

**SUPPORTING INFORMATION**

**Theoretical Study of 9- $\beta$ -D-Erythrofuranosyladenine and Corresponding Carbocyclic Analogues. Evidence for a Base-Activated Conformational Lock**

Akin Akdag, Cynthia M. Carver, Michael L. McKee,\* and Stewart W. Schneller\*

Department of Chemistry, Auburn University, Auburn, Alabama 36849, USA

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Table S1. MMFF94 Relative Energies (kcal/mol) and DFT Total Energies (hartrees)

| Conformer | MMFF94 | B3LYP/6-31G(d,p)<br>//MMFF94 | B3LYP/3-21G<br>//B3LYP/3-21G | B3LYP/6-31G(d,p)<br>//B3LYP/3-21G | B3LYP/6-31+G(d,p)<br>//B3LYP/6-31+G(d,p) |
|-----------|--------|------------------------------|------------------------------|-----------------------------------|------------------------------------------|
| A1        | 0.00   | -849.025622                  | -844.320614                  | -849.023492                       | -849.070692                              |
| A2        | 3.68   | -849.015657                  | -844.304574                  | -849.013348                       | →A1                                      |
| A3        | 4.22   | -849.014809                  | -844.302075                  | -849.013592                       |                                          |
| A4        | 4.43   | -849.013025                  | -844.302744                  | -849.012481                       | -849.063101                              |
| A5        | 4.55   | -849.010556                  | -844.301339                  | -849.009448                       |                                          |
| A6        | 5.19   | -849.014679                  | -844.300057                  | -849.012670                       |                                          |
| A7        | 5.21   | -849.010541                  | -844.296387                  | -849.010627                       |                                          |
| A8        | 5.33   | -849.015975                  | -844.307794                  | -849.014509                       | -849.063228                              |
| A9        | 5.97   | -849.014353                  | -844.300838                  | -849.013494                       |                                          |
| A10       | 6.29   | -849.012107                  | -844.305871                  | -849.011731                       |                                          |
| A11       | 6.32   | -849.013474                  | -844.303233                  | -849.013565                       |                                          |
| A12       | 6.35   | -849.013019                  | -844.300252                  | -849.012281                       |                                          |
| A13       | 6.55   | -849.010584                  | -844.299760                  | -849.009539                       |                                          |
| A14       | 6.71   | -849.011086                  | →A12                         | →A12                              |                                          |
| B1        | 0.00   | -813.123353                  | -808.616237                  | -813.123916                       | -813.168315                              |
| B2        | 0.08   | -813.123818                  | -808.615504                  | -813.123226                       | -813.168951                              |
| B3        | 0.49   | -813.131306                  | -808.631266                  | -813.132520                       | -813.175510                              |
| B4        | 0.66   | -813.124931                  | -808.613246                  | -813.122899                       |                                          |
| B5        | 0.88   | -813.130250                  | →B3                          | →B3                               |                                          |
| B6        | 1.19   | -813.125419                  | -808.614386                  | -813.122987                       |                                          |
| B7        | 1.22   | -813.125619                  | -808.617444                  | -813.125139                       |                                          |
| B8        | 2.03   | -813.123141                  | →B1                          | →B1                               |                                          |
| B9        | 2.38   | -813.119189                  | -808.616877                  | -813.121024                       |                                          |
| B10       | 2.97   | -813.121140                  | -808.612625                  | -813.122391                       |                                          |
| B11       | 3.41   | -813.119955                  | -808.616551                  | -813.122525                       |                                          |
| B12       | 4.07   | -813.120047                  | -808.609077                  | -813.119204                       |                                          |
| B13       | 4.46   | -813.118182                  | -808.611017                  | -813.115966                       |                                          |
| B14       | 4.60   | -813.120050                  | -808.609775                  | -813.120551                       |                                          |
| B15       | 4.67   | -813.120545                  | -808.610671                  | -813.122330                       |                                          |
| B16       | 4.84   | -813.119132                  | -808.611741                  | -813.118731                       |                                          |
| B17       | 5.33   | -813.121765                  | -808.609411                  | -813.118954                       |                                          |
| B18       | 5.77   | -813.117045                  | →B16                         | →B16                              |                                          |
| B19       | 5.80   | -813.120285                  | -808.613450                  | -813.120133                       |                                          |
| B20       | 5.87   | -813.119728                  | →B15                         | →B15                              |                                          |
| B21       | 6.12   | -813.121333                  | -808.609949                  | -813.120680                       |                                          |
| B22       | 6.18   | -813.116483                  | -808.602774                  | -813.117831                       |                                          |
| C1        | 0.00   | -811.885175                  | -807.378747                  | -811.887138                       |                                          |
| C2        | 0.64   | -811.888019                  | -807.380674                  | -811.888597                       | -811.933502                              |
| C3        | 0.80   | -811.895402                  | -807.390510                  | -811.894703                       |                                          |
| C4        | 0.88   | -811.887587                  | →C1                          | →C1                               |                                          |
| C5        | 1.67   | -811.887328                  | →C3                          | →C3                               | -811.939920                              |
| C6        | 2.63   | -811.883119                  | -807.377472                  | -811.888408                       | -811.933379                              |
| C7        | 2.70   | -811.885126                  | -807.376640                  | -811.886692                       |                                          |
| C8        | 2.80   | -811.883280                  | →C1                          | →C1                               |                                          |
| C9        | 2.81   | -811.885514                  | -807.377645                  | -811.888580                       |                                          |
| C10       | 3.79   | -811.884204                  | -807.373229                  | -811.884990                       |                                          |

Table S2. Total energies (hartrees) for **B** with fixed values of the Pseudorotation Angle (P) with the base in the Syn and Anti orientation

| P(deg)           | Base=Syn    |                          |          | Base=Anti   |                          |          |
|------------------|-------------|--------------------------|----------|-------------|--------------------------|----------|
|                  | Energy      | Rel. Energy <sup>b</sup> | $\chi^c$ | Energy      | Rel. Energy <sup>b</sup> | $\chi^c$ |
| 0                | -808.613304 | 11.27                    | 49.7     | -808.609299 | 13.79                    | 215.6    |
| 30               | -808.616237 | 9.43                     | 58.6     | -808.609807 | 13.47                    | 185.6    |
| 60               | -808.611862 | 12.18                    | 60.7     | -808.619330 | 7.49                     | 180.3    |
| 90               | -808.612785 | 11.60                    | 57.2     | -808.625578 | 3.57                     | 172.8    |
| 120              | -808.612399 | 11.84                    | 54.8     | -808.628136 | 1.97                     | 167.8    |
| 146 <sup>a</sup> | -           | -                        | -        | -808.631270 | 0                        | 162.4    |
| 150              | -808.612813 | 11.58                    | 56.8     | -808.629361 | 1.20                     | 167.2    |
| 180              | -808.612115 | 12.02                    | 57.4     | -808.627752 | 2.21                     | 171.7    |
| 210              | -808.613719 | 11.01                    | 56.4     | -808.624463 | 4.27                     | 178.2    |
| 240              | -808.614306 | 10.64                    | 66.0     | -808.616682 | 9.15                     | 181.0    |
| 270              | -808.616877 | 9.03                     | 83.4     | -808.609338 | 13.76                    | 179.1    |
| 300              | -808.614494 | 10.53                    | 67.5     | -808.610764 | 12.87                    | 172.9    |
| 330              | -808.613325 | 11.26                    | 46.0     | -808.609830 | 13.45                    | 187.1    |

- a) Lowest energy conformer of **B** at the B3LYP/3-21G level of theory.  
 b) Energies relative to P=146° in kcal/mol.  
 c)  $\chi$  is the dihedral angle (C5'-C1'-N9-C4)

Table S3. Cartesian Coordinates (Å) for A, B, and C Optimized at the B3LYP/3-21G Level

A1

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 3.540289                | -1.172607 | 0.378214  |
| 2                | 6                | 0              | 3.453933                | 0.356499  | 0.506346  |
| 3                | 1                | 0              | 4.015285                | 0.738326  | 1.367990  |
| 4                | 6                | 0              | 1.937307                | 0.619667  | 0.611826  |
| 5                | 8                | 0              | 3.869906                | 0.946727  | -0.753676 |
| 6                | 6                | 0              | 1.431247                | -0.447591 | -0.388157 |
| 7                | 8                | 0              | 1.690383                | 1.962546  | 0.165482  |
| 8                | 1                | 0              | 1.553564                | 0.387292  | 1.612936  |
| 9                | 7                | 0              | 0.022037                | -0.789652 | -0.199972 |
| 10               | 1                | 0              | 4.314509                | -1.435058 | -0.344060 |
| 11               | 1                | 0              | 1.599826                | -0.063716 | -1.399342 |
| 12               | 8                | 0              | 2.209571                | -1.636575 | -0.125693 |
| 13               | 1                | 0              | 3.716252                | -1.659329 | 1.340211  |
| 14               | 6                | 0              | -0.549641               | -2.064665 | -0.136272 |
| 15               | 6                | 0              | -1.015567               | 0.113919  | -0.129448 |
| 16               | 1                | 0              | 0.676265                | 2.033867  | 0.000311  |
| 17               | 1                | 0              | 3.271820                | 1.756949  | -0.813496 |
| 18               | 7                | 0              | -1.872785               | -2.019967 | -0.031579 |
| 19               | 1                | 0              | 0.069867                | -2.941422 | -0.167328 |
| 20               | 6                | 0              | -2.182264               | -0.655556 | -0.028880 |
| 21               | 1                | 0              | -4.631414               | -1.584163 | 0.171005  |
| 22               | 6                | 0              | -3.397092               | 0.048793  | 0.058445  |
| 23               | 7                | 0              | -3.365727               | 1.408721  | 0.042620  |
| 24               | 7                | 0              | -4.585634               | -0.572213 | 0.157419  |
| 25               | 6                | 0              | -2.182606               | 2.039863  | -0.048240 |
| 26               | 7                | 0              | -0.958536               | 1.465598  | -0.135479 |
| 27               | 1                | 0              | -5.428139               | -0.012896 | 0.216891  |
| 28               | 1                | 0              | -2.205827               | 3.121225  | -0.048093 |

A2

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 3.086573                | -1.207060 | 0.413439  |
| 2                | 6                | 0              | 2.559336                | 0.106086  | 1.047813  |
| 3                | 1                | 0              | 1.790291                | -0.091845 | 1.795372  |
| 4                | 6                | 0              | 1.946516                | 0.813549  | -0.185242 |
| 5                | 8                | 0              | 3.600398                | 0.900296  | 1.643350  |
| 6                | 6                | 0              | 1.363852                | -0.349964 | -0.993144 |
| 7                | 8                | 0              | 3.132021                | 1.347142  | -0.866755 |
| 8                | 1                | 0              | 1.200075                | 1.578435  | 0.033982  |
| 9                | 7                | 0              | 0.001461                | -0.657866 | -0.510728 |
| 10               | 1                | 0              | 4.097962                | -1.028545 | 0.041889  |
| 11               | 1                | 0              | 1.345512                | -0.152321 | -2.067245 |
| 12               | 8                | 0              | 2.188913                | -1.513707 | -0.732796 |
| 13               | 1                | 0              | 3.070452                | -2.056879 | 1.096695  |
| 14               | 6                | 0              | -0.492434               | -1.942047 | -0.247919 |
| 15               | 6                | 0              | -1.060385               | 0.217096  | -0.335280 |
| 16               | 1                | 0              | 2.857395                | 2.097802  | -1.454733 |
| 17               | 1                | 0              | 3.994197                | 1.368824  | 0.846879  |
| 18               | 7                | 0              | -1.775806               | -1.936610 | 0.085635  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 19 | 1 | 0 | 0.152328  | -2.797153 | -0.323534 |
| 20 | 6 | 0 | -2.147644 | -0.588337 | 0.035214  |
| 21 | 1 | 0 | -4.459847 | -1.604264 | 0.749361  |
| 22 | 6 | 0 | -3.366244 | 0.069440  | 0.286078  |
| 23 | 7 | 0 | -3.417081 | 1.419408  | 0.158770  |
| 24 | 7 | 0 | -4.480604 | -0.596801 | 0.648885  |
| 25 | 6 | 0 | -2.296975 | 2.083744  | -0.197165 |
| 26 | 7 | 0 | -1.079347 | 1.559714  | -0.461731 |
| 27 | 1 | 0 | -5.330485 | -0.073421 | 0.819636  |
| 28 | 1 | 0 | -2.384471 | 3.159566  | -0.277260 |

A3

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.243380                | -1.211191 | -1.129357 |
| 2                | 6                | 0              | 2.950752                | -0.952438 | 0.197268  |
| 3                | 1                | 0              | 3.061870                | -1.854108 | 0.808374  |
| 4                | 6                | 0              | 2.046388                | 0.115016  | 0.875513  |
| 5                | 8                | 0              | 4.217129                | -0.233260 | 0.026235  |
| 6                | 6                | 0              | 1.411979                | 0.857135  | -0.355328 |
| 7                | 8                | 0              | 2.808822                | 0.995593  | 1.716585  |
| 8                | 1                | 0              | 1.264404                | -0.371652 | 1.456829  |
| 9                | 7                | 0              | -0.045637               | 0.987057  | -0.225384 |
| 10               | 1                | 0              | 2.903155                | -1.581962 | -1.915500 |
| 11               | 1                | 0              | 1.823276                | 1.866271  | -0.404683 |
| 12               | 8                | 0              | 1.764141                | 0.125639  | -1.555836 |
| 13               | 1                | 0              | 1.391490                | -1.874886 | -0.958264 |
| 14               | 6                | 0              | -0.805394               | 2.157617  | -0.357204 |
| 15               | 6                | 0              | -0.955534               | -0.043458 | -0.039785 |
| 16               | 1                | 0              | 3.727749                | 0.945080  | 1.309952  |
| 17               | 1                | 0              | 4.927647                | -0.862008 | -0.260017 |
| 18               | 7                | 0              | -2.107868               | 1.944599  | -0.248139 |
| 19               | 1                | 0              | -0.332882               | 3.110899  | -0.522615 |
| 20               | 6                | 0              | -2.219098               | 0.563436  | -0.048189 |
| 21               | 1                | 0              | -4.768324               | 1.182735  | 0.010372  |
| 22               | 6                | 0              | -3.332035               | -0.277562 | 0.134076  |
| 23               | 7                | 0              | -3.122594               | -1.606574 | 0.308958  |
| 24               | 7                | 0              | -4.595083               | 0.193607  | 0.140923  |
| 25               | 6                | 0              | -1.855643               | -2.071979 | 0.302550  |
| 26               | 7                | 0              | -0.718917               | -1.360038 | 0.134813  |
| 27               | 1                | 0              | -5.359736               | -0.456279 | 0.275861  |
| 28               | 1                | 0              | -1.737475               | -3.137889 | 0.448353  |

