | 3.266711 | -1.284022 |
| 1 | 5.848115 | 1.723300 | -1.850912 |
| 6 | 3.754229 | 1.759572 | -1.658923 |
| 7 | 2.701788 | 1.403882 | -1.997864 |
| 6 | -1.167440 | -3.813079 | -1.504676 |
| 1 | -1.866154 | -3.981566 | -0.680149 |
| 1 | -0.143514 | -3.975496 | -1.156746 |
| 1 | -1.388774 | -4.502191 | -2.323560 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.294856 | -2.432627 | -1.959500 |
| 7 | -1.408520 | -1.334519 | -2.322086 |
| 6 | -3.127548 | 4.534301 | 0.175611 |
| 1 | -3.838973 | 3.813587 | -0.236848 |
| 1 | -2.951898 | 5.331973 | -0.550519 |
| 1 | -3.538041 | 4.971625 | 1.089172 |
| 6 | -1.878001 | 3.840911 | 0.470445 |
| 7 | -0.887184 | 3.278788 | 0.700489 |
| 6 | 1.582556 | 1.850187 | 2.920400 |
| 1 | 2.033247 | 2.648628 | 3.515281 |
| 1 | 1.170035 | 1.089349 | 3.588768 |
| 1 | 0.778886 | 2.274804 | 2.307751 |
| 6 | 2.587725 | 1.237604 | 2.056018 |
| 7 | 3.367320 | 0.739053 | 1.353468 |
| 6 | -2.401659 | 0.261101 | 2.328962 |
| 1 | -1.762547 | 0.127534 | 3.206747 |
| 1 | -3.393722 | 0.591236 | 2.647893 |
| 1 | -1.973366 | 1.029720 | 1.676743 |
| 6 | -2.505476 | -1.003253 | 1.604807 |
| 7 | -2.566418 | -2.015759 | 1.037023 |
| 6 | -0.361302 | 1.628631 | -2.125351 |
| 6 | -0.013312 | 0.861620 | -0.953316 |
| 7 | 0.256831 | 0.259841 | -0.012165 |
| 1 | -1.451240 | 1.717883 | -2.154934 |
| 1 | 0.008164 | 1.090716 | -3.001713 |
| 1 | 0.120310 | 2.606583 | -2.047706 |
| 1 | 0.481258 | -0.321904 | 0.828342 |

Cartesian coordinates of : PACN9_34

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.156172 | -3.446115 | 1.297202 |
| 1 | 0.933278 | -4.212333 | 1.372170 |
| 1 | -0.720078 | -3.746506 | 1.876017 |
| 1 | 0.531751 | -2.501904 | 1.704981 |
| 6 | -0.213837 | -3.247524 | -0.101010 |
| 7 | -0.471768 | -3.084736 | -1.223031 |
| 6 | 3.234269 | 1.202845 | -2.220518 |
| 1 | 2.954884 | 0.144951 | -2.249712 |
| 1 | 4.233450 | 1.318801 | -2.647936 |
| 1 | 2.520950 | 1.792728 | -2.804602 |
| 6 | 3.221171 | 1.662739 | -0.835264 |
| 7 | 3.201107 | 2.035390 | 0.264844 |
| 6 | -3.344171 | 2.804969 | -1.422450 |
| 1 | -4.057353 | 3.617243 | -1.261100 |
| 1 | -3.871436 | 1.913453 | -1.771437 |
| 1 | -2.613941 | 3.115211 | -2.177350 |
| 6 | -2.643667 | 2.493147 | -0.179964 |
| 7 | -2.061339 | 2.253567 | 0.797119 |
| 6 | -3.831538 | -2.955385 | -0.511981 |
| 1 | -4.915952 | -3.090557 | -0.502982 |
| 1 | -3.439842 | -3.061005 | 0.503736 |
| 1 | -3.375211 | -3.710397 | -1.157329 |
| 6 | -3.496420 | -1.623970 | -1.004838 |
| 7 | -3.232961 | -0.563384 | -1.398967 |
| 6 | 0.652197 | 4.056277 | 0.340145 |
| 1 | 1.626172 | 4.550516 | 0.366921 |
| 1 | 0.631719 | 3.266081 | 1.097633 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.141667 | 4.775521 | 0.556322 |
| 6 | 0.434825 | 3.454790 | -0.971754 |
| 7 | 0.254807 | 2.950717 | -2.004303 |
| 6 | 3.098180 | -3.743529 | -1.485741 |
| 1 | 3.412073 | -4.574377 | -0.848224 |
| 1 | 3.856010 | -3.590475 | -2.258191 |
| 1 | 2.143767 | -3.993395 | -1.958659 |
| 6 | 2.940063 | -2.531616 | -0.684532 |
| 7 | 2.795259 | -1.573321 | -0.042280 |
| 6 | -2.346676 | 0.674948 | 3.545613 |
| 1 | -2.480139 | 0.275119 | 4.553852 |
| 1 | -3.211418 | 1.282991 | 3.270724 |
| 1 | -1.456800 | 1.308853 | 3.509093 |
| 6 | -2.188208 | -0.416784 | 2.590598 |
| 7 | -2.048095 | -1.292573 | 1.839808 |
| 6 | 3.469377 | 0.421267 | 2.997379 |
| 1 | 3.568617 | -0.023424 | 3.990414 |
| 1 | 3.836092 | 1.450409 | 3.002458 |
| 1 | 4.048484 | -0.153379 | 2.267825 |
| 6 | 2.079571 | 0.409416 | 2.570086 |
| 7 | 0.978793 | 0.390277 | 2.202870 |
| 6 | -0.572403 | -0.059951 | -2.774713 |
| 6 | -0.294613 | 0.042007 | -1.358566 |
| 7 | -0.047652 | 0.123058 | -0.240082 |
| 1 | 0.317074 | 0.243317 | -3.333583 |
| 1 | -1.403917 | 0.609971 | -3.009272 |
| 1 | -0.853421 | -1.095399 | -2.990096 |
| 1 | 0.224054 | 0.229820 | 0.788322 |

Cartesian coordinates of : PACN9_35

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.279064 | 0.267709 | 3.344900 |
| 1 | 0.679466 | 1.173865 | 3.213694 |
| 1 | 1.872295 | 0.349674 | 4.259320 |
| 1 | 0.610060 | -0.594778 | 3.412339 |
| 6 | 2.159903 | 0.100800 | 2.192865 |
| 7 | 2.862109 | -0.020605 | 1.274281 |
| 6 | -2.477462 | 3.810984 | 0.590449 |
| 1 | -3.478505 | 4.231654 | 0.714385 |
| 1 | -1.759664 | 4.617934 | 0.425339 |
| 1 | -2.181914 | 3.265864 | 1.490580 |
| 6 | -2.458249 | 2.898034 | -0.548558 |
| 7 | -2.452259 | 2.172354 | -1.456541 |
| 6 | 3.031630 | 3.519258 | 0.374968 |
| 1 | 3.343176 | 4.371276 | 0.984279 |
| 1 | 3.092772 | 3.779442 | -0.684433 |
| 1 | 3.692264 | 2.668412 | 0.568307 |
| 6 | 1.662981 | 3.137803 | 0.707687 |
| 7 | 0.579006 | 2.830072 | 0.991491 |
| 6 | 4.611561 | -0.072215 | -1.668500 |
| 1 | 4.713434 | -0.275485 | -0.598302 |
| 1 | 5.490216 | 0.470529 | -2.026045 |
| 1 | 4.528412 | -1.016762 | -2.213227 |
| 6 | 3.405815 | 0.722210 | -1.879534 |
| 7 | 2.449174 | 1.361558 | -2.041887 |
| 6 | 3.134986 | -3.136150 | 0.495310 |
| 1 | 3.410260 | -4.176258 | 0.303271 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 2.521188 | -3.075714 | 1.399013 |
| 1 | 4.037140 | -2.539097 | 0.652221 |
| 6 | 2.376677 | -2.599376 | -0.630813 |
| 7 | 1.763682 | -2.185044 | -1.527203 |
| 6 | -3.354027 | -1.414505 | 2.664035 |
| 1 | -4.226730 | -1.061034 | 3.218532 |
| 1 | -2.783611 | -2.112896 | 3.282189 |
| 1 | -3.678125 | -1.924346 | 1.751568 |
| 6 | -2.499808 | -0.295076 | 2.291024 |
| 7 | -1.801246 | 0.580037 | 1.983096 |
| 6 | -4.789150 | -0.051724 | -2.321766 |
| 1 | -5.699326 | 0.105333 | -1.737342 |
| 1 | -5.038977 | -0.623875 | -3.218779 |
| 1 | -4.372589 | 0.919034 | -2.603396 |
| 6 | -3.804799 | -0.776262 | -1.523030 |
| 7 | -3.021065 | -1.356304 | -0.889676 |
| 6 | -1.045752 | -3.851673 | -0.395393 |
| 1 | -0.538257 | -4.819634 | -0.371303 |
| 1 | -0.794891 | -3.337912 | -1.327735 |
| 1 | -2.127429 | -3.997838 | -0.356080 |
| 6 | -0.612159 | -3.033252 | 0.733293 |
| 7 | -0.243995 | -2.390700 | 1.629472 |
| 6 | -0.270528 | -0.161241 | -2.859590 |
| 6 | -0.216807 | 0.072316 | -1.435517 |
| 7 | -0.240372 | 0.277564 | -0.306383 |
| 1 | 0.733749 | -0.053692 | -3.274686 |
| 1 | -0.951848 | 0.587096 | -3.278777 |
| 1 | -0.646622 | -1.173217 | -3.033109 |
| 1 | -0.514440 | 0.534069 | 0.660649 |

Cartesian coordinates of : PACN9_36

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.880760 | 3.015358 | -0.256522 |
| 1 | 3.493151 | 3.797698 | -0.913052 |
| 1 | 4.964600 | 3.113818 | -0.156585 |
| 1 | 3.407613 | 3.117893 | 0.724997 |
| 6 | 3.544834 | 1.707982 | -0.810122 |
| 7 | 3.285107 | 0.656766 | -1.233659 |
| 6 | -4.476621 | 0.153706 | 1.230035 |
| 1 | -4.513554 | -0.494954 | 0.348800 |
| 1 | -4.839984 | 1.150598 | 0.966640 |
| 1 | -5.103101 | -0.265318 | 2.021296 |
| 6 | -3.091881 | 0.240435 | 1.675761 |
| 7 | -1.985385 | 0.304692 | 2.023267 |
| 6 | 3.848009 | -2.632547 | -2.070209 |
| 1 | 4.104509 | -2.972216 | -3.076796 |
| 1 | 4.205640 | -3.369894 | -1.346589 |
| 1 | 4.326297 | -1.667141 | -1.881024 |
| 6 | 2.402502 | -2.470588 | -1.947686 |
| 7 | 1.253688 | -2.330850 | -1.841359 |
| 6 | -0.682021 | 3.516251 | 1.226675 |
| 1 | -1.697963 | 3.195214 | 0.979701 |
| 1 | -0.698889 | 4.550316 | 1.580228 |
| 1 | -0.274606 | 2.869200 | 2.009820 |
| 6 | 0.147098 | 3.405013 | 0.031709 |
| 7 | 0.801362 | 3.285630 | -0.921709 |
| 6 | -1.328119 | -3.964189 | -0.709811 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.052747 | -4.712441 | -0.378616 |
| 1 | -0.547676 | -3.841949 | 0.045751 |
| 1 | -0.868602 | -4.285281 | -1.647422 |
| 6 | -1.997370 | -2.683052 | -0.910000 |
| 7 | -2.545400 | -1.669702 | -1.069559 |
| 6 | -4.359023 | 0.712936 | -2.742994 |
| 1 | -4.247499 | -0.370240 | -2.638247 |
| 1 | -4.194059 | 0.997895 | -3.785163 |
| 1 | -5.372783 | 1.006737 | -2.457521 |
| 6 | -3.384101 | 1.370885 | -1.878140 |
| 7 | -2.610495 | 1.878973 | -1.175259 |
| 6 | 3.125534 | -1.021251 | 1.545162 |
| 1 | 3.207389 | -1.707331 | 2.391999 |
| 1 | 4.122141 | -0.747050 | 1.190166 |
| 1 | 2.576063 | -1.517925 | 0.738097 |
| 6 | 2.386730 | 0.175800 | 1.938796 |
| 7 | 1.769520 | 1.115937 | 2.235056 |
| 6 | -0.216865 | -1.196738 | 4.314111 |
| 1 | -1.278615 | -1.203197 | 4.572370 |
| 1 | 0.123658 | -0.158485 | 4.251270 |
| 1 | 0.347887 | -1.723466 | 5.087269 |
| 6 | -0.022071 | -1.837440 | 3.016963 |
| 7 | 0.139520 | -2.317401 | 1.970446 |
| 6 | 0.240471 | 0.541000 | -2.572430 |
| 6 | 0.065410 | 0.304621 | -1.160345 |
| 7 | -0.114306 | 0.128369 | -0.039630 |
| 1 | -0.334462 | -0.218043 | -3.112346 |
| 1 | 1.304768 | 0.459153 | -2.810003 |
| 1 | -0.120371 | 1.552908 | -2.782689 |
| 1 | -0.493727 | 0.047527 | 0.918768 |

Cartesian coordinates of : PACN9_37

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.146800 | 0.664319 | 2.631146 |
| 1 | -2.158005 | 0.464560 | 3.051274 |
| 1 | -3.766117 | -0.222499 | 2.787990 |
| 1 | -3.601935 | 1.525411 | 3.126922 |
| 6 | -3.013599 | 0.924232 | 1.200317 |
| 7 | -2.918673 | 1.136657 | 0.060721 |
| 6 | -2.326041 | 4.193013 | -1.224408 |
| 1 | -3.116762 | 3.451519 | -1.082502 |
| 1 | -2.447452 | 4.683909 | -2.193277 |
| 1 | -2.393850 | 4.946188 | -0.435283 |
| 6 | -1.030737 | 3.522422 | -1.162815 |
| 7 | 0.001407 | 2.988974 | -1.119889 |
| 6 | 3.952917 | -2.538137 | -1.030388 |
| 1 | 4.351865 | -1.750310 | -0.384394 |
| 1 | 4.730791 | -2.884512 | -1.715275 |
| 1 | 3.618204 | -3.366373 | -0.401289 |
| 6 | 2.821636 | -2.006759 | -1.783378 |
| 7 | 1.933267 | -1.570207 | -2.392009 |
| 6 | 2.962502 | 1.775833 | -2.388380 |
| 1 | 3.915673 | 2.203702 | -2.709641 |
| 1 | 2.173527 | 2.525913 | -2.491891 |
| 1 | 2.731600 | 0.906825 | -3.012485 |
| 6 | 3.045691 | 1.359157 | -0.991371 |
| 7 | 3.119310 | 1.023825 | 0.119144 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.544259 | -3.776358 | 0.119120 |
| 1 | 0.177735 | -4.360765 | 0.693869 |
| 1 | -0.008489 | -3.220599 | -0.658211 |
| 1 | -1.274648 | -4.436528 | -0.355135 |
| 6 | -1.225378 | -2.829999 | 0.997337 |
| 7 | -1.772684 | -2.053676 | 1.667737 |
| 6 | 1.684049 | 3.304774 | 2.010330 |
| 1 | 1.556381 | 3.738309 | 1.014022 |
| 1 | 2.741235 | 3.067318 | 2.157341 |
| 1 | 1.355051 | 4.017179 | 2.770835 |
| 6 | 0.899048 | 2.079438 | 2.089731 |
| 7 | 0.285033 | 1.094665 | 2.147845 |
| 6 | 3.025733 | -0.584713 | 3.183454 |
| 1 | 2.297334 | -0.246177 | 3.924877 |
| 1 | 3.488541 | 0.282115 | 2.701545 |
| 1 | 3.794670 | -1.182045 | 3.679663 |
| 6 | 2.351038 | -1.377333 | 2.161333 |
| 7 | 1.818690 | -2.000095 | 1.337377 |
| 6 | -4.714326 | -1.816564 | -0.289477 |
| 1 | -5.446420 | -2.589094 | -0.537182 |
| 1 | -5.171970 | -0.830740 | -0.405462 |
| 1 | -4.387566 | -1.944092 | 0.747827 |
| 6 | -3.550285 | -1.923448 | -1.162740 |
| 7 | -2.610297 | -2.015568 | -1.839260 |
| 6 | -0.696367 | 0.124232 | -2.811989 |
| 6 | -0.360403 | -0.081883 | -1.422611 |
| 7 | -0.099848 | -0.207784 | -0.312039 |
| 1 | -1.716338 | 0.520317 | -2.848057 |
| 1 | -0.644308 | -0.835601 | -3.330456 |
| 1 | 0.017048 | 0.836502 | -3.236216 |
| 1 | 0.084261 | -0.151336 | 0.701940 |

Cartesian coordinates of : PACN9_38

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.504005 | -1.672523 | 0.432587 |
| 1 | -5.569066 | -1.671404 | 0.188173 |
| 1 | -4.359742 | -1.353959 | 1.467513 |
| 1 | -4.108814 | -2.687444 | 0.333773 |
| 6 | -3.781392 | -0.774439 | -0.464719 |
| 7 | -3.210519 | -0.066190 | -1.188349 |
| 6 | 2.922775 | -2.659898 | -2.045079 |
| 1 | 3.021505 | -3.701104 | -2.362493 |
| 1 | 3.913865 | -2.238572 | -1.859239 |
| 1 | 2.436399 | -2.073114 | -2.829153 |
| 6 | 2.118448 | -2.581693 | -0.829504 |
| 7 | 1.472583 | -2.530243 | 0.136171 |
| 6 | -4.480586 | 3.181976 | -0.695668 |
| 1 | -4.683482 | 2.339409 | -1.362786 |
| 1 | -4.557327 | 4.116177 | -1.257491 |
| 1 | -5.220731 | 3.191233 | 0.108403 |
| 6 | -3.138343 | 3.038865 | -0.139476 |
| 7 | -2.066930 | 2.914121 | 0.291678 |
| 6 | 4.048341 | 2.805431 | -1.721863 |
| 1 | 3.942203 | 3.218517 | -2.728210 |
| 1 | 5.112366 | 2.690828 | -1.499493 |
| 1 | 3.593474 | 3.485356 | -0.995956 |
| 6 | 3.374441 | 1.513581 | -1.634674 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 2.825758 | 0.492377 | -1.549887 |
| 6 | 0.023348 | 2.954224 | 2.732683 |
| 1 | -0.620981 | 3.834843 | 2.683264 |
| 1 | 0.599630 | 2.960854 | 3.661274 |
| 1 | -0.599576 | 2.056011 | 2.705403 |
| 6 | 0.927143 | 2.942647 | 1.587474 |
| 7 | 1.651992 | 2.919523 | 0.678857 |
| 6 | -1.505927 | -3.092819 | -1.801619 |
| 1 | -1.081154 | -4.089705 | -1.946095 |
| 1 | -2.542271 | -3.088505 | -2.150521 |
| 1 | -1.475866 | -2.847538 | -0.733629 |
| 6 | -0.728908 | -2.106766 | -2.546305 |
| 7 | -0.091113 | -1.320766 | -3.116933 |
| 6 | 0.209517 | -3.265298 | 3.298297 |
| 1 | -0.178652 | -4.231948 | 3.628533 |
| 1 | 0.418554 | -2.630517 | 4.162799 |
| 1 | 1.130478 | -3.409488 | 2.725337 |
| 6 | -0.756243 | -2.601002 | 2.435728 |
| 7 | -1.510614 | -2.063776 | 1.732056 |
| 6 | 3.559025 | 0.056164 | 1.757613 |
| 1 | 3.672003 | 1.079704 | 1.387866 |
| 1 | 3.661256 | -0.633770 | 0.915263 |
| 1 | 4.326397 | -0.154428 | 2.506742 |
| 6 | 2.231494 | -0.095108 | 2.342125 |
| 7 | 1.171721 | -0.208817 | 2.806036 |
| 6 | -0.203608 | 1.634351 | -1.926252 |
| 6 | -0.230663 | 0.730958 | -0.801990 |
| 7 | -0.284508 | 0.001858 | 0.084092 |
| 1 | 0.449569 | 1.203562 | -2.689848 |
| 1 | 0.159721 | 2.605541 | -1.576210 |
| 1 | -1.230032 | 1.710053 | -2.299918 |
| 1 | -0.427474 | -0.699104 | 0.824493 |

Cartesian coordinates of : PACN9_39

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.985812 | 0.786675 | -2.110441 |
| 1 | 3.373023 | 1.691485 | -2.058517 |
| 1 | 4.531387 | 0.765973 | -3.057097 |
| 1 | 4.697694 | 0.799557 | -1.280423 |
| 6 | 3.121568 | -0.385376 | -2.000921 |
| 7 | 2.435333 | -1.319733 | -1.920189 |
| 6 | -1.984855 | 3.688007 | -0.076852 |
| 1 | -2.722713 | 4.397561 | -0.459186 |
| 1 | -1.011328 | 3.893547 | -0.532999 |
| 1 | -1.899528 | 3.787872 | 1.008473 |
| 6 | -2.378803 | 2.321202 | -0.402594 |
| 7 | -2.678270 | 1.227822 | -0.661106 |
| 6 | -4.683905 | -1.492965 | -1.317129 |
| 1 | -4.771158 | -0.431134 | -1.069308 |
| 1 | -4.853017 | -2.094855 | -0.419762 |
| 1 | -5.431118 | -1.755178 | -2.070201 |
| 6 | -3.341484 | -1.744277 | -1.828958 |
| 7 | -2.272727 | -1.939395 | -2.239917 |
| 6 | -0.400502 | 0.516452 | -3.502755 |
| 1 | -1.469964 | 0.410996 | -3.297880 |
| 1 | 0.061992 | -0.472684 | -3.422281 |
| 1 | -0.250901 | 0.911402 | -4.510710 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.189371 | 1.411398 | -2.514928 |
| 7 | 0.642702 | 2.097586 | -1.691887 |
| 6 | -3.955885 | 0.157031 | 2.246838 |
| 1 | -3.355490 | 1.056031 | 2.415077 |
| 1 | -4.492602 | -0.103964 | 3.162318 |
| 1 | -4.675440 | 0.363078 | 1.449690 |
| 6 | -3.076657 | -0.939176 | 1.848753 |
| 7 | -2.376076 | -1.813830 | 1.540693 |
| 6 | 0.429896 | -0.383057 | 3.503794 |
| 1 | 0.281634 | -0.256680 | 4.579172 |
| 1 | 1.499151 | -0.416024 | 3.275064 |
| 1 | -0.018440 | -1.327458 | 3.178393 |
| 6 | -0.180398 | 0.722044 | 2.775195 |
| 7 | -0.651983 | 1.586806 | 2.155995 |
| 6 | 1.981227 | 3.524753 | 0.995791 |
| 1 | 2.675726 | 4.106923 | 1.606388 |
| 1 | 0.974403 | 3.598310 | 1.418767 |
| 1 | 1.967449 | 3.912827 | -0.025942 |
| 6 | 2.379755 | 2.121004 | 0.973842 |
| 7 | 2.684346 | 0.999009 | 0.956784 |
| 6 | 4.633521 | -1.841650 | 0.892162 |
| 1 | 4.825389 | -2.219525 | -0.115878 |
| 1 | 5.362848 | -2.272826 | 1.582362 |
| 1 | 4.723582 | -0.751433 | 0.898507 |
| 6 | 3.279540 | -2.198966 | 1.300559 |
| 7 | 2.201597 | -2.478635 | 1.630835 |
| 6 | 0.021667 | -3.169412 | -0.371381 |
| 6 | 0.002689 | -1.737168 | -0.211668 |
| 7 | -0.015131 | -0.594420 | -0.092524 |
| 1 | -0.796949 | -3.442043 | -1.043214 |
| 1 | -0.104952 | -3.620845 | 0.616291 |
| 1 | 0.992165 | -3.442016 | -0.796690 |
| 1 | -0.036720 | 0.415506 | 0.022951 |

Cartesian coordinates of : PACN9_40

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.246355 | -2.962973 | 2.632819 |
| 1 | -0.403580 | -3.955060 | 3.063531 |
| 1 | -0.091885 | -2.236551 | 3.435186 |
| 1 | 0.637189 | -2.989693 | 1.985466 |
| 6 | -1.408264 | -2.568200 | 1.842299 |
| 7 | -2.316648 | -2.237013 | 1.197688 |
| 6 | 3.203387 | 2.885980 | -1.757978 |
| 1 | 4.191798 | 3.348801 | -1.700750 |
| 1 | 2.558635 | 3.298632 | -0.977063 |
| 1 | 2.753788 | 3.084611 | -2.733427 |
| 6 | 3.317666 | 1.445598 | -1.560354 |
| 7 | 3.417299 | 0.298735 | -1.394865 |
| 6 | -4.551450 | 0.367081 | 0.710158 |
| 1 | -5.070968 | 0.432134 | -0.250298 |
| 1 | -5.206471 | 0.752915 | 1.495404 |
| 1 | -4.301639 | -0.676524 | 0.923600 |
| 6 | -3.319935 | 1.150119 | 0.656456 |
| 7 | -2.347394 | 1.785404 | 0.618482 |
| 6 | -2.252073 | 2.843204 | -2.516610 |
| 1 | -2.461383 | 3.485333 | -1.657895 |
| 1 | -2.953958 | 2.004607 | -2.514320 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.363918 | 3.414192 | -3.441720 |
| 6 | -0.894835 | 2.317839 | -2.415331 |
| 7 | 0.188514 | 1.902243 | -2.352160 |
| 6 | -0.606658 | 2.974045 | 3.414401 |
| 1 | -1.446861 | 3.374890 | 2.840029 |
| 1 | 0.307600 | 3.507459 | 3.136943 |
| 1 | -0.797077 | 3.087638 | 4.484311 |
| 6 | -0.443458 | 1.570911 | 3.070867 |
| 7 | -0.303429 | 0.462343 | 2.752538 |
| 6 | 4.605193 | -2.904194 | -1.016986 |
| 1 | 4.656086 | -3.622547 | -1.839109 |
| 1 | 5.328179 | -3.194267 | -0.250280 |
| 1 | 4.845378 | -1.904490 | -1.390299 |
| 6 | 3.259221 | -2.882311 | -0.452937 |
| 7 | 2.187647 | -2.849718 | -0.004059 |
| 6 | -4.251132 | -2.662857 | -1.574452 |
| 1 | -5.289431 | -2.323747 | -1.627941 |
| 1 | -4.040928 | -3.041491 | -0.570106 |
| 1 | -4.106089 | -3.463427 | -2.304110 |
| 6 | -3.347892 | -1.551493 | -1.859150 |
| 7 | -2.635343 | -0.658555 | -2.073556 |
| 6 | 3.164707 | -0.012635 | 1.998579 |
| 1 | 3.726945 | -0.371925 | 1.132123 |
| 1 | 2.329648 | -0.698155 | 2.181921 |
| 1 | 3.811436 | 0.008853 | 2.879342 |
| 6 | 2.651267 | 1.324560 | 1.715999 |
| 7 | 2.222268 | 2.380660 | 1.489067 |
| 6 | 0.555160 | -1.181011 | -2.273949 |
| 6 | 0.285068 | -0.661991 | -0.953034 |
| 7 | 0.065694 | -0.283481 | 0.109129 |
| 1 | 1.564077 | -0.866028 | -2.557429 |
| 1 | -0.187320 | -0.766426 | -2.959973 |
| 1 | 0.490340 | -2.271926 | -2.230099 |
| 1 | -0.147545 | 0.027828 | 1.086331 |

