

# Origin of Substituent Effect on Tautomeric Behavior of 1,2,4-triazole Derivatives. Combined Spectroscopic and Theoretical Study

*Tetiana Sergeieva,<sup>†, II</sup> Maria Bilichenko,<sup>†</sup> Sergiy Holodnyak,<sup>II</sup> Yulia V. Monaykina,<sup>II</sup> Sergiy I.  
Okovytyy<sup>\*, †, ‡</sup>, Sergiy I. Kovalenko,<sup>II</sup> Eugene Voronkov<sup>⊥</sup>, Jerzy Leszczynski<sup>‡</sup>*

<sup>†</sup>Department of Chemistry, Oles Honchar Dnipropetrovsk National University, 72 Gagarina  
Ave., Dnipro, 49050, Ukraine

\*e-mail: sokovyty@icnanotox.org, tel.:+380505919276

<sup>‡</sup>Interdisciplinary Nanotoxicity Center, Jackson State University, 1400 J. R. Lynch Str., Jackson,  
Mississippi, 39217, USA

<sup>II</sup>Department of Pharmacy, Zaporihzhya State Medical University, 26 Mayakovsky Ave.,  
Zaporihzhya, 69035, Ukraine

<sup>⊥</sup>Department of Physics, V. Lazaryana Dnepropetrovsk National University of Railway  
Transport, 2 Lazaryana Str., Dnipro, 49010, Ukraine

**Table S1.** The optimized geometries of conformers for **2A-2C**. SMD/PBE1PBE/6-311++G\*\*

2A-T-1c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 5.080256         | -0.335304        | 0.102883  |
| 2                | 6                | 0              | 5.386711         | 0.881816         | -0.485213 |
| 3                | 6                | 0              | 4.371173         | 1.769366         | -0.834739 |
| 4                | 6                | 0              | 3.052882         | 1.406256         | -0.613602 |
| 5                | 6                | 0              | 2.723069         | 0.169988         | -0.047437 |
| 6                | 6                | 0              | 3.754141         | -0.708014        | 0.345905  |
| 7                | 7                | 0              | 3.466004         | -1.948426        | 0.922735  |
| 8                | 6                | 0              | 1.307507         | -0.175081        | 0.070904  |
| 9                | 7                | 0              | 0.813915         | -1.427356        | 0.135990  |
| 10               | 7                | 0              | -0.526040        | -1.418622        | 0.158504  |
| 11               | 6                | 0              | -0.810082        | -0.122472        | 0.115894  |
| 12               | 7                | 0              | 0.293380         | 0.676081         | 0.061578  |
| 13               | 6                | 0              | -2.160516        | 0.454110         | 0.166631  |
| 14               | 6                | 0              | -2.279120        | 1.803585         | 0.510224  |
| 15               | 6                | 0              | -3.510277        | 2.440373         | 0.579702  |
| 16               | 6                | 0              | -4.661361        | 1.717523         | 0.295763  |
| 17               | 6                | 0              | -4.577862        | 0.375163         | -0.054808 |
| 18               | 6                | 0              | -3.339405        | -0.267150        | -0.123695 |
| 19               | 1                | 0              | 5.876638         | -1.011892        | 0.398914  |
| 20               | 1                | 0              | 6.425546         | 1.143510         | -0.658521 |
| 21               | 1                | 0              | 4.605549         | 2.727605         | -1.284558 |
| 22               | 1                | 0              | 2.243320         | 2.069042         | -0.898624 |
| 23               | 1                | 0              | 2.803323         | -1.904818        | 1.687933  |
| 24               | 1                | 0              | 4.294655         | -2.441109        | 1.227788  |
| 25               | 1                | 0              | -1.368813        | 2.350518         | 0.727584  |
| 26               | 1                | 0              | -3.567391        | 3.487779         | 0.854538  |
| 27               | 1                | 0              | -5.635945        | 2.192498         | 0.344588  |
| 28               | 1                | 0              | -5.485684        | -0.170285        | -0.278185 |
| 29               | 8                | 0              | -3.207847        | -1.563449        | -0.471801 |
| 30               | 6                | 0              | -4.372714        | -2.294583        | -0.811830 |
| 31               | 1                | 0              | -4.886419        | -1.850734        | -1.670833 |
| 32               | 1                | 0              | -4.028780        | -3.293996        | -1.074247 |
| 33               | 1                | 0              | -5.063802        | -2.361179        | 0.034638  |
| 34               | 1                | 0              | 1.333345         | -2.294530        | 0.112242  |