A4

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.711455                | 0.358812  | 1.386127  |
| 2                | 6                | 0              | 2.476858                | 0.982310  | -0.004006 |
| 3                | 1                | 0              | 1.637659                | 1.678986  | -0.001541 |
| 4                | 6                | 0              | 2.116369                | -0.268482 | -0.831639 |
| 5                | 8                | 0              | 3.702580                | 1.498745  | -0.608499 |
| 6                | 6                | 0              | 1.342515                | -1.154168 | 0.165654  |
| 7                | 8                | 0              | 3.351349                | -0.977593 | -1.118331 |
| 8                | 1                | 0              | 1.530712                | -0.040030 | -1.727420 |
| 9                | 7                | 0              | -0.107896               | -1.109656 | 0.005773  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 10 | 1 | 0 | 3.718169  | -0.071517 | 1.395942  |
| 11 | 1 | 0 | 1.657959  | -2.189268 | 0.015373  |
| 12 | 8 | 0 | 1.687052  | -0.692359 | 1.510106  |
| 13 | 1 | 0 | 2.568690  | 1.050667  | 2.217873  |
| 14 | 6 | 0 | -0.956549 | -2.226868 | -0.037417 |
| 15 | 6 | 0 | -0.939558 | 0.004810  | 0.004817  |
| 16 | 1 | 0 | 4.024744  | -0.239604 | -1.211683 |
| 17 | 1 | 0 | 3.996072  | 2.310233  | -0.121009 |
| 18 | 7 | 0 | -2.237421 | -1.904135 | -0.087081 |
| 19 | 1 | 0 | -0.555467 | -3.226315 | -0.030943 |
| 20 | 6 | 0 | -2.244917 | -0.504540 | -0.060906 |
| 21 | 1 | 0 | -4.829556 | -0.937014 | -0.172126 |
| 22 | 6 | 0 | -3.298696 | 0.426700  | -0.087895 |
| 23 | 7 | 0 | -2.999680 | 1.749174  | -0.052418 |
| 24 | 7 | 0 | -4.590559 | 0.046771  | -0.148366 |
| 25 | 6 | 0 | -1.703296 | 2.118627  | 0.004423  |
| 26 | 7 | 0 | -0.618866 | 1.313324  | 0.035112  |
| 27 | 1 | 0 | -5.310482 | 0.758644  | -0.163801 |
| 28 | 1 | 0 | -1.510471 | 3.183316  | 0.027042  |

A5

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.073278               | 1.156886  | 0.482521  |
| 2                | 6                | 0              | -2.515685               | -0.181656 | 1.018798  |
| 3                | 1                | 0              | -1.720381               | -0.032439 | 1.754886  |
| 4                | 6                | 0              | -1.968033               | -0.815240 | -0.276432 |
| 5                | 8                | 0              | -3.558739               | -1.090355 | 1.478146  |
| 6                | 6                | 0              | -1.368250               | 0.393711  | -0.992064 |
| 7                | 8                | 0              | -3.115426               | -1.218383 | -1.071372 |
| 8                | 1                | 0              | -1.234996               | -1.610983 | -0.124512 |
| 9                | 7                | 0              | 0.000246                | 0.668147  | -0.505038 |
| 10               | 1                | 0              | -4.074774               | 0.966045  | 0.091157  |
| 11               | 1                | 0              | -1.379548               | 0.267365  | -2.074699 |
| 12               | 8                | 0              | -2.177190               | 1.552170  | -0.628162 |
| 13               | 1                | 0              | -3.081440               | 1.964402  | 1.216947  |
| 14               | 6                | 0              | 0.502501                | 1.945204  | -0.221924 |
| 15               | 6                | 0              | 1.059415                | -0.215374 | -0.341399 |
| 16               | 1                | 0              | -3.754926               | -1.582934 | -0.392882 |
| 17               | 1                | 0              | -4.006415               | -0.706798 | 2.276268  |
| 18               | 7                | 0              | 1.785134                | 1.929679  | 0.113107  |
| 19               | 1                | 0              | -0.137261               | 2.805135  | -0.282696 |
| 20               | 6                | 0              | 2.150009                | 0.580819  | 0.042340  |
| 21               | 1                | 0              | 4.463063                | 1.584957  | 0.765005  |
| 22               | 6                | 0              | 3.366917                | -0.083017 | 0.284863  |
| 23               | 7                | 0              | 3.416534                | -1.430134 | 0.139397  |
| 24               | 7                | 0              | 4.482152                | 0.578286  | 0.658016  |
| 25               | 6                | 0              | 2.293789                | -2.086230 | -0.228192 |
| 26               | 7                | 0              | 1.079081                | -1.555232 | -0.485443 |
| 27               | 1                | 0              | 5.333077                | 0.052753  | 0.815697  |
| 28               | 1                | 0              | 2.378106                | -3.160792 | -0.325396 |

A6

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 1  | 6 | 0 | 2.926285  | -0.504141 | -1.564089 |
| 2  | 6 | 0 | 3.326979  | -0.739543 | -0.103682 |
| 3  | 1 | 0 | 3.764700  | -1.730622 | 0.065690  |
| 4  | 6 | 0 | 2.006394  | -0.529672 | 0.647145  |
| 5  | 8 | 0 | 4.213601  | 0.348222  | 0.288466  |
| 6  | 6 | 0 | 1.430902  | 0.669241  | -0.142876 |
| 7  | 8 | 0 | 2.360412  | -0.180431 | 2.013339  |
| 8  | 1 | 0 | 1.329657  | -1.383162 | 0.562707  |
| 9  | 7 | 0 | 0.001377  | 0.858447  | 0.022120  |
| 10 | 1 | 0 | 3.741525  | -0.004476 | -2.090104 |
| 11 | 1 | 0 | 1.942526  | 1.574008  | 0.199451  |
| 12 | 8 | 0 | 1.729702  | 0.382225  | -1.537930 |
| 13 | 1 | 0 | 2.649740  | -1.435861 | -2.063884 |
| 14 | 6 | 0 | -0.665685 | 2.095987  | 0.020825  |
| 15 | 6 | 0 | -0.996327 | -0.114312 | -0.005231 |
| 16 | 1 | 0 | 1.529046  | -0.033601 | 2.534745  |
| 17 | 1 | 0 | 4.042608  | 0.450366  | 1.270433  |
| 18 | 7 | 0 | -1.981079 | 1.974700  | 0.026710  |
| 19 | 1 | 0 | -0.113502 | 3.020674  | 0.016295  |
| 20 | 6 | 0 | -2.206641 | 0.591461  | 0.009852  |
| 21 | 1 | 0 | -4.701669 | 1.410994  | 0.013407  |
| 22 | 6 | 0 | -3.390813 | -0.168583 | 0.003997  |
| 23 | 7 | 0 | -3.294767 | -1.521602 | -0.010773 |
| 24 | 7 | 0 | -4.611733 | 0.402313  | 0.013225  |
| 25 | 6 | 0 | -2.068821 | -2.086345 | -0.014438 |
| 26 | 7 | 0 | -0.873414 | -1.455497 | -0.009654 |
| 27 | 1 | 0 | -5.430540 | -0.193418 | 0.000355  |
| 28 | 1 | 0 | -2.040145 | -3.168119 | -0.020507 |

A7

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 3.479371                | -1.176027 | -0.612325 |
| 2                | 6                | 0              | 3.614743                | -0.009806 | 0.375699  |
| 3                | 1                | 0              | 4.362433                | -0.181223 | 1.156698  |
| 4                | 6                | 0              | 2.180285                | 0.160695  | 0.918565  |
| 5                | 8                | 0              | 3.807316                | 1.272189  | -0.313881 |
| 6                | 6                | 0              | 1.361962                | -0.109284 | -0.375282 |
| 7                | 8                | 0              | 1.957394                | 1.448517  | 1.495928  |
| 8                | 1                | 0              | 1.944748                | -0.606736 | 1.659480  |
| 9                | 7                | 0              | 0.003162                | -0.539383 | -0.135427 |
| 10               | 1                | 0              | 4.115010                | -1.027457 | -1.490379 |
| 11               | 1                | 0              | 1.329851                | 0.798987  | -0.982525 |
| 12               | 8                | 0              | 2.058341                | -1.217463 | -1.031414 |
| 13               | 1                | 0              | 3.728493                | -2.127386 | -0.132360 |
| 14               | 6                | 0              | -0.424559               | -1.819306 | 0.237397  |
| 15               | 6                | 0              | -1.133901               | 0.246776  | -0.236158 |
| 16               | 1                | 0              | 2.485728                | 2.064660  | 0.909070  |
| 17               | 1                | 0              | 4.742589                | 1.346395  | -0.636273 |
| 18               | 7                | 0              | -1.738756               | -1.890845 | 0.392204  |
| 19               | 1                | 0              | 0.273999                | -2.630340 | 0.332602  |
| 20               | 6                | 0              | -2.199761               | -0.599519 | 0.101454  |
| 21               | 1                | 0              | -4.515750               | -1.715873 | 0.645218  |
| 22               | 6                | 0              | -3.486579               | -0.031268 | 0.076996  |
| 23               | 7                | 0              | -3.616301               | 1.272414  | -0.272102 |
| 24               | 7                | 0              | -4.593235               | -0.740393 | 0.386101  |
| 25               | 6                | 0              | -2.505371               | 1.977359  | -0.586605 |
| 26               | 7                | 0              | -1.228265               | 1.538816  | -0.591861 |
| 27               | 1                | 0              | -5.494215               | -0.280278 | 0.348776  |

28                      1                      0                      -2.660665                      3.011313                      -0.866220

A8

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.155234                | -1.110939 | -1.203323 |
| 2                | 6                | 0              | 2.904371                | -1.012530 | 0.114967  |
| 3                | 1                | 0              | 3.076148                | -1.955065 | 0.629858  |
| 4                | 6                | 0              | 2.052804                | 0.008888  | 0.932280  |
| 5                | 8                | 0              | 4.216737                | -0.372446 | -0.100162 |
| 6                | 6                | 0              | 1.426248                | 0.894651  | -0.208479 |
| 7                | 8                | 0              | 2.903660                | 0.784789  | 1.794731  |
| 8                | 1                | 0              | 1.273253                | -0.492012 | 1.504289  |
| 9                | 7                | 0              | -0.032601               | 0.983209  | -0.155592 |
| 10               | 1                | 0              | 2.757290                | -1.492961 | -2.027189 |
| 11               | 1                | 0              | 1.815612                | 1.907386  | -0.108488 |
| 12               | 8                | 0              | 1.904909                | 0.342273  | -1.482031 |
| 13               | 1                | 0              | 1.212424                | -1.647493 | -1.075298 |
| 14               | 6                | 0              | -0.787183               | 2.162933  | -0.273178 |
| 15               | 6                | 0              | -0.955327               | -0.046783 | -0.012908 |
| 16               | 1                | 0              | 3.810987                | 0.649859  | 1.370049  |
| 17               | 1                | 0              | 4.043849                | 0.271997  | -0.847273 |
| 18               | 7                | 0              | -2.090345               | 1.954019  | -0.199316 |
| 19               | 1                | 0              | -0.305517               | 3.117528  | -0.400991 |
| 20               | 6                | 0              | -2.213902               | 0.569044  | -0.035975 |
| 21               | 1                | 0              | -4.760107               | 1.207323  | -0.016618 |
| 22               | 6                | 0              | -3.337680               | -0.266892 | 0.099886  |
| 23               | 7                | 0              | -3.142194               | -1.602077 | 0.243801  |
| 24               | 7                | 0              | -4.596032               | 0.213720  | 0.090800  |
| 25               | 6                | 0              | -1.880355               | -2.077881 | 0.249799  |
| 26               | 7                | 0              | -0.734726               | -1.369511 | 0.125511  |
| 27               | 1                | 0              | -5.368382               | -0.433633 | 0.191079  |
| 28               | 1                | 0              | -1.771979               | -3.148315 | 0.365433  |

A9

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.286953                | -1.057906 | -1.309443 |
| 2                | 6                | 0              | 2.967413                | -0.986387 | 0.057564  |
| 3                | 1                | 0              | 3.018434                | -1.976043 | 0.531007  |
| 4                | 6                | 0              | 2.026531                | -0.022290 | 0.839018  |
| 5                | 8                | 0              | 4.267478                | -0.367496 | -0.059813 |
| 6                | 6                | 0              | 1.418109                | 0.881495  | -0.271324 |
| 7                | 8                | 0              | 2.816944                | 0.858924  | 1.708914  |
| 8                | 1                | 0              | 1.250544                | -0.571572 | 1.370507  |
| 9                | 7                | 0              | -0.040442               | 1.002367  | -0.132354 |
| 10               | 1                | 0              | 2.996193                | -1.284961 | -2.103559 |
| 11               | 1                | 0              | 1.833881                | 1.886142  | -0.174579 |
| 12               | 8                | 0              | 1.787548                | 0.322666  | -1.548379 |
| 13               | 1                | 0              | 1.448055                | -1.758138 | -1.281041 |
| 14               | 6                | 0              | -0.804783               | 2.170140  | -0.273097 |
| 15               | 6                | 0              | -0.949708               | -0.037305 | 0.004187  |
| 16               | 1                | 0              | 2.934865                | 0.406480  | 2.586790  |
| 17               | 1                | 0              | 4.237322                | 0.368194  | 0.625716  |
| 18               | 7                | 0              | -2.107822               | 1.946072  | -0.208583 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 19 | 1 | 0 | -0.334731 | 3.128758  | -0.413319 |
| 20 | 6 | 0 | -2.216163 | 0.560461  | -0.034174 |
| 21 | 1 | 0 | -4.775004 | 1.152680  | -0.053728 |
| 22 | 6 | 0 | -3.326720 | -0.293320 | 0.099189  |
| 23 | 7 | 0 | -3.109362 | -1.623451 | 0.259564  |
| 24 | 7 | 0 | -4.593901 | 0.164475  | 0.073565  |
| 25 | 6 | 0 | -1.839260 | -2.078194 | 0.287670  |
| 26 | 7 | 0 | -0.703997 | -1.352746 | 0.167765  |
| 27 | 1 | 0 | -5.355315 | -0.496489 | 0.167937  |
| 28 | 1 | 0 | -1.715572 | -3.144998 | 0.421261  |

A10

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.481728               | 1.090547  | 1.038436  |
| 2                | 6                | 0              | -2.302969               | -0.461689 | 1.038256  |
| 3                | 1                | 0              | -1.462614               | -0.759488 | 1.666979  |
| 4                | 6                | 0              | -2.009519               | -0.769528 | -0.465842 |
| 5                | 8                | 0              | -3.490298               | -1.163591 | 1.461829  |
| 6                | 6                | 0              | -1.414220               | 0.536159  | -0.983125 |
| 7                | 8                | 0              | -3.311829               | -0.952292 | -1.124154 |
| 8                | 1                | 0              | -1.392518               | -1.645836 | -0.639265 |
| 9                | 7                | 0              | -0.035991               | 0.747096  | -0.529744 |
| 10               | 1                | 0              | -3.501187               | 1.344932  | 1.324288  |
| 11               | 1                | 0              | -1.495958               | 0.641086  | -2.065853 |
| 12               | 8                | 0              | -2.284614               | 1.545158  | -0.382645 |
| 13               | 1                | 0              | -1.753579               | 1.593079  | 1.678222  |
| 14               | 6                | 0              | 0.532573                | 2.005395  | -0.273411 |
| 15               | 6                | 0              | 0.980553                | -0.186032 | -0.357496 |
| 16               | 1                | 0              | -3.698466               | -0.029622 | -1.178551 |
| 17               | 1                | 0              | -3.943511               | -1.379069 | 0.588322  |
| 18               | 7                | 0              | 1.812926                | 1.929835  | 0.051893  |
| 19               | 1                | 0              | -0.067081               | 2.895848  | -0.333991 |
| 20               | 6                | 0              | 2.111271                | 0.562360  | 0.001480  |
| 21               | 1                | 0              | 4.481066                | 1.460006  | 0.693992  |
| 22               | 6                | 0              | 3.298058                | -0.155487 | 0.241711  |
| 23               | 7                | 0              | 3.279146                | -1.505998 | 0.113323  |
| 24               | 7                | 0              | 4.447742                | 0.452864  | 0.593601  |
| 25               | 6                | 0              | 2.125147                | -2.112019 | -0.236662 |
| 26               | 7                | 0              | 0.933959                | -1.525154 | -0.489754 |
| 27               | 1                | 0              | 5.271683                | -0.113803 | 0.753942  |
| 28               | 1                | 0              | 2.156623                | -3.190070 | -0.323638 |