Cartesian coordinates of : PACN9_41

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.457986 | 1.303112 | 2.790292 |
| 1 | 2.823084 | 2.172604 | 2.985129 |
| 1 | 4.096695 | 1.501210 | 1.924527 |
| 1 | 4.075820 | 1.092843 | 3.666759 |
| 6 | 2.601622 | 0.166892 | 2.486656 |
| 7 | 1.900877 | -0.722175 | 2.222887 |
| 6 | -4.320642 | -2.326190 | -0.465304 |
| 1 | -4.642781 | -1.485733 | 0.157355 |
| 1 | -4.866598 | -3.226905 | -0.173854 |
| 1 | -4.531074 | -2.100171 | -1.513982 |
| 6 | -2.886189 | -2.530049 | -0.285608 |
| 7 | -1.745915 | -2.697861 | -0.136293 |
| 6 | 4.703701 | -1.147170 | -2.154442 |
| 1 | 4.863924 | -0.681410 | -3.130145 |
| 1 | 4.114710 | -2.060216 | -2.275056 |
| 1 | 5.673904 | -1.397113 | -1.717706 |
| 6 | 3.985086 | -0.229168 | -1.274802 |
| 7 | 3.418924 | 0.505409 | -0.573869 |
| 6 | 2.519132 | 3.600858 | -0.751814 |
| 1 | 2.371438 | 4.682999 | -0.791548 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.483000 | 3.345580 | -1.198053 |
| 1 | 2.514884 | 3.264533 | 0.289469 |
| 6 | 1.446333 | 2.919257 | -1.469862 |
| 7 | 0.579203 | 2.380831 | -2.025325 |
| 6 | 1.184354 | -4.052975 | 1.023446 |
| 1 | 1.330081 | -3.355483 | 1.854011 |
| 1 | 1.759856 | -4.963119 | 1.210061 |
| 1 | 0.122775 | -4.298367 | 0.937819 |
| 6 | 1.629426 | -3.422034 | -0.214978 |
| 7 | 1.978254 | -2.907875 | -1.197074 |
| 6 | -1.757788 | 3.235850 | 0.460253 |
| 1 | -1.761466 | 4.317689 | 0.617059 |
| 1 | -2.690540 | 2.805074 | 0.836415 |
| 1 | -1.657513 | 3.018573 | -0.607993 |
| 6 | -0.632227 | 2.635189 | 1.168381 |
| 7 | 0.274966 | 2.160874 | 1.719837 |
| 6 | -4.970898 | 1.660291 | -1.036577 |
| 1 | -4.917549 | 2.729269 | -1.261053 |
| 1 | -5.113085 | 1.519488 | 0.039399 |
| 1 | -5.819401 | 1.233107 | -1.577545 |
| 6 | -3.731165 | 1.000707 | -1.434664 |
| 7 | -2.737850 | 0.471601 | -1.721551 |
| 6 | -1.374748 | -0.848505 | 2.919395 |
| 1 | -0.591440 | -0.125867 | 3.165984 |
| 1 | -0.946278 | -1.639403 | 2.294244 |
| 1 | -1.762501 | -1.289773 | 3.841186 |
| 6 | -2.450525 | -0.180125 | 2.194163 |
| 7 | -3.309303 | 0.352839 | 1.620535 |
| 6 | -0.113680 | -0.775250 | -2.650949 |
| 6 | 0.135146 | -0.495327 | -1.258631 |
| 7 | 0.387180 | -0.306779 | -0.153441 |
| 1 | 0.803153 | -1.211392 | -3.060554 |
| 1 | -0.381754 | 0.159705 | -3.149195 |
| 1 | -0.937351 | -1.492075 | -2.711399 |
| 1 | 0.812130 | -0.265892 | 0.789005 |

Cartesian coordinates of : PACN9_42

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.564523 | 4.063427 | -0.349609 |
| 1 | -0.662606 | 4.623129 | -0.608055 |
| 1 | -2.340190 | 4.752869 | -0.006788 |
| 1 | -1.908847 | 3.524635 | -1.235634 |
| 6 | -1.260153 | 3.096327 | 0.699444 |
| 7 | -1.025620 | 2.328363 | 1.540197 |
| 6 | 1.317876 | -3.906722 | -2.553011 |
| 1 | 1.852962 | -4.859563 | -2.567703 |
| 1 | 1.926726 | -3.147044 | -3.053916 |
| 1 | 0.371232 | -4.027996 | -3.086511 |
| 6 | 1.070459 | -3.490178 | -1.174913 |
| 7 | 0.888622 | -3.135558 | -0.083404 |
| 6 | 1.674893 | 2.190059 | 3.578627 |
| 1 | 2.102341 | 3.131123 | 3.933321 |
| 1 | 1.987600 | 1.375960 | 4.237250 |
| 1 | 0.583262 | 2.255003 | 3.582474 |
| 6 | 2.119986 | 1.917049 | 2.216064 |
| 7 | 2.461700 | 1.688013 | 1.128607 |
| 6 | -0.175648 | -3.364096 | 2.934502 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -0.902754 | -3.629870 | 2.161193 |
| 1 | -0.590121 | -3.558406 | 3.926786 |
| 1 | 0.723912 | -3.965311 | 2.783166 |
| 6 | 0.152935 | -1.951033 | 2.794441 |
| 7 | 0.396375 | -0.820375 | 2.676161 |
| 6 | -3.135982 | -0.210762 | 2.076564 |
| 1 | -3.479908 | 0.688731 | 1.557446 |
| 1 | -2.260168 | 0.064455 | 2.671398 |
| 1 | -3.926191 | -0.586821 | 2.731464 |
| 6 | -2.770411 | -1.225068 | 1.090871 |
| 7 | -2.475009 | -2.013612 | 0.288378 |
| 6 | 3.277221 | 2.635206 | -2.101135 |
| 1 | 3.648934 | 2.430807 | -1.093224 |
| 1 | 3.561624 | 3.646701 | -2.401658 |
| 1 | 3.708636 | 1.911586 | -2.797374 |
| 6 | 1.824152 | 2.502181 | -2.100723 |
| 7 | 0.666249 | 2.399517 | -2.104199 |
| 6 | 3.632299 | -1.213048 | 0.432994 |
| 1 | 4.333986 | -0.444170 | 0.764142 |
| 1 | 4.113419 | -2.194345 | 0.456285 |
| 1 | 2.770355 | -1.217812 | 1.108577 |
| 6 | 3.174704 | -0.919862 | -0.921384 |
| 7 | 2.791161 | -0.712800 | -1.999333 |
| 6 | -5.110049 | -0.480054 | -1.795049 |
| 1 | -4.870617 | -1.476798 | -1.412334 |
| 1 | -5.305816 | -0.542176 | -2.868424 |
| 1 | -6.007843 | -0.108218 | -1.294837 |
| 6 | -3.985120 | 0.415460 | -1.538746 |
| 7 | -3.077937 | 1.107686 | -1.318658 |
| 6 | -0.513423 | -0.493051 | -2.436255 |
| 6 | -0.193145 | -0.153947 | -1.070270 |
| 7 | 0.067118 | 0.071911 | 0.023284 |
| 1 | 0.423901 | -0.740157 | -2.946790 |
| 1 | -0.979690 | 0.378343 | -2.903385 |
| 1 | -1.202197 | -1.345069 | -2.415134 |
| 1 | 0.263024 | 0.197068 | 1.026565 |

 Cartesian coordinates of : PACN9_43

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.379353 | -1.373748 | 3.545272 |
| 1 | -0.911864 | -2.352223 | 3.405823 |
| 1 | -1.997623 | -1.389844 | 4.446268 |
| 1 | -0.599563 | -0.613490 | 3.645821 |
| 6 | -2.199037 | -1.060575 | 2.378790 |
| 7 | -2.854417 | -0.816944 | 1.450559 |
| 6 | 3.956656 | -0.183849 | -2.840868 |
| 1 | 3.784941 | 0.826659 | -3.220548 |
| 1 | 4.573326 | -0.737887 | -3.552999 |
| 1 | 4.469922 | -0.126926 | -1.876512 |
| 6 | 2.677703 | -0.861218 | -2.649793 |
| 7 | 1.663897 | -1.410063 | -2.501574 |
| 6 | 2.781055 | -0.986838 | 3.032711 |
| 1 | 2.729551 | -0.017192 | 3.534153 |
| 1 | 3.475631 | -1.640336 | 3.566508 |
| 1 | 1.779358 | -1.425783 | 3.031037 |
| 6 | 3.219817 | -0.809489 | 1.651392 |
| 7 | 3.575380 | -0.686358 | 0.551733 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.085843 | 3.595100 | 1.396349 |
| 1 | 0.893618 | 4.212085 | 1.800780 |
| 1 | -0.871872 | 3.938752 | 1.793573 |
| 1 | 0.055157 | 3.685625 | 0.307617 |
| 6 | 0.300712 | 2.196642 | 1.757576 |
| 7 | 0.503106 | 1.088688 | 2.045909 |
| 6 | 3.819789 | 2.567364 | 0.434484 |
| 1 | 4.671332 | 1.907727 | 0.247971 |
| 1 | 3.434538 | 2.353512 | 1.436748 |
| 1 | 4.143864 | 3.609745 | 0.380234 |
| 6 | 2.772345 | 2.312855 | -0.550341 |
| 7 | 1.929696 | 2.126552 | -1.327909 |
| 6 | -4.771672 | -2.414254 | -0.938418 |
| 1 | -4.593884 | -2.331205 | 0.137441 |
| 1 | -4.427903 | -3.391625 | -1.286197 |
| 1 | -5.841624 | -2.323855 | -1.142685 |
| 6 | -4.038925 | -1.353482 | -1.622615 |
| 7 | -3.460121 | -0.500276 | -2.157173 |
| 6 | -4.867721 | 1.632130 | 0.087402 |
| 1 | -5.440177 | 2.356656 | 0.671960 |
| 1 | -4.852149 | 0.669323 | 0.606179 |
| 1 | -5.333197 | 1.508052 | -0.893716 |
| 6 | -3.494730 | 2.096436 | -0.080292 |
| 7 | -2.404566 | 2.476097 | -0.211646 |
| 6 | 2.135482 | -3.891691 | -0.426494 |
| 1 | 3.094167 | -3.365035 | -0.458814 |
| 1 | 1.791502 | -4.057516 | -1.450448 |
| 1 | 2.251624 | -4.848304 | 0.088899 |
| 6 | 1.168794 | -3.055774 | 0.272565 |
| 7 | 0.410967 | -2.376009 | 0.832948 |
| 6 | -0.802062 | 1.331690 | -2.717680 |
| 6 | -0.632210 | 0.518093 | -1.537556 |
| 7 | -0.488907 | -0.150756 | -0.616201 |
| 1 | -0.030887 | 1.040545 | -3.437298 |
| 1 | -0.677845 | 2.379601 | -2.435141 |
| 1 | -1.806695 | 1.146404 | -3.108337 |
| 1 | -0.283402 | -0.826329 | 0.140251 |

Cartesian coordinates of : PACN9_44

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.774887 | -2.639234 | 2.140144 |
| 1 | 3.315884 | -2.606221 | 1.189015 |
| 1 | 2.904340 | -3.622681 | 2.598921 |
| 1 | 3.178392 | -1.871472 | 2.805239 |
| 6 | 1.359394 | -2.378802 | 1.894144 |
| 7 | 0.232886 | -2.176539 | 1.690595 |
| 6 | 2.570636 | 4.125687 | -0.196458 |
| 1 | 3.535383 | 4.599491 | -0.394532 |
| 1 | 2.575995 | 3.652830 | 0.789900 |
| 1 | 1.785231 | 4.885201 | -0.206293 |
| 6 | 2.290714 | 3.112230 | -1.209479 |
| 7 | 2.086025 | 2.290653 | -2.005561 |
| 6 | -0.601425 | 0.552769 | 3.478770 |
| 1 | 0.333856 | 0.832383 | 2.981303 |
| 1 | -0.451422 | -0.381808 | 4.025257 |
| 1 | -0.877090 | 1.346168 | 4.178330 |
| 6 | -1.659591 | 0.375226 | 2.487980 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -2.492861 | 0.242883 | 1.688347 |
| 6 | -4.627062 | -0.092556 | -0.998318 |
| 1 | -5.572926 | 0.438784 | -1.130757 |
| 1 | -4.497342 | -0.351895 | 0.056786 |
| 1 | -4.640106 | -1.003733 | -1.602426 |
| 6 | -3.512201 | 0.753760 | -1.411406 |
| 7 | -2.627538 | 1.434052 | -1.735246 |
| 6 | -2.608072 | 3.709473 | 0.643632 |
| 1 | -3.290763 | 2.912728 | 0.954678 |
| 1 | -2.782554 | 3.926073 | -0.412859 |
| 1 | -2.790427 | 4.605249 | 1.242457 |
| 6 | -1.235980 | 3.250008 | 0.831940 |
| 7 | -0.148739 | 2.876177 | 1.003544 |
| 6 | 0.835478 | -4.193934 | -1.535224 |
| 1 | 0.352187 | -4.357886 | -0.567054 |
| 1 | 1.494429 | -5.034881 | -1.765043 |
| 1 | 0.058322 | -4.115921 | -2.299288 |
| 6 | 1.604405 | -2.953561 | -1.483273 |
| 7 | 2.228086 | -1.974179 | -1.427049 |
| 6 | -2.806799 | -3.091162 | 0.881344 |
| 1 | -3.795056 | -3.513849 | 0.681360 |
| 1 | -2.887488 | -2.279502 | 1.609039 |
| 1 | -2.155641 | -3.865320 | 1.295421 |
| 6 | -2.226703 | -2.568794 | -0.351789 |
| 7 | -1.778539 | -2.164802 | -1.345192 |
| 6 | 4.406545 | 0.300848 | -0.425923 |
| 1 | 3.974859 | 0.362398 | -1.428398 |
| 1 | 4.886813 | -0.674524 | -0.309609 |
| 1 | 5.149147 | 1.092077 | -0.293713 |
| 6 | 3.336381 | 0.446939 | 0.554993 |
| 7 | 2.477118 | 0.560711 | 1.330251 |
| 6 | -0.088846 | 0.155485 | -3.015770 |
| 6 | 0.038554 | 0.237455 | -1.581465 |
| 7 | 0.166158 | 0.282918 | -0.442199 |
| 1 | -0.387832 | 1.138391 | -3.388695 |
| 1 | -0.850447 | -0.595177 | -3.245323 |
| 1 | 0.888616 | -0.125536 | -3.419502 |
| 1 | 0.445577 | 0.394481 | 0.530298 |

Cartesian coordinates of : PACN9_45

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.279263 | -2.053420 | -1.362867 |
| 1 | 4.494097 | -1.541148 | -0.420838 |
| 1 | 4.580577 | -1.421492 | -2.203291 |
| 1 | 4.835836 | -2.992916 | -1.406661 |
| 6 | 2.845666 | -2.316440 | -1.435913 |
| 7 | 1.706690 | -2.536829 | -1.498710 |
| 6 | -4.937533 | -1.602799 | -0.337295 |
| 1 | -5.759814 | -1.242779 | -0.961925 |
| 1 | -4.858970 | -0.980453 | 0.558574 |
| 1 | -5.146102 | -2.635460 | -0.046540 |
| 6 | -3.679936 | -1.530699 | -1.075398 |
| 7 | -2.682082 | -1.466347 | -1.666736 |
| 6 | 0.701059 | 3.898937 | -0.202178 |
| 1 | 0.943260 | 3.418178 | -1.154297 |
| 1 | 1.507504 | 4.576472 | 0.089763 |
| 1 | -0.227329 | 4.461248 | -0.325546 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 0.521871 | 2.869355 | 0.815569 |
| 7 | 0.384459 | 2.039343 | 1.618064 |
| 6 | -4.263383 | 1.939799 | -1.517549 |
| 1 | -4.612417 | 1.238596 | -2.281106 |
| 1 | -4.787451 | 2.890656 | -1.642270 |
| 1 | -4.468679 | 1.533615 | -0.523038 |
| 6 | -2.823905 | 2.137996 | -1.654618 |
| 7 | -1.679663 | 2.303445 | -1.769869 |
| 6 | 4.880532 | 1.622078 | -0.551139 |
| 1 | 5.702176 | 1.229131 | -1.156498 |
| 1 | 4.845406 | 1.092597 | 0.405019 |
| 1 | 5.056364 | 2.685872 | -0.372600 |
| 6 | 3.611306 | 1.429394 | -1.246544 |
| 7 | 2.605325 | 1.267930 | -1.804687 |
| 6 | -0.699382 | -3.839297 | 0.304626 |
| 1 | -1.476798 | -4.508011 | 0.682838 |
| 1 | 0.234986 | -4.390886 | 0.179199 |
| 1 | -0.996512 | -3.439706 | -0.669593 |
| 6 | -0.498702 | -2.732527 | 1.234164 |
| 7 | -0.345537 | -1.841993 | 1.965433 |
| 6 | -1.894262 | 0.703199 | 3.688419 |
| 1 | -1.267653 | -0.177217 | 3.857298 |
| 1 | -2.701002 | 0.727269 | 4.425212 |
| 1 | -1.282872 | 1.604424 | 3.782369 |
| 6 | -2.446083 | 0.632569 | 2.339519 |
| 7 | -2.886832 | 0.569754 | 1.266065 |
| 6 | 1.955457 | -0.203602 | 3.728941 |
| 1 | 2.764526 | -0.084538 | 4.453873 |
| 1 | 1.368384 | -1.092522 | 3.973025 |
| 1 | 1.305162 | 0.675599 | 3.755855 |
| 6 | 2.501787 | -0.339221 | 2.382708 |
| 7 | 2.939929 | -0.437144 | 1.310884 |
| 6 | -0.041987 | -0.343509 | -2.991309 |
| 6 | -0.031481 | -0.187676 | -1.557186 |
| 7 | -0.014527 | -0.055579 | -0.417897 |
| 1 | -0.845339 | 0.280929 | -3.391634 |
| 1 | -0.220160 | -1.397057 | -3.219854 |
| 1 | 0.931513 | -0.014467 | -3.365967 |
| 1 | 0.005255 | 0.101163 | 0.589099 |

Cartesian coordinates of : PACN10_ 1

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.375799 | -3.885606 | -1.170864 |
| 1 | -0.771518 | -4.711319 | -0.574269 |
| 1 | -0.250091 | -4.206602 | -2.208221 |
| 1 | -1.085982 | -3.052622 | -1.127579 |
| 6 | 0.909208 | -3.464171 | -0.624250 |
| 7 | 1.930765 | -3.111944 | -0.196000 |
| 6 | 3.144061 | -0.538207 | -2.369905 |
| 1 | 2.751836 | -1.298135 | -1.685495 |
| 1 | 4.236695 | -0.541414 | -2.323547 |
| 1 | 2.821300 | -0.776667 | -3.386429 |
| 6 | 2.634763 | 0.774455 | -1.987276 |
| 7 | 2.214846 | 1.813454 | -1.680998 |
| 6 | -2.243271 | 3.197074 | 2.166428 |
| 1 | -2.704298 | 3.601225 | 3.071135 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.795998 | 3.548877 | 1.290053 |
| 1 | -1.204830 | 3.533296 | 2.101020 |
| 6 | -2.258644 | 1.738351 | 2.204233 |
| 7 | -2.290932 | 0.577134 | 2.240174 |
| 6 | -4.521889 | 0.649988 | -0.266114 |
| 1 | -4.006436 | 1.607070 | -0.389388 |
| 1 | -4.829756 | 0.539435 | 0.777404 |
| 1 | -5.405923 | 0.623106 | -0.908521 |
| 6 | -3.603400 | -0.425456 | -0.627344 |
| 7 | -2.886677 | -1.289536 | -0.927294 |
| 6 | 5.041037 | -2.352929 | 0.835020 |
| 1 | 5.867093 | -2.179313 | 0.140349 |
| 1 | 4.401120 | -3.153836 | 0.454682 |
| 1 | 5.451218 | -2.642945 | 1.805662 |
| 6 | 4.237769 | -1.141952 | 0.972148 |
| 7 | 3.591118 | -0.181159 | 1.072104 |
| 6 | 3.549977 | 3.063256 | 1.196805 |
| 1 | 3.792016 | 2.768648 | 0.172398 |
| 1 | 4.187684 | 2.502685 | 1.884123 |
| 1 | 3.721132 | 4.134946 | 1.326841 |
| 6 | 2.150578 | 2.744953 | 1.458929 |
| 7 | 1.032636 | 2.506346 | 1.670793 |
| 6 | -2.341365 | 0.131899 | -4.006973 |
| 1 | -2.123215 | 0.405054 | -5.042193 |
| 1 | -2.754953 | 0.996723 | -3.477945 |
| 1 | -3.064393 | -0.687535 | -3.984520 |
| 6 | -1.124716 | -0.274996 | -3.319866 |
| 7 | -0.167964 | -0.587870 | -2.741406 |
| 6 | -0.015846 | 4.219097 | -1.060800 |
| 1 | 1.012442 | 3.918454 | -1.278777 |
| 1 | -0.057600 | 4.661677 | -0.061524 |
| 1 | -0.353358 | 4.951976 | -1.798142 |
| 6 | -0.868466 | 3.035295 | -1.110452 |
| 7 | -1.569923 | 2.109017 | -1.158961 |
| 6 | -3.751218 | -2.573328 | 2.193034 |
| 1 | -4.094611 | -3.191429 | 3.026273 |
| 1 | -4.309092 | -2.839054 | 1.291133 |
| 1 | -3.918428 | -1.518180 | 2.428886 |
| 6 | -2.324896 | -2.779979 | 1.965599 |
| 7 | -1.188963 | -2.944788 | 1.787330 |
| 6 | 0.787144 | -0.695839 | 2.508128 |
| 6 | 0.451760 | -0.479090 | 1.120644 |
| 7 | 0.195234 | -0.330894 | 0.011048 |
| 1 | 1.222023 | -1.697818 | 2.584360 |
| 1 | -0.134582 | -0.639960 | 3.093461 |
| 1 | 1.503029 | 0.070686 | 2.813336 |
| 1 | 0.015777 | -0.302224 | -1.014851 |

Cartesian coordinates of : PACN10_ 2

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|-----------|
| 6 | 4.116291 | -2.765820 | -1.720897 |
| 1 | 4.111907 | -2.747082 | -0.627549 |
| 1 | 4.756481 | -1.963775 | -2.097999 |
| 1 | 4.497385 | -3.728038 | -2.071883 |
| 6 | 2.751558 | -2.565243 | -2.195597 |
| 7 | 1.666651 | -2.412457 | -2.581217 |
| 6 | 2.839490 | 3.886070 | -0.253930 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.104169 | 3.404078 | 0.692660 |
| 1 | 2.849115 | 4.971500 | -0.127253 |
| 1 | 3.567140 | 3.599597 | -1.017188 |
| 6 | 1.508374 | 3.440578 | -0.652709 |
| 7 | 0.441354 | 3.091958 | -0.954249 |
| 6 | -0.857918 | 2.089852 | 1.893528 |
| 1 | -0.977191 | 3.174137 | 1.814391 |
| 1 | -1.435063 | 1.716803 | 2.742960 |
| 1 | -1.254238 | 1.622561 | 0.985842 |
| 6 | 0.556130 | 1.756286 | 2.042502 |
| 7 | 1.681968 | 1.485060 | 2.145519 |
| 6 | -3.045672 | -2.142949 | 2.936761 |
| 1 | -3.600216 | -1.337682 | 3.424942 |
| 1 | -2.800447 | -2.924661 | 3.659788 |
| 1 | -3.649584 | -2.562544 | 2.126190 |
| 6 | -1.831212 | -1.605506 | 2.343110 |
| 7 | -0.865818 | -1.186800 | 1.855534 |
| 6 | 4.803135 | 0.385641 | 1.106296 |
| 1 | 5.081077 | -0.663474 | 1.240033 |
| 1 | 4.194313 | 0.707643 | 1.956741 |
| 1 | 5.708513 | 0.995390 | 1.047914 |
| 6 | 4.017148 | 0.534086 | -0.114491 |
| 7 | 3.402405 | 0.669820 | -1.091040 |
| 6 | -2.987253 | 3.298600 | -0.918096 |
| 1 | -2.059486 | 3.870979 | -0.829385 |
| 1 | -3.416644 | 3.136442 | 0.075746 |
| 1 | -3.700004 | 3.852963 | -1.533865 |
| 6 | -2.689230 | 2.007877 | -1.531438 |
| 7 | -2.456840 | 0.975013 | -2.011703 |
| 6 | -1.889886 | -2.376395 | -2.814683 |
| 1 | -2.056046 | -1.400666 | -3.281883 |
| 1 | -2.353878 | -3.154361 | -3.426435 |
| 1 | -0.814691 | -2.574720 | -2.744572 |
| 6 | -2.486926 | -2.366477 | -1.482808 |
| 7 | -2.966313 | -2.356364 | -0.424395 |
| 6 | -5.455345 | -0.333037 | -0.362639 |
| 1 | -5.612706 | -1.393595 | -0.151460 |
| 1 | -4.979988 | -0.244268 | -1.343904 |
| 1 | -6.415631 | 0.188744 | -0.366679 |
| 6 | -4.573711 | 0.244215 | 0.647980 |
| 7 | -3.876527 | 0.718656 | 1.448262 |
| 6 | 2.082439 | -1.384950 | 3.696616 |
| 1 | 2.747793 | -0.567481 | 3.987945 |
| 1 | 2.278817 | -2.258997 | 4.322446 |
| 1 | 1.050048 | -1.054487 | 3.838924 |
| 6 | 2.291410 | -1.713062 | 2.289555 |
| 7 | 2.465519 | -1.968779 | 1.169559 |
| 6 | 0.660230 | 0.516014 | -2.864092 |
| 6 | 0.408876 | 0.029507 | -1.525511 |
| 7 | 0.192702 | -0.363996 | -0.466948 |
| 1 | 1.731022 | 0.723177 | -2.946585 |
| 1 | 0.070070 | 1.423543 | -3.013021 |
| 1 | 0.374049 | -0.265635 | -3.572957 |
| 1 | -0.099366 | -0.722593 | 0.494084 |

 Cartesian coordinates of : PACN10_3

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

| | | | |
|---|-----------|-----------|-----------|
| 6 | -4.658391 | 1.227803 | -1.486998 |
| 1 | -4.598040 | 0.641184 | -2.407088 |
| 1 | -5.451837 | 1.973514 | -1.579682 |
| 1 | -4.879984 | 0.557096 | -0.651125 |
| 6 | -3.378840 | 1.885403 | -1.241006 |
| 7 | -2.362488 | 2.411199 | -1.036122 |
| 6 | -1.953374 | 1.845431 | 2.183219 |
| 1 | -1.201883 | 2.003656 | 1.403810 |
| 1 | -1.437960 | 1.641560 | 3.125655 |
| 1 | -2.555775 | 2.752765 | 2.283109 |
| 6 | -2.807428 | 0.716297 | 1.826770 |
| 7 | -3.476048 | -0.193095 | 1.549138 |
| 6 | 3.801413 | -3.032318 | -0.676760 |
| 1 | 3.138810 | -3.902141 | -0.650322 |
| 1 | 4.794956 | -3.332691 | -0.334595 |
| 1 | 3.876476 | -2.655260 | -1.702051 |
| 6 | 3.270480 | -1.977765 | 0.182360 |
| 7 | 2.853471 | -1.121967 | 0.848404 |
| 6 | 0.676870 | -2.656407 | -2.589694 |
| 1 | -0.206298 | -2.215627 | -3.063441 |
| 1 | 1.035159 | -3.484029 | -3.208068 |
| 1 | 1.465448 | -1.897437 | -2.518617 |
| 6 | 0.312912 | -3.142513 | -1.261209 |
| 7 | 0.022509 | -3.530721 | -0.204699 |
| 6 | -0.116705 | 4.737226 | 0.409580 |
| 1 | -1.180397 | 4.555108 | 0.229846 |
| 1 | 0.095759 | 5.802110 | 0.286417 |
| 1 | 0.145766 | 4.426079 | 1.424876 |
| 6 | 0.666105 | 3.954188 | -0.539977 |
| 7 | 1.288919 | 3.327868 | -1.295015 |
| 6 | 2.727261 | 0.476263 | 3.604634 |
| 1 | 2.724912 | 0.855102 | 4.629631 |
| 1 | 3.756666 | 0.378964 | 3.251374 |
| 1 | 2.258892 | -0.510713 | 3.565426 |
| 6 | 1.990981 | 1.383554 | 2.730828 |
| 7 | 1.397171 | 2.105760 | 2.040600 |
| 6 | -3.448245 | -3.022362 | -0.235505 |
| 1 | -4.201709 | -3.589303 | -0.788323 |
| 1 | -3.912771 | -2.530504 | 0.623789 |
| 1 | -2.662694 | -3.705224 | 0.102808 |
| 6 | -2.853779 | -2.006422 | -1.097503 |
| 7 | -2.378287 | -1.206096 | -1.793465 |
| 6 | -1.337077 | -3.088732 | 2.958734 |
| 1 | -0.999332 | -3.297524 | 3.976770 |
| 1 | -1.115358 | -3.945477 | 2.315158 |
| 1 | -2.414211 | -2.894765 | 2.967223 |
| 6 | -0.648245 | -1.923768 | 2.423945 |
| 7 | -0.113268 | -0.995692 | 1.980993 |
| 6 | 3.958096 | 1.666723 | -0.747979 |
| 1 | 3.219257 | 1.757456 | 0.055347 |
| 1 | 4.100518 | 2.649699 | -1.202523 |
| 1 | 4.903792 | 1.300387 | -0.339789 |
| 6 | 3.455743 | 0.728050 | -1.744738 |
| 7 | 3.046449 | -0.041050 | -2.514911 |
| 6 | -0.108416 | 1.015941 | -2.823503 |
| 6 | 0.087439 | 0.617523 | -1.447103 |
| 7 | 0.247283 | 0.252058 | -0.367620 |
| 1 | 0.816324 | 0.814708 | -3.373763 |
| 1 | -0.331593 | 2.085295 | -2.842367 |
| 1 | -0.950313 | 0.437176 | -3.215917 |
| 1 | 0.266651 | -0.153697 | 0.616736 |