## 2A-T-1c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.714777        | 1.154118         | 0.191869  |
| 2                | 6                | 0              | -5.545985        | 0.051966         | 0.205141  |
| 3                | 6                | 0              | -5.017045        | -1.237299        | 0.106418  |
| 4                | 6                | 0              | -3.647598        | -1.387935        | -0.002768 |
| 5                | 6                | 0              | -2.777546        | -0.287763        | -0.024345 |
| 6                | 6                | 0              | -3.317728        | 1.020536         | 0.076652  |
| 7                | 7                | 0              | -2.531598        | 2.136007         | 0.019831  |
| 8                | 6                | 0              | -1.341176        | -0.499511        | -0.138215 |
| 9                | 7                | 0              | -0.752578        | -1.683021        | -0.408300 |
| 10               | 7                | 0              | 0.584884         | -1.571235        | -0.425393 |
| 11               | 6                | 0              | 0.778489         | -0.288021        | -0.162641 |
| 12               | 7                | 0              | -0.382607        | 0.406283         | 0.016996  |
| 13               | 6                | 0              | 2.081503         | 0.385461         | -0.095091 |
| 14               | 6                | 0              | 2.098400         | 1.780436         | -0.179356 |
| 15               | 6                | 0              | 3.278743         | 2.507728         | -0.121445 |
| 16               | 6                | 0              | 4.481696         | 1.831036         | 0.029822  |
| 17               | 6                | 0              | 4.499432         | 0.444470         | 0.123374  |
| 18               | 6                | 0              | 3.312239         | -0.288946        | 0.063202  |
| 19               | 1                | 0              | -5.134090        | 2.152991         | 0.269163  |
| 20               | 1                | 0              | -6.617996        | 0.195162         | 0.297205  |
| 21               | 1                | 0              | -5.664014        | -2.106580        | 0.123915  |
| 22               | 1                | 0              | -3.242383        | -2.393144        | -0.057532 |
| 23               | 1                | 0              | -1.536161        | 2.006291         | 0.157676  |
| 24               | 1                | 0              | -2.934326        | 3.006342         | 0.326352  |
| 25               | 1                | 0              | 1.150336         | 2.292240         | -0.297646 |
| 26               | 1                | 0              | 3.256601         | 3.589308         | -0.195060 |
| 27               | 1                | 0              | 5.418428         | 2.376981         | 0.076867  |
| 28               | 1                | 0              | 5.446331         | -0.065236        | 0.246074  |
| 29               | 8                | 0              | 3.278729         | -1.633230        | 0.160484  |
| 30               | 6                | 0              | 4.495656         | -2.327545        | 0.371759  |
| 31               | 1                | 0              | 4.977549         | -2.013998        | 1.303500  |
| 32               | 1                | 0              | 4.227161         | -3.380647        | 0.441065  |
| 33               | 1                | 0              | 5.187253         | -2.185414        | -0.464897 |
| 34               | 1                | 0              | -1.177051        | -2.577082        | -0.598753 |

## 2A-T-1c3

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.311831         | 1.370415         | -0.453089 |
| 2                | 6                | 0              | 5.319389         | 0.437316         | -0.306250 |
| 3                | 6                | 0              | 5.018097         | -0.892492        | -0.003352 |
| 4                | 6                | 0              | 3.692749         | -1.256643        | 0.146546  |
| 5                | 6                | 0              | 2.649105         | -0.330262        | 0.009829  |
| 6                | 6                | 0              | 2.956972         | 1.019508         | -0.301077 |
| 7                | 7                | 0              | 1.988427         | 1.977652         | -0.405460 |
| 8                | 6                | 0              | 1.267953         | -0.758646        | 0.181722  |
| 9                | 7                | 0              | 0.882304         | -1.929246        | 0.729892  |
| 10               | 7                | 0              | -0.454950        | -2.041235        | 0.738798  |
| 11               | 6                | 0              | -0.850108        | -0.907311        | 0.180888  |
| 12               | 7                | 0              | 0.175595         | -0.088740        | -0.173052 |
| 13               | 6                | 0              | -2.272435        | -0.636953        | -0.068101 |
| 14               | 6                | 0              | -3.094529        | -1.686982        | -0.477113 |
| 15               | 6                | 0              | -4.449268        | -1.498995        | -0.721299 |
| 16               | 6                | 0              | -4.995063        | -0.233027        | -0.556732 |
| 17               | 6                | 0              | -4.200738        | 0.831429         | -0.143058 |
| 18               | 6                | 0              | -2.841188        | 0.640440         | 0.109333  |
| 19               | 1                | 0              | 4.555780         | 2.401783         | -0.690198 |
| 20               | 1                | 0              | 6.352207         | 0.745702         | -0.434526 |
| 21               | 1                | 0              | 5.804602         | -1.630592        | 0.102553  |
| 22               | 1                | 0              | 3.459891         | -2.296118        | 0.355816  |
| 23               | 1                | 0              | 1.033475         | 1.657264         | -0.522294 |
| 24               | 1                | 0              | 2.241995         | 2.849326         | -0.840875 |
| 25               | 1                | 0              | -2.646213        | -2.665492        | -0.612078 |
| 26               | 1                | 0              | -5.066096        | -2.330010        | -1.044703 |
| 27               | 1                | 0              | -6.049370        | -0.061575        | -0.748670 |
| 28               | 1                | 0              | -4.648819        | 1.807855         | -0.010496 |
| 29               | 8                | 0              | -2.023887        | 1.620269         | 0.550069  |
| 30               | 6                | 0              | -2.572080        | 2.908864         | 0.766046  |
| 31               | 1                | 0              | -3.360091        | 2.885228         | 1.525890  |
| 32               | 1                | 0              | -1.748023        | 3.526356         | 1.120369  |
| 33               | 1                | 0              | -2.969528        | 3.333636         | -0.161421 |
| 34               | 1                | 0              | 1.447525         | -2.654501        | 1.143064  |