A11

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 3.391032                | -1.137119 | 0.677297  |
| 2                | 6                | 0              | 3.435101                | 0.393354  | 0.526008  |
| 3                | 1                | 0              | 3.968281                | 0.891794  | 1.343917  |
| 4                | 6                | 0              | 1.933982                | 0.726585  | 0.504767  |
| 5                | 8                | 0              | 3.916449                | 0.763252  | -0.796694 |
| 6                | 6                | 0              | 1.445924                | -0.390010 | -0.458325 |
| 7                | 8                | 0              | 1.672299                | 2.050225  | 0.073225  |
| 8                | 1                | 0              | 1.527436                | 0.478392  | 1.501410  |
| 9                | 7                | 0              | 0.032795                | -0.735607 | -0.254572 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 10 | 1 | 0 | 4.284625  | -1.622801 | 0.277933  |
| 11 | 1 | 0 | 1.623102  | -0.065826 | -1.485602 |
| 12 | 8 | 0 | 2.223971  | -1.577192 | -0.135902 |
| 13 | 1 | 0 | 3.243927  | -1.428387 | 1.722510  |
| 14 | 6 | 0 | -0.509554 | -2.023836 | -0.198063 |
| 15 | 6 | 0 | -1.026929 | 0.142593  | -0.152117 |
| 16 | 1 | 0 | 0.658440  | 2.113040  | -0.032016 |
| 17 | 1 | 0 | 4.875598  | 0.505369  | -0.859095 |
| 18 | 7 | 0 | -1.831076 | -2.014849 | -0.070483 |
| 19 | 1 | 0 | 0.129977  | -2.884897 | -0.248073 |
| 20 | 6 | 0 | -2.172516 | -0.658958 | -0.042627 |
| 21 | 1 | 0 | -4.585705 | -1.663425 | 0.185689  |
| 22 | 6 | 0 | -3.404554 | 0.009102  | 0.078046  |
| 23 | 7 | 0 | -3.413487 | 1.368038  | 0.084697  |
| 24 | 7 | 0 | -4.572591 | -0.650632 | 0.188592  |
| 25 | 6 | 0 | -2.247349 | 2.031986  | -0.017018 |
| 26 | 7 | 0 | -1.011003 | 1.494598  | -0.135828 |
| 27 | 1 | 0 | -5.430380 | -0.118769 | 0.272561  |
| 28 | 1 | 0 | -2.300347 | 3.112213  | 0.001077  |

A12

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.786155                | 0.106649  | 1.454120  |
| 2                | 6                | 0              | 2.533337                | 0.981813  | 0.207318  |
| 3                | 1                | 0              | 1.714186                | 1.678979  | 0.372567  |
| 4                | 6                | 0              | 2.066951                | -0.083246 | -0.816916 |
| 5                | 8                | 0              | 3.706524                | 1.678521  | -0.248749 |
| 6                | 6                | 0              | 1.341792                | -1.149325 | 0.039798  |
| 7                | 8                | 0              | 3.329271                | -0.645767 | -1.322328 |
| 8                | 1                | 0              | 1.439990                | 0.331476  | -1.607285 |
| 9                | 7                | 0              | -0.113251               | -1.105526 | -0.075357 |
| 10               | 1                | 0              | 3.779878                | -0.346928 | 1.370471  |
| 11               | 1                | 0              | 1.657541                | -2.143881 | -0.291705 |
| 12               | 8                | 0              | 1.729678                | -0.926388 | 1.426459  |
| 13               | 1                | 0              | 2.688089                | 0.648899  | 2.394529  |
| 14               | 6                | 0              | -0.964123               | -2.223314 | -0.072060 |
| 15               | 6                | 0              | -0.945377               | 0.008716  | -0.043809 |
| 16               | 1                | 0              | 3.190784                | -0.987123 | -2.243532 |
| 17               | 1                | 0              | 4.184364                | 0.975976  | -0.783314 |
| 18               | 7                | 0              | -2.245362               | -1.899653 | -0.067592 |
| 19               | 1                | 0              | -0.564411               | -3.223481 | -0.071769 |
| 20               | 6                | 0              | -2.252048               | -0.498977 | -0.049990 |
| 21               | 1                | 0              | -4.845803               | -0.915771 | -0.042693 |
| 22               | 6                | 0              | -3.302174               | 0.437545  | -0.040630 |
| 23               | 7                | 0              | -2.995127               | 1.758851  | -0.029438 |
| 24               | 7                | 0              | -4.597755               | 0.065992  | -0.043376 |
| 25               | 6                | 0              | -1.696304               | 2.124814  | -0.029572 |
| 26               | 7                | 0              | -0.615360               | 1.313329  | -0.038148 |
| 27               | 1                | 0              | -5.312203               | 0.783573  | -0.029849 |
| 28               | 1                | 0              | -1.497471               | 3.188345  | -0.022656 |

A13

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 1  | 6 | 0 | 2.698411  | -0.944738 | -1.304603 |
| 2  | 6 | 0 | 3.489282  | -0.632866 | -0.040775 |
| 3  | 1 | 0 | 4.113678  | -1.434870 | 0.346440  |
| 4  | 6 | 0 | 2.392499  | -0.126497 | 0.957574  |
| 5  | 8 | 0 | 4.361822  | 0.524553  | -0.306421 |
| 6  | 6 | 0 | 1.285072  | 0.414539  | -0.015520 |
| 7  | 8 | 0 | 2.932269  | 0.908696  | 1.794453  |
| 8  | 1 | 0 | 1.999460  | -0.932373 | 1.580663  |
| 9  | 7 | 0 | 0.003293  | -0.260466 | 0.119937  |
| 10 | 1 | 0 | 3.311167  | -0.968678 | -2.205231 |
| 11 | 1 | 0 | 1.102417  | 1.474994  | 0.145418  |
| 12 | 8 | 0 | 1.834638  | 0.262260  | -1.383134 |
| 13 | 1 | 0 | 2.104969  | -1.861197 | -1.214990 |
| 14 | 6 | 0 | -0.305528 | -1.620392 | 0.312696  |
| 15 | 6 | 0 | -1.219593 | 0.390869  | -0.013682 |
| 16 | 1 | 0 | 3.748131  | 1.201479  | 1.275311  |
| 17 | 1 | 0 | 3.818845  | 1.086077  | -0.935470 |
| 18 | 7 | 0 | -1.607250 | -1.856571 | 0.314123  |
| 19 | 1 | 0 | 0.457443  | -2.365935 | 0.452205  |
| 20 | 6 | 0 | -2.197336 | -0.601780 | 0.111676  |
| 21 | 1 | 0 | -4.404715 | -2.027407 | 0.276793  |
| 22 | 6 | 0 | -3.538342 | -0.181751 | 0.022694  |
| 23 | 7 | 0 | -3.793165 | 1.135391  | -0.174411 |
| 24 | 7 | 0 | -4.573196 | -1.040428 | 0.127121  |
| 25 | 6 | 0 | -2.754519 | 1.995122  | -0.274245 |
| 26 | 7 | 0 | -1.437665 | 1.700867  | -0.204608 |
| 27 | 1 | 0 | -5.516326 | -0.678436 | 0.056936  |
| 28 | 1 | 0 | -3.008686 | 3.035685  | -0.427276 |

B1

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.966254               | -0.511919 | 1.258138  |
| 2                | 6                | 0              | -2.575544               | -0.964460 | -0.164397 |
| 3                | 1                | 0              | -1.771632               | -1.704404 | -0.142204 |
| 4                | 6                | 0              | -2.068162               | 0.350757  | -0.795594 |
| 5                | 8                | 0              | -3.716615               | -1.366017 | -0.994080 |
| 6                | 6                | 0              | -1.323318               | 1.085940  | 0.354031  |
| 7                | 8                | 0              | -3.244228               | 1.157001  | -1.094004 |
| 8                | 1                | 0              | -1.428407               | 0.191727  | -1.670364 |
| 9                | 7                | 0              | 0.138816                | 1.098634  | 0.181933  |
| 10               | 1                | 0              | -3.861628               | 0.108623  | 1.158175  |
| 11               | 1                | 0              | -1.663194               | 2.122371  | 0.325044  |
| 12               | 6                | 0              | -1.759776               | 0.363219  | 1.678544  |
| 13               | 1                | 0              | -3.149540               | -1.339749 | 1.948864  |
| 14               | 6                | 0              | 0.958997                | 2.222017  | 0.025069  |
| 15               | 6                | 0              | 0.979953                | -0.002064 | 0.119011  |
| 16               | 1                | 0              | -3.921236               | 0.463086  | -1.359199 |
| 17               | 1                | 0              | -4.230451               | -2.065848 | -0.514118 |
| 18               | 7                | 0              | 2.240136                | 1.914551  | -0.124478 |
| 19               | 1                | 0              | 0.545604                | 3.216351  | 0.031468  |
| 20               | 6                | 0              | 2.269837                | 0.517707  | -0.067670 |
| 21               | 1                | 0              | 5.322588                | -0.735694 | -0.413264 |
| 22               | 6                | 0              | 3.323409                | -0.410069 | -0.164406 |
| 23               | 7                | 0              | 3.038078                | -1.732535 | -0.070926 |
| 24               | 7                | 0              | 4.603182                | -0.026273 | -0.346978 |
| 25               | 6                | 0              | 1.753956                | -2.110124 | 0.110506  |
| 26               | 7                | 0              | 0.669019                | -1.312294 | 0.215620  |
| 27               | 1                | 0              | 4.832100                | 0.957242  | -0.422206 |

|    |   |   |           |           |          |
|----|---|---|-----------|-----------|----------|
| 28 | 1 | 0 | 1.575075  | -3.175365 | 0.178606 |
| 29 | 1 | 0 | -0.942976 | -0.282226 | 2.008121 |
| 30 | 1 | 0 | -2.002752 | 1.075416  | 2.470150 |

B2

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.284737                | 1.387755  | 0.954530  |
| 2                | 6                | 0              | 2.971223                | 0.931575  | -0.333104 |
| 3                | 1                | 0              | 3.149069                | 1.727475  | -1.063948 |
| 4                | 6                | 0              | 2.051460                | -0.189112 | -0.893000 |
| 5                | 8                | 0              | 4.215173                | 0.187653  | -0.037507 |
| 6                | 6                | 0              | 1.414611                | -0.838256 | 0.398978  |
| 7                | 8                | 0              | 2.806228                | -1.129660 | -1.682063 |
| 8                | 1                | 0              | 1.261914                | 0.249432  | -1.504104 |
| 9                | 7                | 0              | -0.055427               | -0.952090 | 0.302050  |
| 10               | 1                | 0              | 2.930366                | 1.998002  | 1.593710  |
| 11               | 1                | 0              | 1.795085                | -1.859060 | 0.459833  |
| 12               | 6                | 0              | 1.881195                | 0.038345  | 1.602863  |
| 13               | 1                | 0              | 1.377869                | 1.936459  | 0.682173  |
| 14               | 6                | 0              | -0.799103               | -2.133135 | 0.409800  |
| 15               | 6                | 0              | -0.977015               | 0.060308  | 0.076976  |
| 16               | 1                | 0              | 3.722790                | -1.062477 | -1.273707 |
| 17               | 1                | 0              | 4.939578                | 0.832695  | 0.167985  |
| 18               | 7                | 0              | -2.104562               | -1.943319 | 0.274785  |
| 19               | 1                | 0              | -0.314037               | -3.079060 | 0.581455  |
| 20               | 6                | 0              | -2.232516               | -0.568020 | 0.063896  |
| 21               | 1                | 0              | -5.383468               | 0.385026  | -0.346360 |
| 22               | 6                | 0              | -3.356009               | 0.250775  | -0.152644 |
| 23               | 7                | 0              | -3.168982               | 1.580776  | -0.337273 |
| 24               | 7                | 0              | -4.609345               | -0.246634 | -0.182578 |
| 25               | 6                | 0              | -1.909837               | 2.069244  | -0.307541 |
| 26               | 7                | 0              | -0.765403               | 1.381454  | -0.106991 |
| 27               | 1                | 0              | -4.763903               | -1.238679 | -0.051079 |
| 28               | 1                | 0              | -1.807985               | 3.135616  | -0.462245 |
| 29               | 1                | 0              | 1.103171                | 0.135487  | 2.361560  |
| 30               | 1                | 0              | 2.771907                | -0.423020 | 2.036821  |

B3

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.756079               | 1.055257  | 0.334266  |
| 2                | 6                | 0              | -3.498021               | -0.468464 | 0.397518  |
| 3                | 1                | 0              | -4.078717               | -0.974235 | 1.178834  |
| 4                | 6                | 0              | -1.972970               | -0.626282 | 0.616779  |
| 5                | 8                | 0              | -3.753615               | -1.020678 | -0.927775 |
| 6                | 6                | 0              | -1.446382               | 0.525144  | -0.287273 |
| 7                | 8                | 0              | -1.639236               | -1.948695 | 0.155058  |
| 8                | 1                | 0              | -1.689834               | -0.430784 | 1.660805  |
| 9                | 7                | 0              | -0.003358               | 0.819829  | -0.146463 |
| 10               | 1                | 0              | -4.433004               | 1.236237  | -0.502478 |
| 11               | 1                | 0              | -1.669019               | 0.213062  | -1.311492 |
| 12               | 6                | 0              | -2.354390               | 1.716550  | 0.097029  |
| 13               | 1                | 0              | -4.209344               | 1.428091  | 1.256072  |
| 14               | 6                | 0              | 0.611471                | 2.080949  | -0.157563 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 15 | 6 | 0 | 1.029274  | -0.099094 | -0.079556 |
| 16 | 1 | 0 | -0.616308 | -1.990402 | 0.044949  |
| 17 | 1 | 0 | -3.104779 | -1.794652 | -0.948963 |
| 18 | 7 | 0 | 1.934898  | 2.016557  | -0.093002 |
| 19 | 1 | 0 | 0.033124  | 2.985205  | -0.215589 |
| 20 | 6 | 0 | 2.214119  | 0.649749  | -0.044621 |
| 21 | 1 | 0 | 5.460074  | -0.012357 | 0.118469  |
| 22 | 6 | 0 | 3.424281  | -0.064009 | 0.028595  |
| 23 | 7 | 0 | 3.381507  | -1.421822 | 0.058910  |
| 24 | 7 | 0 | 4.619763  | 0.551123  | 0.068594  |
| 25 | 6 | 0 | 2.186904  | -2.037681 | 0.021560  |
| 26 | 7 | 0 | 0.970356  | -1.449891 | -0.045753 |
| 27 | 1 | 0 | 4.672035  | 1.562552  | 0.045137  |
| 28 | 1 | 0 | 2.195059  | -3.118867 | 0.050397  |
| 29 | 1 | 0 | -1.982794 | 2.161170  | 1.026929  |
| 30 | 1 | 0 | -2.385098 | 2.486671  | -0.677744 |