Cartesian coordinates of : PACN10_ 4

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.535553 | -1.495670 | 2.527089 |
| 1 | -3.293945 | -1.036073 | 3.164936 |
| 1 | -1.605186 | -0.929143 | 2.627519 |
| 1 | -2.359509 | -2.530939 | 2.831978 |
| 6 | -2.972476 | -1.455969 | 1.135059 |
| 7 | -3.313545 | -1.431132 | 0.023642 |
| 6 | 2.625503 | -2.507693 | -1.807202 |
| 1 | 2.149129 | -2.667198 | -0.835088 |
| 1 | 3.711859 | -2.497429 | -1.686350 |
| 1 | 2.327157 | -3.315206 | -2.479506 |
| 6 | 2.174616 | -1.228420 | -2.345007 |
| 7 | 1.824191 | -0.200563 | -2.760492 |
| 6 | 2.919642 | 1.997974 | 2.870903 |
| 1 | 3.729541 | 1.275215 | 3.002786 |
| 1 | 2.718320 | 2.510806 | 3.814437 |
| 1 | 3.210119 | 2.725010 | 2.105466 |
| 6 | 1.728189 | 1.310079 | 2.396905 |
| 7 | 0.787325 | 0.771858 | 1.986121 |
| 6 | -1.274814 | 3.712196 | 1.194713 |
| 1 | -1.538936 | 3.897581 | 0.148553 |
| 1 | -0.198658 | 3.526254 | 1.261430 |
| 1 | -1.529499 | 4.591826 | 1.791311 |
| 6 | -2.012708 | 2.546850 | 1.671743 |
| 7 | -2.602105 | 1.613075 | 2.032901 |
| 6 | -1.881815 | -4.553275 | -0.194044 |
| 1 | -1.723235 | -5.618363 | -0.380450 |
| 1 | -2.943773 | -4.318090 | -0.300824 |
| 1 | -1.556302 | -4.308372 | 0.821591 |
| 6 | -1.104011 | -3.756470 | -1.136472 |
| 7 | -0.475260 | -3.125401 | -1.882064 |
| 6 | 4.649892 | 1.371759 | -1.263521 |
| 1 | 4.650597 | 2.393323 | -0.875246 |
| 1 | 4.013418 | 1.335484 | -2.152786 |
| 1 | 5.668806 | 1.078447 | -1.528544 |
| 6 | 4.111428 | 0.462355 | -0.256165 |
| 7 | 3.687699 | -0.273936 | 0.537499 |
| 6 | -5.141569 | 1.325976 | -0.320555 |
| 1 | -5.956796 | 2.034241 | -0.487814 |
| 1 | -4.956924 | 1.218729 | 0.752523 |
| 1 | -5.409055 | 0.348701 | -0.729672 |
| 6 | -3.921326 | 1.808448 | -0.958313 |
| 7 | -2.946549 | 2.203108 | -1.453932 |
| 6 | 0.443421 | 2.945416 | -2.544865 |
| 1 | -0.621548 | 2.906068 | -2.287378 |
| 1 | 0.700320 | 2.096532 | -3.186310 |
| 1 | 0.646228 | 3.877790 | -3.078141 |
| 6 | 1.249533 | 2.879400 | -1.329236 |
| 7 | 1.881632 | 2.831774 | -0.354549 |
| 6 | 2.662777 | -2.459643 | 2.732918 |
| 1 | 3.499948 | -2.657263 | 2.059630 |
| 1 | 2.636574 | -3.209218 | 3.527581 |
| 1 | 2.809701 | -1.467332 | 3.168115 |
| 6 | 1.409085 | -2.478955 | 1.985258 |
| 7 | 0.404106 | -2.501767 | 1.401767 |
| 6 | -1.499599 | -0.351011 | -2.622571 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -0.896724 | -0.109265 | -1.330143 |
| 7 | -0.424954 | 0.098169 | -0.302004 |
| 1 | -2.423299 | -0.914075 | -2.451095 |
| 1 | -0.803135 | -0.940593 | -3.223487 |
| 1 | -1.726255 | 0.611949 | -3.087780 |
| 1 | 0.015616 | 0.300554 | 0.651436 |

Cartesian coordinates of : PACN10_ 5

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.396120 | -1.336965 | -2.522054 |
| 1 | 4.751654 | -0.337142 | -2.784229 |
| 1 | 4.912915 | -2.077802 | -3.137082 |
| 1 | 4.609713 | -1.529126 | -1.465342 |
| 6 | 2.954381 | -1.418200 | -2.735582 |
| 7 | 1.804545 | -1.490020 | -2.886154 |
| 6 | 1.957386 | 4.201035 | 0.680928 |
| 1 | 2.714644 | 4.220281 | -0.106787 |
| 1 | 2.271632 | 3.513971 | 1.471966 |
| 1 | 1.834039 | 5.205655 | 1.093107 |
| 6 | 0.691347 | 3.728668 | 0.131500 |
| 7 | -0.325449 | 3.367969 | -0.300411 |
| 6 | -4.537090 | -1.443809 | -1.904034 |
| 1 | -5.175400 | -2.301177 | -2.132098 |
| 1 | -4.425342 | -0.819604 | -2.793486 |
| 1 | -4.988654 | -0.848126 | -1.105669 |
| 6 | -3.224456 | -1.901793 | -1.461605 |
| 7 | -2.185836 | -2.281148 | -1.103731 |
| 6 | -2.112262 | 1.469411 | 2.063288 |
| 1 | -1.576387 | 1.877366 | 1.198778 |
| 1 | -1.388995 | 0.948193 | 2.696849 |
| 1 | -2.554831 | 2.293559 | 2.630080 |
| 6 | -3.153042 | 0.543261 | 1.625680 |
| 7 | -3.980735 | -0.193654 | 1.274911 |
| 6 | 4.574341 | 0.880025 | 0.984736 |
| 1 | 4.425713 | -0.159843 | 1.291067 |
| 1 | 4.353552 | 1.540390 | 1.828661 |
| 1 | 5.611819 | 1.029365 | 0.674360 |
| 6 | 3.669141 | 1.176721 | -0.121366 |
| 7 | 2.959763 | 1.420000 | -1.008859 |
| 6 | 2.116328 | -0.915019 | 3.663512 |
| 1 | 3.140415 | -1.197531 | 3.405263 |
| 1 | 1.458671 | -1.756881 | 3.431148 |
| 1 | 2.055825 | -0.679806 | 4.729005 |
| 6 | 1.706588 | 0.238756 | 2.868665 |
| 7 | 1.380757 | 1.161224 | 2.240309 |
| 6 | -2.734571 | -3.311950 | 1.977954 |
| 1 | -2.651192 | -4.069727 | 1.194146 |
| 1 | -3.642745 | -2.723484 | 1.811916 |
| 1 | -2.774866 | -3.790430 | 2.959562 |
| 6 | -1.590445 | -2.416085 | 1.895519 |
| 7 | -0.687631 | -1.689726 | 1.810681 |
| 6 | 1.016953 | -3.610851 | -0.486910 |
| 1 | 1.492207 | -4.100555 | -1.340669 |
| 1 | 0.137939 | -3.063622 | -0.845324 |
| 1 | 0.700731 | -4.367477 | 0.236822 |
| 6 | 1.959085 | -2.689824 | 0.141657 |
| 7 | 2.702646 | -1.945580 | 0.636817 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -3.809688 | 3.364186 | -0.559580 |
| 1 | -4.390673 | 4.002736 | -1.229625 |
| 1 | -2.972504 | 3.937899 | -0.150635 |
| 1 | -4.457146 | 3.021497 | 0.253341 |
| 6 | -3.282829 | 2.214350 | -1.287842 |
| 7 | -2.854737 | 1.293517 | -1.852246 |
| 6 | 0.135628 | 1.111205 | -2.667098 |
| 6 | 0.046409 | 0.454674 | -1.384067 |
| 7 | -0.024012 | -0.069006 | -0.363100 |
| 1 | 1.194544 | 1.260161 | -2.892484 |
| 1 | -0.392483 | 2.065326 | -2.594730 |
| 1 | -0.334370 | 0.463811 | -3.412320 |
| 1 | -0.141523 | -0.599699 | 0.527068 |

Cartesian coordinates of : PACN10_ 6

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.855236 | 4.520610 | -1.466738 |
| 1 | -0.096712 | 4.395121 | -1.991654 |
| 1 | 1.669309 | 4.082183 | -2.051947 |
| 1 | 1.049467 | 5.586529 | -1.323312 |
| 6 | 0.776103 | 3.843823 | -0.176733 |
| 7 | 0.710209 | 3.296991 | 0.846040 |
| 6 | 3.164199 | 1.637359 | 2.176039 |
| 1 | 4.052186 | 1.660363 | 2.812912 |
| 1 | 2.291557 | 1.984341 | 2.735463 |
| 1 | 3.300890 | 2.300172 | 1.316968 |
| 6 | 2.924622 | 0.278075 | 1.704802 |
| 7 | 2.740776 | -0.806663 | 1.327864 |
| 6 | -1.373111 | -3.706336 | -2.114238 |
| 1 | -0.982988 | -3.945041 | -1.120117 |
| 1 | -0.565282 | -3.784460 | -2.846276 |
| 1 | -2.170228 | -4.406044 | -2.378864 |
| 6 | -1.891943 | -2.341992 | -2.098883 |
| 7 | -2.329092 | -1.265087 | -2.083765 |
| 6 | -3.905669 | -2.333184 | 0.759127 |
| 1 | -3.058931 | -3.023891 | 0.707473 |
| 1 | -4.458744 | -2.368411 | -0.183631 |
| 1 | -4.567268 | -2.630004 | 1.576832 |
| 6 | -3.404241 | -0.980560 | 0.983300 |
| 7 | -3.020528 | 0.101667 | 1.159226 |
| 6 | 4.579586 | -0.374250 | -1.685455 |
| 1 | 4.495146 | -0.991967 | -0.786093 |
| 1 | 5.599131 | 0.009475 | -1.772948 |
| 1 | 4.343810 | -0.985185 | -2.560481 |
| 6 | 3.633898 | 0.734040 | -1.591452 |
| 7 | 2.888212 | 1.621756 | -1.510293 |
| 6 | 2.382606 | -3.800762 | -0.216066 |
| 1 | 2.702422 | -3.299517 | 0.701923 |
| 1 | 3.213392 | -4.373468 | -0.636357 |
| 1 | 1.555920 | -4.478580 | 0.015076 |
| 6 | 1.936863 | -2.788538 | -1.168052 |
| 7 | 1.589729 | -1.990856 | -1.938580 |
| 6 | -1.762011 | 2.633734 | 2.731681 |
| 1 | -1.269268 | 3.518064 | 3.142205 |
| 1 | -2.683899 | 2.416747 | 3.276336 |
| 1 | -1.996202 | 2.809855 | 1.676356 |
| 6 | -0.865435 | 1.489470 | 2.801282 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.153909 | 0.569008 | 2.811580 |
| 6 | 0.566952 | -2.478578 | 3.480824 |
| 1 | 1.509357 | -1.928359 | 3.414553 |
| 1 | 0.746786 | -3.483104 | 3.872251 |
| 1 | -0.105078 | -1.935085 | 4.148858 |
| 6 | -0.026657 | -2.558876 | 2.150034 |
| 7 | -0.492906 | -2.638414 | 1.087550 |
| 6 | -4.449805 | 1.551356 | -1.401159 |
| 1 | -5.069522 | 2.076459 | -2.132308 |
| 1 | -4.924989 | 1.594398 | -0.418144 |
| 1 | -4.334771 | 0.504759 | -1.698080 |
| 6 | -3.128374 | 2.166909 | -1.333017 |
| 7 | -2.078043 | 2.663206 | -1.295461 |
| 6 | 0.067093 | 0.833507 | -2.620726 |
| 6 | 0.022372 | 0.522774 | -1.209724 |
| 7 | -0.005459 | 0.270230 | -0.090567 |
| 1 | -0.936738 | 0.699316 | -3.030602 |
| 1 | 0.779443 | 0.149516 | -3.090191 |
| 1 | 0.394852 | 1.870416 | -2.731245 |
| 1 | -0.039676 | 0.131061 | 0.930817 |

Cartesian coordinates of : PACN10_7

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.361759 | 3.641083 | -0.624907 |
| 1 | -3.134012 | 3.562628 | 0.441986 |
| 1 | -4.384564 | 4.002724 | -0.756960 |
| 1 | -2.663613 | 4.339140 | -1.093774 |
| 6 | -3.214149 | 2.322660 | -1.231617 |
| 7 | -3.101266 | 1.274381 | -1.719179 |
| 6 | 4.800327 | 0.052469 | 0.581963 |
| 1 | 4.734756 | -0.055903 | -0.504843 |
| 1 | 4.894535 | -0.942333 | 1.025819 |
| 1 | 5.678188 | 0.650852 | 0.838545 |
| 6 | 3.586044 | 0.700669 | 1.069981 |
| 7 | 2.623062 | 1.226572 | 1.452982 |
| 6 | -0.534855 | -3.977472 | 0.447157 |
| 1 | 0.472392 | -3.869471 | 0.859845 |
| 1 | -0.826268 | -5.030846 | 0.456341 |
| 1 | -1.241266 | -3.398824 | 1.051140 |
| 6 | -0.552613 | -3.461405 | -0.917714 |
| 7 | -0.564940 | -3.022532 | -1.994496 |
| 6 | -3.417332 | -0.512843 | 3.207025 |
| 1 | -2.682837 | -1.321906 | 3.240547 |
| 1 | -4.324206 | -0.892196 | 2.730992 |
| 1 | -3.643469 | -0.173024 | 4.220729 |
| 6 | -2.871895 | 0.587131 | 2.418655 |
| 7 | -2.427307 | 1.465831 | 1.802089 |
| 6 | 3.027826 | 3.452248 | -1.587114 |
| 1 | 2.196488 | 4.039786 | -1.983497 |
| 1 | 3.968617 | 3.800156 | -2.021037 |
| 1 | 3.054050 | 3.577100 | -0.500064 |
| 6 | 2.823398 | 2.041150 | -1.898200 |
| 7 | 2.683309 | 0.911531 | -2.132165 |
| 6 | 2.794814 | -2.469685 | -2.456189 |
| 1 | 3.557621 | -3.233082 | -2.629989 |
| 1 | 3.113727 | -1.520155 | -2.894614 |
| 1 | 1.856067 | -2.789471 | -2.919198 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 2.585844 | -2.290277 | -1.022009 |
| 7 | 2.422694 | -2.156833 | 0.121774 |
| 6 | 0.144792 | 3.265360 | 1.907824 |
| 1 | 0.177267 | 2.266348 | 2.350251 |
| 1 | -0.728965 | 3.796151 | 2.293807 |
| 1 | 1.061650 | 3.798846 | 2.171187 |
| 6 | 0.043604 | 3.140067 | 0.457306 |
| 7 | -0.034039 | 3.047201 | -0.699200 |
| 6 | 2.369952 | -1.551765 | 3.596085 |
| 1 | 2.990115 | -2.030966 | 2.831675 |
| 1 | 2.226003 | -2.235505 | 4.436238 |
| 1 | 2.858039 | -0.638007 | 3.945305 |
| 6 | 1.090784 | -1.215012 | 2.989242 |
| 7 | 0.081710 | -0.946617 | 2.483062 |
| 6 | -3.967297 | -1.937450 | -2.138481 |
| 1 | -3.205593 | -2.422475 | -2.757571 |
| 1 | -4.164147 | -0.932238 | -2.519973 |
| 1 | -4.884412 | -2.531079 | -2.169613 |
| 6 | -3.475983 | -1.840680 | -0.767437 |
| 7 | -3.065673 | -1.777829 | 0.318170 |
| 6 | -0.389702 | 0.190767 | -2.648559 |
| 6 | -0.367384 | 0.004388 | -1.216230 |
| 7 | -0.350083 | -0.163793 | -0.080731 |
| 1 | -1.313328 | -0.249021 | -3.034344 |
| 1 | 0.490244 | -0.296586 | -3.076570 |
| 1 | -0.371468 | 1.267416 | -2.845478 |
| 1 | -0.320388 | -0.391843 | 0.946309 |

Cartesian coordinates of : PACN10_ 8

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -3.377166 | 2.332908 | 0.576413 |
| 1 | -4.290381 | 1.836740 | 0.913066 |
| 1 | -3.520084 | 3.416476 | 0.561253 |
| 1 | -2.566789 | 2.077959 | 1.265550 |
| 6 | -3.020767 | 1.860638 | -0.757427 |
| 7 | -2.726829 | 1.504102 | -1.823944 |
| 6 | -0.245641 | 2.927952 | 3.645693 |
| 1 | 0.614313 | 3.096736 | 4.298749 |
| 1 | -1.161065 | 2.973770 | 4.241081 |
| 1 | -0.273557 | 3.697524 | 2.867783 |
| 6 | -0.134972 | 1.629617 | 2.992355 |
| 7 | -0.047927 | 0.608534 | 2.446367 |
| 6 | 4.676724 | -0.836771 | -1.744363 |
| 1 | 4.760024 | -0.036019 | -2.483442 |
| 1 | 5.458631 | -1.579685 | -1.920377 |
| 1 | 4.789711 | -0.412341 | -0.742772 |
| 6 | 3.360822 | -1.459570 | -1.843454 |
| 7 | 2.315376 | -1.960401 | -1.922732 |
| 6 | 0.330465 | -4.376187 | -1.069217 |
| 1 | -0.141437 | -3.886297 | -1.924454 |
| 1 | -0.174931 | -5.324024 | -0.867165 |
| 1 | 1.383177 | -4.555509 | -1.298100 |
| 6 | 0.223780 | -3.498238 | 0.091491 |
| 7 | 0.135554 | -2.807095 | 1.022220 |
| 6 | -0.176064 | 3.759855 | -2.356312 |
| 1 | -0.231360 | 4.827230 | -2.585176 |
| 1 | -1.039765 | 3.250693 | -2.795305 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 0.747205 | 3.347798 | -2.775275 |
| 6 | -0.181369 | 3.555614 | -0.910587 |
| 7 | -0.185856 | 3.382337 | 0.239207 |
| 6 | 3.082917 | 2.648730 | 0.659188 |
| 1 | 4.035241 | 2.250677 | 1.017106 |
| 1 | 2.286305 | 2.298616 | 1.322226 |
| 1 | 3.106736 | 3.741527 | 0.658880 |
| 6 | 2.817270 | 2.157952 | -0.689006 |
| 7 | 2.592311 | 1.784486 | -1.766461 |
| 6 | -2.175946 | -2.280058 | 3.112625 |
| 1 | -2.914023 | -2.253264 | 3.918137 |
| 1 | -1.206545 | -1.934808 | 3.482749 |
| 1 | -2.057352 | -3.303731 | 2.750913 |
| 6 | -2.596412 | -1.413905 | 2.016067 |
| 7 | -2.935935 | -0.707915 | 1.158149 |
| 6 | 2.329605 | -2.031773 | 3.170934 |
| 1 | 1.316391 | -1.784294 | 3.499668 |
| 1 | 3.031932 | -1.905890 | 3.998715 |
| 1 | 2.335209 | -3.070917 | 2.834735 |
| 6 | 2.692758 | -1.151755 | 2.064931 |
| 7 | 2.984066 | -0.434609 | 1.198590 |
| 6 | -4.547396 | -1.320695 | -1.792330 |
| 1 | -5.238266 | -2.144724 | -1.987191 |
| 1 | -4.718115 | -0.521208 | -2.517671 |
| 1 | -4.713052 | -0.931074 | -0.783902 |
| 6 | -3.168613 | -1.786993 | -1.894233 |
| 7 | -2.072648 | -2.163371 | -1.976505 |
| 6 | 0.037483 | -0.084606 | -2.872252 |
| 6 | 0.026492 | -0.100190 | -1.426949 |
| 7 | 0.017602 | -0.073457 | -0.278772 |
| 1 | 0.099843 | -1.118576 | -3.220340 |
| 1 | 0.917554 | 0.481385 | -3.194225 |
| 1 | -0.895977 | 0.377077 | -3.209609 |
| 1 | 0.006613 | -0.035275 | 0.760158 |

Cartesian coordinates of : PACN10_ 9

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.836724 | -2.365838 | -2.301676 |
| 1 | -1.929297 | -2.629497 | -2.852279 |
| 1 | -3.309543 | -1.492930 | -2.763200 |
| 1 | -3.538904 | -3.203409 | -2.325147 |
| 6 | -2.482670 | -2.046830 | -0.920952 |
| 7 | -2.206210 | -1.779751 | 0.177344 |
| 6 | -2.442446 | 3.728278 | -0.700309 |
| 1 | -1.489101 | 4.092369 | -1.095551 |
| 1 | -3.001877 | 4.567609 | -0.279262 |
| 1 | -3.028866 | 3.274605 | -1.505561 |
| 6 | -2.184836 | 2.727099 | 0.331459 |
| 7 | -1.975529 | 1.915946 | 1.138606 |
| 6 | 4.007802 | 2.711142 | -1.705899 |
| 1 | 3.528459 | 3.684852 | -1.834363 |
| 1 | 4.956105 | 2.695237 | -2.248773 |
| 1 | 4.190914 | 2.535419 | -0.641863 |
| 6 | 3.123250 | 1.664758 | -2.206204 |
| 7 | 2.417228 | 0.830777 | -2.601374 |
| 6 | -0.177873 | -4.527828 | 0.347667 |
| 1 | -1.110494 | -4.412519 | 0.905167 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 0.239742 | -5.520518 | 0.533516 |
| 1 | -0.383307 | -4.412399 | -0.721447 |
| 6 | 0.772612 | -3.499004 | 0.757155 |
| 7 | 1.541505 | -2.683834 | 1.064574 |
| 6 | -5.078406 | 0.225067 | 0.730872 |
| 1 | -6.129699 | 0.516694 | 0.792512 |
| 1 | -4.502691 | 0.762372 | 1.490694 |
| 1 | -4.987690 | -0.849931 | 0.910402 |
| 6 | -4.537437 | 0.547725 | -0.585445 |
| 7 | -4.087051 | 0.805629 | -1.625201 |
| 6 | 1.374907 | 3.060969 | 1.987539 |
| 1 | 2.447232 | 3.056435 | 2.197543 |
| 1 | 0.950873 | 2.103412 | 2.308320 |
| 1 | 0.892956 | 3.872018 | 2.539512 |
| 6 | 1.150915 | 3.233064 | 0.556328 |
| 7 | 0.946451 | 3.363056 | -0.580772 |
| 6 | -2.203021 | -0.470625 | 3.479526 |
| 1 | -2.335204 | -1.059523 | 4.390435 |
| 1 | -2.725744 | -0.948831 | 2.645663 |
| 1 | -2.600514 | 0.537002 | 3.625233 |
| 6 | -0.790646 | -0.384282 | 3.134578 |
| 7 | 0.333656 | -0.317963 | 2.848871 |
| 6 | 3.712972 | -1.171897 | 2.924132 |
| 1 | 4.047671 | -2.122581 | 2.502631 |
| 1 | 2.761949 | -1.334982 | 3.438464 |
| 1 | 4.460311 | -0.794404 | 3.626312 |
| 6 | 3.501214 | -0.207928 | 1.849685 |
| 7 | 3.325659 | 0.565113 | 0.998508 |
| 6 | 3.076500 | -2.160212 | -1.850081 |
| 1 | 3.172272 | -1.439252 | -1.030716 |
| 1 | 3.629041 | -1.787478 | -2.715512 |
| 1 | 3.479950 | -3.125287 | -1.532621 |
| 6 | 1.665164 | -2.302376 | -2.190440 |
| 7 | 0.532862 | -2.415620 | -2.428251 |
| 6 | -0.615966 | 0.778441 | -2.174282 |
| 6 | 0.027298 | 0.336491 | -0.960337 |
| 7 | 0.511290 | -0.018324 | 0.018302 |
| 1 | -1.703444 | 0.765127 | -2.022950 |
| 1 | -0.318722 | 0.099819 | -2.980458 |
| 1 | -0.258280 | 1.790545 | -2.393264 |
| 1 | 0.841226 | -0.332455 | 0.942420 |

Cartesian coordinates of : PACN10_10

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.710036 | -3.715164 | -2.658515 |
| 1 | 1.343131 | -4.489242 | -3.099434 |
| 1 | -0.077596 | -3.440092 | -3.364249 |
| 1 | 0.245801 | -4.096056 | -1.743451 |
| 6 | 1.511244 | -2.539194 | -2.331592 |
| 7 | 2.160967 | -1.614199 | -2.061289 |
| 6 | 3.001073 | -3.242754 | 1.004977 |
| 1 | 3.384321 | -2.912341 | 1.972831 |
| 1 | 3.450873 | -2.615998 | 0.230628 |
| 1 | 3.259413 | -4.292210 | 0.841260 |
| 6 | 1.551376 | -3.075352 | 0.965809 |
| 7 | 0.394239 | -2.971210 | 0.918716 |
| 6 | -3.015868 | 2.148124 | 1.932073 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -3.835118 | 2.470447 | 2.579810 |
| 1 | -2.942007 | 2.812399 | 1.066504 |
| 1 | -2.067135 | 2.199018 | 2.473967 |
| 6 | -3.245915 | 0.781404 | 1.476703 |
| 7 | -3.422353 | -0.311873 | 1.121901 |
| 6 | 4.716406 | 0.694285 | -1.154982 |
| 1 | 4.311772 | -0.315370 | -1.268546 |
| 1 | 5.254625 | 0.757202 | -0.206082 |
| 1 | 5.400013 | 0.913755 | -1.978906 |
| 6 | 3.608194 | 1.644557 | -1.157552 |
| 7 | 2.721806 | 2.396756 | -1.162500 |
| 6 | -2.798487 | -3.169789 | -0.150788 |
| 1 | -3.843634 | -2.904408 | 0.023755 |
| 1 | -2.240353 | -3.064233 | 0.782448 |
| 1 | -2.727507 | -4.203584 | -0.499914 |
| 6 | -2.221051 | -2.269519 | -1.143407 |
| 7 | -1.764641 | -1.569813 | -1.951827 |
| 6 | -1.584122 | -2.134944 | 3.718771 |
| 1 | -1.516075 | -2.084163 | 4.808171 |
| 1 | -1.151993 | -3.076563 | 3.366784 |
| 1 | -2.633837 | -2.077631 | 3.413764 |
| 6 | -0.857424 | -1.031156 | 3.108693 |
| 7 | -0.294505 | -0.160493 | 2.588364 |
| 6 | 2.580082 | 2.145432 | 2.719733 |
| 1 | 1.569775 | 2.180906 | 3.136072 |
| 1 | 2.676171 | 2.961593 | 1.997914 |
| 1 | 3.318859 | 2.263278 | 3.516401 |
| 6 | 2.776435 | 0.871448 | 2.036988 |
| 7 | 2.927575 | -0.140412 | 1.485300 |
| 6 | 0.078674 | 4.654663 | -1.083340 |
| 1 | 1.013240 | 4.436559 | -1.608707 |
| 1 | 0.041959 | 5.719073 | -0.838010 |
| 1 | -0.776294 | 4.401096 | -1.717404 |
| 6 | 0.023957 | 3.853114 | 0.135018 |
| 7 | -0.018520 | 3.202393 | 1.096775 |
| 6 | -4.372965 | 0.524883 | -2.174385 |
| 1 | -4.590571 | -0.102722 | -1.304908 |
| 1 | -4.079589 | -0.116176 | -3.009435 |
| 1 | -5.263362 | 1.097110 | -2.446586 |
| 6 | -3.277417 | 1.431522 | -1.843900 |
| 7 | -2.411685 | 2.159781 | -1.576671 |
| 6 | 0.305266 | 0.946238 | -2.583031 |
| 6 | 0.229192 | 0.616500 | -1.176814 |
| 7 | 0.155508 | 0.366199 | -0.059211 |
| 1 | 0.132509 | 2.020539 | -2.691312 |
| 1 | -0.472938 | 0.377186 | -3.099841 |
| 1 | 1.298036 | 0.676302 | -2.949400 |
| 1 | 0.066644 | 0.198631 | 0.976207 |