## 2A-T-1c4

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.969693         | -0.084316        | 0.114413  |
| 2                | 6                | 0              | 5.075734         | 1.274578         | 0.366401  |
| 3                | 6                | 0              | 3.930272         | 2.051128         | 0.527554  |
| 4                | 6                | 0              | 2.687107         | 1.453105         | 0.403031  |
| 5                | 6                | 0              | 2.560440         | 0.088553         | 0.120447  |
| 6                | 6                | 0              | 3.720951         | -0.703914        | 0.001001  |
| 7                | 7                | 0              | 3.636075         | -2.071884        | -0.275841 |
| 8                | 6                | 0              | 1.215966         | -0.446892        | -0.085941 |
| 9                | 7                | 0              | 0.920439         | -1.560264        | -0.785889 |
| 10               | 7                | 0              | -0.405062        | -1.745806        | -0.854048 |
| 11               | 6                | 0              | -0.878001        | -0.716276        | -0.164331 |
| 12               | 7                | 0              | 0.083421         | 0.107823         | 0.326606  |
| 13               | 6                | 0              | -2.321001        | -0.567950        | 0.078889  |
| 14               | 6                | 0              | -3.060556        | -1.685918        | 0.461290  |
| 15               | 6                | 0              | -4.427817        | -1.606810        | 0.699986  |
| 16               | 6                | 0              | -5.068043        | -0.383901        | 0.553723  |
| 17               | 6                | 0              | -4.356750        | 0.746187         | 0.162005  |
| 18               | 6                | 0              | -2.985574        | 0.663400         | -0.084331 |
| 19               | 1                | 0              | 5.865369         | -0.690636        | 0.016733  |
| 20               | 1                | 0              | 6.058969         | 1.726040         | 0.450765  |
| 21               | 1                | 0              | 4.007169         | 3.112336         | 0.735931  |
| 22               | 1                | 0              | 1.780668         | 2.040411         | 0.499525  |
| 23               | 1                | 0              | 2.996782         | -2.576871        | 0.326550  |
| 24               | 1                | 0              | 4.536844         | -2.531337        | -0.264383 |
| 25               | 1                | 0              | -2.539001        | -2.629735        | 0.580552  |
| 26               | 1                | 0              | -4.981181        | -2.488434        | 1.003655  |
| 27               | 1                | 0              | -6.133511        | -0.297676        | 0.741354  |
| 28               | 1                | 0              | -4.879674        | 1.686457         | 0.041092  |
| 29               | 8                | 0              | -2.240734        | 1.706405         | -0.508696 |
| 30               | 6                | 0              | -2.881644        | 2.953306         | -0.712539 |
| 31               | 1                | 0              | -3.313313        | 3.336558         | 0.217704  |
| 32               | 1                | 0              | -2.104483        | 3.634542         | -1.055710 |
| 33               | 1                | 0              | -3.662699        | 2.880229         | -1.476440 |
| 34               | 1                | 0              | 1.565159         | -2.167884        | -1.273152 |

## 2A-T-2c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 5.090952         | 0.381655         | -0.005690 |
| 2                | 6                | 0              | 5.402211         | -0.964696        | -0.039916 |
| 3                | 6                | 0              | 4.387877         | -1.923883        | -0.042287 |
| 4                | 6                | 0              | 3.070086         | -1.501442        | -0.018305 |
| 5                | 6                | 0              | 2.725047         | -0.143715        | 0.012518  |
| 6                | 6                | 0              | 3.756801         | 0.827446         | 0.027458  |
| 7                | 7                | 0              | 3.499029         | 2.171224         | 0.120561  |
| 8                | 6                | 0              | 1.305340         | 0.210747         | 0.012288  |
| 9                | 7                | 0              | 0.851971         | 1.462545         | -0.010815 |
| 10               | 7                | 0              | -0.477752        | 1.303928         | -0.019793 |
| 11               | 6                | 0              | -0.802090        | -0.001396        | 0.001934  |
| 12               | 7                | 0              | 0.313638         | -0.719065        | 0.021741  |
| 13               | 6                | 0              | -2.156049        | -0.546924        | 0.005112  |
| 14               | 6                | 0              | -2.313257        | -1.934991        | 0.021603  |
| 15               | 6                | 0              | -3.570516        | -2.518879        | 0.026192  |
| 16               | 6                | 0              | -4.698074        | -1.705684        | 0.014221  |
| 17               | 6                | 0              | -4.572429        | -0.321596        | -0.002162 |
| 18               | 6                | 0              | -3.307987        | 0.264879         | -0.006807 |
| 19               | 1                | 0              | 5.884455         | 1.123616         | 0.001741  |
| 20               | 1                | 0              | 6.443860         | -1.269838        | -0.064423 |
| 21               | 1                | 0              | 4.624956         | -2.981679        | -0.067403 |
| 22               | 1                | 0              | 2.263292         | -2.226043        | -0.028217 |
| 23               | 1                | 0              | 2.554995         | 2.479101         | -0.071754 |
| 24               | 1                | 0              | 4.241212         | 2.799185         | -0.142525 |
| 25               | 1                | 0              | -1.418739        | -2.547283        | 0.030862  |
| 26               | 1                | 0              | -3.669606        | -3.598347        | 0.038914  |
| 27               | 1                | 0              | -5.690053        | -2.145152        | 0.017578  |
| 28               | 1                | 0              | -5.462208        | 0.294599         | -0.011112 |
| 29               | 8                | 0              | -3.110136        | 1.604172         | -0.022278 |
| 30               | 6                | 0              | -4.241487        | 2.465262         | -0.033636 |
| 31               | 1                | 0              | -4.850619        | 2.322066         | 0.863155  |
| 32               | 1                | 0              | -3.842497        | 3.477798         | -0.044794 |
| 33               | 1                | 0              | -4.848370        | 2.301403         | -0.928407 |
| 34               | 1                | 0              | -1.116352        | 2.086075         | -0.032374 |