B4

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.421113               | 1.389489  | -1.007992 |
| 2                | 6                | 0              | -3.089909               | 0.896709  | 0.277071  |
| 3                | 1                | 0              | -3.366799               | 1.698495  | 0.972988  |
| 4                | 6                | 0              | -2.030436               | -0.045469 | 0.878254  |
| 5                | 8                | 0              | -4.230082               | 0.071770  | -0.106656 |
| 6                | 6                | 0              | -1.426185               | -0.775588 | -0.372891 |
| 7                | 8                | 0              | -2.757819               | -0.946229 | 1.767633  |
| 8                | 1                | 0              | -1.253692               | 0.529732  | 1.387960  |
| 9                | 7                | 0              | 0.036997                | -0.939957 | -0.268703 |
| 10               | 1                | 0              | -3.131153               | 1.893450  | -1.666690 |
| 11               | 1                | 0              | -1.855466               | -1.778983 | -0.412598 |
| 12               | 6                | 0              | -1.870148               | 0.072419  | -1.614597 |
| 13               | 1                | 0              | -1.588158               | 2.049677  | -0.748698 |
| 14               | 6                | 0              | 0.768140                | -2.124477 | -0.420752 |
| 15               | 6                | 0              | 0.971994                | 0.061965  | -0.054156 |
| 16               | 1                | 0              | -2.112649               | -1.532976 | 2.240608  |
| 17               | 1                | 0              | -4.303962               | -0.592690 | 0.638303  |
| 18               | 7                | 0              | 2.077861                | -1.946090 | -0.310300 |
| 19               | 1                | 0              | 0.274181                | -3.062478 | -0.611407 |
| 20               | 6                | 0              | 2.222229                | -0.574539 | -0.079260 |
| 21               | 1                | 0              | 5.385006                | 0.369500  | 0.266508  |
| 22               | 6                | 0              | 3.354063                | 0.237747  | 0.123587  |
| 23               | 7                | 0              | 3.174411                | 1.565355  | 0.331636  |
| 24               | 7                | 0              | 4.606737                | -0.261225 | 0.118400  |
| 25               | 6                | 0              | 1.916986                | 2.060163  | 0.338871  |
| 26               | 7                | 0              | 0.765152                | 1.379070  | 0.155208  |
| 27               | 1                | 0              | 4.759948                | -1.249440 | -0.040467 |
| 28               | 1                | 0              | 1.823497                | 3.124277  | 0.512184  |
| 29               | 1                | 0              | -1.040639               | 0.225840  | -2.306301 |
| 30               | 1                | 0              | -2.688727               | -0.449331 | -2.112699 |

B6

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |          |           |
|------------------|------------------|----------------|-------------------------|----------|-----------|
|                  |                  |                | X                       | Y        | Z         |
| 1                | 6                | 0              | -2.343247               | 1.315755 | -1.106585 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 2  | 6 | 0 | -3.028699 | 0.957198  | 0.215966  |
| 3  | 1 | 0 | -3.231346 | 1.828807  | 0.854158  |
| 4  | 6 | 0 | -2.028146 | -0.029837 | 0.871915  |
| 5  | 8 | 0 | -4.235984 | 0.198364  | -0.079959 |
| 6  | 6 | 0 | -1.427392 | -0.830051 | -0.326638 |
| 7  | 8 | 0 | -2.755891 | -0.994556 | 1.716307  |
| 8  | 1 | 0 | -1.244273 | 0.500946  | 1.414030  |
| 9  | 7 | 0 | 0.039999  | -0.961358 | -0.226305 |
| 10 | 1 | 0 | -3.027383 | 1.817974  | -1.793643 |
| 11 | 1 | 0 | -1.832856 | -1.842251 | -0.276826 |
| 12 | 6 | 0 | -1.895242 | -0.078419 | -1.616066 |
| 13 | 1 | 0 | -1.465992 | 1.935049  | -0.898623 |
| 14 | 6 | 0 | 0.781296  | -2.141699 | -0.357684 |
| 15 | 6 | 0 | 0.966197  | 0.053830  | -0.038848 |
| 16 | 1 | 0 | -2.875054 | -0.589764 | 2.617591  |
| 17 | 1 | 0 | -4.225020 | -0.523220 | 0.620850  |
| 18 | 7 | 0 | 2.089844  | -1.948180 | -0.264422 |
| 19 | 1 | 0 | 0.293755  | -3.088991 | -0.514591 |
| 20 | 6 | 0 | 2.222366  | -0.571150 | -0.062462 |
| 21 | 1 | 0 | 5.379696  | 0.402856  | 0.241693  |
| 22 | 6 | 0 | 3.348465  | 0.253734  | 0.116732  |
| 23 | 7 | 0 | 3.159790  | 1.583531  | 0.303904  |
| 24 | 7 | 0 | 4.604937  | -0.235592 | 0.109578  |
| 25 | 6 | 0 | 1.898466  | 2.066838  | 0.314122  |
| 26 | 7 | 0 | 0.750971  | 1.372814  | 0.151453  |
| 27 | 1 | 0 | 4.763431  | -1.225736 | -0.031341 |
| 28 | 1 | 0 | 1.796631  | 3.132819  | 0.471036  |
| 29 | 1 | 0 | -1.105287 | -0.042718 | -2.367629 |
| 30 | 1 | 0 | -2.774475 | -0.591943 | -2.009641 |

B7

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.957792               | -0.432078 | 1.295760  |
| 2                | 6                | 0              | -2.572287               | -0.965007 | -0.092334 |
| 3                | 1                | 0              | -1.785501               | -1.719686 | -0.032927 |
| 4                | 6                | 0              | -2.054495               | 0.308777  | -0.810255 |
| 5                | 8                | 0              | -3.797588               | -1.431538 | -0.761767 |
| 6                | 6                | 0              | -1.319882               | 1.120427  | 0.293087  |
| 7                | 8                | 0              | -3.231674               | 1.077034  | -1.184380 |
| 8                | 1                | 0              | -1.398903               | 0.096476  | -1.663971 |
| 9                | 7                | 0              | 0.143811                | 1.118597  | 0.129588  |
| 10               | 1                | 0              | -3.867467               | 0.161600  | 1.168781  |
| 11               | 1                | 0              | -1.658507               | 2.152911  | 0.195783  |
| 12               | 6                | 0              | -1.762901               | 0.481591  | 1.658670  |
| 13               | 1                | 0              | -3.130350               | -1.226458 | 2.024262  |
| 14               | 6                | 0              | 0.980009                | 2.230801  | -0.019250 |
| 15               | 6                | 0              | 0.972560                | 0.007852  | 0.091943  |
| 16               | 1                | 0              | -3.929803               | 0.359108  | -1.299590 |
| 17               | 1                | 0              | -3.532472               | -2.034931 | -1.507416 |
| 18               | 7                | 0              | 2.260334                | 1.906963  | -0.141505 |
| 19               | 1                | 0              | 0.578699                | 3.230032  | -0.028056 |
| 20               | 6                | 0              | 2.272196                | 0.510556  | -0.072924 |
| 21               | 1                | 0              | 5.316624                | -0.782185 | -0.338480 |
| 22               | 6                | 0              | 3.316362                | -0.430483 | -0.139549 |
| 23               | 7                | 0              | 3.012994                | -1.748728 | -0.041266 |
| 24               | 7                | 0              | 4.604226                | -0.063803 | -0.297339 |
| 25               | 6                | 0              | 1.720945                | -2.109524 | 0.114966  |
| 26               | 7                | 0              | 0.643482                | -1.298204 | 0.190087  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 27 | 1 | 0 | 4.847169  | 0.916362  | -0.372583 |
| 28 | 1 | 0 | 1.528202  | -3.172062 | 0.188526  |
| 29 | 1 | 0 | -0.940747 | -0.129794 | 2.037494  |
| 30 | 1 | 0 | -2.015077 | 1.243421  | 2.399717  |

B9

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.966541               | -0.511513 | 1.258216  |
| 2                | 6                | 0              | -2.575874               | -0.964450 | -0.164205 |
| 3                | 1                | 0              | -1.772164               | -1.704602 | -0.141832 |
| 4                | 6                | 0              | -2.068088               | 0.350538  | -0.795620 |
| 5                | 8                | 0              | -3.716997               | -1.365952 | -0.993874 |
| 6                | 6                | 0              | -1.323260               | 1.085822  | 0.353967  |
| 7                | 8                | 0              | -3.243969               | 1.156949  | -1.094356 |
| 8                | 1                | 0              | -1.428250               | 0.191194  | -1.670270 |
| 9                | 7                | 0              | 0.138879                | 1.098583  | 0.181890  |
| 10               | 1                | 0              | -3.861596               | 0.109455  | 1.158067  |
| 11               | 1                | 0              | -1.663212               | 2.122224  | 0.324909  |
| 12               | 6                | 0              | -1.759679               | 0.363138  | 1.678520  |
| 13               | 1                | 0              | -3.150241               | -1.339148 | 1.949069  |
| 14               | 6                | 0              | 0.959060                | 2.221978  | 0.025098  |
| 15               | 6                | 0              | 0.980022                | -0.002098 | 0.118920  |
| 16               | 1                | 0              | -3.921043               | 0.463018  | -1.359436 |
| 17               | 1                | 0              | -4.232119               | -2.064110 | -0.512843 |
| 18               | 7                | 0              | 2.240212                | 1.914533  | -0.124384 |
| 19               | 1                | 0              | 0.545659                | 3.216309  | 0.031514  |
| 20               | 6                | 0              | 2.269916                | 0.517685  | -0.067652 |
| 21               | 1                | 0              | 5.322719                | -0.735687 | -0.413003 |
| 22               | 6                | 0              | 3.323497                | -0.410084 | -0.164393 |
| 23               | 7                | 0              | 3.038159                | -1.732552 | -0.071004 |
| 24               | 7                | 0              | 4.603295                | -0.026277 | -0.346780 |
| 25               | 6                | 0              | 1.754021                | -2.110151 | 0.110305  |
| 26               | 7                | 0              | 0.669084                | -1.312331 | 0.215441  |
| 27               | 1                | 0              | 4.832241                | 0.957236  | -0.421913 |
| 28               | 1                | 0              | 1.575152                | -3.175392 | 0.178442  |
| 29               | 1                | 0              | -0.943050               | -0.282680 | 2.007782  |
| 30               | 1                | 0              | -2.002215               | 1.075314  | 2.470277  |

B10

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.124065               | -0.461292 | 1.502349  |
| 2                | 6                | 0              | -2.368988               | -1.058092 | 0.095082  |
| 3                | 1                | 0              | -1.713362               | -1.902920 | -0.100110 |
| 4                | 6                | 0              | -2.095079               | 0.117377  | -0.925279 |
| 5                | 8                | 0              | -3.803232               | -1.427460 | -0.006028 |
| 6                | 6                | 0              | -1.396203               | 1.225535  | -0.104183 |
| 7                | 8                | 0              | -3.375045               | 0.688745  | -1.302653 |
| 8                | 1                | 0              | -1.510777               | -0.200875 | -1.794442 |
| 9                | 7                | 0              | 0.080740                | 1.125135  | -0.071240 |
| 10               | 1                | 0              | -2.934369               | -0.761816 | 2.169591  |
| 11               | 1                | 0              | -1.636000               | 2.184537  | -0.566555 |
| 12               | 6                | 0              | -2.049072               | 1.073764  | 1.292360  |
| 13               | 1                | 0              | -1.171571               | -0.838716 | 1.882068  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 14 | 6 | 0 | 0.937403  | 2.233823  | -0.036077 |
| 15 | 6 | 0 | 0.908066  | 0.008733  | -0.075715 |
| 16 | 1 | 0 | -4.028878 | 0.032792  | -0.891281 |
| 17 | 1 | 0 | -3.882004 | -2.162006 | -0.672646 |
| 18 | 7 | 0 | 2.221184  | 1.906969  | -0.015995 |
| 19 | 1 | 0 | 0.543838  | 3.236360  | -0.034444 |
| 20 | 6 | 0 | 2.219843  | 0.511051  | -0.041051 |
| 21 | 1 | 0 | 5.282813  | -0.761227 | -0.017946 |
| 22 | 6 | 0 | 3.269998  | -0.425319 | -0.043417 |
| 23 | 7 | 0 | 2.967534  | -1.746263 | -0.077100 |
| 24 | 7 | 0 | 4.564096  | -0.048039 | -0.013319 |
| 25 | 6 | 0 | 1.667730  | -2.110130 | -0.107272 |
| 26 | 7 | 0 | 0.586478  | -1.302285 | -0.108516 |
| 27 | 1 | 0 | 4.804901  | 0.935320  | 0.009104  |
| 28 | 1 | 0 | 1.471266  | -3.174297 | -0.132773 |
| 29 | 1 | 0 | -1.497822 | 1.598784  | 2.075251  |
| 30 | 1 | 0 | -3.059847 | 1.482457  | 1.206029  |

B11

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.022216               | -0.416596 | 1.319033  |
| 2                | 6                | 0              | -2.668274               | -0.980086 | -0.079865 |
| 3                | 1                | 0              | -1.895671               | -1.746147 | 0.008421  |
| 4                | 6                | 0              | -2.050952               | 0.257518  | -0.779886 |
| 5                | 8                | 0              | -3.781998               | -1.500183 | -0.830487 |
| 6                | 6                | 0              | -1.318319               | 1.059033  | 0.341746  |
| 7                | 8                | 0              | -3.238825               | 1.010995  | -1.229840 |
| 8                | 1                | 0              | -1.391794               | -0.002397 | -1.611784 |
| 9                | 7                | 0              | 0.142223                | 1.091987  | 0.168934  |
| 10               | 1                | 0              | -3.883603               | 0.251285  | 1.207022  |
| 11               | 1                | 0              | -1.675634               | 2.090234  | 0.291969  |
| 12               | 6                | 0              | -1.753356               | 0.382652  | 1.689810  |
| 13               | 1                | 0              | -3.259298               | -1.203174 | 2.038256  |
| 14               | 6                | 0              | 0.963891                | 2.219854  | 0.049917  |
| 15               | 6                | 0              | 0.986436                | -0.006319 | 0.099413  |
| 16               | 1                | 0              | -2.989432               | 1.567745  | -2.012871 |
| 17               | 1                | 0              | -4.198785               | -0.667992 | -1.203145 |
| 18               | 7                | 0              | 2.247022                | 1.915906  | -0.087838 |
| 19               | 1                | 0              | 0.551704                | 3.214527  | 0.078235  |
| 20               | 6                | 0              | 2.278043                | 0.517542  | -0.058383 |
| 21               | 1                | 0              | 5.333616                | -0.739921 | -0.371994 |
| 22               | 6                | 0              | 3.331933                | -0.410810 | -0.155780 |
| 23               | 7                | 0              | 3.041871                | -1.733856 | -0.092215 |
| 24               | 7                | 0              | 4.615821                | -0.028352 | -0.309433 |
| 25               | 6                | 0              | 1.754364                | -2.113907 | 0.061513  |
| 26               | 7                | 0              | 0.669644                | -1.315350 | 0.164989  |
| 27               | 1                | 0              | 4.851890                | 0.955160  | -0.356095 |
| 28               | 1                | 0              | 1.572494                | -3.179616 | 0.106660  |
| 29               | 1                | 0              | -0.966594               | -0.312928 | 1.991903  |
| 30               | 1                | 0              | -1.907677               | 1.121081  | 2.479873  |