Cartesian coordinates of : PACN10_11

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|----------|-----------|
| 6 | 3.158675 | 3.132993 | -2.250168 |
| 1 | 2.481837 | 3.927350 | -2.572350 |
| 1 | 4.069719 | 3.150396 | -2.853766 |
| 1 | 3.402875 | 3.300588 | -1.196984 |
| 6 | 2.494628 | 1.840061 | -2.382911 |
| 7 | 1.988466 | 0.797918 | -2.481604 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 1.851588 | -2.426737 | -3.104435 |
| 1 | 1.899161 | -3.368531 | -3.656984 |
| 1 | 2.536615 | -2.466644 | -2.251965 |
| 1 | 2.147188 | -1.599422 | -3.753413 |
| 6 | 0.496045 | -2.200598 | -2.612523 |
| 7 | -0.583320 | -2.039570 | -2.212180 |
| 6 | -2.880392 | -0.310309 | 2.577468 |
| 1 | -3.387434 | -0.561901 | 3.512346 |
| 1 | -3.603223 | 0.073720 | 1.852304 |
| 1 | -2.133460 | 0.467040 | 2.768830 |
| 6 | -2.226095 | -1.490858 | 2.023645 |
| 7 | -1.692087 | -2.414060 | 1.562265 |
| 6 | -5.022699 | 2.736469 | -0.421281 |
| 1 | -5.023540 | 3.488478 | -1.214339 |
| 1 | -5.753866 | 3.023961 | 0.338457 |
| 1 | -5.294963 | 1.762815 | -0.838554 |
| 6 | -3.694216 | 2.635980 | 0.174813 |
| 7 | -2.636641 | 2.537453 | 0.645699 |
| 6 | 0.452123 | -4.387429 | 0.364891 |
| 1 | -0.017178 | -4.627057 | 1.321249 |
| 1 | 1.047621 | -5.235335 | 0.016510 |
| 1 | -0.339324 | -4.162813 | -0.355662 |
| 6 | 1.302510 | -3.210104 | 0.515409 |
| 7 | 2.002279 | -2.286731 | 0.614653 |
| 6 | 2.931416 | -0.881188 | 3.766733 |
| 1 | 3.590353 | -0.010946 | 3.827454 |
| 1 | 3.363164 | -1.617481 | 3.080962 |
| 1 | 2.816086 | -1.327662 | 4.757273 |
| 6 | 1.640024 | -0.473414 | 3.235390 |
| 7 | 0.627278 | -0.150539 | 2.771933 |
| 6 | 0.402722 | 3.381252 | 1.971796 |
| 1 | 1.261635 | 2.793985 | 2.308060 |
| 1 | -0.526697 | 2.856763 | 2.215683 |
| 1 | 0.403180 | 4.355881 | 2.466453 |
| 6 | 0.478871 | 3.550845 | 0.525000 |
| 7 | 0.531055 | 3.661795 | -0.630790 |
| 6 | 4.475528 | -0.412314 | -0.285222 |
| 1 | 3.951827 | -0.681784 | -1.206787 |
| 1 | 4.618451 | -1.316091 | 0.311848 |
| 1 | 5.445785 | 0.028147 | -0.529218 |
| 6 | 3.660037 | 0.546500 | 0.454341 |
| 7 | 3.021421 | 1.326835 | 1.032355 |
| 6 | -3.551710 | -3.051683 | -1.281457 |
| 1 | -3.170818 | -3.209827 | -2.292849 |
| 1 | -4.518854 | -3.547268 | -1.165762 |
| 1 | -2.837458 | -3.463757 | -0.562626 |
| 6 | -3.691623 | -1.621422 | -1.031179 |
| 7 | -3.816238 | -0.484520 | -0.823145 |
| 6 | -1.168883 | 1.171706 | -2.033333 |
| 6 | -0.641280 | 0.676076 | -0.783705 |
| 7 | -0.224985 | 0.309169 | 0.222970 |
| 1 | -0.663159 | 0.654443 | -2.852015 |
| 1 | -0.963313 | 2.247360 | -2.068267 |
| 1 | -2.243777 | 0.968528 | -2.048969 |
| 1 | 0.117347 | 0.057853 | 1.188360 |

Cartesian coordinates of : PACN10_12

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|---|---|---|
|----|---|---|---|

```
-----  
6      -1.617610      3.592689      0.440310  
1      -2.650748      3.732781      0.766291  
1      -1.101630      4.555392      0.396670  
1      -1.111797      2.939967      1.158864  
6      -1.593960      2.955369      -0.872431  
7      -1.546473      2.446967      -1.917150  
6      4.638134      1.286893      0.635032  
1      4.531509      1.446646      -0.442104  
1      5.672824      1.020443      0.865189  
1      4.376311      2.214009      1.152190  
6      3.736312      0.215085      1.048336  
7      3.025920      -0.646215      1.371162  
6      -2.387778      -3.791937      -1.019996  
1      -3.376025      -3.554978      -1.419022  
1      -2.302192      -4.866096      -0.837218  
1      -1.634259      -3.490624      -1.754228  
6      -2.164446      -3.054006      0.219350  
7      -1.955476      -2.474242      1.204903  
6      -3.385995      -0.583345      3.280401  
1      -2.390325      -0.922538      3.577750  
1      -3.984899      -1.462294      3.031386  
1      -3.857279      -0.034250      4.099339  
6      -3.259746      0.275313      2.107445  
7      -3.150016      0.970957      1.183178  
6      1.858418      3.142128      -2.279989  
1      2.289602      4.138869      -2.404437  
1      0.866808      3.120898      -2.743363  
1      2.500528      2.398452      -2.759869  
6      1.734552      2.824665      -0.859550  
7      1.634982      2.580733      0.273255  
6      4.107489      -2.396150      -1.769491  
1      4.165439      -2.579183      -0.692096  
1      5.112589      -2.395460      -2.198632  
1      3.510734      -3.190448      -2.223843  
6      3.463929      -1.106323      -1.997246  
7      2.969046      -0.067978      -2.163009  
6      1.890717      1.734440      3.709186  
1      2.690484      1.040120      3.980393  
1      1.525435      2.242525      4.604916  
1      2.270411      2.473121      2.995856  
6      0.812487      1.001286      3.062879  
7      -0.035051      0.420903      2.523750  
6      1.160363      -3.242891      1.721635  
1      0.550379      -4.089946      2.045058  
1      0.751393      -2.323937      2.152168  
1      2.190802      -3.362405      2.063859  
6      1.129318      -3.139084      0.266120  
7      1.084676      -3.053005      -0.892725  
6      -4.748094      1.320906      -1.781938  
1      -4.410850      2.031544      -2.540874  
1      -4.645892      1.774616      -0.792115  
1      -5.794462      1.062608      -1.962659  
6      -3.918079      0.122336      -1.834543  
7      -3.256809      -0.831912      -1.881433  
6      -0.171018      -0.415871      -2.682179  
6      -0.270945      -0.251114      -1.250015  
7      -0.346442      -0.131261      -0.110384  
1      0.249508      -1.408664      -2.874017  
1      0.499421      0.352936      -3.075564  
1      -1.173506      -0.317375      -3.105915  
1      -0.375107      0.006304      0.935303
```

Cartesian coordinates of : PACN10_13

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -5.086919 | -0.200171 | -0.354097 |
| 1 | -5.379372 | -1.073566 | 0.233149 |
| 1 | -4.655348 | -0.539085 | -1.299432 |
| 1 | -5.964210 | 0.422172 | -0.548600 |
| 6 | -4.083046 | 0.566211 | 0.376573 |
| 7 | -3.294466 | 1.192270 | 0.957676 |
| 6 | 2.547528 | 2.133448 | 1.022382 |
| 1 | 2.598367 | 2.802612 | 1.884906 |
| 1 | 1.616203 | 2.336368 | 0.481920 |
| 1 | 3.403865 | 2.305942 | 0.362616 |
| 6 | 2.560409 | 0.745957 | 1.474757 |
| 7 | 2.575350 | -0.365604 | 1.816807 |
| 6 | -1.043866 | -2.273739 | -2.590162 |
| 1 | -0.165569 | -2.143470 | -3.228065 |
| 1 | -1.687250 | -3.049856 | -3.012931 |
| 1 | -0.720730 | -2.583637 | -1.590454 |
| 6 | -1.775277 | -1.014077 | -2.495871 |
| 7 | -2.339265 | -0.002690 | -2.404271 |
| 6 | -2.385285 | -5.047371 | 0.693976 |
| 1 | -1.304451 | -5.169626 | 0.806383 |
| 1 | -2.729330 | -5.617619 | -0.172602 |
| 1 | -2.890046 | -5.423952 | 1.587212 |
| 6 | -2.679402 | -3.629052 | 0.512128 |
| 7 | -2.898446 | -2.496198 | 0.371065 |
| 6 | 2.981889 | -2.756809 | -0.247826 |
| 1 | 3.654594 | -2.703852 | 0.612387 |
| 1 | 2.985577 | -1.784590 | -0.750834 |
| 1 | 3.322037 | -3.532431 | -0.938773 |
| 6 | 1.633974 | -3.061661 | 0.221150 |
| 7 | 0.557673 | -3.310868 | 0.582351 |
| 6 | -1.835216 | 4.046044 | 2.141001 |
| 1 | -1.410527 | 4.679913 | 1.357580 |
| 1 | -2.021562 | 4.650402 | 3.032242 |
| 1 | -2.775416 | 3.610478 | 1.790896 |
| 6 | -0.908465 | 2.962924 | 2.451083 |
| 7 | -0.169429 | 2.102507 | 2.701928 |
| 6 | -2.806072 | 3.262030 | -1.689461 |
| 1 | -3.416670 | 3.546823 | -0.828081 |
| 1 | -3.209697 | 2.346127 | -2.129363 |
| 1 | -2.821835 | 4.066328 | -2.429391 |
| 6 | -1.434463 | 3.009375 | -1.258611 |
| 7 | -0.335253 | 2.833967 | -0.923760 |
| 6 | 2.688608 | 2.160731 | -2.902723 |
| 1 | 3.742214 | 2.041090 | -2.636089 |
| 1 | 2.289940 | 3.082605 | -2.466193 |
| 1 | 2.578882 | 2.198890 | -3.989280 |
| 6 | 1.934244 | 1.042494 | -2.360033 |
| 7 | 1.310565 | 0.176132 | -1.904383 |
| 6 | 6.074246 | -0.726904 | 1.037592 |
| 1 | 5.336929 | -0.924550 | 1.822357 |
| 1 | 6.851257 | -0.068350 | 1.433890 |
| 1 | 6.536705 | -1.666757 | 0.724597 |
| 6 | 5.408294 | -0.091931 | -0.096645 |
| 7 | 4.855993 | 0.410367 | -0.986845 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.110067 | -0.876513 | 2.592058 |
| 6 | -0.686357 | -0.478444 | 1.271950 |
| 7 | -0.308522 | -0.187965 | 0.226931 |
| 1 | -2.107020 | -0.465337 | 2.775670 |
| 1 | -0.390826 | -0.465620 | 3.307103 |
| 1 | -1.122822 | -1.969753 | 2.623854 |
| 1 | 0.208166 | -0.006361 | -0.674473 |

Cartesian coordinates of : PACN10_14

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.886239 | -1.301466 | -4.007744 |
| 1 | -0.749707 | -0.246037 | -4.257287 |
| 1 | -1.294920 | -1.835845 | -4.869087 |
| 1 | 0.078485 | -1.741750 | -3.733962 |
| 6 | -1.798847 | -1.405489 | -2.873924 |
| 7 | -2.509940 | -1.499115 | -1.958807 |
| 6 | 2.600304 | 0.810551 | -2.666129 |
| 1 | 2.245655 | 1.840219 | -2.565408 |
| 1 | 1.734618 | 0.151208 | -2.792097 |
| 1 | 3.244265 | 0.730043 | -3.545455 |
| 6 | 3.335154 | 0.426494 | -1.465045 |
| 7 | 3.900432 | 0.119541 | -0.497584 |
| 6 | -0.854826 | -1.630853 | 3.941148 |
| 1 | -1.795591 | -2.030440 | 3.551268 |
| 1 | -2.587842 | 0.523556 | 1.182926 |
| 1 | -0.928532 | -1.521649 | 5.026177 |
| 6 | -0.586534 | -0.333419 | 3.326606 |
| 7 | -0.358507 | 0.693327 | 2.830240 |
| 6 | -2.951550 | 1.169456 | 0.379111 |
| 1 | -4.043248 | 1.215047 | 0.431195 |
| 1 | -0.034825 | -2.316794 | 3.705275 |
| 1 | -2.655592 | 0.743979 | -0.586068 |
| 6 | -2.388828 | 2.506460 | 0.532328 |
| 7 | -1.935656 | 3.570053 | 0.650770 |
| 6 | 3.951317 | -3.304427 | -0.562018 |
| 1 | 4.493059 | -2.411599 | -0.236021 |
| 1 | 4.599780 | -3.927003 | -1.183375 |
| 1 | 3.637123 | -3.865893 | 0.321423 |
| 6 | 2.777754 | -2.889272 | -1.323414 |
| 7 | 1.845883 | -2.551095 | -1.931323 |
| 6 | 3.223224 | 0.407849 | 2.750539 |
| 1 | 3.709807 | 0.890426 | 1.898226 |
| 1 | 3.955454 | 0.243014 | 3.545069 |
| 1 | 2.413809 | 1.041902 | 3.126364 |
| 6 | 2.664312 | -0.866760 | 2.312500 |
| 7 | 2.205948 | -1.878494 | 1.969567 |
| 6 | -0.426356 | 4.290549 | -2.264259 |
| 1 | 0.641344 | 4.502267 | -2.153353 |
| 1 | -0.959103 | 4.656597 | -1.381520 |
| 1 | -0.801924 | 4.797666 | -3.156449 |
| 6 | -0.629124 | 2.849678 | -2.379653 |
| 7 | -0.772848 | 1.699068 | -2.461359 |
| 6 | 0.828758 | 3.975113 | 2.184183 |
| 1 | 0.253519 | 3.441585 | 2.948184 |
| 1 | 0.237593 | 4.825228 | 1.835212 |
| 1 | 1.781911 | 4.315102 | 2.596840 |
| 6 | 1.050761 | 3.052802 | 1.082157 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 1.208820 | 2.291263 | 0.220429 |
| 6 | -5.407412 | -2.098234 | -0.138561 |
| 1 | -5.845034 | -3.099614 | -0.149366 |
| 1 | -4.997627 | -1.870107 | -1.126537 |
| 1 | -6.186599 | -1.374476 | 0.114345 |
| 6 | -4.328605 | -2.034882 | 0.841481 |
| 7 | -3.462144 | -1.973842 | 1.613410 |
| 6 | -0.464666 | -2.629025 | 0.221307 |
| 6 | -0.045363 | -1.271264 | -0.037629 |
| 7 | 0.292680 | -0.183595 | -0.198357 |
| 1 | -1.442555 | -2.600404 | 0.716421 |
| 1 | 0.296733 | -3.085193 | 0.862780 |
| 1 | -0.538866 | -3.164409 | -0.728294 |
| 1 | 0.656714 | 0.820427 | -0.174236 |

Cartesian coordinates of : PACN10_15

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.079312 | -2.948620 | -2.063728 |
| 1 | 0.992810 | -1.907342 | -2.385021 |
| 1 | 0.373789 | -3.558035 | -2.633532 |
| 1 | 2.103612 | -3.287582 | -2.237454 |
| 6 | 0.763314 | -3.034682 | -0.641744 |
| 7 | 0.516072 | -3.110501 | 0.491918 |
| 6 | -4.631512 | 1.222203 | 1.881154 |
| 1 | -4.663933 | 0.943742 | 0.824273 |
| 1 | -5.300173 | 2.066335 | 2.067206 |
| 1 | -4.942873 | 0.362424 | 2.478775 |
| 6 | -3.261275 | 1.586791 | 2.223076 |
| 7 | -2.167727 | 1.883459 | 2.484520 |
| 6 | -2.920810 | 0.064795 | -3.705514 |
| 1 | -3.068893 | -0.401496 | -4.682731 |
| 1 | -2.276592 | 0.942641 | -3.807848 |
| 1 | -3.879493 | 0.391650 | -3.297330 |
| 6 | -2.293354 | -0.880822 | -2.788384 |
| 7 | -1.778978 | -1.638307 | -2.073263 |
| 6 | 1.338801 | 2.658925 | 2.652380 |
| 1 | 1.568456 | 3.630752 | 3.097206 |
| 1 | 1.852139 | 1.871056 | 3.210839 |
| 1 | 0.255788 | 2.493214 | 2.699494 |
| 6 | 1.788548 | 2.627815 | 1.263560 |
| 7 | 2.136306 | 2.612236 | 0.154220 |
| 6 | -2.814002 | -3.953420 | 0.129464 |
| 1 | -2.081224 | -4.521942 | 0.707748 |
| 1 | -2.443135 | -3.828965 | -0.891518 |
| 1 | -3.765682 | -4.490495 | 0.115521 |
| 6 | -2.993104 | -2.633448 | 0.725640 |
| 7 | -3.142917 | -1.584653 | 1.203427 |
| 6 | -1.284606 | 3.696328 | -0.346333 |
| 1 | -1.650082 | 4.670886 | -0.679867 |
| 1 | -0.294171 | 3.513544 | -0.774180 |
| 1 | -1.208244 | 3.694529 | 0.745874 |
| 6 | -2.204764 | 2.641263 | -0.759698 |
| 7 | -2.926188 | 1.785984 | -1.073381 |
| 6 | 2.518030 | 2.012158 | -3.273761 |
| 1 | 3.177957 | 1.196929 | -3.581807 |
| 1 | 3.015067 | 2.617077 | -2.508363 |
| 1 | 2.274218 | 2.636848 | -4.136448 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 1.307817 | 1.458035 | -2.685723 |
| 7 | 0.355477 | 1.022175 | -2.187271 |
| 6 | 3.554072 | -2.865206 | 1.700830 |
| 1 | 2.833581 | -3.644454 | 1.960685 |
| 1 | 4.497611 | -3.045625 | 2.222012 |
| 1 | 3.719605 | -2.889262 | 0.619223 |
| 6 | 3.019756 | -1.557670 | 2.068761 |
| 7 | 2.611853 | -0.506554 | 2.350937 |
| 6 | 4.904122 | 0.964400 | 0.042927 |
| 1 | 4.846222 | 1.966817 | -0.389298 |
| 1 | 5.924980 | 0.584372 | -0.046216 |
| 1 | 4.624243 | 1.027549 | 1.098616 |
| 6 | 3.972243 | 0.073538 | -0.642834 |
| 7 | 3.235386 | -0.648010 | -1.179175 |
| 6 | -0.510854 | -0.813031 | 2.691503 |
| 6 | -0.407237 | -0.307032 | 1.340047 |
| 7 | -0.305896 | 0.084192 | 0.263960 |
| 1 | -1.559406 | -0.772642 | 2.992936 |
| 1 | 0.113403 | -0.201124 | 3.347489 |
| 1 | -0.149741 | -1.846542 | 2.677576 |
| 1 | -0.170542 | 0.411074 | -0.734828 |

Cartesian coordinates of : PACN10_16

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.187839 | 1.154396 | 1.714177 |
| 1 | -4.720720 | 1.228852 | 2.665620 |
| 1 | -4.477879 | 0.234004 | 1.198581 |
| 1 | -4.456195 | 2.002348 | 1.078491 |
| 6 | -2.745446 | 1.138392 | 1.944173 |
| 7 | -1.601137 | 1.108854 | 2.145390 |
| 6 | 2.670655 | -3.302844 | 1.928840 |
| 1 | 3.555511 | -2.662571 | 1.853665 |
| 1 | 2.653155 | -3.993776 | 1.081625 |
| 1 | 2.696605 | -3.862743 | 2.866908 |
| 6 | 1.488945 | -2.453933 | 1.876665 |
| 7 | 0.555545 | -1.764489 | 1.819759 |
| 6 | 4.589515 | -1.211788 | -1.628870 |
| 1 | 4.586078 | -0.528507 | -2.481143 |
| 1 | 5.252870 | -2.055647 | -1.835051 |
| 1 | 4.938164 | -0.672253 | -0.743778 |
| 6 | 3.233409 | -1.691280 | -1.382154 |
| 7 | 2.159920 | -2.090719 | -1.182288 |
| 6 | -4.294248 | -0.746078 | -2.409461 |
| 1 | -5.360350 | -0.509619 | -2.456822 |
| 1 | -4.134048 | -1.637624 | -1.796976 |
| 1 | -3.912776 | -0.937763 | -3.415213 |
| 6 | -3.561133 | 0.366730 | -1.814900 |
| 7 | -2.988845 | 1.260055 | -1.338507 |
| 6 | 1.836733 | 1.464355 | 2.317386 |
| 1 | 2.208675 | 2.189015 | 3.047203 |
| 1 | 1.030445 | 0.880468 | 2.771011 |
| 1 | 1.420046 | 1.999856 | 1.456489 |
| 6 | 2.918399 | 0.582521 | 1.888510 |
| 7 | 3.777090 | -0.120248 | 1.541785 |
| 6 | 3.710219 | 3.560386 | -0.048014 |
| 1 | 4.273010 | 3.192658 | 0.815440 |
| 1 | 2.823229 | 4.102947 | 0.292414 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 4.347380 | 4.235651 | -0.624439 |
| 6 | 3.287306 | 2.434848 | -0.874942 |
| 7 | 2.941798 | 1.530593 | -1.517035 |
| 6 | -2.373851 | -2.347571 | 3.015562 |
| 1 | -1.807249 | -1.502488 | 3.417052 |
| 1 | -1.801291 | -3.264049 | 3.178717 |
| 1 | -3.334404 | -2.429856 | 3.530873 |
| 6 | -2.586118 | -2.141536 | 1.585435 |
| 7 | -2.760401 | -1.955473 | 0.451348 |
| 6 | -0.664772 | -3.689118 | -1.450552 |
| 1 | -0.304904 | -3.314047 | -0.487818 |
| 1 | 0.127439 | -4.281565 | -1.914303 |
| 1 | -1.553908 | -4.304630 | -1.292608 |
| 6 | -0.995544 | -2.553031 | -2.303816 |
| 7 | -1.263952 | -1.643246 | -2.975013 |
| 6 | -2.232350 | 4.228428 | 0.294826 |
| 1 | -2.350249 | 5.266662 | -0.025428 |
| 1 | -2.456132 | 4.154880 | 1.362898 |
| 1 | -2.915765 | 3.588913 | -0.271352 |
| 6 | -0.864966 | 3.782256 | 0.051259 |
| 7 | 0.226761 | 3.437899 | -0.147973 |
| 6 | 0.093569 | 1.134651 | -2.584802 |
| 6 | 0.031260 | 0.508042 | -1.285110 |
| 7 | -0.018259 | -0.004605 | -0.257810 |
| 1 | 0.433447 | 2.165087 | -2.452384 |
| 1 | -0.901650 | 1.089463 | -3.032914 |
| 1 | 0.812273 | 0.573686 | -3.189452 |
| 1 | 0.007106 | -0.564658 | 0.619827 |

Cartesian coordinates of : PACN10_17

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.402418 | -0.714450 | 0.218820 |
| 1 | 4.769401 | 0.220358 | 0.650122 |
| 1 | 5.245350 | -1.328730 | -0.107764 |
| 1 | 3.828303 | -1.248166 | 0.981018 |
| 6 | 3.522539 | -0.429235 | -0.909960 |
| 7 | 2.827350 | -0.218098 | -1.817350 |
| 6 | 2.100009 | -1.741598 | 3.557336 |
| 1 | 2.484538 | -2.603572 | 3.004498 |
| 1 | 1.968938 | -2.003616 | 4.610077 |
| 1 | 2.802199 | -0.906475 | 3.472048 |
| 6 | 0.830822 | -1.339186 | 2.969982 |
| 7 | -0.168596 | -1.007446 | 2.481121 |
| 6 | -3.138877 | 0.699719 | 3.239031 |
| 1 | -3.190870 | 1.163472 | 4.227210 |
| 1 | -2.761250 | -0.322669 | 3.323481 |
| 1 | -4.135052 | 0.662181 | 2.792784 |
| 6 | -2.241217 | 1.458625 | 2.374934 |
| 7 | -1.512452 | 2.060867 | 1.698696 |
| 6 | -2.191078 | 4.130073 | -0.935342 |
| 1 | -1.891960 | 4.055628 | 0.113950 |
| 1 | -3.097027 | 4.735836 | -1.017301 |
| 1 | -1.384793 | 4.593100 | -1.509270 |
| 6 | -2.437601 | 2.787064 | -1.447852 |
| 7 | -2.639655 | 1.720957 | -1.862440 |
| 6 | 1.914762 | -3.572751 | -2.212478 |
| 1 | 2.435783 | -4.523471 | -2.351546 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 2.456953 | -2.782070 | -2.739995 |
| 1 | 0.901253 | -3.652944 | -2.616714 |
| 6 | 1.842554 | -3.243042 | -0.791514 |
| 7 | 1.790313 | -2.972159 | 0.338006 |
| 6 | -1.598195 | -3.784286 | 0.866286 |
| 1 | -0.596096 | -3.907806 | 1.287198 |
| 1 | -2.149078 | -4.725285 | 0.941240 |
| 1 | -2.126797 | -3.001901 | 1.419551 |
| 6 | -1.484815 | -3.378423 | -0.530610 |
| 7 | -1.386858 | -3.035667 | -1.637549 |
| 6 | 1.230615 | 3.594980 | 1.852769 |
| 1 | 0.583475 | 3.828589 | 1.003385 |
| 1 | 2.051444 | 4.315095 | 1.910492 |
| 1 | 0.632790 | 3.644907 | 2.765625 |
| 6 | 1.763263 | 2.245711 | 1.685067 |
| 7 | 2.215844 | 1.183640 | 1.546838 |
| 6 | -4.369624 | -1.121890 | -1.891785 |
| 1 | -5.411937 | -1.446096 | -1.837723 |
| 1 | -3.790429 | -1.866834 | -2.446822 |
| 1 | -4.306987 | -0.157121 | -2.401677 |
| 6 | -3.812030 | -0.988619 | -0.549453 |
| 7 | -3.352700 | -0.899536 | 0.514492 |
| 6 | 3.432658 | 3.024969 | -1.659618 |
| 1 | 3.822108 | 2.397337 | -2.464861 |
| 1 | 3.845755 | 2.673323 | -0.708382 |
| 1 | 3.733911 | 4.062216 | -1.826007 |
| 6 | 1.976843 | 2.922995 | -1.618580 |
| 7 | 0.818152 | 2.852190 | -1.568451 |
| 6 | -0.314681 | -0.100797 | -2.741242 |
| 6 | -0.312378 | -0.110998 | -1.296008 |
| 7 | -0.319770 | -0.157967 | -0.149171 |
| 1 | -1.299546 | -0.436580 | -3.077783 |
| 1 | 0.473675 | -0.772287 | -3.091800 |
| 1 | -0.126742 | 0.922904 | -3.076722 |
| 1 | -0.364634 | -0.309959 | 0.883643 |

Cartesian coordinates of : PACN10_18

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.199847 | -1.624355 | -1.818062 |
| 1 | 3.952649 | -1.349672 | -2.846823 |
| 1 | 5.090479 | -2.257686 | -1.814875 |
| 1 | 4.394150 | -0.714480 | -1.241860 |
| 6 | 3.077031 | -2.336580 | -1.214755 |
| 7 | 2.188582 | -2.906434 | -0.728137 |
| 6 | 2.727915 | -1.505908 | 2.679002 |
| 1 | 2.611071 | -2.486955 | 2.210141 |
| 1 | 1.843021 | -1.313013 | 3.290777 |
| 1 | 3.626960 | -1.491663 | 3.300466 |
| 6 | 2.828121 | -0.488632 | 1.638921 |
| 7 | 2.930282 | 0.318175 | 0.807476 |
| 6 | -2.111741 | 3.727644 | 1.736221 |
| 1 | -1.414888 | 3.461110 | 2.537226 |
| 1 | -3.015131 | 4.165801 | 2.167636 |
| 1 | -1.629625 | 4.455333 | 1.078680 |
| 6 | -2.445951 | 2.524533 | 0.979709 |
| 7 | -2.707883 | 1.554152 | 0.395740 |
| 6 | -1.288865 | 2.645481 | -2.692280 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.017465 | 3.458200 | -2.628270 |
| 1 | -0.627604 | 2.819217 | -3.545357 |
| 1 | -0.691691 | 2.623200 | -1.774655 |
| 6 | -1.982587 | 1.372894 | -2.858238 |
| 7 | -2.533689 | 0.357501 | -2.981536 |
| 6 | -0.650466 | -4.765854 | 0.468323 |
| 1 | -1.573650 | -4.611911 | -0.098923 |
| 1 | -0.770723 | -5.634983 | 1.119866 |
| 1 | 0.186762 | -4.943065 | -0.214032 |
| 6 | -0.376134 | -3.572616 | 1.261129 |
| 7 | -0.155363 | -2.613611 | 1.878175 |
| 6 | -2.260639 | -0.624778 | 3.015938 |
| 1 | -3.092229 | -0.004080 | 3.359745 |
| 1 | -2.098136 | -1.454927 | 3.707212 |
| 1 | -2.490291 | -1.032869 | 2.025366 |
| 6 | -1.048107 | 0.177666 | 2.916561 |
| 7 | -0.090454 | 0.828147 | 2.799986 |
| 6 | 3.293832 | 2.486933 | -1.878088 |
| 1 | 3.676245 | 2.207685 | -0.891528 |
| 1 | 2.765094 | 3.440350 | -1.798785 |
| 1 | 4.122029 | 2.589807 | -2.583931 |
| 6 | 2.373105 | 1.449300 | -2.332030 |
| 7 | 1.655575 | 0.613868 | -2.702879 |
| 6 | 2.330581 | 3.156201 | 2.289504 |
| 1 | 3.350968 | 2.914562 | 1.979977 |
| 1 | 2.014097 | 2.447507 | 3.060714 |
| 1 | 2.296870 | 4.174808 | 2.684140 |
| 6 | 1.430165 | 3.021763 | 1.151102 |
| 7 | 0.706415 | 2.901150 | 0.249220 |
| 6 | -4.931895 | -0.663111 | -1.101182 |
| 1 | -5.852171 | -0.974897 | -0.600914 |
| 1 | -5.045948 | -0.760664 | -2.183363 |
| 1 | -4.711016 | 0.381136 | -0.864870 |
| 6 | -3.815047 | -1.488178 | -0.654468 |
| 7 | -2.930194 | -2.152051 | -0.295957 |
| 6 | -0.432469 | -1.878274 | -2.102102 |
| 6 | -0.272871 | -0.912667 | -1.040386 |
| 7 | -0.122814 | -0.126492 | -0.216226 |
| 1 | -1.408887 | -1.716843 | -2.566761 |
| 1 | -0.359666 | -2.880359 | -1.673039 |
| 1 | 0.374302 | -1.704880 | -2.820555 |
| 1 | 0.048284 | 0.564620 | 0.516651 |