## 2A-T-2c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.749595        | 1.122793         | -0.039045 |
| 2                | 6                | 0              | -5.561299        | 0.012207         | 0.093504  |
| 3                | 6                | 0              | -5.001848        | -1.264549        | 0.174886  |
| 4                | 6                | 0              | -3.625038        | -1.393354        | 0.128083  |
| 5                | 6                | 0              | -2.777569        | -0.285059        | -0.004462 |
| 6                | 6                | 0              | -3.347864        | 1.008073         | -0.095840 |
| 7                | 7                | 0              | -2.586120        | 2.134367         | -0.289127 |
| 8                | 6                | 0              | -1.329480        | -0.508256        | -0.032477 |
| 9                | 7                | 0              | -0.800750        | -1.727513        | -0.089321 |
| 10               | 7                | 0              | 0.514503         | -1.483714        | -0.071180 |
| 11               | 6                | 0              | 0.766994         | -0.166083        | -0.009495 |
| 12               | 7                | 0              | -0.395107        | 0.480047         | 0.015220  |
| 13               | 6                | 0              | 2.084507         | 0.458614         | 0.023989  |
| 14               | 6                | 0              | 2.162714         | 1.852606         | 0.079119  |
| 15               | 6                | 0              | 3.384879         | 2.505946         | 0.113723  |
| 16               | 6                | 0              | 4.556940         | 1.758609         | 0.093501  |
| 17               | 6                | 0              | 4.510203         | 0.370475         | 0.039028  |
| 18               | 6                | 0              | 3.281432         | -0.285696        | 0.004187  |
| 19               | 1                | 0              | -5.190458        | 2.113399         | -0.106735 |
| 20               | 1                | 0              | -6.638446        | 0.141366         | 0.135059  |
| 21               | 1                | 0              | -5.631793        | -2.140672        | 0.281011  |
| 22               | 1                | 0              | -3.169537        | -2.374997        | 0.201715  |
| 23               | 1                | 0              | -1.597227        | 2.048484         | -0.086622 |
| 24               | 1                | 0              | -3.016618        | 3.016388         | -0.062053 |
| 25               | 1                | 0              | 1.236650         | 2.415869         | 0.094459  |
| 26               | 1                | 0              | 3.422239         | 3.588549         | 0.156030  |
| 27               | 1                | 0              | 5.522124         | 2.253445         | 0.120214  |
| 28               | 1                | 0              | 5.433075         | -0.194926        | 0.024514  |
| 29               | 8                | 0              | 3.159698         | -1.633001        | -0.048794 |
| 30               | 6                | 0              | 4.337736         | -2.428987        | -0.068431 |
| 31               | 1                | 0              | 4.928352         | -2.274771        | 0.838837  |
| 32               | 1                | 0              | 3.996195         | -3.461575        | -0.109549 |
| 33               | 1                | 0              | 4.943553         | -2.208532        | -0.951714 |
| 34               | 1                | 0              | 1.200364         | -2.224349        | -0.105595 |

## 2A-T-2c3

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.362724        | 1.273437         | -0.652364 |
| 2                | 6                | 0              | -5.351402        | 0.473428         | -0.112254 |
| 3                | 6                | 0              | -5.022731        | -0.737829        | 0.499991  |
| 4                | 6                | 0              | -3.692691        | -1.113909        | 0.561831  |
| 5                | 6                | 0              | -2.668873        | -0.320836        | 0.026170  |
| 6                | 6                | 0              | -3.005673        | 0.901736         | -0.605045 |
| 7                | 7                | 0              | -2.066772        | 1.700476         | -1.209399 |
| 8                | 6                | 0              | -1.283923        | -0.782693        | 0.152019  |
| 9                | 7                | 0              | -0.974799        | -1.977316        | 0.645275  |
| 10               | 7                | 0              | 0.363028         | -1.980210        | 0.598764  |
| 11               | 6                | 0              | 0.837687         | -0.827889        | 0.094463  |
| 12               | 7                | 0              | -0.190842        | -0.045989        | -0.199040 |
| 13               | 6                | 0              | 2.265615         | -0.584822        | -0.119222 |
| 14               | 6                | 0              | 3.056665         | -1.604342        | -0.650851 |
| 15               | 6                | 0              | 4.418049         | -1.428220        | -0.861630 |
| 16               | 6                | 0              | 4.998080         | -0.209309        | -0.537031 |
| 17               | 6                | 0              | 4.233612         | 0.822252         | -0.002207 |
| 18               | 6                | 0              | 2.866693         | 0.646061         | 0.215168  |
| 19               | 1                | 0              | -4.625175        | 2.211692         | -1.132953 |
| 20               | 1                | 0              | -6.386789        | 0.795228         | -0.167862 |
| 21               | 1                | 0              | -5.792691        | -1.370986        | 0.926551  |
| 22               | 1                | 0              | -3.414489        | -2.045361        | 1.043122  |
| 23               | 1                | 0              | -1.099263        | 1.526485         | -0.962871 |
| 24               | 1                | 0              | -2.325865        | 2.659457         | -1.376698 |
| 25               | 1                | 0              | 2.587897         | -2.544180        | -0.925102 |
| 26               | 1                | 0              | 5.012600         | -2.230395        | -1.283350 |
| 27               | 1                | 0              | 6.059045         | -0.049269        | -0.698913 |
| 28               | 1                | 0              | 4.710310         | 1.760584         | 0.250918  |
| 29               | 8                | 0              | 2.069702         | 1.586369         | 0.757400  |
| 30               | 6                | 0              | 2.645308         | 2.829817         | 1.123766  |
| 31               | 1                | 0              | 3.064768         | 3.344145         | 0.253525  |
| 32               | 1                | 0              | 1.830580         | 3.423032         | 1.535591  |
| 33               | 1                | 0              | 3.421037         | 2.699756         | 1.884985  |
| 34               | 1                | 0              | 0.883953         | -2.771162        | 0.947833  |