B12

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 1  | 6 | 0 | -3.151481 | 1.675833  | 0.424398  |
| 2  | 6 | 0 | -3.668196 | 0.209056  | 0.370820  |
| 3  | 1 | 0 | -4.441118 | -0.017822 | 1.111842  |
| 4  | 6 | 0 | -2.408445 | -0.674309 | 0.535654  |
| 5  | 8 | 0 | -4.106909 | -0.170987 | -0.987912 |
| 6  | 6 | 0 | -1.352059 | 0.170408  | -0.218755 |
| 7  | 8 | 0 | -2.613955 | -2.003954 | 0.014028  |
| 8  | 1 | 0 | -2.117558 | -0.752842 | 1.586802  |
| 9  | 7 | 0 | 0.005446  | -0.358303 | -0.057284 |
| 10 | 1 | 0 | -3.528828 | 2.205574  | -0.454974 |
| 11 | 1 | 0 | -1.633880 | 0.171703  | -1.278145 |
| 12 | 6 | 0 | -1.588651 | 1.574826  | 0.378730  |
| 13 | 1 | 0 | -3.492688 | 2.192554  | 1.324700  |
| 14 | 6 | 0 | 0.346593  | -1.718065 | 0.048188  |
| 15 | 6 | 0 | 1.201960  | 0.342661  | -0.096813 |
| 16 | 1 | 0 | -3.234692 | -1.844287 | -0.758790 |
| 17 | 1 | 0 | -5.012398 | 0.197393  | -1.156794 |
| 18 | 7 | 0 | 1.657119  | -1.913537 | 0.103415  |
| 19 | 1 | 0 | -0.433207 | -2.459694 | 0.061926  |
| 20 | 6 | 0 | 2.207801  | -0.630154 | 0.013639  |
| 21 | 1 | 0 | 5.524369  | -0.642165 | 0.090683  |
| 22 | 6 | 0 | 3.538103  | -0.173592 | 0.004941  |
| 23 | 7 | 0 | 3.773140  | 1.156089  | -0.113692 |
| 24 | 7 | 0 | 4.585483  | -1.019998 | 0.107868  |
| 25 | 6 | 0 | 2.716142  | 1.993528  | -0.219478 |
| 26 | 7 | 0 | 1.406200  | 1.670315  | -0.219784 |
| 27 | 1 | 0 | 4.423764  | -2.015815 | 0.192655  |
| 28 | 1 | 0 | 2.951571  | 3.045866  | -0.316336 |
| 29 | 1 | 0 | -1.176608 | 1.595126  | 1.392869  |
| 30 | 1 | 0 | -1.104118 | 2.360829  | -0.196968 |

B13

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.038793               | -1.307510 | 0.848446  |
| 2                | 6                | 0              | -3.529808               | -0.491101 | -0.352128 |
| 3                | 1                | 0              | -4.070995               | -1.067093 | -1.110049 |
| 4                | 6                | 0              | -2.250723               | 0.198504  | -0.924647 |
| 5                | 8                | 0              | -4.324186               | 0.660340  | 0.117756  |
| 6                | 6                | 0              | -1.282811               | 0.320318  | 0.316907  |
| 7                | 8                | 0              | -2.582553               | 1.461644  | -1.527105 |
| 8                | 1                | 0              | -1.783452               | -0.436383 | -1.681669 |
| 9                | 7                | 0              | 0.025900                | -0.313978 | 0.067815  |
| 10               | 1                | 0              | -3.852806               | -1.608778 | 1.514771  |
| 11               | 1                | 0              | -1.057001               | 1.375366  | 0.478173  |
| 12               | 6                | 0              | -2.035457               | -0.331043 | 1.514039  |
| 13               | 1                | 0              | -2.529132               | -2.210076 | 0.490822  |
| 14               | 6                | 0              | 0.334068                | -1.630467 | -0.296084 |
| 15               | 6                | 0              | 1.239709                | 0.348870  | 0.166918  |
| 16               | 1                | 0              | -3.394337               | 1.745863  | -1.006981 |
| 17               | 1                | 0              | -5.256734               | 0.370421  | 0.288895  |
| 18               | 7                | 0              | 1.638914                | -1.839784 | -0.431796 |
| 19               | 1                | 0              | -0.429499               | -2.374696 | -0.440394 |
| 20               | 6                | 0              | 2.222101                | -0.601647 | -0.143591 |
| 21               | 1                | 0              | 5.535280                | -0.608998 | -0.356327 |
| 22               | 6                | 0              | 3.558908                | -0.160377 | -0.111245 |
| 23               | 7                | 0              | 3.810961                | 1.130500  | 0.213547  |
| 24               | 7                | 0              | 4.594263                | -0.980671 | -0.391879 |
| 25               | 6                | 0              | 2.769216                | 1.948385  | 0.495041  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 26 | 7 | 0 | 1.457254  | 1.634646  | 0.494986  |
| 27 | 1 | 0 | 4.424203  | -1.947037 | -0.640531 |
| 28 | 1 | 0 | 3.021470  | 2.969835  | 0.748857  |
| 29 | 1 | 0 | -1.351556 | -0.809191 | 2.216451  |
| 30 | 1 | 0 | -2.611030 | 0.446300  | 2.022131  |

B14

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.594056               | 1.226140  | 0.882575  |
| 2                | 6                | 0              | -2.378184               | -0.312199 | 1.067379  |
| 3                | 1                | 0              | -1.598521               | -0.521678 | 1.805323  |
| 4                | 6                | 0              | -1.968851               | -0.848810 | -0.342925 |
| 5                | 8                | 0              | -3.611643               | -1.043051 | 1.384089  |
| 6                | 6                | 0              | -1.384649               | 0.389504  | -1.054217 |
| 7                | 8                | 0              | -3.184611               | -1.160734 | -1.080483 |
| 8                | 1                | 0              | -1.268726               | -1.684205 | -0.308410 |
| 9                | 7                | 0              | -0.022688               | 0.698743  | -0.544406 |
| 10               | 1                | 0              | -3.594179               | 1.517690  | 1.217488  |
| 11               | 1                | 0              | -1.347401               | 0.223221  | -2.132889 |
| 12               | 6                | 0              | -2.402129               | 1.476286  | -0.640795 |
| 13               | 1                | 0              | -1.849208               | 1.779834  | 1.460726  |
| 14               | 6                | 0              | 0.523932                | 1.966385  | -0.295335 |
| 15               | 6                | 0              | 1.020933                | -0.203756 | -0.352598 |
| 16               | 1                | 0              | -3.845595               | -1.355361 | -0.348101 |
| 17               | 1                | 0              | -4.020873               | -0.657638 | 2.200494  |
| 18               | 7                | 0              | 1.802939                | 1.928364  | 0.051374  |
| 19               | 1                | 0              | -0.063084               | 2.861962  | -0.386264 |
| 20               | 6                | 0              | 2.130467                | 0.570784  | 0.018946  |
| 21               | 1                | 0              | 5.300667                | -0.004790 | 0.810711  |
| 22               | 6                | 0              | 3.333313                | -0.112632 | 0.278058  |
| 23               | 7                | 0              | 3.357312                | -1.461482 | 0.154835  |
| 24               | 7                | 0              | 4.460095                | 0.534122  | 0.642980  |
| 25               | 6                | 0              | 2.221868                | -2.098220 | -0.210615 |
| 26               | 7                | 0              | 1.020503                | -1.546713 | -0.480198 |
| 27               | 1                | 0              | 4.460382                | 1.542670  | 0.731707  |
| 28               | 1                | 0              | 2.285201                | -3.175279 | -0.295986 |
| 29               | 1                | 0              | -2.111088               | 2.497867  | -0.890367 |
| 30               | 1                | 0              | -3.320530               | 1.213846  | -1.168227 |

B15

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.395322               | -0.053546 | 1.282153  |
| 2                | 6                | 0              | -3.294192               | -0.705541 | -0.111892 |
| 3                | 1                | 0              | -2.958145               | -1.748133 | -0.038278 |
| 4                | 6                | 0              | -2.233254               | 0.179000  | -0.808049 |
| 5                | 8                | 0              | -4.501733               | -0.579712 | -0.928027 |
| 6                | 6                | 0              | -1.199592               | 0.515150  | 0.300198  |
| 7                | 8                | 0              | -2.897183               | 1.431833  | -1.134785 |
| 8                | 1                | 0              | -1.770603               | -0.297871 | -1.679633 |
| 9                | 7                | 0              | 0.069519                | -0.211237 | 0.148922  |
| 10               | 1                | 0              | -3.895277               | 0.908136  | 1.138016  |
| 11               | 1                | 0              | -0.948769               | 1.572879  | 0.209781  |
| 12               | 6                | 0              | -1.912795               | 0.187165  | 1.662190  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 13 | 1 | 0 | -3.935029 | -0.658798 | 2.015870  |
| 14 | 6 | 0 | 0.296940  | -1.588895 | 0.042607  |
| 15 | 6 | 0 | 1.316972  | 0.389764  | 0.085050  |
| 16 | 1 | 0 | -3.816301 | 1.133293  | -1.406824 |
| 17 | 1 | 0 | -5.285713 | -0.857495 | -0.386291 |
| 18 | 7 | 0 | 1.583045  | -1.893250 | -0.083318 |
| 19 | 1 | 0 | -0.510957 | -2.300428 | 0.060624  |
| 20 | 6 | 0 | 2.238311  | -0.657009 | -0.057218 |
| 21 | 1 | 0 | 5.537478  | -0.890682 | -0.345937 |
| 22 | 6 | 0 | 3.595954  | -0.294269 | -0.144820 |
| 23 | 7 | 0 | 3.923585  | 1.019417  | -0.086178 |
| 24 | 7 | 0 | 4.578469  | -1.209461 | -0.284873 |
| 25 | 6 | 0 | 2.935286  | 1.933834  | 0.053168  |
| 26 | 7 | 0 | 1.609393  | 1.700378  | 0.146493  |
| 27 | 1 | 0 | 4.352570  | -2.194981 | -0.334080 |
| 28 | 1 | 0 | 3.247130  | 2.969402  | 0.093971  |
| 29 | 1 | 0 | -1.473110 | -0.722834 | 2.082027  |
| 30 | 1 | 0 | -1.789870 | 0.995713  | 2.385604  |

B16

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.524842               | -0.456468 | 1.096982  |
| 2                | 6                | 0              | -3.367003               | -0.538513 | -0.442153 |
| 3                | 1                | 0              | -3.138928               | -1.567651 | -0.739454 |
| 4                | 6                | 0              | -2.128484               | 0.366251  | -0.687481 |
| 5                | 8                | 0              | -4.504166               | -0.089811 | -1.199979 |
| 6                | 6                | 0              | -1.221384               | 0.199775  | 0.570434  |
| 7                | 8                | 0              | -2.732543               | 1.707016  | -0.703007 |
| 8                | 1                | 0              | -1.596051               | 0.144301  | -1.617376 |
| 9                | 7                | 0              | 0.079318                | -0.413085 | 0.269303  |
| 10               | 1                | 0              | -3.902871               | 0.543440  | 1.333568  |
| 11               | 1                | 0              | -0.988587               | 1.197073  | 0.950929  |
| 12               | 6                | 0              | -2.073517               | -0.614083 | 1.601930  |
| 13               | 1                | 0              | -4.208337               | -1.210606 | 1.491865  |
| 14               | 6                | 0              | 0.396862                | -1.732137 | -0.080970 |
| 15               | 6                | 0              | 1.271996                | 0.292249  | 0.230515  |
| 16               | 1                | 0              | -2.058859               | 2.364351  | -1.018815 |
| 17               | 1                | 0              | -4.378075               | 0.904728  | -1.217075 |
| 18               | 7                | 0              | 1.690857                | -1.902984 | -0.324674 |
| 19               | 1                | 0              | -0.352204               | -2.502926 | -0.134720 |
| 20               | 6                | 0              | 2.255392                | -0.637393 | -0.131077 |
| 21               | 1                | 0              | 5.536873                | -0.541327 | -0.628030 |
| 22               | 6                | 0              | 3.573452                | -0.151971 | -0.232296 |
| 23               | 7                | 0              | 3.803821                | 1.160498  | 0.019918  |
| 24               | 7                | 0              | 4.610089                | -0.945396 | -0.571710 |
| 25               | 6                | 0              | 2.762962                | 1.954940  | 0.357977  |
| 26               | 7                | 0              | 1.465863                | 1.599340  | 0.482512  |
| 27               | 1                | 0              | 4.458280                | -1.928117 | -0.762290 |
| 28               | 1                | 0              | 2.999027                | 2.993932  | 0.548585  |
| 29               | 1                | 0              | -1.778460               | -1.668027 | 1.565638  |
| 30               | 1                | 0              | -1.920375               | -0.251317 | 2.620447  |

B17

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 1  | 6 | 0 | -2.711262 | 1.354716  | 0.641258  |
| 2  | 6 | 0 | -2.455836 | -0.118730 | 1.125682  |
| 3  | 1 | 0 | -1.693532 | -0.137482 | 1.906892  |
| 4  | 6 | 0 | -1.932611 | -0.867607 | -0.144894 |
| 5  | 8 | 0 | -3.636297 | -0.779347 | 1.634450  |
| 6  | 6 | 0 | -1.364416 | 0.234883  | -1.060650 |
| 7  | 8 | 0 | -3.157964 | -1.373803 | -0.796342 |
| 8  | 1 | 0 | -1.215019 | -1.663745 | 0.053806  |
| 9  | 7 | 0 | -0.026700 | 0.641227  | -0.567701 |
| 10 | 1 | 0 | -3.748268 | 1.609483  | 0.867038  |
| 11 | 1 | 0 | -1.273522 | -0.111866 | -2.093798 |
| 12 | 6 | 0 | -2.415041 | 1.353959  | -0.884745 |
| 13 | 1 | 0 | -2.050071 | 2.049248  | 1.167806  |
| 14 | 6 | 0 | 0.471036  | 1.929930  | -0.324293 |
| 15 | 6 | 0 | 1.041223  | -0.222955 | -0.355353 |
| 16 | 1 | 0 | -2.945288 | -2.227014 | -1.255230 |
| 17 | 1 | 0 | -4.025415 | -1.188212 | 0.802325  |
| 18 | 7 | 0 | 1.748577  | 1.935600  | 0.030812  |
| 19 | 1 | 0 | -0.147722 | 2.803001  | -0.421061 |
| 20 | 6 | 0 | 2.122107  | 0.588689  | 0.015137  |
| 21 | 1 | 0 | 5.296469  | 0.100520  | 0.850659  |
| 22 | 6 | 0 | 3.340506  | -0.059267 | 0.292397  |
| 23 | 7 | 0 | 3.399370  | -1.409703 | 0.184069  |
| 24 | 7 | 0 | 4.446869  | 0.617735  | 0.660835  |
| 25 | 6 | 0 | 2.286066  | -2.082333 | -0.180593 |
| 26 | 7 | 0 | 1.070625  | -1.567125 | -0.467243 |
| 27 | 1 | 0 | 4.420223  | 1.626148  | 0.748640  |
| 28 | 1 | 0 | 2.380055  | -3.158463 | -0.248911 |
| 29 | 1 | 0 | -2.104439 | 2.320521  | -1.287570 |
| 30 | 1 | 0 | -3.301201 | 1.011203  | -1.424530 |