Cartesian coordinates of : PACN10_19

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.717741 | 1.548207 | -1.496987 |
| 1 | 4.279461 | 2.484742 | -1.850285 |
| 1 | 5.705147 | 1.415470 | -1.946319 |
| 1 | 4.811673 | 1.578816 | -0.407134 |
| 6 | 3.848489 | 0.433853 | -1.858110 |
| 7 | 3.174250 | -0.467786 | -2.142904 |
| 6 | -2.217069 | 1.625283 | 3.628051 |
| 1 | -2.985315 | 2.278458 | 3.206181 |
| 1 | -1.904467 | 2.004214 | 4.604145 |
| 1 | -2.615179 | 0.611056 | 3.736692 |
| 6 | -1.082980 | 1.561807 | 2.718646 |
| 7 | -0.185720 | 1.481330 | 1.986827 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -4.744532 | -0.627110 | 1.217922 |
| 1 | -5.798652 | -0.360588 | 1.106269 |
| 1 | -4.530483 | -0.836865 | 2.269503 |
| 1 | -4.529230 | -1.526096 | 0.632980 |
| 6 | -3.895205 | 0.463814 | 0.746894 |
| 7 | -3.226565 | 1.335620 | 0.367570 |
| 6 | -4.253150 | 0.023813 | -3.046807 |
| 1 | -3.688871 | 0.260440 | -3.951808 |
| 1 | -4.378247 | 0.945582 | -2.470529 |
| 1 | -5.231226 | -0.384559 | -3.313285 |
| 6 | -3.508558 | -0.939622 | -2.242427 |
| 7 | -2.932288 | -1.703071 | -1.582134 |
| 6 | 4.342381 | -2.933586 | -0.453468 |
| 1 | 4.713061 | -2.024589 | 0.029781 |
| 1 | 4.572587 | -2.882164 | -1.520304 |
| 1 | 4.823771 | -3.810269 | -0.013004 |
| 6 | 2.896993 | -3.010870 | -0.270456 |
| 7 | 1.747996 | -3.074428 | -0.108011 |
| 6 | 1.716021 | -1.358807 | 2.905983 |
| 1 | 0.792545 | -0.816926 | 3.127603 |
| 1 | 2.229106 | -1.604423 | 3.839392 |
| 1 | 1.455827 | -2.280806 | 2.377913 |
| 6 | 2.581557 | -0.544030 | 2.057206 |
| 7 | 3.271411 | 0.098385 | 1.376813 |
| 6 | -1.388474 | 3.482142 | -1.320713 |
| 1 | -1.139127 | 3.168247 | -0.303233 |
| 1 | -2.380736 | 3.940079 | -1.315083 |
| 1 | -0.641483 | 4.199046 | -1.668793 |
| 6 | -1.391281 | 2.311347 | -2.191173 |
| 7 | -1.400024 | 1.376629 | -2.881444 |
| 6 | 2.773974 | 3.313114 | 1.625382 |
| 1 | 3.791733 | 2.915581 | 1.665077 |
| 1 | 2.196498 | 2.862355 | 2.437450 |
| 1 | 2.797698 | 4.398566 | 1.749560 |
| 6 | 2.155155 | 2.961505 | 0.350860 |
| 7 | 1.662081 | 2.678385 | -0.662777 |
| 6 | -1.558902 | -3.740111 | 0.773680 |
| 1 | -0.533741 | -3.874260 | 0.414700 |
| 1 | -2.236262 | -3.684195 | -0.082765 |
| 1 | -1.833883 | -4.585062 | 1.410344 |
| 6 | -1.645035 | -2.496392 | 1.533625 |
| 7 | -1.717270 | -1.511088 | 2.147312 |
| 6 | 0.139162 | -1.531069 | -2.412076 |
| 6 | 0.153633 | -0.710050 | -1.224131 |
| 7 | 0.161727 | -0.046126 | -0.286031 |
| 1 | -0.345150 | -2.481766 | -2.173888 |
| 1 | 1.176133 | -1.679749 | -2.725807 |
| 1 | -0.431600 | -0.989732 | -3.173443 |
| 1 | 0.129711 | 0.585022 | 0.550133 |

Cartesian coordinates of : PACN10_20

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.844066 | -2.261575 | -2.505126 |
| 1 | -1.017328 | -1.794284 | -3.045978 |
| 1 | -2.516904 | -2.757264 | -3.209738 |
| 1 | -1.430769 | -2.994189 | -1.806338 |
| 6 | -2.573216 | -1.245957 | -1.754482 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -3.160465 | -0.448369 | -1.144554 |
| 6 | -3.989899 | 1.559500 | 1.545243 |
| 1 | -4.860757 | 1.484288 | 2.201779 |
| 1 | -4.245060 | 1.199780 | 0.543760 |
| 1 | -3.678281 | 2.605637 | 1.480281 |
| 6 | -2.893648 | 0.749823 | 2.070299 |
| 7 | -2.030966 | 0.097085 | 2.495564 |
| 6 | 4.616259 | 1.092637 | 1.946495 |
| 1 | 5.671327 | 1.245322 | 1.705803 |
| 1 | 4.503601 | 0.895813 | 3.015288 |
| 1 | 4.041986 | 1.986461 | 1.688461 |
| 6 | 4.088259 | -0.035280 | 1.188052 |
| 7 | 3.678080 | -0.937204 | 0.579910 |
| 6 | 3.482252 | -4.071344 | -0.818784 |
| 1 | 3.229006 | -4.955721 | -0.228539 |
| 1 | 4.138977 | -3.418274 | -0.237213 |
| 1 | 3.996903 | -4.390554 | -1.728568 |
| 6 | 2.271043 | -3.331721 | -1.159784 |
| 7 | 1.312357 | -2.728937 | -1.421158 |
| 6 | -2.884001 | 2.375261 | -2.720914 |
| 1 | -3.019678 | 3.391166 | -3.100315 |
| 1 | -3.855764 | 1.920619 | -2.511512 |
| 1 | -2.357129 | 1.767283 | -3.463213 |
| 6 | -2.083055 | 2.386566 | -1.505341 |
| 7 | -1.428339 | 2.372342 | -0.544473 |
| 6 | 1.154515 | 4.018398 | -1.873612 |
| 1 | 1.969129 | 4.630152 | -2.269176 |
| 1 | 0.401958 | 4.668446 | -1.419856 |
| 1 | 0.691388 | 3.453951 | -2.689241 |
| 6 | 1.663585 | 3.084381 | -0.873022 |
| 7 | 2.066301 | 2.331946 | -0.083845 |
| 6 | -4.273873 | -2.433023 | 1.622061 |
| 1 | -4.628365 | -1.628024 | 0.970006 |
| 1 | -4.195155 | -2.062036 | 2.647258 |
| 1 | -4.984327 | -3.262775 | 1.590356 |
| 6 | -2.963235 | -2.874385 | 1.156129 |
| 7 | -1.925001 | -3.221407 | 0.767702 |
| 6 | 0.164363 | 2.708357 | 2.778931 |
| 1 | -0.616317 | 2.755655 | 3.542638 |
| 1 | -0.301033 | 2.618743 | 1.791689 |
| 1 | 0.760770 | 3.624063 | 2.809011 |
| 6 | 1.020727 | 1.551909 | 3.021170 |
| 7 | 1.703442 | 0.629637 | 3.203296 |
| 6 | 2.605122 | 0.018138 | -2.655358 |
| 1 | 3.236622 | 0.856973 | -2.960955 |
| 1 | 2.841370 | -0.859205 | -3.262435 |
| 1 | 2.797713 | -0.214661 | -1.602486 |
| 6 | 1.199834 | 0.370261 | -2.823308 |
| 7 | 0.083108 | 0.673172 | -2.941135 |
| 6 | 0.747240 | -1.991897 | 1.795550 |
| 6 | 0.351521 | -0.939655 | 0.892552 |
| 7 | 0.010594 | -0.082971 | 0.204971 |
| 1 | 1.821995 | -1.903879 | 1.976082 |
| 1 | 0.475405 | -2.950417 | 1.347075 |
| 1 | 0.188616 | -1.832618 | 2.724886 |
| 1 | -0.382049 | 0.740127 | -0.273264 |

Cartesian coordinates of : PACN10_21

Atomic number (AN) and Cartesian coordinates

file:///home/alma/Documents/Papers/ALMA/P_MeCN/P_MeCN_Paper/Submission/P_MeCN_Geometries.ooo

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -4.478155 | 1.655865 | -1.612679 |
| 1 | -5.267060 | 2.411788 | -1.589588 |
| 1 | -4.738593 | 0.833741 | -0.938901 |
| 1 | -4.375012 | 1.265222 | -2.628104 |
| 6 | -3.211526 | 2.240445 | -1.182851 |
| 7 | -2.207993 | 2.711041 | -0.833366 |
| 6 | -2.555352 | 1.702231 | 2.573754 |
| 1 | -3.248215 | 1.906312 | 3.394127 |
| 1 | -2.464952 | 2.584532 | 1.934453 |
| 1 | -1.562380 | 1.478922 | 2.974538 |
| 6 | -3.033965 | 0.572867 | 1.784414 |
| 7 | -3.408446 | -0.334945 | 1.161541 |
| 6 | 4.910778 | -0.230074 | -1.590849 |
| 1 | 5.650837 | -0.878502 | -2.066321 |
| 1 | 4.976618 | -0.331653 | -0.503619 |
| 1 | 5.103417 | 0.809934 | -1.866110 |
| 6 | 3.565842 | -0.605148 | -2.013394 |
| 7 | 2.493622 | -0.903350 | -2.347300 |
| 6 | 3.370697 | 1.874814 | 1.922097 |
| 1 | 3.509515 | 2.823251 | 2.447193 |
| 1 | 4.246851 | 1.236562 | 2.059452 |
| 1 | 2.493236 | 1.365412 | 2.331334 |
| 6 | 3.153799 | 2.122934 | 0.500496 |
| 7 | 2.962886 | 2.331764 | -0.627480 |
| 6 | 0.278989 | -3.086368 | -2.871654 |
| 1 | 0.074960 | -2.085630 | -3.260660 |
| 1 | -0.395311 | -3.809605 | -3.338422 |
| 1 | 1.315383 | -3.339297 | -3.104489 |
| 6 | 0.079078 | -3.090150 | -1.425627 |
| 7 | -0.119138 | -3.110439 | -0.280073 |
| 6 | 2.300491 | -3.462663 | 2.133552 |
| 1 | 1.437907 | -3.868961 | 1.597113 |
| 1 | 2.039762 | -3.306109 | 3.183981 |
| 1 | 3.130767 | -4.171008 | 2.075568 |
| 6 | 2.682868 | -2.189901 | 1.528837 |
| 7 | 2.989549 | -1.173694 | 1.056984 |
| 6 | -1.790031 | -3.112895 | 2.754178 |
| 1 | -2.818371 | -2.804179 | 2.540574 |
| 1 | -1.725660 | -3.484826 | 3.779689 |
| 1 | -1.491329 | -3.898167 | 2.052432 |
| 6 | -0.910314 | -1.969022 | 2.565760 |
| 7 | -0.217822 | -1.056353 | 2.380512 |
| 6 | 0.413255 | 4.868935 | -0.099786 |
| 1 | 1.296872 | 4.696468 | -0.723200 |
| 1 | 0.481737 | 5.863306 | 0.348451 |
| 1 | -0.490881 | 4.808601 | -0.712803 |
| 6 | 0.353964 | 3.846927 | 0.940808 |
| 7 | 0.320891 | 3.019912 | 1.756552 |
| 6 | -3.536459 | -2.592962 | -1.079241 |
| 1 | -3.749343 | -3.393084 | -1.792914 |
| 1 | -4.469723 | -2.200963 | -0.668342 |
| 1 | -2.931847 | -2.984975 | -0.256190 |
| 6 | -2.795847 | -1.519343 | -1.734500 |
| 7 | -2.197621 | -0.677483 | -2.267376 |
| 6 | 0.350123 | 1.509788 | -2.247238 |
| 6 | 0.296422 | 0.815441 | -0.981191 |
| 7 | 0.247794 | 0.271089 | 0.029294 |
| 1 | 0.255074 | 2.581454 | -2.052276 |
| 1 | -0.489589 | 1.159037 | -2.854681 |
| 1 | 1.309809 | 1.286453 | -2.719124 |

1 0.181535 -0.207153 0.962489

Cartesian coordinates of : PACN10_22

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.059360 | -3.521496 | -1.470755 |
| 1 | 3.205228 | -3.403351 | -0.392749 |
| 1 | 3.836200 | -2.970287 | -2.007255 |
| 1 | 3.119320 | -4.580312 | -1.734718 |
| 6 | 1.748163 | -2.988306 | -1.824322 |
| 7 | 0.701247 | -2.570651 | -2.105043 |
| 6 | 3.804113 | 3.180980 | -0.798965 |
| 1 | 4.077231 | 2.711510 | 0.151158 |
| 1 | 4.159581 | 4.214246 | -0.816549 |
| 1 | 4.263712 | 2.618552 | -1.615352 |
| 6 | 2.351918 | 3.148544 | -0.938946 |
| 7 | 1.193946 | 3.131903 | -1.038539 |
| 6 | -3.451020 | 0.212593 | 2.986978 |
| 1 | -3.862323 | 1.089220 | 2.477673 |
| 1 | -3.634825 | 0.290863 | 4.061300 |
| 1 | -3.919675 | -0.697107 | 2.599194 |
| 6 | -2.023611 | 0.150137 | 2.713965 |
| 7 | -0.891274 | 0.090954 | 2.466279 |
| 6 | -2.362715 | -3.358499 | -1.810685 |
| 1 | -2.128130 | -2.629557 | -2.590853 |
| 1 | -3.345358 | -3.799791 | -1.997214 |
| 1 | -1.597600 | -4.137337 | -1.829768 |
| 6 | -2.360962 | -2.690481 | -0.512484 |
| 7 | -2.401201 | -2.151149 | 0.517046 |
| 6 | 4.562154 | -0.822797 | 0.924079 |
| 1 | 3.845675 | -1.237704 | 1.637112 |
| 1 | 5.052636 | 0.037300 | 1.386388 |
| 1 | 5.310126 | -1.575266 | 0.658440 |
| 6 | 3.838836 | -0.394561 | -0.268402 |
| 7 | 3.277857 | -0.063831 | -1.231344 |
| 6 | 0.549119 | 3.034061 | 2.378823 |
| 1 | -0.236505 | 2.860404 | 1.636594 |
| 1 | 0.903243 | 4.064307 | 2.287883 |
| 1 | 0.134295 | 2.878764 | 3.377940 |
| 6 | 1.652774 | 2.106530 | 2.150059 |
| 7 | 2.530619 | 1.372269 | 1.949376 |
| 6 | -4.819181 | 0.115186 | -0.718237 |
| 1 | -4.849549 | 1.055919 | -0.161058 |
| 1 | -4.682747 | -0.712296 | -0.015496 |
| 1 | -5.758167 | -0.017725 | -1.261308 |
| 6 | -3.694173 | 0.142334 | -1.648134 |
| 7 | -2.792289 | 0.165369 | -2.380565 |
| 6 | -2.083690 | 3.628244 | -1.840554 |
| 1 | -2.321043 | 2.940970 | -2.659104 |
| 1 | -1.038847 | 3.941017 | -1.915411 |
| 1 | -2.735221 | 4.503355 | -1.906340 |
| 6 | -2.290927 | 2.943852 | -0.567882 |
| 7 | -2.473988 | 2.385122 | 0.435296 |
| 6 | -0.219973 | -3.070306 | 3.114877 |
| 1 | -0.020183 | -4.104549 | 3.406177 |
| 1 | -1.229245 | -2.993386 | 2.700352 |
| 1 | -0.141722 | -2.425558 | 3.994021 |
| 6 | 0.744646 | -2.638693 | 2.107564 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 1.518591 | -2.298695 | 1.310266 |
| 6 | 0.378153 | 0.471135 | -2.682251 |
| 6 | 0.193452 | 0.252054 | -1.265496 |
| 7 | 0.049978 | 0.097461 | -0.136460 |
| 1 | -0.181763 | -0.293504 | -3.224802 |
| 1 | 1.450526 | 0.394405 | -2.886727 |
| 1 | 0.005885 | 1.470152 | -2.925564 |
| 1 | -0.133776 | -0.007596 | 0.886448 |

Cartesian coordinates of : PACN10_23

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 4.724850 | -0.778997 | 0.057749 |
| 1 | 4.948329 | 0.163146 | 0.566254 |
| 1 | 5.644623 | -1.190663 | -0.365276 |
| 1 | 4.310207 | -1.485347 | 0.784263 |
| 6 | 3.741054 | -0.551169 | -0.996616 |
| 7 | 2.957158 | -0.380862 | -1.837268 |
| 6 | 1.983143 | -3.806790 | -1.827772 |
| 1 | 0.979387 | -3.958194 | -2.236369 |
| 1 | 2.505058 | -4.766238 | -1.787364 |
| 1 | 2.539664 | -3.119800 | -2.472891 |
| 6 | 1.877195 | -3.233136 | -0.488704 |
| 7 | 1.795039 | -2.760098 | 0.570169 |
| 6 | 0.619727 | 4.086722 | 1.428004 |
| 1 | 0.586168 | 4.739882 | 0.551128 |
| 1 | 1.571325 | 3.547342 | 1.440335 |
| 1 | 0.532419 | 4.693862 | 2.332595 |
| 6 | -0.474413 | 3.121638 | 1.364299 |
| 7 | -1.359895 | 2.370521 | 1.318004 |
| 6 | 3.386148 | 2.917642 | -1.250709 |
| 1 | 3.948466 | 2.394352 | -2.028232 |
| 1 | 3.632739 | 2.490581 | -0.273698 |
| 1 | 3.651619 | 3.978032 | -1.266465 |
| 6 | 1.954993 | 2.755772 | -1.486268 |
| 7 | 0.811669 | 2.650285 | -1.664665 |
| 6 | -1.571767 | -3.646848 | 1.192833 |
| 1 | -1.745042 | -4.707881 | 1.389702 |
| 1 | -2.404451 | -3.054673 | 1.583078 |
| 1 | -0.647517 | -3.328078 | 1.684950 |
| 6 | -1.453574 | -3.414294 | -0.242672 |
| 7 | -1.346099 | -3.209800 | -1.382384 |
| 6 | -4.335129 | -1.358634 | -1.885075 |
| 1 | -5.321889 | -1.826036 | -1.836262 |
| 1 | -3.638681 | -2.043078 | -2.379870 |
| 1 | -4.390605 | -0.428186 | -2.454508 |
| 6 | -3.848376 | -1.073220 | -0.538847 |
| 7 | -3.455938 | -0.865738 | 0.535210 |
| 6 | 2.360077 | -0.779905 | 3.368584 |
| 1 | 3.382256 | -0.865594 | 3.747583 |
| 1 | 2.038532 | -1.734979 | 2.944344 |
| 1 | 1.689319 | -0.511570 | 4.188095 |
| 6 | 2.298106 | 0.242461 | 2.328275 |
| 7 | 2.267557 | 1.052162 | 1.494111 |
| 6 | -3.058327 | 0.342144 | 3.472081 |
| 1 | -2.985004 | 0.705042 | 4.500081 |
| 1 | -3.815879 | -0.441404 | 3.398864 |
| 1 | -3.331783 | 1.162148 | 2.801285 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -1.775224 | -0.174968 | 3.023521 |
| 7 | -0.750796 | -0.567129 | 2.638797 |
| 6 | -2.388194 | 3.927978 | -1.509870 |
| 1 | -2.828224 | 4.097916 | -0.524156 |
| 1 | -2.914292 | 4.529964 | -2.254985 |
| 1 | -1.331828 | 4.211919 | -1.491175 |
| 6 | -2.482364 | 2.513223 | -1.851649 |
| 7 | -2.561666 | 1.390992 | -2.139311 |
| 6 | -0.158333 | -0.425602 | -2.675781 |
| 6 | -0.195502 | -0.294309 | -1.237046 |
| 7 | -0.223078 | -0.231931 | -0.091045 |
| 1 | 0.612891 | -1.155229 | -2.935924 |
| 1 | 0.082479 | 0.553023 | -3.100706 |
| 1 | -1.146023 | -0.753922 | -3.009663 |
| 1 | -0.316464 | -0.253398 | 0.947640 |

Cartesian coordinates of : PACN10_24

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 3.666066 | 0.807293 | -2.883973 |
| 1 | 3.964691 | -0.194836 | -3.199588 |
| 1 | 4.073307 | 0.993085 | -1.886610 |
| 1 | 4.054590 | 1.545407 | -3.590327 |
| 6 | 2.210343 | 0.892650 | -2.824106 |
| 7 | 1.051785 | 0.981421 | -2.784831 |
| 6 | 3.154528 | -0.184456 | 2.059727 |
| 1 | 4.133409 | -0.632810 | 1.870549 |
| 1 | 2.379212 | -0.952202 | 1.965520 |
| 1 | 3.132993 | 0.220968 | 3.075147 |
| 6 | 2.907892 | 0.882922 | 1.095275 |
| 7 | 2.704332 | 1.750705 | 0.348880 |
| 6 | -3.130610 | 2.343377 | 2.417252 |
| 1 | -2.809240 | 1.894338 | 3.360669 |
| 1 | -4.123399 | 2.782272 | 2.543375 |
| 1 | -2.420961 | 3.125198 | 2.129429 |
| 6 | -3.157929 | 1.327772 | 1.369414 |
| 7 | -3.178829 | 0.529971 | 0.524524 |
| 6 | 0.857905 | 3.199078 | 3.099892 |
| 1 | 0.055289 | 3.919982 | 2.918925 |
| 1 | 1.646731 | 3.358060 | 2.357889 |
| 1 | 1.260237 | 3.352652 | 4.104298 |
| 6 | 0.339915 | 1.841334 | 2.960531 |
| 7 | -0.070402 | 0.761666 | 2.829652 |
| 6 | -2.373435 | 1.741786 | -2.757004 |
| 1 | -1.355834 | 2.066725 | -2.992913 |
| 1 | -2.619449 | 2.036900 | -1.732588 |
| 1 | -3.079545 | 2.204392 | -3.451308 |
| 6 | -2.439266 | 0.288830 | -2.868317 |
| 7 | -2.486938 | -0.868945 | -2.952617 |
| 6 | -4.722216 | -2.199039 | -1.035494 |
| 1 | -4.724645 | -2.399953 | -2.109457 |
| 1 | -4.850860 | -1.124848 | -0.875798 |
| 1 | -5.537337 | -2.745468 | -0.554586 |
| 6 | -3.440798 | -2.603000 | -0.468250 |
| 7 | -2.419130 | -2.920344 | -0.014608 |
| 6 | -1.429597 | -2.228324 | 2.872662 |
| 1 | -2.072495 | -3.111372 | 2.891099 |
| 1 | -1.925856 | -1.441599 | 2.295581 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -1.241412 | -1.869565 | 3.887403 |
| 6 | -0.165280 | -2.559520 | 2.226113 |
| 7 | 0.843232 | -2.813668 | 1.706530 |
| 6 | 3.784875 | -3.917151 | 0.401136 |
| 1 | 4.770506 | -3.821947 | 0.864165 |
| 1 | 3.798765 | -4.768739 | -0.283910 |
| 1 | 3.027793 | -4.083036 | 1.172978 |
| 6 | 3.450154 | -2.695510 | -0.324374 |
| 7 | 3.171033 | -1.717160 | -0.886816 |
| 6 | 1.074347 | 4.085909 | -1.498803 |
| 1 | 0.990131 | 5.158471 | -1.306715 |
| 1 | 0.810608 | 3.875710 | -2.538986 |
| 1 | 2.099377 | 3.751335 | -1.312660 |
| 6 | 0.188423 | 3.343243 | -0.612316 |
| 7 | -0.511723 | 2.746463 | 0.098273 |
| 6 | 0.108331 | -2.288952 | -1.620629 |
| 6 | -0.105181 | -1.114180 | -0.810958 |
| 7 | -0.267166 | -0.163231 | -0.185314 |
| 1 | 0.315850 | -3.129304 | -0.951015 |
| 1 | 0.956898 | -2.089158 | -2.281072 |
| 1 | -0.808067 | -2.467918 | -2.191598 |
| 1 | -0.425448 | 0.754735 | 0.249734 |

Cartesian coordinates of : PACN10_25

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.513652 | 3.318601 | -1.482303 |
| 1 | -2.534363 | 3.705914 | -1.531637 |
| 1 | -0.806337 | 4.061588 | -1.857612 |
| 1 | -1.274527 | 3.088379 | -0.440386 |
| 6 | -1.410303 | 2.096877 | -2.273163 |
| 7 | -1.333347 | 1.121110 | -2.899779 |
| 6 | 2.605672 | 3.418748 | 1.580414 |
| 1 | 3.641298 | 3.072040 | 1.632214 |
| 1 | 2.047200 | 2.955713 | 2.398904 |
| 1 | 2.575875 | 4.506221 | 1.683885 |
| 6 | 2.011628 | 3.013406 | 0.310034 |
| 7 | 1.538100 | 2.687435 | -0.699995 |
| 6 | -1.277461 | -3.629415 | 0.825662 |
| 1 | -1.902209 | -3.637720 | -0.071733 |
| 1 | -1.473831 | -4.525662 | 1.419988 |
| 1 | -0.221536 | -3.617854 | 0.533790 |
| 6 | -1.584942 | -2.436235 | 1.608871 |
| 7 | -1.821801 | -1.487390 | 2.238281 |
| 6 | -4.827875 | -0.714427 | 1.227249 |
| 1 | -5.889029 | -0.488670 | 1.094442 |
| 1 | -4.617227 | -0.873003 | 2.288339 |
| 1 | -4.575372 | -1.629178 | 0.683238 |
| 6 | -4.010977 | 0.384148 | 0.718418 |
| 7 | -3.368581 | 1.261336 | 0.307096 |
| 6 | 4.611398 | 1.642133 | -1.519603 |
| 1 | 4.712420 | 1.689394 | -0.430800 |
| 1 | 4.166607 | 2.571775 | -1.883003 |
| 1 | 5.596372 | 1.508351 | -1.974059 |
| 6 | 3.744080 | 0.519310 | -1.859385 |
| 7 | 3.070865 | -0.389019 | -2.125310 |
| 6 | 4.671474 | -2.621881 | -0.354969 |
| 1 | 4.937563 | -1.668438 | 0.111680 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 4.877307 | -2.561463 | -1.426487 |
| 1 | 5.261982 | -3.427194 | 0.088875 |
| 6 | 3.248838 | -2.868542 | -0.146897 |
| 7 | 2.116751 | -3.061771 | 0.030066 |
| 6 | -2.335647 | 1.723805 | 3.519873 |
| 1 | -2.750080 | 0.724263 | 3.687558 |
| 1 | -3.089867 | 2.359608 | 3.049075 |
| 1 | -2.026136 | 2.158658 | 4.473365 |
| 6 | -1.194186 | 1.585929 | 2.628228 |
| 7 | -0.290568 | 1.445700 | 1.913746 |
| 6 | 1.709710 | -1.273609 | 2.924672 |
| 1 | 1.518956 | -2.216657 | 2.403115 |
| 1 | 0.754131 | -0.773681 | 3.106756 |
| 1 | 2.199548 | -1.480628 | 3.879674 |
| 6 | 2.565664 | -0.431521 | 2.092853 |
| 7 | 3.245867 | 0.229910 | 1.421071 |
| 6 | -4.251795 | -0.139837 | -3.052597 |
| 1 | -3.665126 | 0.075256 | -3.948819 |
| 1 | -4.388037 | 0.792951 | -2.496715 |
| 1 | -5.224936 | -0.550137 | -3.333700 |
| 6 | -3.528677 | -1.089247 | -2.213294 |
| 7 | -2.966458 | -1.840884 | -1.527805 |
| 6 | 0.276355 | -1.631328 | -2.392039 |
| 6 | 0.242139 | -0.800824 | -1.210869 |
| 7 | 0.192223 | -0.147702 | -0.265888 |
| 1 | -0.695745 | -2.123536 | -2.489203 |
| 1 | 1.090056 | -2.351989 | -2.281168 |
| 1 | 0.460657 | -0.978789 | -3.249913 |
| 1 | 0.104373 | 0.506848 | 0.553029 |