## 2A-T-2c4

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.996406        | 0.003018         | -0.001345 |
| 2                | 6                | 0              | -5.069052        | 1.242011         | -0.609994 |
| 3                | 6                | 0              | -3.903879        | 1.918964         | -0.974494 |
| 4                | 6                | 0              | -2.680134        | 1.322940         | -0.724337 |
| 5                | 6                | 0              | -2.576490        | 0.066018         | -0.113810 |
| 6                | 6                | 0              | -3.760192        | -0.613111        | 0.267187  |
| 7                | 7                | 0              | -3.736681        | -1.817048        | 0.924039  |
| 8                | 6                | 0              | -1.241064        | -0.497530        | 0.085937  |
| 9                | 7                | 0              | -1.009581        | -1.694522        | 0.617878  |
| 10               | 7                | 0              | 0.326440         | -1.789789        | 0.577527  |
| 11               | 6                | 0              | 0.867227         | -0.678507        | 0.042516  |
| 12               | 7                | 0              | -0.103316        | 0.158808         | -0.279077 |
| 13               | 6                | 0              | 2.309511         | -0.529679        | -0.172043 |
| 14               | 6                | 0              | 3.028402         | -1.590389        | -0.724100 |
| 15               | 6                | 0              | 4.396784         | -1.498879        | -0.945197 |
| 16               | 6                | 0              | 5.056232         | -0.324257        | -0.609771 |
| 17               | 6                | 0              | 4.364342         | 0.746023         | -0.052461 |
| 18               | 6                | 0              | 2.990970         | 0.654250         | 0.176108  |
| 19               | 1                | 0              | -5.906446        | -0.516199        | 0.285722  |
| 20               | 1                | 0              | -6.041756        | 1.684828         | -0.800955 |
| 21               | 1                | 0              | -3.953602        | 2.892199         | -1.449931 |
| 22               | 1                | 0              | -1.760141        | 1.823025         | -1.005957 |
| 23               | 1                | 0              | -2.869051        | -2.336442        | 0.913414  |
| 24               | 1                | 0              | -4.585516        | -2.359187        | 0.915734  |
| 25               | 1                | 0              | 2.497286         | -2.493955        | -1.006613 |
| 26               | 1                | 0              | 4.935189         | -2.331402        | -1.383245 |
| 27               | 1                | 0              | 6.123734         | -0.229627        | -0.780042 |
| 28               | 1                | 0              | 4.902741         | 1.648042         | 0.208666  |
| 29               | 8                | 0              | 2.260849         | 1.634321         | 0.741891  |
| 30               | 6                | 0              | 2.919391         | 2.830016         | 1.126834  |
| 31               | 1                | 0              | 3.363034         | 3.334210         | 0.262641  |
| 32               | 1                | 0              | 2.148971         | 3.466082         | 1.559450  |
| 33               | 1                | 0              | 3.692504         | 2.634036         | 1.876544  |
| 34               | 1                | 0              | 0.794381         | -2.597645        | 0.960688  |