B19

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.709645               | 1.354571  | 0.643560  |
| 2                | 6                | 0              | -2.456381               | -0.119946 | 1.125740  |
| 3                | 1                | 0              | -1.694805               | -0.140860 | 1.907617  |
| 4                | 6                | 0              | -1.932758               | -0.867386 | -0.145739 |
| 5                | 8                | 0              | -3.638096               | -0.779975 | 1.632186  |
| 6                | 6                | 0              | -1.364492               | 0.236102  | -1.060251 |
| 7                | 8                | 0              | -3.157880               | -1.372950 | -0.798262 |
| 8                | 1                | 0              | -1.215182               | -1.663712 | 0.052177  |
| 9                | 7                | 0              | -0.026603               | 0.641718  | -0.567135 |
| 10               | 1                | 0              | -3.745895               | 1.611082  | 0.870820  |
| 11               | 1                | 0              | -1.273977               | -0.109449 | -2.093837 |
| 12               | 6                | 0              | -2.414893               | 1.355143  | -0.882671 |
| 13               | 1                | 0              | -2.046416               | 2.047118  | 1.170172  |
| 14               | 6                | 0              | 0.471781                | 1.930278  | -0.324491 |
| 15               | 6                | 0              | 1.041050                | -0.222835 | -0.354854 |
| 16               | 1                | 0              | -2.945296               | -2.226444 | -1.256684 |
| 17               | 1                | 0              | -4.026334               | -1.187879 | 0.799185  |
| 18               | 7                | 0              | 1.749452                | 1.935591  | 0.030200  |
| 19               | 1                | 0              | -0.146610               | 2.803594  | -0.421396 |
| 20               | 6                | 0              | 2.122405                | 0.588532  | 0.014991  |
| 21               | 1                | 0              | 5.296833                | 0.099323  | 0.849712  |
| 22               | 6                | 0              | 3.340642                | -0.059837 | 0.292088  |
| 23               | 7                | 0              | 3.398928                | -1.410320 | 0.184235  |
| 24               | 7                | 0              | 4.447383                | 0.616827  | 0.660012  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 25 | 6 | 0 | 2.285264  | -2.082644 | -0.179836 |
| 26 | 7 | 0 | 1.069955  | -1.567027 | -0.466322 |
| 27 | 1 | 0 | 4.421202  | 1.625279  | 0.747436  |
| 28 | 1 | 0 | 2.378813  | -3.158831 | -0.247831 |
| 29 | 1 | 0 | -2.104632 | 2.322020  | -1.284989 |
| 30 | 1 | 0 | -3.301533 | 1.012777  | -1.421933 |

B21

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.525224               | -0.457718 | 1.096440  |
| 2                | 6                | 0              | -3.368217               | -0.536967 | -0.442919 |
| 3                | 1                | 0              | -3.141920               | -1.565901 | -0.742281 |
| 4                | 6                | 0              | -2.128290               | 0.366261  | -0.687208 |
| 5                | 8                | 0              | -4.505025               | -0.085004 | -1.199328 |
| 6                | 6                | 0              | -1.221520               | 0.197158  | 0.570678  |
| 7                | 8                | 0              | -2.730222               | 1.707958  | -0.701552 |
| 8                | 1                | 0              | -1.596081               | 0.144315  | -1.617235 |
| 9                | 7                | 0              | 0.079510                | -0.414632 | 0.268889  |
| 10               | 1                | 0              | -3.901522               | 0.542329  | 1.335237  |
| 11               | 1                | 0              | -0.989333               | 1.193794  | 0.953281  |
| 12               | 6                | 0              | -2.073903               | -0.618735 | 1.600244  |
| 13               | 1                | 0              | -4.209749               | -1.211537 | 1.490146  |
| 14               | 6                | 0              | 0.397884                | -1.733131 | -0.082695 |
| 15               | 6                | 0              | 1.271735                | 0.291500  | 0.230790  |
| 16               | 1                | 0              | -2.055318               | 2.364641  | -1.016106 |
| 17               | 1                | 0              | -4.376927               | 0.909308  | -1.215334 |
| 18               | 7                | 0              | 1.691999                | -1.902923 | -0.326503 |
| 19               | 1                | 0              | -0.350682               | -2.504349 | -0.137208 |
| 20               | 6                | 0              | 2.255741                | -0.637174 | -0.131614 |
| 21               | 1                | 0              | 5.537198                | -0.538564 | -0.628224 |
| 22               | 6                | 0              | 3.573512                | -0.150830 | -0.232231 |
| 23               | 7                | 0              | 3.803027                | 1.161538  | 0.021292  |
| 24               | 7                | 0              | 4.610666                | -0.943267 | -0.572355 |
| 25               | 6                | 0              | 2.761637                | 1.955003  | 0.360001  |
| 26               | 7                | 0              | 1.464748                | 1.598467  | 0.484072  |
| 27               | 1                | 0              | 4.459480                | -1.925881 | -0.763966 |
| 28               | 1                | 0              | 2.997047                | 2.993940  | 0.551720  |
| 29               | 1                | 0              | -1.780329               | -1.672972 | 1.560559  |
| 30               | 1                | 0              | -1.919681               | -0.259254 | 2.619760  |

B22

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.424301               | -0.168686 | 1.245663  |
| 2                | 6                | 0              | -3.294360               | -0.687701 | -0.194500 |
| 3                | 1                | 0              | -2.999159               | -1.743620 | -0.218574 |
| 4                | 6                | 0              | -2.200474               | 0.241021  | -0.789255 |
| 5                | 8                | 0              | -4.571058               | -0.455353 | -0.884412 |
| 6                | 6                | 0              | -1.200424               | 0.484166  | 0.373510  |
| 7                | 8                | 0              | -2.856178               | 1.511246  | -1.051120 |
| 8                | 1                | 0              | -1.701566               | -0.169934 | -1.676865 |
| 9                | 7                | 0              | 0.073128                | -0.229506 | 0.197901  |
| 10               | 1                | 0              | -3.941492               | 0.792267  | 1.184183  |
| 11               | 1                | 0              | -0.947863               | 1.545366  | 0.373475  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 12 | 6 | 0 | -1.954128 | 0.046748  | 1.681053  |
| 13 | 1 | 0 | -3.979179 | -0.846662 | 1.896732  |
| 14 | 6 | 0 | 0.308565  | -1.602123 | 0.054695  |
| 15 | 6 | 0 | 1.314509  | 0.382535  | 0.119994  |
| 16 | 1 | 0 | -3.807416 | 1.240616  | -1.237765 |
| 17 | 1 | 0 | -4.579845 | -0.997245 | -1.719832 |
| 18 | 7 | 0 | 1.593861  | -1.893987 | -0.105804 |
| 19 | 1 | 0 | -0.492640 | -2.320974 | 0.079228  |
| 20 | 6 | 0 | 2.240383  | -0.653515 | -0.065672 |
| 21 | 1 | 0 | 5.534762  | -0.854049 | -0.426597 |
| 22 | 6 | 0 | 3.593244  | -0.278159 | -0.173633 |
| 23 | 7 | 0 | 3.912174  | 1.036391  | -0.092640 |
| 24 | 7 | 0 | 4.579557  | -1.181963 | -0.354957 |
| 25 | 6 | 0 | 2.920354  | 1.939644  | 0.088808  |
| 26 | 7 | 0 | 1.598655  | 1.693602  | 0.204853  |
| 27 | 1 | 0 | 4.360885  | -2.168307 | -0.417683 |
| 28 | 1 | 0 | 3.225269  | 2.976443  | 0.146650  |
| 29 | 1 | 0 | -1.521795 | -0.891764 | 2.042279  |
| 30 | 1 | 0 | -1.853903 | 0.795389  | 2.469581  |

C1

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.540202                | -0.120388 | -0.131014 |
| 2                | 7                | 0              | 2.235780                | 1.896445  | -0.010420 |
| 3                | 1                | 0              | -3.937802               | 0.140903  | -1.347953 |
| 4                | 7                | 0              | 0.088441                | 1.151336  | 0.049288  |
| 5                | 6                | 0              | 0.958648                | 2.247982  | 0.037346  |
| 6                | 1                | 0              | -1.710051               | 2.201878  | -0.090840 |
| 7                | 1                | 0              | 0.582978                | 3.257086  | 0.060523  |
| 8                | 6                | 0              | 1.590254                | -2.111247 | -0.076551 |
| 9                | 7                | 0              | 0.528795                | -1.278534 | -0.019722 |
| 10               | 1                | 0              | 4.809463                | 0.855671  | -0.123261 |
| 11               | 6                | 0              | 2.210339                | 0.498201  | -0.031427 |
| 12               | 8                | 0              | -3.240304               | 0.869617  | -1.377834 |
| 13               | 7                | 0              | 2.898677                | -1.775855 | -0.109295 |
| 14               | 1                | 0              | 5.237328                | -0.853116 | -0.179857 |
| 15               | 1                | 0              | 1.369165                | -3.170450 | -0.100917 |
| 16               | 6                | 0              | 3.236440                | -0.463140 | -0.090434 |
| 17               | 6                | 0              | 0.891524                | 0.020188  | 0.005759  |
| 18               | 6                | 0              | -1.386155               | 1.186958  | 0.148738  |
| 19               | 1                | 0              | -2.787277               | -1.044320 | 2.328217  |
| 20               | 6                | 0              | -2.080086               | 0.199174  | -0.836547 |
| 21               | 6                | 0              | -2.565634               | -1.003831 | 0.062362  |
| 22               | 1                | 0              | -4.543645               | -0.923329 | 0.401332  |
| 23               | 1                | 0              | -1.604001               | 1.272562  | 2.423393  |
| 24               | 8                | 0              | -3.966083               | -1.328484 | -0.301216 |
| 25               | 6                | 0              | -2.437552               | -0.476135 | 1.474511  |
| 26               | 1                | 0              | -1.949227               | -1.885206 | -0.104277 |
| 27               | 1                | 0              | -1.385355               | -0.137785 | -1.611048 |
| 28               | 6                | 0              | -1.830068               | 0.709519  | 1.527115  |

C2

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |   |   |
|------------------|------------------|----------------|-------------------------|---|---|
|                  |                  |                | X                       | Y | Z |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 1  | 7 | 0 | 4.540278  | -0.120485 | -0.126653 |
| 2  | 7 | 0 | 2.238544  | 1.892372  | -0.052143 |
| 3  | 1 | 0 | -4.036353 | 0.214984  | -1.012377 |
| 4  | 7 | 0 | 0.088634  | 1.152194  | 0.022205  |
| 5  | 6 | 0 | 0.961550  | 2.245953  | -0.012137 |
| 6  | 1 | 0 | -1.689779 | 2.226943  | -0.148228 |
| 7  | 1 | 0 | 0.587146  | 3.255769  | -0.008209 |
| 8  | 6 | 0 | 1.594212  | -2.114208 | -0.034353 |
| 9  | 7 | 0 | 0.531685  | -1.282048 | 0.002921  |
| 10 | 1 | 0 | 4.806055  | 0.856600  | -0.135177 |
| 11 | 6 | 0 | 2.210118  | 0.494997  | -0.044570 |
| 12 | 8 | 0 | -3.314032 | 0.854500  | -1.312306 |
| 13 | 7 | 0 | 2.902055  | -1.779173 | -0.072926 |
| 14 | 1 | 0 | 5.240186  | -0.851617 | -0.154539 |
| 15 | 1 | 0 | 1.374247  | -3.174049 | -0.035247 |
| 16 | 6 | 0 | 3.237408  | -0.465732 | -0.081592 |
| 17 | 6 | 0 | 0.889888  | 0.019311  | 0.001716  |
| 18 | 6 | 0 | -1.387072 | 1.213080  | 0.121896  |
| 19 | 1 | 0 | -2.904828 | -0.913689 | 2.327820  |
| 20 | 6 | 0 | -2.108731 | 0.215768  | -0.835173 |
| 21 | 6 | 0 | -2.523783 | -0.985817 | 0.091390  |
| 22 | 1 | 0 | -3.882906 | -2.072623 | -0.928134 |
| 23 | 1 | 0 | -1.667467 | 1.389475  | 2.385353  |
| 24 | 8 | 0 | -3.913487 | -1.379207 | -0.214662 |
| 25 | 6 | 0 | -2.487152 | -0.388675 | 1.479676  |
| 26 | 1 | 0 | -1.814521 | -1.810963 | -0.001312 |
| 27 | 1 | 0 | -1.453794 | -0.093862 | -1.655357 |
| 28 | 6 | 0 | -1.860806 | 0.787101  | 1.507701  |

C3

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.578250                | 0.463734  | 0.218057  |
| 2                | 7                | 0              | 1.925704                | 2.015095  | 0.058120  |
| 3                | 1                | 0              | -0.756645               | -1.969671 | -0.034831 |
| 4                | 7                | 0              | -0.020927               | 0.868613  | -0.196220 |
| 5                | 6                | 0              | 0.606634                | 2.112912  | -0.062574 |
| 6                | 1                | 0              | -1.537863               | 0.090963  | -1.422943 |
| 7                | 1                | 0              | 0.045844                | 3.029965  | -0.056785 |
| 8                | 6                | 0              | 2.084951                | -2.043852 | -0.144825 |
| 9                | 7                | 0              | 0.884902                | -1.421049 | -0.219697 |
| 10               | 1                | 0              | 4.660205                | 1.471411  | 0.282145  |
| 11               | 6                | 0              | 2.182138                | 0.642754  | 0.001155  |
| 12               | 8                | 0              | -1.756843               | -1.884792 | 0.182513  |
| 13               | 7                | 0              | 3.290355                | -1.463195 | -0.009726 |
| 14               | 1                | 0              | 5.399018                | -0.128322 | 0.264002  |
| 15               | 1                | 0              | 2.068329                | -3.124206 | -0.194197 |
| 16               | 6                | 0              | 3.370173                | -0.108698 | 0.071869  |
| 17               | 6                | 0              | 0.988477                | -0.073747 | -0.151187 |
| 18               | 6                | 0              | -1.442818               | 0.532479  | -0.423269 |
| 19               | 1                | 0              | -4.479995               | 1.801347  | 0.392145  |
| 20               | 6                | 0              | -1.974494               | -0.527171 | 0.596641  |
| 21               | 6                | 0              | -3.512072               | -0.271916 | 0.574721  |
| 22               | 1                | 0              | -3.390980               | -1.792796 | -0.602638 |
| 23               | 1                | 0              | -2.261642               | 2.670159  | -0.637717 |
| 24               | 8                | 0              | -4.059347               | -1.036642 | -0.536382 |
| 25               | 6                | 0              | -3.579504               | 1.217077  | 0.262668  |
| 26               | 1                | 0              | -3.982881               | -0.535693 | 1.529578  |
| 27               | 1                | 0              | -1.562526               | -0.283945 | 1.584324  |

28                      6                      0                      -2.436706                      1.670140                      -0.262844