Cartesian coordinates of : PACN10_26

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.193284 | 0.573693 | 2.998523 |
| 1 | -1.197566 | 0.238162 | 3.303827 |
| 1 | -2.808583 | 0.747478 | 3.884911 |
| 1 | -2.098001 | 1.508125 | 2.435387 |
| 6 | -2.805448 | -0.441105 | 2.147184 |
| 7 | -3.277752 | -1.240282 | 1.446833 |
| 6 | -1.449200 | 4.086065 | -2.037643 |
| 1 | -1.636081 | 4.037280 | -0.962058 |
| 1 | -2.330124 | 4.489246 | -2.543329 |
| 1 | -0.587774 | 4.732786 | -2.219578 |
| 6 | -1.164084 | 2.741179 | -2.524730 |
| 7 | -0.936055 | 1.667539 | -2.907483 |
| 6 | 0.652449 | -4.438224 | -3.395695 |
| 1 | 1.366523 | -5.265463 | -3.382423 |
| 1 | 1.137135 | -3.541852 | -3.792474 |
| 1 | -0.191909 | -4.709933 | -4.034177 |
| 6 | 0.186397 | -4.156916 | -2.041689 |
| 7 | -0.179642 | -3.919596 | -0.964549 |
| 6 | 2.821339 | -2.331030 | 0.087108 |
| 1 | 3.441188 | -2.705771 | -0.731688 |
| 1 | 1.769330 | -2.495295 | -0.162704 |
| 1 | 3.056755 | -2.870216 | 1.008565 |
| 6 | 3.060265 | -0.903820 | 0.271065 |
| 7 | 3.254307 | 0.234084 | 0.411289 |
| 6 | -5.639773 | 0.908597 | -0.135575 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -6.315427 | 1.489529 | 0.497133 |
| 1 | -5.579128 | -0.115059 | 0.246301 |
| 1 | -6.034147 | 0.893360 | -1.154662 |
| 6 | -4.305273 | 1.501364 | -0.120526 |
| 7 | -3.232636 | 1.948397 | -0.095822 |
| 6 | 2.512704 | 1.216014 | -2.949625 |
| 1 | 3.074144 | 1.278192 | -3.885314 |
| 1 | 3.175900 | 1.416541 | -2.102986 |
| 1 | 1.707481 | 1.955219 | -2.948856 |
| 6 | 1.939418 | -0.116179 | -2.801431 |
| 7 | 1.494694 | -1.183025 | -2.673902 |
| 6 | 2.859801 | 0.161133 | 3.820373 |
| 1 | 2.883229 | 0.436381 | 4.877527 |
| 1 | 3.846831 | 0.314838 | 3.375277 |
| 1 | 2.576565 | -0.891495 | 3.719389 |
| 6 | 1.878505 | 0.961601 | 3.103093 |
| 7 | 1.097417 | 1.573980 | 2.500414 |
| 6 | 3.365576 | 3.630738 | 1.049104 |
| 1 | 4.027980 | 4.392490 | 0.630437 |
| 1 | 3.906142 | 2.684165 | 1.142361 |
| 1 | 3.023653 | 3.954935 | 2.035614 |
| 6 | 2.214581 | 3.426972 | 0.175475 |
| 7 | 1.297421 | 3.256951 | -0.517350 |
| 6 | -1.214573 | -3.904673 | 2.111498 |
| 1 | -0.684963 | -4.747140 | 1.661760 |
| 1 | -2.075069 | -3.655871 | 1.484381 |
| 1 | -1.561756 | -4.170303 | 3.113255 |
| 6 | -0.324575 | -2.749741 | 2.187090 |
| 7 | 0.380057 | -1.827268 | 2.265086 |
| 6 | -1.556076 | -0.907653 | -1.355916 |
| 6 | -0.750003 | -0.069315 | -0.501071 |
| 7 | -0.123548 | 0.581783 | 0.209972 |
| 1 | -1.764610 | -1.841251 | -0.823524 |
| 1 | -0.995698 | -1.095422 | -2.276341 |
| 1 | -2.479387 | -0.364633 | -1.577180 |
| 1 | 0.395061 | 1.120834 | 0.940084 |

 Cartesian coordinates of : PACN10_27

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.574130 | 4.145400 | -0.232141 |
| 1 | 0.651984 | 3.625645 | -1.191543 |
| 1 | 1.376284 | 4.884317 | -0.157768 |
| 1 | -0.397673 | 4.641478 | -0.185797 |
| 6 | 0.693669 | 3.173617 | 0.850627 |
| 7 | 0.816049 | 2.394459 | 1.704855 |
| 6 | -2.626011 | 2.056685 | 2.240936 |
| 1 | -1.651034 | 1.711118 | 2.597782 |
| 1 | -3.217228 | 2.425165 | 3.083169 |
| 1 | -2.463310 | 2.865563 | 1.523117 |
| 6 | -3.322898 | 0.956201 | 1.582145 |
| 7 | -3.871561 | 0.070763 | 1.065737 |
| 6 | 1.971309 | -4.084745 | -0.485780 |
| 1 | 2.065370 | -5.058835 | 0.001053 |
| 1 | 2.707510 | -3.390703 | -0.070359 |
| 1 | 2.147738 | -4.192202 | -1.558598 |
| 6 | 0.632044 | -3.548280 | -0.263817 |
| 7 | -0.442534 | -3.148732 | -0.074375 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -3.724932 | -2.687703 | -0.979608 |
| 1 | -2.980554 | -3.355506 | -0.537389 |
| 1 | -4.353746 | -3.251028 | -1.673720 |
| 1 | -4.345618 | -2.250900 | -0.192125 |
| 6 | -3.033174 | -1.615713 | -1.687106 |
| 7 | -2.493895 | -0.760197 | -2.259185 |
| 6 | 4.304297 | 2.066401 | 0.972068 |
| 1 | 4.877111 | 1.148704 | 1.133298 |
| 1 | 3.611381 | 2.206192 | 1.808363 |
| 1 | 4.988799 | 2.916878 | 0.921715 |
| 6 | 3.538401 | 1.960052 | -0.266388 |
| 7 | 2.924164 | 1.884681 | -1.249637 |
| 6 | 2.215128 | -0.184787 | 3.545201 |
| 1 | 1.700265 | -0.974437 | 4.097937 |
| 1 | 1.564727 | 0.692327 | 3.484951 |
| 1 | 3.141715 | 0.072372 | 4.065980 |
| 6 | 2.514086 | -0.644768 | 2.191941 |
| 7 | 2.766295 | -0.999758 | 1.113719 |
| 6 | -4.466546 | 1.785399 | -1.990381 |
| 1 | -5.153500 | 2.629999 | -2.085335 |
| 1 | -4.870226 | 1.058064 | -1.279708 |
| 1 | -4.342765 | 1.297689 | -2.960399 |
| 6 | -3.168146 | 2.245508 | -1.509112 |
| 7 | -2.136998 | 2.613499 | -1.118109 |
| 6 | -2.423966 | -2.688615 | 2.679808 |
| 1 | -3.408803 | -2.297871 | 2.405755 |
| 1 | -2.423646 | -2.976282 | 3.734051 |
| 1 | -2.186555 | -3.557406 | 2.058817 |
| 6 | -1.425679 | -1.658961 | 2.431802 |
| 7 | -0.637093 | -0.836201 | 2.209339 |
| 6 | 4.681996 | -1.002309 | -1.805587 |
| 1 | 4.742520 | -0.977391 | -0.713005 |
| 1 | 4.999908 | -0.037858 | -2.210061 |
| 1 | 5.337798 | -1.787415 | -2.190452 |
| 6 | 3.299330 | -1.266024 | -2.190543 |
| 7 | 2.199729 | -1.493249 | -2.488352 |
| 6 | 0.171711 | 0.772779 | -2.828743 |
| 6 | 0.110879 | 0.370513 | -1.442184 |
| 7 | 0.061013 | 0.082068 | -0.331403 |
| 1 | 1.160797 | 1.201168 | -3.014406 |
| 1 | -0.626646 | 1.500419 | -3.000247 |
| 1 | 0.014876 | -0.115576 | -3.445155 |
| 1 | -0.057410 | -0.208914 | 0.663125 |

Cartesian coordinates of : PACN10_28

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.649228 | -3.271130 | -1.929994 |
| 1 | -3.246475 | -2.824737 | -2.729587 |
| 1 | -3.025958 | -2.935100 | -0.959771 |
| 1 | -2.718013 | -4.359956 | -1.994577 |
| 6 | -1.259181 | -2.847810 | -2.066578 |
| 7 | -0.152430 | -2.515597 | -2.187343 |
| 6 | 2.960823 | -3.186328 | -1.749252 |
| 1 | 2.330008 | -3.492461 | -0.910433 |
| 1 | 3.960277 | -3.618366 | -1.649519 |
| 1 | 2.500319 | -3.533393 | -2.677010 |
| 6 | 3.047817 | -1.730005 | -1.761731 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | 3.139553 | -0.570864 | -1.762143 |
| 6 | -3.280002 | 0.033861 | 2.956997 |
| 1 | -2.734806 | -0.204857 | 3.874239 |
| 1 | -4.346890 | -0.152161 | 3.108296 |
| 1 | -3.112969 | 1.086868 | 2.712147 |
| 6 | -2.775665 | -0.786524 | 1.860362 |
| 7 | -2.383942 | -1.441609 | 0.983115 |
| 6 | -1.999239 | 3.734040 | -1.575781 |
| 1 | -0.957950 | 4.023540 | -1.741912 |
| 1 | -2.620027 | 4.630047 | -1.495541 |
| 1 | -2.351983 | 3.128370 | -2.416910 |
| 6 | -2.088970 | 2.949835 | -0.347389 |
| 7 | -2.176535 | 2.313720 | 0.621700 |
| 6 | -0.317661 | -3.022000 | 3.161030 |
| 1 | 0.186825 | -3.724667 | 3.828889 |
| 1 | -1.234474 | -3.476059 | 2.777018 |
| 1 | -0.566966 | -2.108735 | 3.709506 |
| 6 | 0.558674 | -2.668886 | 2.049221 |
| 7 | 1.264993 | -2.383157 | 1.171486 |
| 6 | 4.412871 | -1.077208 | 1.370720 |
| 1 | 3.814024 | -1.980738 | 1.223888 |
| 1 | 4.955581 | -1.149554 | 2.316588 |
| 1 | 5.128043 | -0.978846 | 0.549482 |
| 6 | 3.525144 | 0.081303 | 1.388569 |
| 7 | 2.830512 | 1.012402 | 1.402518 |
| 6 | 3.929465 | 2.837495 | -1.038004 |
| 1 | 4.165769 | 1.803625 | -1.307066 |
| 1 | 4.312068 | 3.041067 | -0.034865 |
| 1 | 4.388821 | 3.523332 | -1.754271 |
| 6 | 2.480150 | 3.003628 | -1.046028 |
| 7 | 1.325425 | 3.137159 | -1.063538 |
| 6 | 0.514177 | 2.903035 | 2.553940 |
| 1 | 0.703215 | 3.070582 | 1.488132 |
| 1 | 1.426894 | 3.123589 | 3.112469 |
| 1 | -0.302574 | 3.548526 | 2.886326 |
| 6 | 0.151569 | 1.504882 | 2.740275 |
| 7 | -0.133845 | 0.383224 | 2.853585 |
| 6 | -4.829355 | 0.216193 | -0.712415 |
| 1 | -5.015910 | -0.792365 | -0.332872 |
| 1 | -5.705939 | 0.563740 | -1.264790 |
| 1 | -4.642207 | 0.887067 | 0.132430 |
| 6 | -3.655729 | 0.207744 | -1.580301 |
| 7 | -2.721748 | 0.213705 | -2.271068 |
| 6 | 0.317592 | 0.654158 | -2.737995 |
| 6 | 0.222269 | 0.331945 | -1.331712 |
| 7 | 0.150488 | 0.086356 | -0.213104 |
| 1 | -0.218574 | 1.589508 | -2.916883 |
| 1 | -0.140703 | -0.162030 | -3.301730 |
| 1 | 1.377195 | 0.758918 | -2.985948 |
| 1 | 0.102952 | -0.141505 | 0.784222 |

Cartesian coordinates of : PACN10_29

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|----------|-----------|
| 6 | 4.577534 | 1.369382 | -0.068675 |
| 1 | 5.230488 | 0.498638 | 0.026862 |
| 1 | 4.099793 | 1.556484 | 0.897119 |
| 1 | 5.162236 | 2.244500 | -0.363570 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 3.539593 | 1.104302 | -1.059981 |
| 7 | 2.714882 | 0.907678 | -1.855197 |
| 6 | 3.840846 | -2.173721 | -2.415740 |
| 1 | 4.251828 | -3.108124 | -2.805888 |
| 1 | 4.358943 | -1.903821 | -1.490214 |
| 1 | 3.982124 | -1.375885 | -3.149148 |
| 6 | 2.417623 | -2.330231 | -2.132913 |
| 7 | 1.286217 | -2.460729 | -1.900719 |
| 6 | -2.440038 | -0.798902 | 3.619900 |
| 1 | -3.386141 | -1.087416 | 4.085313 |
| 1 | -1.813685 | -0.295486 | 4.360298 |
| 1 | -1.924221 | -1.690942 | 3.254020 |
| 6 | -2.686272 | 0.094306 | 2.491962 |
| 7 | -2.886662 | 0.797544 | 1.588793 |
| 6 | 2.583006 | 0.933152 | 3.710198 |
| 1 | 3.463391 | 0.400119 | 3.336848 |
| 1 | 2.503032 | 0.794955 | 4.791195 |
| 1 | 2.669008 | 1.997012 | 3.472714 |
| 6 | 1.403133 | 0.409017 | 3.039460 |
| 7 | 0.478114 | -0.015844 | 2.481883 |
| 6 | -4.115362 | 2.936072 | -0.776206 |
| 1 | -4.273911 | 2.400938 | 0.164092 |
| 1 | -4.679772 | 2.449432 | -1.576156 |
| 1 | -4.453667 | 3.970111 | -0.673086 |
| 6 | -2.692150 | 2.904037 | -1.094975 |
| 7 | -1.559835 | 2.889015 | -1.354038 |
| 6 | -5.057642 | -1.058713 | 0.045647 |
| 1 | -5.906935 | -1.578292 | -0.404987 |
| 1 | -5.412727 | -0.182767 | 0.595242 |
| 1 | -4.546032 | -1.725731 | 0.746551 |
| 6 | -4.114463 | -0.641747 | -0.987248 |
| 7 | -3.362537 | -0.322988 | -1.813481 |
| 6 | 1.533726 | -3.212854 | 1.485407 |
| 1 | 0.678858 | -2.748958 | 1.986678 |
| 1 | 1.941431 | -4.010077 | 2.112199 |
| 1 | 1.186020 | -3.630442 | 0.536404 |
| 6 | 2.556415 | -2.204778 | 1.225820 |
| 7 | 3.366257 | -1.395317 | 1.024453 |
| 6 | -1.832528 | -3.353928 | -1.759064 |
| 1 | -1.643687 | -2.503814 | -2.420603 |
| 1 | -2.826157 | -3.757253 | -1.971688 |
| 1 | -1.072885 | -4.116154 | -1.945498 |
| 6 | -1.763632 | -2.909439 | -0.369811 |
| 7 | -1.726815 | -2.547659 | 0.734318 |
| 6 | 1.344523 | 4.257211 | -1.054866 |
| 1 | 1.361314 | 3.597248 | -1.927261 |
| 1 | 2.149501 | 4.992019 | -1.137599 |
| 1 | 0.378284 | 4.764427 | -1.027198 |
| 6 | 1.523644 | 3.459073 | 0.154254 |
| 7 | 1.701952 | 2.821916 | 1.109491 |
| 6 | -0.287988 | 0.433402 | -2.745502 |
| 6 | -0.221683 | 0.277208 | -1.309587 |
| 7 | -0.175956 | 0.131357 | -0.171073 |
| 1 | 0.162698 | 1.394382 | -3.004087 |
| 1 | -1.341803 | 0.410627 | -3.037947 |
| 1 | 0.279598 | -0.382771 | -3.201339 |
| 1 | -0.075953 | 0.035143 | 0.871243 |

Cartesian coordinates of : PACN10_30

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 2.351543 | 0.889099 | 3.436897 |
| 1 | 2.312804 | 1.764926 | 2.783661 |
| 1 | 3.327922 | 0.840446 | 3.926565 |
| 1 | 1.570089 | 0.966826 | 4.196695 |
| 6 | 2.135133 | -0.308603 | 2.631429 |
| 7 | 1.967610 | -1.262715 | 1.988392 |
| 6 | 2.304901 | -4.091005 | -0.045181 |
| 1 | 2.164623 | -5.139997 | 0.227673 |
| 1 | 2.686593 | -3.534433 | 0.815964 |
| 1 | 3.019219 | -4.022971 | -0.869447 |
| 6 | 1.031495 | -3.505677 | -0.451846 |
| 7 | 0.007909 | -3.054234 | -0.766744 |
| 6 | -4.720938 | 1.084684 | -1.290578 |
| 1 | -4.940763 | 0.139465 | -0.785996 |
| 1 | -4.530499 | 0.886419 | -2.347774 |
| 1 | -5.569426 | 1.766090 | -1.188740 |
| 6 | -3.532819 | 1.672336 | -0.681214 |
| 7 | -2.600515 | 2.152642 | -0.180407 |
| 6 | -0.072626 | 4.084687 | -0.068565 |
| 1 | 0.717041 | 4.823795 | 0.089146 |
| 1 | -0.015948 | 3.321609 | 0.714760 |
| 1 | -1.053000 | 4.563379 | -0.019682 |
| 6 | 0.099618 | 3.442612 | -1.367396 |
| 7 | 0.267585 | 2.914821 | -2.389176 |
| 6 | 4.914171 | -0.870019 | 0.516811 |
| 1 | 4.774232 | -1.659189 | 1.260789 |
| 1 | 4.751310 | 0.099973 | 0.997356 |
| 1 | 5.932692 | -0.916431 | 0.123356 |
| 6 | 3.946049 | -1.033497 | -0.563482 |
| 7 | 3.177622 | -1.154205 | -1.426632 |
| 6 | -3.344885 | -3.323278 | -1.502992 |
| 1 | -2.511233 | -3.828339 | -1.006217 |
| 1 | -3.693145 | -3.936500 | -2.337808 |
| 1 | -4.161414 | -3.180116 | -0.790071 |
| 6 | -2.883740 | -2.026304 | -1.986390 |
| 7 | -2.520574 | -0.989891 | -2.364975 |
| 6 | -3.113717 | 1.887605 | 3.029263 |
| 1 | -3.841539 | 1.177650 | 2.623093 |
| 1 | -3.291722 | 2.871020 | 2.586759 |
| 1 | -3.211449 | 1.942095 | 4.116245 |
| 6 | -1.782447 | 1.431290 | 2.659215 |
| 7 | -0.731952 | 1.050680 | 2.341461 |
| 6 | -1.415557 | -2.475159 | 2.181489 |
| 1 | -0.446056 | -2.013243 | 1.967879 |
| 1 | -1.410997 | -3.488407 | 1.770932 |
| 1 | -1.563515 | -2.523198 | 3.263629 |
| 6 | -2.490715 | -1.699006 | 1.569993 |
| 7 | -3.353132 | -1.073715 | 1.104502 |
| 6 | 3.585969 | 2.320514 | -2.223743 |
| 1 | 3.906716 | 1.347039 | -2.607518 |
| 1 | 4.428576 | 3.015987 | -2.253649 |
| 1 | 2.774021 | 2.706236 | -2.848044 |
| 6 | 3.105315 | 2.167516 | -0.852926 |
| 7 | 2.717356 | 2.031950 | 0.234749 |
| 6 | 0.413374 | -0.234208 | -2.726026 |
| 6 | 0.168970 | 0.011150 | -1.324360 |
| 7 | -0.009348 | 0.221721 | -0.208804 |
| 1 | 0.401403 | -1.316633 | -2.884853 |
| 1 | 1.393601 | 0.176843 | -2.980716 |

| | | | |
|---|-----------|----------|-----------|
| 1 | -0.380094 | 0.253368 | -3.297265 |
| 1 | -0.192546 | 0.488500 | 0.784322 |

Cartesian coordinates of : PACN10_31

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.500970 | -2.976537 | 1.840776 |
| 1 | -1.837636 | -3.455013 | 1.115506 |
| 1 | -3.462820 | -3.495246 | 1.872656 |
| 1 | -2.026525 | -3.023298 | 2.823625 |
| 6 | -2.700174 | -1.582878 | 1.453160 |
| 7 | -2.890282 | -0.481148 | 1.133859 |
| 6 | -4.063611 | 2.004127 | -0.561656 |
| 1 | -3.514698 | 2.423489 | 0.286185 |
| 1 | -4.749289 | 1.237458 | -0.192339 |
| 1 | -4.624544 | 2.796835 | -1.062925 |
| 6 | -3.106264 | 1.406123 | -1.486249 |
| 7 | -2.344553 | 0.939926 | -2.230351 |
| 6 | 4.948358 | -0.059485 | -1.426094 |
| 1 | 4.804434 | -0.437026 | -0.409783 |
| 1 | 5.886603 | 0.497174 | -1.490631 |
| 1 | 4.970013 | -0.907721 | -2.113915 |
| 6 | 3.827624 | 0.812755 | -1.758102 |
| 7 | 2.935850 | 1.515816 | -2.008119 |
| 6 | 2.100904 | -1.318409 | 3.755243 |
| 1 | 1.929571 | -1.909766 | 4.658194 |
| 1 | 1.872390 | -0.266787 | 3.950633 |
| 1 | 3.148023 | -1.389875 | 3.453646 |
| 6 | 1.244585 | -1.793166 | 2.673468 |
| 7 | 0.543809 | -2.166466 | 1.824710 |
| 6 | -3.872531 | -2.046273 | -2.077439 |
| 1 | -4.299948 | -1.484196 | -1.241006 |
| 1 | -4.458696 | -2.952920 | -2.246939 |
| 1 | -3.901992 | -1.420193 | -2.972744 |
| 6 | -2.488790 | -2.392325 | -1.764212 |
| 7 | -1.391140 | -2.672829 | -1.504337 |
| 6 | 0.022400 | 3.553202 | -2.210874 |
| 1 | 0.992548 | 3.042849 | -2.199376 |
| 1 | 0.166263 | 4.588203 | -2.531748 |
| 1 | -0.644474 | 3.048304 | -2.917158 |
| 6 | -0.578191 | 3.520065 | -0.880414 |
| 7 | -1.058021 | 3.486059 | 0.177828 |
| 6 | -2.287641 | 2.355448 | 3.177679 |
| 1 | -2.227581 | 2.528977 | 4.254842 |
| 1 | -3.173272 | 1.753332 | 2.951771 |
| 1 | -2.347117 | 3.312151 | 2.650336 |
| 6 | -1.110624 | 1.640775 | 2.707662 |
| 7 | -0.185424 | 1.068494 | 2.303719 |
| 6 | 2.469157 | 3.039205 | 1.093398 |
| 1 | 1.430115 | 3.170903 | 1.410312 |
| 1 | 2.552614 | 3.271938 | 0.026914 |
| 1 | 3.110190 | 3.718681 | 1.660833 |
| 6 | 2.877999 | 1.655110 | 1.312383 |
| 7 | 3.189408 | 0.546288 | 1.467614 |
| 6 | 1.300723 | -4.431469 | -0.573535 |
| 1 | 2.035014 | -5.186117 | -0.280821 |
| 1 | 0.706041 | -4.801676 | -1.411882 |
| 1 | 0.635651 | -4.214779 | 0.266455 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 1.978721 | -3.198751 | -0.960189 |
| 7 | 2.526675 | -2.222556 | -1.272152 |
| 6 | 0.506391 | -0.290641 | -2.800514 |
| 6 | 0.397409 | -0.053105 | -1.376893 |
| 7 | 0.307507 | 0.152828 | -0.249971 |
| 1 | -0.325693 | -0.930300 | -3.102290 |
| 1 | 1.465972 | -0.778386 | -2.987707 |
| 1 | 0.454501 | 0.669656 | -3.319441 |
| 1 | 0.204707 | 0.365837 | 0.773632 |

Cartesian coordinates of : PACN10_32

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -0.812562 | 4.074511 | -0.670396 |
| 1 | -0.815610 | 3.379103 | -1.514225 |
| 1 | 0.116371 | 4.647871 | -0.696432 |
| 1 | -1.670701 | 4.746093 | -0.756294 |
| 6 | -0.900655 | 3.320825 | 0.577038 |
| 7 | -1.002198 | 2.726060 | 1.570955 |
| 6 | 2.365342 | 2.165802 | 2.227212 |
| 1 | 2.214396 | 2.937053 | 1.466594 |
| 1 | 3.058550 | 2.530971 | 2.989349 |
| 1 | 1.397573 | 1.942320 | 2.683857 |
| 6 | 2.902710 | 0.964120 | 1.595568 |
| 7 | 3.336512 | 0.012668 | 1.087377 |
| 6 | -1.916714 | -3.714577 | -0.009555 |
| 1 | -1.183211 | -3.494159 | -0.788774 |
| 1 | -2.743782 | -4.287351 | -0.437719 |
| 1 | -1.431212 | -4.300055 | 0.774713 |
| 6 | -2.421665 | -2.461911 | 0.545236 |
| 7 | -2.841593 | -1.467200 | 0.977221 |
| 6 | -2.078736 | 0.348579 | 3.903187 |
| 1 | -2.179263 | 1.436974 | 3.854136 |
| 1 | -1.938793 | 0.037110 | 4.941209 |
| 1 | -2.975388 | -0.128034 | 3.495164 |
| 6 | -0.937815 | -0.047869 | 3.092713 |
| 7 | -0.039868 | -0.352458 | 2.423223 |
| 6 | 4.476320 | 1.876253 | -1.795493 |
| 1 | 4.806189 | 1.132904 | -1.063450 |
| 1 | 5.146548 | 2.739186 | -1.774635 |
| 1 | 4.490527 | 1.421458 | -2.788948 |
| 6 | 3.115658 | 2.288966 | -1.467806 |
| 7 | 2.036176 | 2.620839 | -1.192639 |
| 6 | 4.091302 | -2.592251 | -1.125982 |
| 1 | 4.346714 | -2.220259 | -0.129115 |
| 1 | 5.005658 | -2.796116 | -1.688946 |
| 1 | 3.509233 | -3.512010 | -1.029902 |
| 6 | 3.296413 | -1.578768 | -1.811207 |
| 7 | 2.682994 | -0.761825 | -2.364164 |
| 6 | -4.258555 | 1.566799 | 0.930626 |
| 1 | -3.634660 | 2.043131 | 1.693353 |
| 1 | -4.503422 | 0.550890 | 1.251691 |
| 1 | -5.173349 | 2.149435 | 0.795802 |
| 6 | -3.508055 | 1.508823 | -0.319419 |
| 7 | -2.911278 | 1.478219 | -1.316152 |
| 6 | 2.518471 | -2.668848 | 2.738173 |
| 1 | 2.127772 | -1.820835 | 3.307857 |
| 1 | 3.572338 | -2.480382 | 2.516249 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 2.424452 | -3.584348 | 3.327373 |
| 6 | 1.766178 | -2.786476 | 1.493291 |
| 7 | 1.166941 | -2.874379 | 0.501432 |
| 6 | -4.663756 | -1.205734 | -2.322694 |
| 1 | -4.895793 | -0.222542 | -2.739701 |
| 1 | -4.879267 | -1.196283 | -1.249119 |
| 1 | -5.282322 | -1.963058 | -2.810550 |
| 6 | -3.248236 | -1.501891 | -2.521566 |
| 7 | -2.120255 | -1.742814 | -2.659727 |
| 6 | -0.067884 | 0.550602 | -2.856320 |
| 6 | 0.021928 | 0.186786 | -1.460394 |
| 7 | 0.088263 | -0.075826 | -0.343586 |
| 1 | 0.706943 | 1.295552 | -3.057453 |
| 1 | -1.072907 | 0.943559 | -3.036188 |
| 1 | 0.105042 | -0.346313 | -3.455574 |
| 1 | 0.143388 | -0.287297 | 0.678810 |