## 2A-T-3c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -5.083729        | 0.361290         | 0.068066  |
| 2                | 6                | 0              | -5.369077        | -0.899284        | 0.554064  |
| 3                | 6                | 0              | -4.341468        | -1.811240        | 0.804667  |
| 4                | 6                | 0              | -3.036284        | -1.430587        | 0.552082  |
| 5                | 6                | 0              | -2.714283        | -0.158509        | 0.056483  |
| 6                | 6                | 0              | -3.761129        | 0.768707         | -0.190101 |
| 7                | 7                | 0              | -3.515021        | 2.038084         | -0.625751 |
| 8                | 6                | 0              | -1.327533        | 0.192943         | -0.210746 |
| 9                | 7                | 0              | -0.886877        | 1.310581         | -0.762320 |
| 10               | 7                | 0              | 0.470574         | 1.252311         | -0.844645 |
| 11               | 6                | 0              | 0.850172         | 0.101327         | -0.340791 |
| 12               | 7                | 0              | -0.250346        | -0.594634        | 0.064533  |
| 13               | 6                | 0              | 2.205286         | -0.447512        | -0.257473 |
| 14               | 6                | 0              | 2.419908         | -1.779460        | -0.615272 |
| 15               | 6                | 0              | 3.683343         | -2.352735        | -0.552459 |
| 16               | 6                | 0              | 4.753489         | -1.579166        | -0.123809 |
| 17               | 6                | 0              | 4.566924         | -0.251353        | 0.245554  |
| 18               | 6                | 0              | 3.297525         | 0.325624         | 0.187351  |
| 19               | 1                | 0              | -5.887238        | 1.067073         | -0.121135 |
| 20               | 1                | 0              | -6.401813        | -1.177195        | 0.739652  |
| 21               | 1                | 0              | -4.558197        | -2.802754        | 1.184881  |
| 22               | 1                | 0              | -2.246040        | -2.151152        | 0.737118  |
| 23               | 1                | 0              | -2.585120        | 2.242804         | -0.975017 |
| 24               | 1                | 0              | -4.287892        | 2.568710         | -0.992105 |
| 25               | 1                | 0              | 1.580745         | -2.369192        | -0.971070 |
| 26               | 1                | 0              | 3.827881         | -3.386929        | -0.843152 |
| 27               | 1                | 0              | 5.749935         | -2.005620        | -0.071895 |
| 28               | 1                | 0              | 5.415247         | 0.328585         | 0.585858  |
| 29               | 8                | 0              | 3.038127         | 1.594079         | 0.558836  |
| 30               | 6                | 0              | 4.107142         | 2.385740         | 1.049529  |
| 31               | 1                | 0              | 4.881260         | 2.523939         | 0.288145  |
| 32               | 1                | 0              | 3.670208         | 3.351411         | 1.298418  |
| 33               | 1                | 0              | 4.549053         | 1.944248         | 1.948536  |
| 34               | 1                | 0              | -0.243057        | -1.485666        | 0.535485  |

## 2A-T-3c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.409857        | -1.821170        | -0.883389 |
| 2                | 6                | 0              | -5.269462        | -0.974010        | -1.565488 |
| 3                | 6                | 0              | -4.833276        | 0.281176         | -1.983863 |
| 4                | 6                | 0              | -3.522819        | 0.657402         | -1.737436 |
| 5                | 6                | 0              | -2.634527        | -0.193838        | -1.071392 |
| 6                | 6                | 0              | -3.090943        | -1.445323        | -0.609690 |
| 7                | 7                | 0              | -2.232449        | -2.319843        | 0.066365  |
| 8                | 6                | 0              | -1.247374        | 0.238110         | -0.912797 |
| 9                | 7                | 0              | -0.821956        | 1.484626         | -0.910016 |
| 10               | 7                | 0              | 0.535713         | 1.467835         | -0.806189 |
| 11               | 6                | 0              | 0.923334         | 0.212322         | -0.745580 |
| 12               | 7                | 0              | -0.174469        | -0.591935        | -0.808222 |
| 13               | 6                | 0              | 2.288375         | -0.315372        | -0.686750 |
| 14               | 6                | 0              | 2.621321         | -1.419154        | -1.474062 |
| 15               | 6                | 0              | 3.897021         | -1.967644        | -1.455420 |
| 16               | 6                | 0              | 4.861930         | -1.400830        | -0.633972 |
| 17               | 6                | 0              | 4.557016         | -0.304140        | 0.165046  |
| 18               | 6                | 0              | 3.274256         | 0.245347         | 0.151813  |
| 19               | 1                | 0              | -4.761932        | -2.788047        | -0.535769 |
| 20               | 1                | 0              | -6.288551        | -1.292037        | -1.760348 |
| 21               | 1                | 0              | -5.503590        | 0.951774         | -2.509769 |
| 22               | 1                | 0              | -3.152454        | 1.617336         | -2.079889 |
| 23               | 1                | 0              | -1.725587        | -1.890388        | 0.831255  |
| 24               | 1                | 0              | -2.704573        | -3.147290        | 0.405316  |
| 25               | 1                | 0              | 1.867053         | -1.841967        | -2.130432 |
| 26               | 1                | 0              | 4.132803         | -2.820543        | -2.081494 |
| 27               | 1                | 0              | 5.866638         | -1.809893        | -0.607271 |
| 28               | 1                | 0              | 5.323058         | 0.115581         | 0.804432  |
| 29               | 8                | 0              | 2.904117         | 1.285584         | 0.923728  |
| 30               | 6                | 0              | 3.860531         | 1.841837         | 1.810195  |
| 31               | 1                | 0              | 4.713647         | 2.257197         | 1.264556  |
| 32               | 1                | 0              | 3.345036         | 2.643226         | 2.336934  |
| 33               | 1                | 0              | 4.212189         | 1.098789         | 2.533114  |
| 34               | 1                | 0              | -0.215420        | -1.602218        | -0.772734 |