C6

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.608769                | -0.791092 | -0.439028 |
| 2                | 7                | 0              | 1.716891                | -1.857939 | -0.450221 |
| 3                | 1                | 0              | -3.247091               | 1.640508  | -1.251022 |
| 4                | 7                | 0              | 0.017628                | -0.460944 | 0.117146  |
| 5                | 6                | 0              | 0.404749                | -1.745476 | -0.286289 |
| 6                | 1                | 0              | -1.174003               | 1.100239  | 0.688493  |
| 7                | 1                | 0              | -0.314597               | -2.533535 | -0.428300 |
| 8                | 6                | 0              | 2.601985                | 1.973208  | 0.573103  |
| 9                | 7                | 0              | 1.313966                | 1.568434  | 0.583391  |
| 10               | 1                | 0              | 4.503814                | -1.758371 | -0.718639 |
| 11               | 6                | 0              | 2.220453                | -0.588713 | -0.139706 |
| 12               | 8                | 0              | -2.380423               | 1.248902  | -1.592444 |
| 13               | 7                | 0              | 3.690622                | 1.239271  | 0.246724  |
| 14               | 1                | 0              | 5.521409                | -0.353715 | -0.408322 |
| 15               | 1                | 0              | 2.787681                | 3.000492  | 0.858422  |
| 16               | 6                | 0              | 3.523847                | -0.056397 | -0.115871 |
| 17               | 6                | 0              | 1.182661                | 0.283271  | 0.214658  |
| 18               | 6                | 0              | -1.328112               | 0.060146  | 0.381402  |
| 19               | 1                | 0              | -4.068112               | -1.548114 | 1.657923  |
| 20               | 6                | 0              | -2.289312               | 0.019342  | -0.866599 |
| 21               | 6                | 0              | -3.685734               | -0.360783 | -0.253374 |
| 22               | 1                | 0              | -4.205531               | 1.272901  | 0.797267  |
| 23               | 1                | 0              | -1.596148               | -1.084292 | 2.337802  |
| 24               | 8                | 0              | -4.455704               | 0.901420  | -0.093744 |
| 25               | 6                | 0              | -3.342723               | -1.001736 | 1.069857  |
| 26               | 1                | 0              | -4.287421               | -0.975731 | -0.921933 |
| 27               | 1                | 0              | -1.946128               | -0.783893 | -1.525708 |
| 28               | 6                | 0              | -2.074479               | -0.760055 | 1.422394  |

C7

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.444915                | -1.117120 | -0.568719 |
| 2                | 7                | 0              | 1.496999                | -1.891212 | -0.104747 |
| 3                | 1                | 0              | -3.361109               | 1.762539  | 0.532064  |
| 4                | 7                | 0              | -0.011885               | -0.265977 | 0.387033  |
| 5                | 6                | 0              | 0.226209                | -1.630983 | 0.172604  |
| 6                | 1                | 0              | -0.992345               | 1.398125  | 1.102106  |
| 7                | 1                | 0              | -0.562413               | -2.357726 | 0.253240  |
| 8                | 6                | 0              | 2.788519                | 1.953082  | 0.152480  |
| 9                | 7                | 0              | 1.481653                | 1.680566  | 0.360311  |
| 10               | 1                | 0              | 4.236243                | -2.103646 | -0.659514 |
| 11               | 6                | 0              | 2.129786                | -0.642357 | -0.069662 |
| 12               | 8                | 0              | -3.037261               | 1.793302  | -0.412069 |
| 13               | 7                | 0              | 3.771246                | 1.075451  | -0.151920 |
| 14               | 1                | 0              | 5.387093                | -0.770031 | -0.699848 |
| 15               | 1                | 0              | 3.084685                | 2.990423  | 0.238157  |
| 16               | 6                | 0              | 3.464591                | -0.240516 | -0.268586 |
| 17               | 6                | 0              | 1.211079                | 0.370437  | 0.234241  |
| 18               | 6                | 0              | -1.277123               | 0.429182  | 0.683223  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 19 | 1 | 0 | -3.927532 | -1.656886 | 1.244977  |
| 20 | 6 | 0 | -2.154866 | 0.624474  | -0.582112 |
| 21 | 6 | 0 | -3.093149 | -0.626607 | -0.626117 |
| 22 | 1 | 0 | -4.402686 | 0.703312  | -1.113238 |
| 23 | 1 | 0 | -1.989039 | -0.554558 | 2.627922  |
| 24 | 8 | 0 | -4.364915 | -0.297393 | -1.220863 |
| 25 | 6 | 0 | -3.164406 | -0.993375 | 0.861327  |
| 26 | 1 | 0 | -2.644298 | -1.445699 | -1.197654 |
| 27 | 1 | 0 | -1.582011 | 0.800520  | -1.489086 |
| 28 | 6 | 0 | -2.182253 | -0.427603 | 1.571039  |

C9

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.472707                | -0.856066 | -0.691785 |
| 2                | 7                | 0              | 1.627293                | -1.932747 | -0.188455 |
| 3                | 1                | 0              | -2.327812               | 2.646114  | 0.094220  |
| 4                | 7                | 0              | -0.002283               | -0.491265 | 0.464094  |
| 5                | 6                | 0              | 0.347437                | -1.808239 | 0.142796  |
| 6                | 1                | 0              | -1.120387               | 0.838481  | 1.607859  |
| 7                | 1                | 0              | -0.375799               | -2.603099 | 0.180313  |
| 8                | 6                | 0              | 2.562965                | 1.995641  | 0.262754  |
| 9                | 7                | 0              | 1.295869                | 1.589518  | 0.499724  |
| 10               | 1                | 0              | 4.353953                | -1.851580 | -0.833166 |
| 11               | 6                | 0              | 2.145169                | -0.636054 | -0.085718 |
| 12               | 8                | 0              | -2.869618               | 1.815243  | 0.088316  |
| 13               | 7                | 0              | 3.612052                | 1.234694  | -0.122059 |
| 14               | 1                | 0              | 5.372189                | -0.413526 | -0.834582 |
| 15               | 1                | 0              | 2.763720                | 3.051254  | 0.393741  |
| 16               | 6                | 0              | 3.426970                | -0.096663 | -0.305455 |
| 17               | 6                | 0              | 1.148553                | 0.264226  | 0.313719  |
| 18               | 6                | 0              | -1.310399               | 0.071287  | 0.852968  |
| 19               | 1                | 0              | -4.040553               | -1.946339 | 0.493406  |
| 20               | 6                | 0              | -2.033681               | 0.704273  | -0.372349 |
| 21               | 6                | 0              | -3.079509               | -0.366645 | -0.843402 |
| 22               | 1                | 0              | -4.309461               | 1.111961  | -0.761365 |
| 23               | 1                | 0              | -2.162968               | -1.509068 | 2.264507  |
| 24               | 8                | 0              | -4.303824               | 0.253461  | -1.285252 |
| 25               | 6                | 0              | -3.230768               | -1.235104 | 0.404037  |
| 26               | 1                | 0              | -2.680111               | -0.958191 | -1.673832 |
| 27               | 1                | 0              | -1.332614               | 1.007993  | -1.152920 |
| 28               | 6                | 0              | -2.275420               | -1.014817 | 1.308428  |

C10

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | -4.612741               | 0.310459  | 0.098509  |
| 2                | 7                | 0              | -2.029427               | 1.958644  | 0.070270  |
| 3                | 1                | 0              | 1.704293                | -0.178502 | 2.588312  |
| 4                | 7                | 0              | -0.017022               | 0.901945  | -0.046229 |
| 5                | 6                | 0              | -0.714353               | 2.115582  | 0.027857  |
| 6                | 1                | 0              | 1.907638                | 1.669549  | 0.172758  |
| 7                | 1                | 0              | -0.190115               | 3.056277  | 0.048489  |
| 8                | 6                | 0              | -1.999195               | -2.098989 | -0.079699 |
| 9                | 7                | 0              | -0.823923               | -1.434379 | -0.099195 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 10 | 1 | 0 | -4.731401 | 1.315384  | 0.135724  |
| 11 | 6 | 0 | -2.215862 | 0.573571  | 0.017647  |
| 12 | 8 | 0 | 2.464649  | -0.077014 | 1.961645  |
| 13 | 7 | 0 | -3.241645 | -1.571208 | -0.021383 |
| 14 | 1 | 0 | -5.413505 | -0.309349 | 0.103460  |
| 15 | 1 | 0 | -1.940252 | -3.179174 | -0.112410 |
| 16 | 6 | 0 | -3.376239 | -0.223297 | 0.031865  |
| 17 | 6 | 0 | -0.984470 | -0.095605 | -0.056983 |
| 18 | 6 | 0 | 1.441629  | 0.747551  | -0.191322 |
| 19 | 1 | 0 | 3.530460  | -0.708933 | -2.451575 |
| 20 | 6 | 0 | 2.047110  | -0.440098 | 0.617823  |
| 21 | 6 | 0 | 3.345451  | -0.777648 | -0.169035 |
| 22 | 1 | 0 | 4.203262  | 0.197150  | 1.283413  |
| 23 | 1 | 0 | 1.456402  | 0.884607  | -2.477549 |
| 24 | 8 | 0 | 4.416474  | 0.091339  | 0.308738  |
| 25 | 6 | 0 | 2.966705  | -0.386169 | -1.587726 |
| 26 | 1 | 0 | 3.606824  | -1.838716 | -0.069909 |
| 27 | 1 | 0 | 1.344125  | -1.275937 | 0.580027  |
| 28 | 6 | 0 | 1.913657  | 0.434238  | -1.606695 |

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Table S4. Cartesian Coordinates (Å) for A, B, and C Optimized at the B3LYP/6-31+G(d,p) Level

A1

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 3.419468                | -1.217035 | 0.461529  |
| 2                | 6                | 0              | 3.446148                | 0.306388  | 0.541567  |
| 3                | 1                | 0              | 3.930547                | 0.660947  | 1.461512  |
| 4                | 6                | 0              | 1.951089                | 0.658385  | 0.511873  |
| 5                | 8                | 0              | 4.103808                | 0.826234  | -0.604034 |
| 6                | 6                | 0              | 1.409764                | -0.428380 | -0.446756 |
| 7                | 8                | 0              | 1.770584                | 1.980239  | 0.070596  |
| 8                | 1                | 0              | 1.514343                | 0.496240  | 1.508986  |
| 9                | 7                | 0              | 0.002012                | -0.765166 | -0.203721 |
| 10               | 1                | 0              | 4.263070                | -1.598381 | -0.118625 |
| 11               | 1                | 0              | 1.508227                | -0.091882 | -1.487893 |
| 12               | 8                | 0              | 2.187436                | -1.580907 | -0.215912 |
| 13               | 1                | 0              | 3.413991                | -1.679735 | 1.454992  |
| 14               | 6                | 0              | -0.575106               | -2.023002 | -0.151759 |
| 15               | 6                | 0              | -1.041047               | 0.132109  | -0.132238 |
| 16               | 1                | 0              | 0.801553                | 2.118444  | -0.045536 |
| 17               | 1                | 0              | 3.726135                | 1.705068  | -0.772191 |
| 18               | 7                | 0              | -1.884498               | -1.995969 | -0.034468 |
| 19               | 1                | 0              | 0.037606                | -2.910614 | -0.196204 |
| 20               | 6                | 0              | -2.194825               | -0.649145 | -0.023309 |
| 21               | 1                | 0              | -4.651160               | -1.579900 | 0.200924  |
| 22               | 6                | 0              | -3.414131               | 0.054394  | 0.077653  |
| 23               | 7                | 0              | -3.390628               | 1.403140  | 0.058632  |
| 24               | 7                | 0              | -4.605206               | -0.573316 | 0.193156  |
| 25               | 6                | 0              | -2.210551               | 2.026240  | -0.049540 |
| 26               | 7                | 0              | -0.991390               | 1.478005  | -0.147951 |
| 27               | 1                | 0              | -5.447872               | -0.023511 | 0.252290  |
| 28               | 1                | 0              | -2.247955               | 3.112215  | -0.057122 |

A4

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.769385                | 0.136668  | 1.442820  |
| 2                | 6                | 0              | 2.608431                | 0.938553  | 0.149834  |
| 3                | 1                | 0              | 1.853354                | 1.719105  | 0.265065  |
| 4                | 6                | 0              | 2.092281                | -0.132416 | -0.839870 |
| 5                | 8                | 0              | 3.867767                | 1.475625  | -0.261936 |
| 6                | 6                | 0              | 1.332027                | -1.117608 | 0.074415  |
| 7                | 8                | 0              | 3.177310                | -0.838833 | -1.423311 |
| 8                | 1                | 0              | 1.441259                | 0.287514  | -1.614576 |
| 9                | 7                | 0              | -0.116885               | -1.071009 | -0.038854 |
| 10               | 1                | 0              | 3.750552                | -0.356270 | 1.458898  |
| 11               | 1                | 0              | 1.627970                | -2.138721 | -0.187126 |
| 12               | 8                | 0              | 1.710671                | -0.828246 | 1.419442  |
| 13               | 1                | 0              | 2.650432                | 0.736373  | 2.347798  |
| 14               | 6                | 0              | -0.949588               | -2.178467 | -0.039049 |
| 15               | 6                | 0              | -0.959312               | 0.028901  | -0.029538 |
| 16               | 1                | 0              | 3.926606                | -0.220713 | -1.460619 |
| 17               | 1                | 0              | 3.729577                | 2.333244  | -0.682454 |
| 18               | 7                | 0              | -2.227144               | -1.888349 | -0.052094 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 19 | 1 | 0 | -0.536466 | -3.178690 | -0.032891 |
| 20 | 6 | 0 | -2.252302 | -0.504211 | -0.046370 |
| 21 | 1 | 0 | -4.853511 | -0.932598 | -0.029395 |
| 22 | 6 | 0 | -3.313117 | 0.426055  | -0.053973 |
| 23 | 7 | 0 | -3.021593 | 1.740615  | -0.041564 |
| 24 | 7 | 0 | -4.611573 | 0.044065  | -0.082525 |
| 25 | 6 | 0 | -1.731408 | 2.109545  | -0.028698 |
| 26 | 7 | 0 | -0.641410 | 1.333165  | -0.023336 |
| 27 | 1 | 0 | -5.329956 | 0.748691  | -0.025990 |
| 28 | 1 | 0 | -1.553941 | 3.182177  | -0.021084 |

A8

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.305434                | -1.125477 | -1.175278 |
| 2                | 6                | 0              | 3.031862                | -0.924977 | 0.144723  |
| 3                | 1                | 0              | 3.204027                | -1.850318 | 0.698247  |
| 4                | 6                | 0              | 2.073186                | 0.038892  | 0.887319  |
| 5                | 8                | 0              | 4.315278                | -0.305837 | -0.015490 |
| 6                | 6                | 0              | 1.410187                | 0.832174  | -0.284736 |
| 7                | 8                | 0              | 2.727237                | 0.875597  | 1.814556  |
| 8                | 1                | 0              | 1.312531                | -0.532398 | 1.423512  |
| 9                | 7                | 0              | -0.041444               | 0.935938  | -0.185420 |
| 10               | 1                | 0              | 2.957600                | -1.440047 | -1.993398 |
| 11               | 1                | 0              | 1.779770                | 1.860864  | -0.297963 |
| 12               | 8                | 0              | 1.809509                | 0.196340  | -1.494776 |
| 13               | 1                | 0              | 1.471319                | -1.827020 | -1.061086 |
| 14               | 6                | 0              | -0.774570               | 2.103351  | -0.325767 |
| 15               | 6                | 0              | -0.976177               | -0.072567 | -0.017097 |
| 16               | 1                | 0              | 3.661377                | 0.912022  | 1.545695  |
| 17               | 1                | 0              | 4.292306                | 0.258859  | -0.802349 |
| 18               | 7                | 0              | -2.071615               | 1.934388  | -0.246124 |
| 19               | 1                | 0              | -0.277748               | 3.052697  | -0.477693 |
| 20               | 6                | 0              | -2.216709               | 0.571452  | -0.053627 |
| 21               | 1                | 0              | -4.769420               | 1.232047  | -0.019062 |
| 22               | 6                | 0              | -3.352588               | -0.251331 | 0.103263  |
| 23               | 7                | 0              | -3.174741               | -1.575279 | 0.273098  |
| 24               | 7                | 0              | -4.612253               | 0.242309  | 0.084151  |
| 25               | 6                | 0              | -1.922163               | -2.057250 | 0.285680  |
| 26               | 7                | 0              | -0.770478               | -1.389250 | 0.148057  |
| 27               | 1                | 0              | -5.388217               | -0.385975 | 0.220764  |
| 28               | 1                | 0              | -1.836803               | -3.131879 | 0.425797  |