Cartesian coordinates of : PACN10_33

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.095080 | -3.788583 | 0.716599 |
| 1 | -0.519559 | -4.713510 | 0.805392 |
| 1 | -2.133447 | -3.963188 | 1.008684 |
| 1 | -0.655912 | -3.034033 | 1.377363 |
| 6 | -1.042222 | -3.303446 | -0.658691 |
| 7 | -0.981988 | -2.911405 | -1.751783 |
| 6 | -3.886018 | 2.285472 | 0.440946 |
| 1 | -3.989813 | 2.713171 | -0.559981 |
| 1 | -4.450544 | 2.889182 | 1.156197 |
| 1 | -4.282552 | 1.266327 | 0.420615 |
| 6 | -2.476158 | 2.242690 | 0.820880 |
| 7 | -1.359478 | 2.211532 | 1.142563 |
| 6 | 4.510616 | 1.977896 | -0.986021 |
| 1 | 5.344018 | 2.182584 | -1.662753 |
| 1 | 4.878075 | 1.907657 | 0.040470 |
| 1 | 3.776814 | 2.786185 | -1.049871 |
| 6 | 3.860750 | 0.726380 | -1.358947 |
| 7 | 3.351535 | -0.269570 | -1.672215 |
| 6 | 2.664256 | -1.461164 | 3.394277 |
| 1 | 2.839303 | -1.187985 | 4.437656 |
| 1 | 3.365630 | -0.925344 | 2.747522 |
| 1 | 2.796793 | -2.536227 | 3.253540 |
| 6 | 1.320169 | -1.081413 | 2.989337 |
| 7 | 0.260017 | -0.760318 | 2.636724 |
| 6 | -4.018100 | -1.642349 | -2.141198 |
| 1 | -5.024601 | -1.441557 | -2.516860 |
| 1 | -4.072887 | -2.067755 | -1.135305 |
| 1 | -3.513244 | -2.352777 | -2.800519 |
| 6 | -3.250289 | -0.403316 | -2.080249 |
| 7 | -2.645471 | 0.588738 | -2.034656 |
| 6 | -1.261758 | 3.842848 | -2.043307 |
| 1 | -1.592206 | 4.427735 | -1.179952 |
| 1 | -1.966459 | 3.024282 | -2.221296 |
| 1 | -1.223077 | 4.491461 | -2.922077 |
| 6 | 0.059475 | 3.281415 | -1.776963 |
| 7 | 1.112614 | 2.834161 | -1.571792 |
| 6 | -2.723809 | -0.259207 | 3.529636 |
| 1 | -3.706218 | -0.003168 | 3.934792 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -2.079600 | 0.624489 | 3.516911 |
| 1 | -2.255955 | -1.017406 | 4.162221 |
| 6 | -2.858135 | -0.768066 | 2.167853 |
| 7 | -2.970997 | -1.154401 | 1.077342 |
| 6 | 1.473159 | 3.766566 | 1.827353 |
| 1 | 0.577508 | 3.715518 | 2.450170 |
| 1 | 1.196499 | 4.172176 | 0.850693 |
| 1 | 2.215557 | 4.416555 | 2.297378 |
| 6 | 2.022857 | 2.426001 | 1.650432 |
| 7 | 2.482370 | 1.366846 | 1.518280 |
| 6 | 2.649520 | -3.553515 | -1.934825 |
| 1 | 1.724828 | -3.738369 | -2.491570 |
| 1 | 3.246843 | -4.468712 | -1.922909 |
| 1 | 3.217081 | -2.751929 | -2.415522 |
| 6 | 2.320632 | -3.148984 | -0.571246 |
| 7 | 2.042842 | -2.830645 | 0.511313 |
| 6 | 0.482632 | -0.248291 | -2.683242 |
| 6 | 0.316703 | -0.192762 | -1.247305 |
| 7 | 0.166194 | -0.160478 | -0.109591 |
| 1 | -0.508222 | -0.210809 | -3.142798 |
| 1 | 0.984187 | -1.187339 | -2.931030 |
| 1 | 1.101577 | 0.598312 | -2.990126 |
| 1 | 0.090932 | -0.205758 | 0.927745 |

Cartesian coordinates of : PACN10_34

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.924947 | -3.979989 | 1.710043 |
| 1 | 0.909242 | -4.452726 | 2.695276 |
| 1 | 1.859033 | -3.424016 | 1.587775 |
| 1 | 0.858468 | -4.751971 | 0.938242 |
| 6 | -0.198650 | -3.057306 | 1.578175 |
| 7 | -1.102793 | -2.335551 | 1.471488 |
| 6 | -4.347025 | -1.206040 | 1.609346 |
| 1 | -4.981767 | -1.173737 | 2.498448 |
| 1 | -3.553085 | -1.943926 | 1.752466 |
| 1 | -4.954477 | -1.483660 | 0.743371 |
| 6 | -3.739235 | 0.101175 | 1.381798 |
| 7 | -3.271678 | 1.150038 | 1.206031 |
| 6 | 1.605973 | 3.770391 | -1.895993 |
| 1 | 2.090127 | 3.093663 | -2.607630 |
| 1 | 2.105780 | 4.741835 | -1.930058 |
| 1 | 0.552482 | 3.888033 | -2.162659 |
| 6 | 1.700190 | 3.204393 | -0.553281 |
| 7 | 1.799165 | 2.744616 | 0.509926 |
| 6 | 3.367540 | -2.970490 | -1.391759 |
| 1 | 3.681091 | -2.468458 | -0.471491 |
| 1 | 3.828370 | -2.472845 | -2.248913 |
| 1 | 3.681896 | -4.017233 | -1.369942 |
| 6 | 1.914404 | -2.886365 | -1.500203 |
| 7 | 0.756150 | -2.836979 | -1.583621 |
| 6 | -2.620384 | -3.664964 | -1.175460 |
| 1 | -3.190172 | -4.244179 | -1.906391 |
| 1 | -2.960159 | -3.912084 | -0.165765 |
| 1 | -1.556417 | -3.902675 | -1.261991 |
| 6 | -2.803279 | -2.237446 | -1.418081 |
| 7 | -2.963581 | -1.103574 | -1.618118 |
| 6 | -4.138499 | 2.267822 | -1.638792 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.296577 | 1.187093 | -1.697297 |
| 1 | -4.543109 | 2.752920 | -2.530673 |
| 1 | -4.640663 | 2.651447 | -0.747509 |
| 6 | -2.706529 | 2.525972 | -1.535426 |
| 7 | -1.564869 | 2.734388 | -1.466379 |
| 6 | 2.844356 | 0.799248 | 3.220064 |
| 1 | 2.613567 | 1.789220 | 2.815613 |
| 1 | 3.875357 | 0.771087 | 3.582998 |
| 1 | 2.158748 | 0.587295 | 4.044041 |
| 6 | 2.658043 | -0.192182 | 2.165458 |
| 7 | 2.532847 | -0.979152 | 1.318559 |
| 6 | -1.150183 | 3.325862 | 2.270202 |
| 1 | -0.408301 | 4.058813 | 2.596751 |
| 1 | -2.085085 | 3.456716 | 2.819979 |
| 1 | -1.348833 | 3.453100 | 1.200664 |
| 6 | -0.642127 | 1.976806 | 2.471996 |
| 7 | -0.233662 | 0.894510 | 2.586634 |
| 6 | 4.765727 | 0.954381 | -0.332013 |
| 1 | 4.360657 | 1.647314 | 0.412453 |
| 1 | 5.601065 | 1.428020 | -0.853801 |
| 1 | 5.119324 | 0.052339 | 0.175284 |
| 6 | 3.710870 | 0.605686 | -1.278927 |
| 7 | 2.870623 | 0.334973 | -2.034386 |
| 6 | -0.176245 | 0.158247 | -2.703153 |
| 6 | -0.139197 | 0.093730 | -1.258623 |
| 7 | -0.118801 | 0.046024 | -0.112316 |
| 1 | 0.277737 | 1.101369 | -3.017769 |
| 1 | -1.223464 | 0.109041 | -3.013212 |
| 1 | 0.393371 | -0.685625 | -3.099763 |
| 1 | -0.132190 | 0.085217 | 0.924547 |

Cartesian coordinates of : PACN10_35

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.829994 | 4.035762 | -1.392570 |
| 1 | 0.872955 | 3.973866 | -1.918668 |
| 1 | 2.558793 | 3.364981 | -1.859052 |
| 1 | 2.205352 | 5.060940 | -1.443735 |
| 6 | 1.632454 | 3.639093 | -0.002521 |
| 7 | 1.481165 | 3.311974 | 1.102101 |
| 6 | -1.433396 | 2.838570 | 2.600678 |
| 1 | -1.553059 | 3.136211 | 3.645458 |
| 1 | -2.413994 | 2.739242 | 2.125399 |
| 1 | -0.839413 | 3.586456 | 2.068463 |
| 6 | -0.743322 | 1.559853 | 2.518790 |
| 7 | -0.216085 | 0.526635 | 2.434058 |
| 6 | -0.617264 | -3.786137 | -1.717381 |
| 1 | 0.333846 | -4.320964 | -1.669412 |
| 1 | -0.547044 | -3.043713 | -2.516804 |
| 1 | -1.426241 | -4.490441 | -1.930352 |
| 6 | -0.871358 | -3.108358 | -0.449481 |
| 7 | -1.105133 | -2.568086 | 0.553229 |
| 6 | -3.828255 | 2.415656 | -1.695867 |
| 1 | -3.882340 | 1.950247 | -2.683791 |
| 1 | -4.325718 | 3.388235 | -1.727899 |
| 1 | -4.321756 | 1.773430 | -0.961124 |
| 6 | -2.430045 | 2.578859 | -1.311201 |
| 7 | -1.315475 | 2.717959 | -1.012711 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 3.723936 | 1.090391 | 1.708457 |
| 1 | 4.335612 | 0.263337 | 2.077242 |
| 1 | 2.712650 | 1.000338 | 2.117487 |
| 1 | 4.147646 | 2.046070 | 2.026865 |
| 6 | 3.654018 | 1.042892 | 0.251467 |
| 7 | 3.588348 | 1.017239 | -0.909195 |
| 6 | 4.529136 | -2.165221 | -1.239398 |
| 1 | 4.503981 | -2.075686 | -0.149671 |
| 1 | 5.088948 | -1.324544 | -1.656724 |
| 1 | 5.011709 | -3.104221 | -1.521667 |
| 6 | 3.159175 | -2.134244 | -1.739099 |
| 7 | 2.067856 | -2.114127 | -2.137777 |
| 6 | -3.075750 | -1.459473 | 2.842755 |
| 1 | -3.738619 | -1.245228 | 3.684793 |
| 1 | -2.032067 | -1.409486 | 3.165627 |
| 1 | -3.271712 | -2.466202 | 2.465321 |
| 6 | -3.282464 | -0.482436 | 1.778272 |
| 7 | -3.445819 | 0.307695 | 0.941850 |
| 6 | 0.841209 | -2.618946 | 3.364729 |
| 1 | -0.045631 | -3.104428 | 2.947735 |
| 1 | 0.532264 | -1.753730 | 3.958076 |
| 1 | 1.381520 | -3.323901 | 4.001393 |
| 6 | 1.696105 | -2.168230 | 2.271308 |
| 7 | 2.376872 | -1.804139 | 1.402935 |
| 6 | -4.223345 | -1.739709 | -1.495271 |
| 1 | -4.695731 | -2.348617 | -2.270173 |
| 1 | -4.938563 | -1.001943 | -1.121813 |
| 1 | -3.919296 | -2.377940 | -0.659522 |
| 6 | -3.047968 | -1.061031 | -2.033554 |
| 7 | -2.107747 | -0.535825 | -2.469202 |
| 6 | 0.816501 | 0.646800 | -2.753718 |
| 6 | 0.574811 | 0.305000 | -1.371338 |
| 7 | 0.392679 | 0.058749 | -0.265094 |
| 1 | 0.195819 | 1.514360 | -2.997448 |
| 1 | 0.534651 | -0.207494 | -3.373308 |
| 1 | 1.884539 | 0.862155 | -2.861332 |
| 1 | 0.209249 | -0.062388 | 0.746928 |

Cartesian coordinates of : PACN10_36

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.885947 | 0.050561 | -3.055747 |
| 1 | -3.061566 | -0.814586 | -3.698945 |
| 1 | -3.541205 | 0.876525 | -3.344298 |
| 1 | -3.094937 | -0.232908 | -2.018238 |
| 6 | -1.491388 | 0.466438 | -3.159978 |
| 7 | -0.383928 | 0.816075 | -3.214446 |
| 6 | 2.764929 | 1.822514 | -2.458773 |
| 1 | 2.032485 | 1.479527 | -3.195458 |
| 1 | 3.532771 | 1.057483 | -2.312110 |
| 1 | 3.237820 | 2.742671 | -2.812079 |
| 6 | 2.082837 | 2.067691 | -1.191123 |
| 7 | 1.534597 | 2.265021 | -0.184124 |
| 6 | -1.132342 | -2.030074 | 3.144471 |
| 1 | -0.450067 | -2.123800 | 3.992988 |
| 1 | -2.127156 | -2.385179 | 3.425065 |
| 1 | -1.197922 | -0.975415 | 2.860091 |
| 6 | -0.626167 | -2.807557 | 2.018586 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.220089 | -3.421362 | 1.119179 |
| 6 | -4.798828 | 1.077752 | 1.425134 |
| 1 | -4.113239 | 1.778080 | 1.909859 |
| 1 | -5.620732 | 0.829349 | 2.100994 |
| 1 | -5.192132 | 1.547228 | 0.520473 |
| 6 | -4.059585 | -0.128874 | 1.068891 |
| 7 | -3.464772 | -1.088944 | 0.791105 |
| 6 | 6.524020 | -2.238698 | -0.856361 |
| 1 | 7.467203 | -1.746381 | -0.606992 |
| 1 | 6.565366 | -2.579974 | -1.893686 |
| 1 | 6.389378 | -3.104192 | -0.202887 |
| 6 | 5.413062 | -1.306168 | -0.683044 |
| 7 | 4.529692 | -0.564026 | -0.544836 |
| 6 | 3.814752 | 1.072732 | 2.245516 |
| 1 | 3.848088 | 1.644228 | 3.177488 |
| 1 | 3.807492 | 1.758612 | 1.393796 |
| 1 | 4.703237 | 0.440998 | 2.178846 |
| 6 | 2.610562 | 0.247487 | 2.206333 |
| 7 | 1.639556 | -0.390640 | 2.189283 |
| 6 | -0.964810 | 4.006139 | -1.790919 |
| 1 | -0.248931 | 4.412925 | -1.072564 |
| 1 | -1.557317 | 4.818753 | -2.218690 |
| 1 | -0.417576 | 3.493250 | -2.588272 |
| 6 | -1.839213 | 3.044458 | -1.127130 |
| 7 | -2.541731 | 2.272235 | -0.616687 |
| 6 | 0.597489 | 2.930245 | 3.168344 |
| 1 | 0.259228 | 3.895308 | 3.553767 |
| 1 | 1.295390 | 3.088826 | 2.340346 |
| 1 | 1.094868 | 2.376832 | 3.969762 |
| 6 | -0.537390 | 2.160346 | 2.674003 |
| 7 | -1.440470 | 1.547767 | 2.276616 |
| 6 | -2.848646 | -4.275011 | -0.585567 |
| 1 | -2.157084 | -5.001191 | -0.151568 |
| 1 | -3.600593 | -4.792504 | -1.186512 |
| 1 | -3.337486 | -3.719913 | 0.220091 |
| 6 | -2.103033 | -3.334256 | -1.414176 |
| 7 | -1.510374 | -2.584072 | -2.074970 |
| 6 | 1.173762 | -1.414829 | -1.107583 |
| 6 | 0.099485 | -0.699107 | -0.466490 |
| 7 | -0.735032 | -0.100674 | 0.046915 |
| 1 | 1.056272 | -1.301764 | -2.190155 |
| 1 | 1.086993 | -2.468797 | -0.822940 |
| 1 | 2.124517 | -0.996222 | -0.756117 |
| 1 | -1.396591 | 0.471839 | 0.585374 |

Cartesian coordinates of : PACN10_37

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|----------|
| 6 | 2.013032 | 2.977649 | 2.097389 |
| 1 | 2.126852 | 3.374315 | 3.109271 |
| 1 | 1.455254 | 3.687346 | 1.479866 |
| 1 | 2.996285 | 2.807079 | 1.648898 |
| 6 | 1.287598 | 1.716222 | 2.127928 |
| 7 | 0.712493 | 0.706491 | 2.137248 |
| 6 | 3.379148 | -1.472352 | 2.807689 |
| 1 | 4.033637 | -1.276761 | 3.660837 |
| 1 | 3.504965 | -2.508312 | 2.481746 |
| 1 | 2.333271 | -1.328829 | 3.091896 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 3.700499 | -0.564209 | 1.710923 |
| 7 | 3.959159 | 0.169926 | 0.847902 |
| 6 | -4.734366 | 1.437726 | 0.524993 |
| 1 | -4.101534 | 2.008147 | 1.212522 |
| 1 | -5.071174 | 0.523168 | 1.021364 |
| 1 | -5.602386 | 2.040585 | 0.246698 |
| 6 | -3.956468 | 1.096843 | -0.662195 |
| 7 | -3.337980 | 0.833113 | -1.609678 |
| 6 | -1.295203 | 3.666869 | -1.609345 |
| 1 | -1.673282 | 4.688316 | -1.701681 |
| 1 | -1.889992 | 3.007370 | -2.249664 |
| 1 | -0.246188 | 3.633668 | -1.915114 |
| 6 | -1.404066 | 3.213783 | -0.225929 |
| 7 | -1.511155 | 2.842736 | 0.870611 |
| 6 | 3.858591 | -2.703831 | -1.066758 |
| 1 | 3.289011 | -3.039362 | -0.195238 |
| 1 | 4.798939 | -2.255732 | -0.734875 |
| 1 | 4.071609 | -3.557547 | -1.714914 |
| 6 | 3.071215 | -1.710636 | -1.790069 |
| 7 | 2.451768 | -0.923769 | -2.378686 |
| 6 | -4.271249 | -2.405127 | -1.169851 |
| 1 | -4.713468 | -3.403783 | -1.212986 |
| 1 | -4.826393 | -1.736526 | -1.832787 |
| 1 | -4.322013 | -2.023586 | -0.145267 |
| 6 | -2.872137 | -2.455916 | -1.582331 |
| 7 | -1.755885 | -2.513153 | -1.899724 |
| 6 | -2.171243 | 0.678737 | 3.510571 |
| 1 | -1.348903 | 0.336934 | 4.143733 |
| 1 | -3.092384 | 0.714461 | 4.098517 |
| 1 | -1.931122 | 1.674272 | 3.125335 |
| 6 | -2.333659 | -0.235678 | 2.384069 |
| 7 | -2.486981 | -0.957968 | 1.485676 |
| 6 | -1.087641 | -4.109244 | 0.974583 |
| 1 | -1.191450 | -4.621472 | 0.014921 |
| 1 | -1.988206 | -3.518333 | 1.165699 |
| 1 | -0.955135 | -4.845441 | 1.771467 |
| 6 | 0.064466 | -3.214016 | 0.927027 |
| 7 | 0.992472 | -2.514615 | 0.902913 |
| 6 | 4.154635 | 1.850114 | -2.091804 |
| 1 | 4.682237 | 1.230538 | -1.361688 |
| 1 | 4.710741 | 2.774714 | -2.266149 |
| 1 | 4.056660 | 1.295631 | -3.028330 |
| 6 | 2.828040 | 2.155634 | -1.567358 |
| 7 | 1.773812 | 2.413464 | -1.150137 |
| 6 | -0.405334 | 0.070547 | -3.016034 |
| 6 | -0.252281 | -0.009414 | -1.581436 |
| 7 | -0.129232 | -0.033897 | -0.440893 |
| 1 | -0.113265 | -0.891819 | -3.442897 |
| 1 | 0.263887 | 0.856875 | -3.379445 |
| 1 | -1.454152 | 0.289926 | -3.235750 |
| 1 | 0.076933 | 0.005651 | 0.575006 |

 Cartesian coordinates of : PACN10_38

 Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|----------|-----------|----------|
| 6 | 2.782174 | -2.631714 | 0.868621 |
| 1 | 3.069746 | -2.372870 | 1.890209 |
| 1 | 3.083974 | -1.812518 | 0.209242 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.281244 | -3.555667 | 0.564909 |
| 6 | 1.335577 | -2.805502 | 0.794692 |
| 7 | 0.185691 | -2.958409 | 0.722642 |
| 6 | 7.458259 | -0.973540 | -0.897579 |
| 1 | 7.392402 | -1.766841 | -1.646220 |
| 1 | 7.902442 | -1.380134 | 0.014301 |
| 1 | 8.101323 | -0.177441 | -1.280849 |
| 6 | 6.126687 | -0.444311 | -0.612194 |
| 7 | 5.068522 | -0.022065 | -0.385251 |
| 6 | 2.240191 | 1.600994 | -1.614950 |
| 1 | 3.305047 | 1.563770 | -1.370669 |
| 1 | 1.689298 | 2.134905 | -0.832106 |
| 1 | 2.081475 | 2.118128 | -2.564449 |
| 6 | 1.714204 | 0.245517 | -1.704529 |
| 7 | 1.255613 | -0.821965 | -1.761379 |
| 6 | -3.431732 | 1.401148 | -2.868973 |
| 1 | -3.494183 | 1.500123 | -3.955555 |
| 1 | -4.094920 | 2.134044 | -2.400748 |
| 1 | -3.739811 | 0.392151 | -2.578821 |
| 6 | -2.059999 | 1.623360 | -2.421989 |
| 7 | -0.968538 | 1.808341 | -2.069136 |
| 6 | 3.624345 | 2.402567 | 1.706841 |
| 1 | 4.083589 | 2.669857 | 2.661954 |
| 1 | 3.001315 | 3.233499 | 1.362769 |
| 1 | 4.409711 | 2.192559 | 0.975353 |
| 6 | 2.786305 | 1.219140 | 1.868253 |
| 7 | 2.108898 | 0.283854 | 1.998923 |
| 6 | -3.028960 | -3.873800 | 1.178981 |
| 1 | -3.657685 | -3.838429 | 0.284312 |
| 1 | -3.452430 | -4.587533 | 1.889951 |
| 1 | -2.018096 | -4.184513 | 0.900696 |
| 6 | -2.957092 | -2.546164 | 1.780344 |
| 7 | -2.913299 | -1.488176 | 2.258497 |
| 6 | -1.559614 | 4.580032 | -0.270059 |
| 1 | -2.498744 | 4.027511 | -0.176914 |
| 1 | -1.291372 | 4.662626 | -1.326405 |
| 1 | -1.674331 | 5.578933 | 0.158207 |
| 6 | -0.514792 | 3.849484 | 0.439115 |
| 7 | 0.323760 | 3.278017 | 1.006218 |
| 6 | -0.807896 | -3.493385 | -2.328360 |
| 1 | -1.123828 | -3.831924 | -3.318226 |
| 1 | -0.837180 | -4.328530 | -1.623291 |
| 1 | 0.213152 | -3.104435 | -2.373330 |
| 6 | -1.687800 | -2.428762 | -1.858791 |
| 7 | -2.393274 | -1.582326 | -1.485821 |
| 6 | -5.143612 | -0.134024 | 0.285105 |
| 1 | -5.457126 | -0.531643 | 1.253489 |
| 1 | -4.675636 | -0.934701 | -0.296010 |
| 1 | -6.015726 | 0.252351 | -0.249446 |
| 6 | -4.169274 | 0.933782 | 0.488593 |
| 7 | -3.402218 | 1.794996 | 0.633292 |
| 6 | -0.972554 | 0.899963 | 2.860788 |
| 6 | -0.792161 | 0.413813 | 1.514351 |
| 7 | -0.650871 | 0.026854 | 0.444230 |
| 1 | -0.237399 | 1.689942 | 3.035695 |
| 1 | -0.826398 | 0.062694 | 3.548258 |
| 1 | -1.994276 | 1.281551 | 2.945543 |
| 1 | -0.479095 | -0.352889 | -0.486908 |

Cartesian coordinates of : PACN10_39

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -1.859289 | 3.856926 | 1.493320 |
| 1 | -1.428321 | 4.775499 | 1.900021 |
| 1 | -2.805764 | 3.634583 | 1.991497 |
| 1 | -2.050153 | 3.972556 | 0.422174 |
| 6 | -0.941325 | 2.741512 | 1.676022 |
| 7 | -0.204738 | 1.854021 | 1.810678 |
| 6 | -1.849234 | -0.589930 | 3.561823 |
| 1 | -2.433757 | 0.303495 | 3.322146 |
| 1 | -0.859812 | -0.294165 | 3.920745 |
| 1 | -2.361530 | -1.165873 | 4.336692 |
| 6 | -1.693992 | -1.399967 | 2.357497 |
| 7 | -1.587055 | -2.040083 | 1.392692 |
| 6 | -2.267633 | -3.743906 | -1.540859 |
| 1 | -1.569754 | -4.368713 | -2.102798 |
| 1 | -3.295219 | -4.047251 | -1.760966 |
| 1 | -2.060384 | -3.858505 | -0.472896 |
| 6 | -2.073286 | -2.344181 | -1.903128 |
| 7 | -1.953278 | -1.222490 | -2.184799 |
| 6 | -4.632618 | -1.046463 | -0.032433 |
| 1 | -4.046582 | -1.911958 | 0.291746 |
| 1 | -4.768732 | -1.092973 | -1.116647 |
| 1 | -5.610079 | -1.062279 | 0.456298 |
| 6 | -3.915730 | 0.174798 | 0.323686 |
| 7 | -3.362972 | 1.153383 | 0.619059 |
| 6 | 1.628654 | 4.316609 | -0.398535 |
| 1 | 0.593199 | 4.317072 | -0.750517 |
| 1 | 2.156795 | 5.183097 | -0.804217 |
| 1 | 1.644952 | 4.365919 | 0.694305 |
| 6 | 2.270971 | 3.084541 | -0.844899 |
| 7 | 2.792852 | 2.108318 | -1.198120 |
| 6 | 5.319793 | -0.216454 | -1.812371 |
| 1 | 6.294786 | -0.139713 | -1.324524 |
| 1 | 4.980854 | 0.783069 | -2.099813 |
| 1 | 5.421196 | -0.841086 | -2.703609 |
| 6 | 4.344932 | -0.801795 | -0.896399 |
| 7 | 3.557655 | -1.255152 | -0.171744 |
| 6 | 3.192155 | 0.882669 | 2.322003 |
| 1 | 4.207927 | 0.486922 | 2.399156 |
| 1 | 3.088826 | 1.753695 | 2.974591 |
| 1 | 3.012756 | 1.176601 | 1.282379 |
| 6 | 2.227139 | -0.140849 | 2.709403 |
| 7 | 1.432758 | -0.934438 | 3.007098 |
| 6 | 1.605897 | -3.771109 | 1.320196 |
| 1 | 2.513798 | -3.189433 | 1.499579 |
| 1 | 1.803234 | -4.832010 | 1.494193 |
| 1 | 0.829293 | -3.418039 | 2.003768 |
| 6 | 1.174475 | -3.564123 | -0.056628 |
| 7 | 0.834047 | -3.404343 | -1.156529 |
| 6 | -3.204449 | 1.885739 | -2.744155 |
| 1 | -3.286250 | 2.354702 | -3.727928 |
| 1 | -4.002754 | 2.257966 | -2.096468 |
| 1 | -3.292917 | 0.800434 | -2.846409 |
| 6 | -1.908995 | 2.194789 | -2.147423 |
| 7 | -0.878505 | 2.454333 | -1.676391 |
| 6 | 1.142942 | -0.513907 | -2.535588 |
| 6 | 0.752364 | -0.257370 | -1.170284 |
| 7 | 0.451412 | -0.019433 | -0.087514 |
| 1 | 1.314977 | -1.589379 | -2.646851 |

| | | | |
|---|----------|-----------|-----------|
| 1 | 2.048857 | 0.066824 | -2.734777 |
| 1 | 0.322380 | -0.191236 | -3.183152 |
| 1 | 0.186309 | 0.426193 | 0.813771 |