## 2A-T-3c3

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.310999         | 1.313388         | 0.182566  |
| 2                | 6                | 0              | 5.262389         | 0.447319         | -0.332328 |
| 3                | 6                | 0              | 4.919152         | -0.864594        | -0.653079 |
| 4                | 6                | 0              | 3.609671         | -1.280240        | -0.476343 |
| 5                | 6                | 0              | 2.630071         | -0.414863        | 0.023394  |
| 6                | 6                | 0              | 2.988779         | 0.900780         | 0.384755  |
| 7                | 7                | 0              | 2.045808         | 1.797604         | 0.887532  |
| 8                | 6                | 0              | 1.259146         | -0.909465        | 0.126837  |
| 9                | 7                | 0              | 0.904521         | -2.170898        | 0.275963  |
| 10               | 7                | 0              | -0.452164        | -2.231807        | 0.257685  |
| 11               | 6                | 0              | -0.913903        | -1.005877        | 0.099695  |
| 12               | 7                | 0              | 0.137494         | -0.147845        | 0.020136  |
| 13               | 6                | 0              | -2.325318        | -0.641968        | 0.029262  |
| 14               | 6                | 0              | -3.283405        | -1.654601        | 0.133122  |
| 15               | 6                | 0              | -4.639790        | -1.376079        | 0.073337  |
| 16               | 6                | 0              | -5.058763        | -0.061035        | -0.094351 |
| 17               | 6                | 0              | -4.129435        | 0.966618         | -0.201535 |
| 18               | 6                | 0              | -2.765252        | 0.686325         | -0.141122 |
| 19               | 1                | 0              | 4.589521         | 2.327756         | 0.453360  |
| 20               | 1                | 0              | 6.280065         | 0.796764         | -0.473810 |
| 21               | 1                | 0              | 5.660669         | -1.548965        | -1.049711 |
| 22               | 1                | 0              | 3.312483         | -2.288135        | -0.744344 |
| 23               | 1                | 0              | 1.424050         | 1.410663         | 1.586109  |
| 24               | 1                | 0              | 2.456757         | 2.653691         | 1.233594  |
| 25               | 1                | 0              | -2.935351        | -2.672978        | 0.263268  |
| 26               | 1                | 0              | -5.363798        | -2.178760        | 0.156756  |
| 27               | 1                | 0              | -6.116512        | 0.175427         | -0.143479 |
| 28               | 1                | 0              | -4.472950        | 1.984708         | -0.332154 |
| 29               | 8                | 0              | -1.808138        | 1.641573         | -0.238775 |
| 30               | 6                | 0              | -2.204286        | 2.994154         | -0.420473 |
| 31               | 1                | 0              | -2.802635        | 3.344586         | 0.425346  |
| 32               | 1                | 0              | -1.280735        | 3.567728         | -0.474917 |
| 33               | 1                | 0              | -2.765849        | 3.116001         | -1.351042 |
| 34               | 1                | 0              | 0.069437         | 0.850375         | -0.130408 |

## 2A-T-3c4

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.967905         | -0.085065        | 0.019138  |
| 2                | 6                | 0              | 5.048382         | 1.292542         | -0.036591 |
| 3                | 6                | 0              | 3.888019         | 2.068810         | -0.069915 |
| 4                | 6                | 0              | 2.659959         | 1.432989         | -0.052944 |
| 5                | 6                | 0              | 2.545340         | 0.036115         | 0.000038  |
| 6                | 6                | 0              | 3.727251         | -0.749595        | 0.043203  |
| 7                | 7                | 0              | 3.687373         | -2.110221        | 0.147399  |
| 8                | 6                | 0              | 1.230776         | -0.587702        | -0.005090 |
| 9                | 7                | 0              | 0.969493         | -1.884770        | -0.036293 |
| 10               | 7                | 0              | -0.376953        | -2.056262        | -0.046272 |
| 11               | 6                | 0              | -0.932091        | -0.861733        | -0.018196 |
| 12               | 7                | 0              | 0.046338         | 0.082695         | 0.007944  |
| 13               | 6                | 0              | -2.368196        | -0.602964        | -0.012226 |
| 14               | 6                | 0              | -3.243377        | -1.692885        | -0.032271 |
| 15               | 6                | 0              | -4.617850        | -1.516596        | -0.027817 |
| 16               | 6                | 0              | -5.139767        | -0.228075        | -0.002236 |
| 17               | 6                | 0              | -4.294622        | 0.874769         | 0.018510  |
| 18               | 6                | 0              | -2.912053        | 0.697278         | 0.013588  |
| 19               | 1                | 0              | 5.874431         | -0.682371        | 0.050095  |
| 20               | 1                | 0              | 6.023698         | 1.768635         | -0.054158 |
| 21               | 1                | 0              | 3.943523         | 3.150368         | -0.113495 |
| 22               | 1                | 0              | 1.763275         | 2.043065         | -0.090546 |
| 23               | 1                | 0              | 2.797504         | -2.567207        | -0.020070 |
| 24               | 1                | 0              | 4.528779         | -2.622902        | -0.058880 |
| 25               | 1                | 0              | -2.815998        | -2.688956        | -0.051433 |
| 26               | 1                | 0              | -5.276401        | -2.377656        | -0.043733 |
| 27               | 1                | 0              | -6.213323        | -0.071498        | 0.001921  |
| 28               | 1                | 0              | -4.717371        | 1.870914         | 0.038440  |
| 29               | 8                | 0              | -2.033528        | 1.730336         | 0.032613  |
| 30               | 6                | 0              | -2.536017        | 3.060032         | 0.055052  |
| 31               | 1                | 0              | -3.131486        | 3.238375         | 0.954761  |
| 32               | 1                | 0              | -1.660551        | 3.706657         | 0.064263  |
| 33               | 1                | 0              | -3.134102        | 3.267209         | -0.836706 |
| 34               | 1                | 0              | -0.139454        | 1.075055         | 0.035729  |