B1

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.068614               | -0.426461 | 1.309457  |
| 2                | 6                | 0              | -2.772228               | -0.915989 | -0.116235 |
| 3                | 1                | 0              | -2.065357               | -1.754159 | -0.086217 |
| 4                | 6                | 0              | -2.068248               | 0.280325  | -0.787338 |
| 5                | 8                | 0              | -3.917063               | -1.252657 | -0.903249 |
| 6                | 6                | 0              | -1.310416               | 0.993566  | 0.367357  |
| 7                | 8                | 0              | -3.018864               | 1.211789  | -1.298370 |
| 8                | 1                | 0              | -1.387160               | -0.041763 | -1.584029 |
| 9                | 7                | 0              | 0.142525                | 1.023157  | 0.200766  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 10 | 1 | 0 | -3.919487 | 0.263708  | 1.280689  |
| 11 | 1 | 0 | -1.634773 | 2.036451  | 0.345159  |
| 12 | 6 | 0 | -1.768193 | 0.304869  | 1.685959  |
| 13 | 1 | 0 | -3.310223 | -1.240127 | 2.001346  |
| 14 | 6 | 0 | 0.932286  | 2.152530  | 0.090445  |
| 15 | 6 | 0 | 1.011943  | -0.047397 | 0.113294  |
| 16 | 1 | 0 | -3.736934 | 0.697581  | -1.699682 |
| 17 | 1 | 0 | -4.318116 | -2.063919 | -0.569047 |
| 18 | 7 | 0 | 2.213703  | 1.902294  | -0.052237 |
| 19 | 1 | 0 | 0.490839  | 3.140186  | 0.121827  |
| 20 | 6 | 0 | 2.281825  | 0.521359  | -0.039961 |
| 21 | 1 | 0 | 5.360216  | -0.653544 | -0.462449 |
| 22 | 6 | 0 | 3.359044  | -0.382188 | -0.159222 |
| 23 | 7 | 0 | 3.103879  | -1.703415 | -0.123113 |
| 24 | 7 | 0 | 4.641564  | 0.033301  | -0.295909 |
| 25 | 6 | 0 | 1.831450  | -2.107174 | 0.028247  |
| 26 | 7 | 0 | 0.728884  | -1.360472 | 0.153646  |
| 27 | 1 | 0 | 4.843274  | 1.013569  | -0.413392 |
| 28 | 1 | 0 | 1.684440  | -3.184172 | 0.049887  |
| 29 | 1 | 0 | -1.009915 | -0.418668 | 1.997701  |
| 30 | 1 | 0 | -1.896378 | 1.027106  | 2.497075  |

B2

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.797148               | 1.472112  | -0.779567 |
| 2                | 6                | 0              | -3.280287               | 0.665153  | 0.429393  |
| 3                | 1                | 0              | -3.670191               | 1.287256  | 1.243975  |
| 4                | 6                | 0              | -2.032825               | -0.121812 | 0.855097  |
| 5                | 8                | 0              | -4.252676               | -0.336431 | 0.071790  |
| 6                | 6                | 0              | -1.402226               | -0.553605 | -0.499695 |
| 7                | 8                | 0              | -2.296199               | -1.193928 | 1.736375  |
| 8                | 1                | 0              | -1.343659               | 0.554814  | 1.368206  |
| 9                | 7                | 0              | 0.037779                | -0.782869 | -0.408565 |
| 10               | 1                | 0              | -3.628818               | 1.811929  | -1.405579 |
| 11               | 1                | 0              | -1.837621               | -1.517586 | -0.775635 |
| 12               | 6                | 0              | -1.813831               | 0.537131  | -1.530742 |
| 13               | 1                | 0              | -2.269296               | 2.362043  | -0.418731 |
| 14               | 6                | 0              | 0.696661                | -1.984297 | -0.585651 |
| 15               | 6                | 0              | 1.022016                | 0.139607  | -0.109722 |
| 16               | 1                | 0              | -3.140457               | -1.584384 | 1.460260  |
| 17               | 1                | 0              | -5.111142               | 0.079873  | -0.072108 |
| 18               | 7                | 0              | 1.999942                | -1.911871 | -0.436961 |
| 19               | 1                | 0              | 0.147007                | -2.885792 | -0.822579 |
| 20               | 6                | 0              | 2.222087                | -0.580502 | -0.137014 |
| 21               | 1                | 0              | 5.413230                | 0.132283  | 0.438285  |
| 22               | 6                | 0              | 3.394260                | 0.153100  | 0.141908  |
| 23               | 7                | 0              | 3.287741                | 1.466580  | 0.416223  |
| 24               | 7                | 0              | 4.625789                | -0.414557 | 0.126630  |
| 25               | 6                | 0              | 2.066443                | 2.026982  | 0.407773  |
| 26               | 7                | 0              | 0.886222                | 1.449916  | 0.157050  |
| 27               | 1                | 0              | 4.714094                | -1.414428 | 0.035967  |
| 28               | 1                | 0              | 2.039951                | 3.089450  | 0.636803  |
| 29               | 1                | 0              | -0.943011               | 1.087031  | -1.891496 |
| 30               | 1                | 0              | -2.292311               | 0.066775  | -2.394009 |

B3

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.688037               | 1.085796  | 0.452804  |
| 2                | 6                | 0              | -3.502801               | -0.439382 | 0.416744  |
| 3                | 1                | 0              | -4.020863               | -0.949730 | 1.239855  |
| 4                | 6                | 0              | -1.980344               | -0.660475 | 0.506783  |
| 5                | 8                | 0              | -3.987167               | -0.923032 | -0.833806 |
| 6                | 6                | 0              | -1.422290               | 0.514932  | -0.334111 |
| 7                | 8                | 0              | -1.687986               | -1.954627 | 0.034404  |
| 8                | 1                | 0              | -1.655312               | -0.531630 | 1.552911  |
| 9                | 7                | 0              | 0.017654                | 0.786128  | -0.150410 |
| 10               | 1                | 0              | -4.469162               | 1.361248  | -0.259742 |
| 11               | 1                | 0              | -1.587963               | 0.272284  | -1.389843 |
| 12               | 6                | 0              | -2.308859               | 1.706470  | 0.088196  |
| 13               | 1                | 0              | -4.012296               | 1.420803  | 1.442576  |
| 14               | 6                | 0              | 0.629025                | 2.029642  | -0.187305 |
| 15               | 6                | 0              | 1.056716                | -0.122130 | -0.075394 |
| 16               | 1                | 0              | -0.706176               | -2.050358 | -0.006231 |
| 17               | 1                | 0              | -3.535903               | -1.768098 | -0.995086 |
| 18               | 7                | 0              | 1.940250                | 1.991928  | -0.120317 |
| 19               | 1                | 0              | 0.047496                | 2.936339  | -0.265978 |
| 20               | 6                | 0              | 2.226753                | 0.643539  | -0.048477 |
| 21               | 1                | 0              | 5.483533                | 0.006196  | 0.125595  |
| 22               | 6                | 0              | 3.443785                | -0.065626 | 0.041092  |
| 23               | 7                | 0              | 3.411405                | -1.412199 | 0.088011  |
| 24               | 7                | 0              | 4.641855                | 0.558953  | 0.082291  |
| 25               | 6                | 0              | 2.221034                | -2.024509 | 0.050592  |
| 26               | 7                | 0              | 1.006687                | -1.466708 | -0.028360 |
| 27               | 1                | 0              | 4.693730                | 1.563871  | 0.030043  |
| 28               | 1                | 0              | 2.245391                | -3.110161 | 0.089638  |
| 29               | 1                | 0              | -1.870370               | 2.192658  | 0.966427  |
| 30               | 1                | 0              | -2.385738               | 2.461589  | -0.698996 |

C2

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.569264                | -0.059405 | -0.192136 |
| 2                | 7                | 0              | 2.205965                | 1.891977  | -0.024547 |
| 3                | 1                | 0              | -4.005799               | 0.475991  | -1.229058 |
| 4                | 7                | 0              | 0.091971                | 1.090489  | 0.098282  |
| 5                | 6                | 0              | 0.929603                | 2.189807  | 0.055534  |
| 6                | 1                | 0              | -1.651227               | 2.178600  | 0.075923  |
| 7                | 1                | 0              | 0.525863                | 3.193583  | 0.084650  |
| 8                | 6                | 0              | 1.673219                | -2.099658 | -0.041325 |
| 9                | 7                | 0              | 0.593053                | -1.315293 | 0.036486  |
| 10               | 1                | 0              | 4.819980                | 0.916164  | -0.204722 |
| 11               | 6                | 0              | 2.220123                | 0.509745  | -0.035212 |
| 12               | 8                | 0              | -3.203279               | 1.017092  | -1.329072 |
| 13               | 7                | 0              | 2.966067                | -1.741868 | -0.113302 |
| 14               | 1                | 0              | 5.280463                | -0.770230 | -0.257228 |
| 15               | 1                | 0              | 1.486689                | -3.170811 | -0.048384 |
| 16               | 6                | 0              | 3.269488                | -0.430553 | -0.114752 |
| 17               | 6                | 0              | 0.923332                | -0.013035 | 0.040933  |
| 18               | 6                | 0              | -1.371690               | 1.132923  | 0.236882  |
| 19               | 1                | 0              | -3.029464               | -1.068469 | 2.256152  |
| 20               | 6                | 0              | -2.129664               | 0.256225  | -0.801794 |
| 21               | 6                | 0              | -2.664215               | -0.967186 | 0.015960  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 22 | 1 | 0 | -4.024381 | -2.016338 | -0.966955 |
| 23 | 1 | 0 | -1.608923 | 1.103952  | 2.509064  |
| 24 | 8 | 0 | -4.021091 | -1.281067 | -0.341127 |
| 25 | 6 | 0 | -2.577638 | -0.504840 | 1.446470  |
| 26 | 1 | 0 | -2.019443 | -1.839209 | -0.139551 |
| 27 | 1 | 0 | -1.463434 | -0.052975 | -1.615348 |
| 28 | 6 | 0 | -1.855825 | 0.609945  | 1.574565  |

C3

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | 4.588880                | 0.496077  | 0.296557  |
| 2                | 7                | 0              | 1.900911                | 1.990794  | 0.108583  |
| 3                | 1                | 0              | -0.881759               | -2.049533 | -0.030246 |
| 4                | 7                | 0              | -0.004297               | 0.816014  | -0.226174 |
| 5                | 6                | 0              | 0.595750                | 2.049075  | -0.042244 |
| 6                | 1                | 0              | -1.450263               | 0.045300  | -1.502962 |
| 7                | 1                | 0              | 0.015851                | 2.960025  | -0.021542 |
| 8                | 6                | 0              | 2.147196                | -2.022965 | -0.202484 |
| 9                | 7                | 0              | 0.943646                | -1.441677 | -0.296849 |
| 10               | 1                | 0              | 4.654662                | 1.496676  | 0.395098  |
| 11               | 6                | 0              | 2.186944                | 0.642071  | 0.018118  |
| 12               | 8                | 0              | -1.832776               | -1.898332 | 0.167115  |
| 13               | 7                | 0              | 3.337475                | -1.436213 | -0.017788 |
| 14               | 1                | 0              | 5.415454                | -0.077669 | 0.356193  |
| 15               | 1                | 0              | 2.162435                | -3.106556 | -0.282657 |
| 16               | 6                | 0              | 3.388909                | -0.094101 | 0.101312  |
| 17               | 6                | 0              | 1.022510                | -0.102388 | -0.186626 |
| 18               | 6                | 0              | -1.412283               | 0.480196  | -0.495005 |
| 19               | 1                | 0              | -4.391918               | 1.886358  | 0.348047  |
| 20               | 6                | 0              | -1.986618               | -0.544860 | 0.526076  |
| 21               | 6                | 0              | -3.496292               | -0.200197 | 0.614756  |
| 22               | 1                | 0              | -3.810023               | -1.807951 | -0.419874 |
| 23               | 1                | 0              | -2.196272               | 2.611986  | -0.811460 |
| 24               | 8                | 0              | -4.262673               | -0.952966 | -0.322320 |
| 25               | 6                | 0              | -3.517288               | 1.257898  | 0.217700  |
| 26               | 1                | 0              | -3.885277               | -0.375807 | 1.627611  |
| 27               | 1                | 0              | -1.522080               | -0.336285 | 1.501341  |
| 28               | 6                | 0              | -2.381081               | 1.633416  | -0.379638 |

C6

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | -4.606574               | -0.798677 | 0.372570  |
| 2                | 7                | 0              | -1.709587               | -1.850829 | 0.403058  |
| 3                | 1                | 0              | 2.979655                | 1.620954  | 1.492522  |
| 4                | 7                | 0              | -0.010381               | -0.450887 | -0.114269 |
| 5                | 6                | 0              | -0.410611               | -1.724323 | 0.252367  |
| 6                | 1                | 0              | 1.200093                | 1.098125  | -0.633455 |
| 7                | 1                | 0              | 0.306066                | -2.522970 | 0.388650  |
| 8                | 6                | 0              | -2.579126               | 1.969729  | -0.534443 |
| 9                | 7                | 0              | -1.299336               | 1.583055  | -0.549690 |
| 10               | 1                | 0              | -4.499672               | -1.735536 | 0.728002  |
| 11               | 6                | 0              | -2.203652               | -0.590126 | 0.118220  |
| 12               | 8                | 0              | 2.273331                | 1.007184  | 1.757143  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 13 | 7 | 0 | -3.668974 | 1.241922  | -0.234181 |
| 14 | 1 | 0 | -5.499398 | -0.335523 | 0.440651  |
| 15 | 1 | 0 | -2.769063 | 3.007093  | -0.797682 |
| 16 | 6 | 0 | -3.508476 | -0.053041 | 0.094736  |
| 17 | 6 | 0 | -1.170462 | 0.294187  | -0.208252 |
| 18 | 6 | 0 | 1.339477  | 0.045423  | -0.361779 |
| 19 | 1 | 0 | 4.113600  | -1.392192 | -1.749361 |
| 20 | 6 | 0 | 2.309491  | -0.069083 | 0.856701  |
| 21 | 6 | 0 | 3.708232  | -0.284881 | 0.209578  |
| 22 | 1 | 0 | 4.181598  | 1.368649  | -0.777072 |
| 23 | 1 | 0 | 1.603823  | -1.028648 | -2.361529 |
| 24 | 8 | 0 | 4.398991  | 0.976415  | 0.080545  |
| 25 | 6 | 0 | 3.373437  | -0.903525 | -1.123535 |
| 26 | 1 | 0 | 4.360903  | -0.894333 | 0.840236  |
| 27 | 1 | 0 | 2.040287  | -0.972576 | 1.416741  |
| 28 | 6 | 0 | 2.086271  | -0.710012 | -1.442196 |

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