Cartesian coordinates of : PACN10_40

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -2.985188 | -2.966481 | -2.245237 |
| 1 | -2.055891 | -3.201877 | -2.773259 |
| 1 | -3.449383 | -2.074559 | -2.676373 |
| 1 | -3.672457 | -3.811424 | -2.336302 |
| 6 | -2.683161 | -2.711838 | -0.840620 |
| 7 | -2.436185 | -2.509501 | 0.276480 |
| 6 | -3.487164 | -1.041679 | 2.911380 |
| 1 | -3.949064 | -0.748985 | 3.857520 |
| 1 | -2.727191 | -1.807474 | 3.086102 |
| 1 | -4.241733 | -1.456814 | 2.239501 |
| 6 | -2.854051 | 0.113639 | 2.285330 |
| 7 | -2.343466 | 1.039740 | 1.802919 |
| 6 | 4.431733 | 1.291041 | -0.323433 |
| 1 | 4.013072 | 1.641766 | 0.624894 |
| 1 | 5.044268 | 2.078525 | -0.770831 |
| 1 | 5.052893 | 0.410966 | -0.138049 |
| 6 | 3.333746 | 0.940057 | -1.218338 |
| 7 | 2.462822 | 0.685743 | -1.943926 |
| 6 | 3.125535 | -2.677490 | -2.345508 |
| 1 | 3.677243 | -2.439325 | -1.432261 |
| 1 | 3.333072 | -1.914025 | -3.099847 |
| 1 | 3.434013 | -3.655478 | -2.723461 |
| 6 | 1.697795 | -2.687950 | -2.042230 |
| 7 | 0.557991 | -2.708114 | -1.813211 |
| 6 | -3.982287 | 2.760254 | -0.643458 |
| 1 | -5.050935 | 2.850139 | -0.433110 |
| 1 | -3.680502 | 3.532667 | -1.354653 |
| 1 | -3.412946 | 2.884146 | 0.281641 |
| 6 | -3.690723 | 1.442264 | -1.197440 |
| 7 | -3.462382 | 0.393057 | -1.641640 |
| 6 | -0.424149 | 3.521501 | 2.263909 |
| 1 | -0.942330 | 3.088784 | 3.122352 |
| 1 | -1.144907 | 3.632523 | 1.449074 |
| 1 | -0.007769 | 4.495622 | 2.533408 |
| 6 | 0.645478 | 2.627351 | 1.830479 |
| 7 | 1.513370 | 1.940418 | 1.473504 |
| 6 | 0.441693 | -3.851141 | 1.512539 |
| 1 | 0.334540 | -4.561832 | 2.335763 |
| 1 | 1.455623 | -3.904107 | 1.104461 |
| 1 | -0.279358 | -4.084064 | 0.723964 |
| 6 | 0.193612 | -2.494584 | 1.979668 |
| 7 | 0.013446 | -1.399676 | 2.327549 |
| 6 | 3.123070 | -0.332329 | 3.194955 |
| 1 | 3.639949 | -0.936236 | 3.945010 |
| 1 | 2.081535 | -0.181411 | 3.491840 |
| 1 | 3.607589 | 0.644583 | 3.115332 |
| 6 | 3.151003 | -1.007588 | 1.901195 |
| 7 | 3.169904 | -1.553410 | 0.875190 |
| 6 | 1.713736 | 4.059375 | -1.528144 |
| 1 | 1.679789 | 5.148776 | -1.608302 |
| 1 | 2.205737 | 3.645362 | -2.411971 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 2.283396 | 3.775319 | -0.637417 |
| 6 | 0.360018 | 3.522212 | -1.420691 |
| 7 | -0.720461 | 3.105436 | -1.322614 |
| 6 | -0.620303 | 0.122154 | -2.756754 |
| 6 | -0.472415 | 0.039995 | -1.320976 |
| 7 | -0.341102 | -0.032668 | -0.183473 |
| 1 | 0.380121 | 0.099191 | -3.196449 |
| 1 | -1.139668 | 1.053269 | -2.996468 |
| 1 | -1.215685 | -0.733429 | -3.085997 |
| 1 | -0.258455 | -0.210331 | 0.828689 |

Cartesian coordinates of : PACN10_41

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.506604 | 4.803609 | -1.027901 |
| 1 | 0.310143 | 5.138605 | -0.005306 |
| 1 | 0.455877 | 5.658578 | -1.706671 |
| 1 | 1.503167 | 4.355577 | -1.076713 |
| 6 | -0.477110 | 3.796334 | -1.411426 |
| 7 | -1.271358 | 3.003970 | -1.713473 |
| 6 | -3.090784 | -2.018528 | 2.232277 |
| 1 | -3.415910 | -2.412545 | 3.198277 |
| 1 | -2.867132 | -2.846865 | 1.553071 |
| 1 | -3.877339 | -1.391714 | 1.801766 |
| 6 | -1.891302 | -1.208623 | 2.390040 |
| 7 | -0.930525 | -0.562307 | 2.482392 |
| 6 | 4.493833 | 0.491430 | -1.285212 |
| 1 | 4.445213 | -0.080913 | -0.353783 |
| 1 | 5.367580 | 1.148144 | -1.270209 |
| 1 | 4.575376 | -0.196622 | -2.130655 |
| 6 | 3.274172 | 1.282592 | -1.413355 |
| 7 | 2.314170 | 1.930282 | -1.508946 |
| 6 | 1.691117 | -2.077722 | 3.372706 |
| 1 | 2.533874 | -2.596482 | 3.837145 |
| 1 | 0.975038 | -2.802415 | 2.974612 |
| 1 | 1.186937 | -1.455846 | 4.116315 |
| 6 | 2.164136 | -1.237838 | 2.276843 |
| 7 | 2.559038 | -0.581980 | 1.401425 |
| 6 | -5.151705 | -0.917317 | -1.312426 |
| 1 | -5.471219 | -0.446643 | -2.245680 |
| 1 | -5.220462 | -0.187234 | -0.501352 |
| 1 | -5.804138 | -1.769259 | -1.104436 |
| 6 | -3.766234 | -1.361619 | -1.427626 |
| 7 | -2.663807 | -1.717930 | -1.517581 |
| 6 | -0.603806 | -4.103208 | -1.799135 |
| 1 | -1.671263 | -4.303141 | -1.912955 |
| 1 | -0.032448 | -5.011929 | -2.006517 |
| 1 | -0.317617 | -3.324335 | -2.510986 |
| 6 | -0.326533 | -3.639814 | -0.442419 |
| 7 | -0.074512 | -3.286062 | 0.635851 |
| 6 | -2.892666 | 3.542579 | 1.181188 |
| 1 | -3.536536 | 3.862410 | 2.004433 |
| 1 | -3.118260 | 4.133219 | 0.289710 |
| 1 | -1.844283 | 3.683449 | 1.457968 |
| 6 | -3.116769 | 2.129171 | 0.896747 |
| 7 | -3.318221 | 1.005216 | 0.682229 |
| 6 | 3.367880 | -3.309802 | -0.337713 |
| 1 | 4.158058 | -2.731602 | 0.149557 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 3.810997 | -4.158053 | -0.865546 |
| 1 | 2.676067 | -3.674667 | 0.427997 |
| 6 | 2.637417 | -2.458377 | -1.272313 |
| 7 | 2.053891 | -1.787001 | -2.019906 |
| 6 | 2.988427 | 2.810038 | 1.755395 |
| 1 | 3.349554 | 3.484307 | 0.973250 |
| 1 | 3.459475 | 1.830738 | 1.631399 |
| 1 | 3.250201 | 3.219270 | 2.734374 |
| 6 | 1.540520 | 2.659362 | 1.644050 |
| 7 | 0.386486 | 2.558302 | 1.556058 |
| 6 | -0.347950 | 0.219816 | -2.735401 |
| 6 | -0.260640 | 0.161097 | -1.294185 |
| 7 | -0.194432 | 0.113198 | -0.149627 |
| 1 | -1.297070 | 0.695304 | -2.994810 |
| 1 | -0.287361 | -0.797212 | -3.128717 |
| 1 | 0.489552 | 0.822529 | -3.098795 |
| 1 | -0.242821 | 0.046458 | 0.883496 |

Cartesian coordinates of : PACN10_42

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.014768 | -4.000067 | 0.309389 |
| 1 | 2.059776 | -3.735697 | 0.122848 |
| 1 | 0.455246 | -3.895619 | -0.623953 |
| 1 | 0.950980 | -5.028984 | 0.672517 |
| 6 | 0.461703 | -3.083577 | 1.299386 |
| 7 | 0.037417 | -2.337524 | 2.084413 |
| 6 | 4.255847 | -1.347292 | -2.370835 |
| 1 | 4.622477 | -1.251668 | -1.344736 |
| 1 | 4.369157 | -0.392374 | -2.891326 |
| 1 | 4.832188 | -2.113499 | -2.895322 |
| 6 | 2.845116 | -1.717048 | -2.328518 |
| 7 | 1.722571 | -2.013460 | -2.293623 |
| 6 | -0.446029 | 3.415850 | 2.727430 |
| 1 | 0.104648 | 4.285556 | 3.094326 |
| 1 | -1.152640 | 3.070541 | 3.485674 |
| 1 | -0.996926 | 3.678867 | 1.819546 |
| 6 | 0.474521 | 2.332943 | 2.408082 |
| 7 | 1.205282 | 1.465893 | 2.151574 |
| 6 | -3.992264 | 2.690412 | 0.214513 |
| 1 | -3.731990 | 3.519652 | -0.447315 |
| 1 | -3.332907 | 2.708657 | 1.087029 |
| 1 | -5.032723 | 2.787937 | 0.534575 |
| 6 | -3.801410 | 1.423409 | -0.483635 |
| 7 | -3.658999 | 0.406551 | -1.028671 |
| 6 | 2.833119 | -1.035705 | 3.466063 |
| 1 | 3.142652 | -0.053657 | 3.832586 |
| 1 | 3.393727 | -1.815501 | 3.987643 |
| 1 | 1.763291 | -1.165244 | 3.654034 |
| 6 | 3.072645 | -1.120506 | 2.028822 |
| 7 | 3.252050 | -1.183509 | 0.881857 |
| 6 | 4.097284 | 1.879714 | 0.186058 |
| 1 | 4.593963 | 2.843558 | 0.048810 |
| 1 | 4.836751 | 1.075938 | 0.137068 |
| 1 | 3.611399 | 1.846983 | 1.165204 |
| 6 | 3.090181 | 1.683484 | -0.852979 |
| 7 | 2.300485 | 1.540737 | -1.693882 |
| 6 | -4.374198 | -2.840146 | -1.826193 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | -4.776616 | -1.823648 | -1.857900 |
| 1 | -4.958982 | -3.443857 | -1.126951 |
| 1 | -4.440633 | -3.290402 | -2.819822 |
| 6 | -2.981682 | -2.779535 | -1.392675 |
| 7 | -1.876679 | -2.717794 | -1.038648 |
| 6 | 0.462237 | 3.989389 | -2.760892 |
| 1 | 0.783964 | 3.190333 | -3.433724 |
| 1 | 1.354913 | 4.493150 | -2.381961 |
| 1 | -0.155408 | 4.707277 | -3.306036 |
| 6 | -0.291608 | 3.419103 | -1.647264 |
| 7 | -0.896916 | 2.965931 | -0.764366 |
| 6 | -3.281168 | -1.596047 | 2.015067 |
| 1 | -2.538525 | -2.371841 | 1.811569 |
| 1 | -3.990918 | -1.544516 | 1.183441 |
| 1 | -3.814408 | -1.832437 | 2.939379 |
| 6 | -2.606171 | -0.309807 | 2.144742 |
| 7 | -2.088054 | 0.725837 | 2.240425 |
| 6 | -0.656493 | -0.098519 | -2.490354 |
| 6 | -0.264894 | -0.134097 | -1.101203 |
| 7 | 0.060224 | -0.114660 | -0.000830 |
| 1 | -1.645333 | 0.365493 | -2.554899 |
| 1 | -0.673970 | -1.123796 | -2.866958 |
| 1 | 0.105247 | 0.481833 | -3.022181 |
| 1 | 0.390916 | 0.029208 | 0.959050 |

Cartesian coordinates of : PACN10_43

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 0.931525 | 1.038609 | 4.130506 |
| 1 | 1.565999 | 0.626090 | 4.919464 |
| 1 | 0.257696 | 1.785701 | 4.557044 |
| 1 | 1.547909 | 1.513812 | 3.361911 |
| 6 | 0.150150 | -0.026355 | 3.509807 |
| 7 | -0.459503 | -0.890074 | 3.026468 |
| 6 | -1.348542 | -4.069642 | 1.859837 |
| 1 | -1.894466 | -4.821245 | 2.435685 |
| 1 | -0.778036 | -3.427655 | 2.536808 |
| 1 | -0.661628 | -4.561462 | 1.167081 |
| 6 | -2.286362 | -3.240508 | 1.110382 |
| 7 | -3.049367 | -2.591336 | 0.521655 |
| 6 | 6.730987 | -1.173655 | -0.824313 |
| 1 | 7.274294 | -0.727506 | -1.661007 |
| 1 | 6.981531 | -2.235808 | -0.766944 |
| 1 | 7.043015 | -0.683933 | 0.101418 |
| 6 | 5.291860 | -1.008099 | -1.019178 |
| 7 | 4.148171 | -0.875809 | -1.177322 |
| 6 | -5.577636 | -1.904192 | -1.667081 |
| 1 | -6.608213 | -1.762827 | -1.331966 |
| 1 | -5.096664 | -2.674121 | -1.057964 |
| 1 | -5.584480 | -2.217311 | -2.714073 |
| 6 | -4.830152 | -0.658967 | -1.521636 |
| 7 | -4.234550 | 0.331368 | -1.399266 |
| 6 | 2.583723 | -1.854966 | 1.775407 |
| 1 | 3.539782 | -2.324546 | 1.530368 |
| 1 | 2.234662 | -2.219716 | 2.745444 |
| 1 | 2.711685 | -0.769424 | 1.817101 |
| 6 | 1.598924 | -2.178203 | 0.747630 |
| 7 | 0.818003 | -2.465744 | -0.063723 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | -2.259938 | 2.095015 | -3.366143 |
| 1 | -2.021912 | 2.536596 | -4.337085 |
| 1 | -3.309375 | 2.273769 | -3.122323 |
| 1 | -2.097322 | 1.013743 | -3.404642 |
| 6 | -1.404453 | 2.670446 | -2.333579 |
| 7 | -0.708548 | 3.111010 | -1.514015 |
| 6 | 1.918712 | -2.070733 | -3.279898 |
| 1 | 2.105569 | -2.788040 | -2.475292 |
| 1 | 2.873490 | -1.685273 | -3.644264 |
| 1 | 1.376339 | -2.558742 | -4.093283 |
| 6 | 1.120963 | -0.985309 | -2.729287 |
| 7 | 0.468862 | -0.139817 | -2.275172 |
| 6 | 0.524452 | 4.541054 | 1.299109 |
| 1 | 1.536753 | 4.318361 | 1.648590 |
| 1 | 0.238001 | 5.540595 | 1.635626 |
| 1 | 0.497188 | 4.499768 | 0.206627 |
| 6 | -0.404097 | 3.547202 | 1.827778 |
| 7 | -1.135594 | 2.755349 | 2.260537 |
| 6 | 2.592568 | 2.250208 | -1.506073 |
| 1 | 1.728468 | 2.549790 | -2.104681 |
| 1 | 3.157388 | 1.477226 | -2.034311 |
| 1 | 3.234836 | 3.118292 | -1.333817 |
| 6 | 2.127656 | 1.713206 | -0.231332 |
| 7 | 1.764847 | 1.295782 | 0.791179 |
| 6 | -3.127949 | 0.493968 | 1.601292 |
| 6 | -2.035731 | 0.346709 | 0.666111 |
| 7 | -1.184253 | 0.229905 | -0.095458 |
| 1 | -3.623784 | 1.446745 | 1.398377 |
| 1 | -2.718170 | 0.491770 | 2.613464 |
| 1 | -3.811514 | -0.344977 | 1.447426 |
| 1 | -0.475482 | 0.131154 | -0.860979 |

Cartesian coordinates of : PACN10_44

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.574221 | 3.092037 | -2.358016 |
| 1 | 0.482490 | 3.010184 | -2.391960 |
| 1 | 2.015120 | 2.291027 | -2.958176 |
| 1 | 1.869827 | 4.061174 | -2.768085 |
| 6 | 2.046287 | 2.967951 | -0.982158 |
| 7 | 2.424774 | 2.872387 | 0.112477 |
| 6 | 4.971719 | 1.041417 | 0.533376 |
| 1 | 5.943839 | 0.564065 | 0.681004 |
| 1 | 4.977702 | 2.037199 | 0.983827 |
| 1 | 4.769059 | 1.155315 | -0.535542 |
| 6 | 3.916045 | 0.232489 | 1.136595 |
| 7 | 3.084315 | -0.426789 | 1.611263 |
| 6 | -4.357856 | -1.923244 | 0.801670 |
| 1 | -3.839490 | -1.847993 | 1.762879 |
| 1 | -4.944312 | -2.845094 | 0.771623 |
| 1 | -5.022679 | -1.063626 | 0.687472 |
| 6 | -3.367383 | -1.921993 | -0.270236 |
| 7 | -2.571122 | -1.939110 | -1.116259 |
| 6 | -2.861949 | 1.209432 | 3.352912 |
| 1 | -2.372902 | 2.135561 | 3.665494 |
| 1 | -2.223354 | 0.358914 | 3.607059 |
| 1 | -3.820774 | 1.118749 | 3.870011 |
| 6 | -3.071676 | 1.227349 | 1.908007 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -3.246434 | 1.236724 | 0.758719 |
| 6 | 3.772926 | -2.414319 | -1.473972 |
| 1 | 4.772763 | -2.443950 | -1.914631 |
| 1 | 3.176128 | -3.249502 | -1.848286 |
| 1 | 3.854722 | -2.495334 | -0.384798 |
| 6 | 3.106511 | -1.161339 | -1.815264 |
| 7 | 2.584775 | -0.154303 | -2.068785 |
| 6 | -0.757080 | -4.629281 | 0.213776 |
| 1 | -1.079233 | -5.270947 | -0.610094 |
| 1 | -1.643985 | -4.191531 | 0.686874 |
| 1 | -0.253662 | -5.241439 | 0.971753 |
| 6 | 0.157510 | -3.540293 | -0.271944 |
| 7 | 0.537863 | -3.353919 | -1.476212 |
| 6 | 2.149482 | 2.293482 | 3.490140 |
| 1 | 2.665941 | 1.434617 | 3.926456 |
| 1 | 1.800028 | 2.959432 | 4.282758 |
| 1 | 2.829808 | 2.835916 | 2.825673 |
| 6 | 1.030817 | 1.825940 | 2.686906 |
| 7 | 0.156340 | 1.459073 | 2.021421 |
| 6 | 0.709543 | -2.587262 | 0.781715 |
| 1 | 0.122780 | -4.059897 | -2.095254 |
| 1 | 1.259269 | -1.775301 | 0.294329 |
| 1 | 1.418062 | -3.112857 | 1.436429 |
| 6 | -0.344378 | -2.014020 | 1.623033 |
| 7 | -1.201976 | -1.564883 | 2.265221 |
| 6 | -4.329886 | 3.172652 | -1.880043 |
| 1 | -5.042086 | 2.891096 | -2.659658 |
| 1 | -4.369167 | 4.255421 | -1.737187 |
| 1 | -4.591385 | 2.671730 | -0.944516 |
| 6 | -2.981827 | 2.770863 | -2.267519 |
| 7 | -1.909053 | 2.452550 | -2.578947 |
| 6 | -0.506014 | -0.336838 | -2.842893 |
| 6 | -0.434557 | 0.134893 | -1.478679 |
| 7 | -0.355590 | 0.509950 | -0.394199 |
| 1 | -0.056217 | -1.334895 | -2.868725 |
| 1 | 0.049103 | 0.359836 | -3.476826 |
| 1 | -1.556917 | -0.378354 | -3.136963 |
| 1 | -0.252480 | 0.889213 | 0.609722 |

Cartesian coordinates of : PACN10_45

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | 1.971649 | -0.554185 | 3.734977 |
| 1 | 1.300122 | -1.371423 | 4.014716 |
| 1 | 1.414011 | 0.386325 | 3.738949 |
| 1 | 2.796389 | -0.502313 | 4.450150 |
| 6 | 2.488300 | -0.785688 | 2.389640 |
| 7 | 2.898880 | -0.988890 | 1.320607 |
| 6 | -2.353508 | 0.771773 | 2.588915 |
| 1 | -1.884605 | 1.244964 | 3.455298 |
| 1 | -3.322938 | 0.346807 | 2.858322 |
| 1 | -2.490718 | 1.519177 | 1.802358 |
| 6 | -1.476719 | -0.274642 | 2.081944 |
| 7 | -0.755815 | -1.100645 | 1.693179 |
| 6 | 4.010238 | -2.706692 | -1.607797 |
| 1 | 5.037051 | -2.889030 | -1.935123 |
| 1 | 3.359795 | -3.495966 | -1.992417 |
| 1 | 3.965123 | -2.706395 | -0.514351 |

| | | | |
|---|-----------|-----------|-----------|
| 6 | 3.550567 | -1.411297 | -2.098370 |
| 7 | 3.207140 | -0.372621 | -2.488593 |
| 6 | 5.222389 | 1.137768 | -0.280573 |
| 1 | 4.997135 | 0.176044 | 0.189482 |
| 1 | 5.967639 | 1.671510 | 0.314536 |
| 1 | 5.614924 | 0.964281 | -1.285772 |
| 6 | 3.995894 | 1.923440 | -0.368516 |
| 7 | 3.025593 | 2.557503 | -0.442438 |
| 6 | -6.912133 | -1.285003 | 0.430129 |
| 1 | -6.938086 | -2.244838 | 0.951924 |
| 1 | -7.324120 | -1.415993 | -0.573567 |
| 1 | -7.531280 | -0.568962 | 0.976198 |
| 6 | -5.536591 | -0.796712 | 0.348117 |
| 7 | -4.443248 | -0.407703 | 0.283719 |
| 6 | -3.991440 | 2.098052 | -1.953499 |
| 1 | -3.911723 | 1.132052 | -2.458626 |
| 1 | -4.095081 | 2.892647 | -2.696777 |
| 1 | -4.867402 | 2.094360 | -1.300530 |
| 6 | -2.786454 | 2.313363 | -1.159679 |
| 7 | -1.823831 | 2.500778 | -0.535793 |
| 6 | 0.596600 | 4.380202 | 0.948793 |
| 1 | -0.288892 | 4.448872 | 0.310645 |
| 1 | 1.499234 | 4.453021 | 0.336187 |
| 1 | 0.583173 | 5.191016 | 1.681617 |
| 6 | 0.589435 | 3.088940 | 1.627420 |
| 7 | 0.580142 | 2.060260 | 2.167777 |
| 6 | 1.198629 | -3.950673 | 1.495480 |
| 1 | 0.888130 | -4.998215 | 1.516530 |
| 1 | 0.619853 | -3.384005 | 2.231564 |
| 1 | 2.261714 | -3.882445 | 1.743286 |
| 6 | 0.962972 | -3.376267 | 0.174581 |
| 7 | 0.773920 | -2.909481 | -0.872824 |
| 6 | -2.432959 | -2.612275 | -1.306012 |
| 1 | -1.838771 | -3.432960 | -1.714283 |
| 1 | -3.497769 | -2.818213 | -1.440855 |
| 1 | -2.217615 | -2.509837 | -0.238376 |
| 6 | -2.082141 | -1.370621 | -1.988214 |
| 7 | -1.809857 | -0.386252 | -2.542215 |
| 6 | 0.764069 | 1.827654 | -2.504575 |
| 6 | 0.712615 | 0.921503 | -1.383282 |
| 7 | 0.651009 | 0.190303 | -0.501980 |
| 1 | -0.072244 | 1.577468 | -3.165428 |
| 1 | 1.727006 | 1.688108 | -3.004136 |
| 1 | 0.671872 | 2.848496 | -2.123289 |
| 1 | 0.502068 | -0.449149 | 0.284813 |

Cartesian coordinates of : PACN10_46

Atomic number (AN) and Cartesian coordinates

| AN | X | Y | Z |
|----|-----------|-----------|-----------|
| 6 | -7.296240 | 0.238359 | -0.480220 |
| 1 | -7.845825 | -0.593424 | -0.032622 |
| 1 | -7.539206 | 0.291583 | -1.544328 |
| 1 | -7.607924 | 1.167898 | 0.002493 |
| 6 | -5.858933 | 0.039931 | -0.303194 |
| 7 | -4.716454 | -0.118409 | -0.161129 |
| 6 | 1.003863 | 1.421217 | 4.085520 |
| 1 | 0.086863 | 2.016396 | 4.113071 |
| 1 | 1.641073 | 1.693453 | 4.930528 |

| | | | |
|---|-----------|-----------|-----------|
| 1 | 0.744552 | 0.360771 | 4.146449 |
| 6 | 1.703819 | 1.661560 | 2.827786 |
| 7 | 2.252437 | 1.858354 | 1.822390 |
| 6 | -3.169334 | -2.692223 | -1.834922 |
| 1 | -3.255389 | -1.744160 | -2.371596 |
| 1 | -4.105703 | -2.892770 | -1.308329 |
| 1 | -2.971833 | -3.500851 | -2.543309 |
| 6 | -2.074109 | -2.593506 | -0.874908 |
| 7 | -1.200392 | -2.533054 | -0.110950 |
| 6 | -2.552218 | -0.977947 | 2.427956 |
| 1 | -1.870575 | -1.829791 | 2.492559 |
| 1 | -3.370831 | -1.222501 | 1.746087 |
| 1 | -2.953257 | -0.744971 | 3.417874 |
| 6 | -1.825894 | 0.173534 | 1.904304 |
| 7 | -1.243394 | 1.100674 | 1.512648 |
| 6 | 0.243790 | 4.131461 | 0.585335 |
| 1 | -0.319036 | 3.505227 | 1.283787 |
| 1 | -0.357179 | 4.995753 | 0.289497 |
| 1 | 1.157226 | 4.476782 | 1.077454 |
| 6 | 0.588735 | 3.335077 | -0.588872 |
| 7 | 0.854023 | 2.715326 | -1.535460 |
| 6 | -2.699480 | 2.460872 | -1.290927 |
| 1 | -2.472691 | 2.508718 | -0.221769 |
| 1 | -3.783877 | 2.467675 | -1.425750 |
| 1 | -2.261266 | 3.322291 | -1.802593 |
| 6 | -2.142698 | 1.229583 | -1.840574 |
| 7 | -1.702956 | 0.254929 | -2.294001 |
| 6 | 1.156802 | -4.077296 | 1.821016 |
| 1 | 0.699234 | -4.227926 | 0.839636 |
| 1 | 0.634164 | -4.672204 | 2.574271 |
| 1 | 2.205930 | -4.377812 | 1.773423 |
| 6 | 1.062912 | -2.661284 | 2.148572 |
| 7 | 0.972533 | -1.529520 | 2.398147 |
| 6 | 5.321389 | -2.548030 | -1.263997 |
| 1 | 5.618289 | -3.198189 | -2.090746 |
| 1 | 5.914014 | -2.801974 | -0.381553 |
| 1 | 5.502688 | -1.504091 | -1.532804 |
| 6 | 3.900149 | -2.720713 | -0.977322 |
| 7 | 2.767835 | -2.858797 | -0.753963 |
| 6 | 4.163364 | 3.109791 | -0.758942 |
| 1 | 3.681023 | 3.236485 | 0.214335 |
| 1 | 3.653370 | 3.727254 | -1.502826 |
| 1 | 5.211875 | 3.410942 | -0.692684 |
| 6 | 4.071817 | 1.705985 | -1.146112 |
| 7 | 4.013765 | 0.588802 | -1.459842 |
| 6 | 1.290040 | -0.409730 | -2.746263 |
| 6 | 1.125561 | -0.315111 | -1.315729 |
| 7 | 1.001369 | -0.243798 | -0.177994 |
| 1 | 0.509598 | -1.066037 | -3.139070 |
| 1 | 2.291392 | -0.800463 | -2.944110 |
| 1 | 1.177806 | 0.597550 | -3.159654 |
| 1 | 0.914109 | -0.312335 | 0.842310 |