## 2B-T-1c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 5.382217         | -0.377419        | 0.111191  |
| 2                | 6                | 0              | 4.055278         | -0.809398        | 0.203278  |
| 3                | 6                | 0              | 5.687929         | 0.949437         | -0.148424 |
| 4                | 6                | 0              | 4.670197         | 1.887391         | -0.308491 |
| 5                | 6                | 0              | 3.351480         | 1.470190         | -0.235871 |
| 6                | 6                | 0              | 3.024027         | 0.129679         | -0.004237 |
| 7                | 7                | 0              | 3.766876         | -2.155791        | 0.447999  |
| 8                | 6                | 0              | 1.611769         | -0.244702        | -0.033585 |
| 9                | 7                | 0              | 0.583043         | 0.578172         | 0.120091  |
| 10               | 7                | 0              | 1.137582         | -1.481106        | -0.288292 |
| 11               | 7                | 0              | -0.201131        | -1.485911        | -0.315086 |
| 12               | 6                | 0              | -0.501044        | -0.219957        | -0.058962 |
| 13               | 6                | 0              | -1.882111        | 0.267986         | 0.028787  |
| 14               | 6                | 0              | -2.130653        | 1.627309         | 0.251007  |
| 15               | 6                | 0              | -2.948931        | -0.614994        | -0.108964 |
| 16               | 6                | 0              | -4.262740        | -0.153447        | -0.028856 |
| 17               | 6                | 0              | -4.514409        | 1.201538         | 0.191381  |
| 18               | 6                | 0              | -3.439241        | 2.077127         | 0.328968  |
| 19               | 8                | 0              | -5.227143        | -1.094359        | -0.175876 |
| 20               | 6                | 0              | -6.579753        | -0.680731        | -0.096344 |
| 21               | 1                | 0              | 6.179368         | -1.099056        | 0.263701  |
| 22               | 1                | 0              | 6.727511         | 1.254311         | -0.211637 |
| 23               | 1                | 0              | 4.903729         | 2.928711         | -0.499699 |
| 24               | 1                | 0              | 2.540841         | 2.175622         | -0.381296 |
| 25               | 1                | 0              | 4.594291         | -2.703067        | 0.644355  |
| 26               | 1                | 0              | 3.088458         | -2.304300        | 1.186088  |
| 27               | 1                | 0              | 1.674440         | -2.313659        | -0.492235 |
| 28               | 1                | 0              | -1.298788        | 2.312843         | 0.358720  |
| 29               | 1                | 0              | -2.772084        | -1.671022        | -0.279096 |
| 30               | 1                | 0              | -5.526564        | 1.580421         | 0.256905  |
| 31               | 1                | 0              | -3.637237        | 3.130378         | 0.500092  |
| 32               | 1                | 0              | -7.177381        | -1.579904        | -0.238134 |
| 33               | 1                | 0              | -6.806010        | -0.246411        | 0.883047  |
| 34               | 1                | 0              | -6.822105        | 0.042401         | -0.882050 |

## 2B-T-1c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.968328        | 1.215611         | -0.038030 |
| 2                | 6                | 0              | -3.574519        | 1.020411         | -0.089183 |
| 3                | 6                | 0              | -5.840573        | 0.154582         | 0.098179  |
| 4                | 6                | 0              | -5.358709        | -1.153523        | 0.192402  |
| 5                | 6                | 0              | -3.993744        | -1.364412        | 0.148154  |
| 6                | 6                | 0              | -3.082406        | -0.307324        | 0.004704  |
| 7                | 7                | 0              | -2.746852        | 2.090911         | -0.271098 |
| 8                | 6                | 0              | -1.653141        | -0.580247        | -0.036803 |
| 9                | 7                | 0              | -0.664788        | 0.307535         | 0.029148  |
| 10               | 7                | 0              | -1.102166        | -1.808363        | -0.140609 |
| 11               | 7                | 0              | 0.237227         | -1.741070        | -0.137762 |
| 12               | 6                | 0              | 0.466932         | -0.443142        | -0.032874 |
| 13               | 6                | 0              | 1.816279         | 0.129799         | 0.010963  |
| 14               | 6                | 0              | 1.985989         | 1.516513         | 0.093399  |
| 15               | 6                | 0              | 2.931987         | -0.701125        | -0.029464 |
| 16               | 6                | 0              | 4.216940         | -0.160280        | 0.010296  |
| 17               | 6                | 0              | 4.390121         | 1.222314         | 0.091808  |
| 18               | 6                | 0              | 3.266662         | 2.045176         | 0.132568  |
| 19               | 8                | 0              | 5.233982         | -1.054632        | -0.034263 |
| 20               | 6                | 0              | 6.560444         | -0.558232        | 0.005524  |
| 21               | 1                | 0              | -5.350919        | 2.229485         | -0.109943 |
| 22               | 1                | 0              | -6.908444        | 0.345339         | 0.136092  |
| 23               | 1                | 0              | -6.038672        | -1.989484        | 0.307710  |
| 24               | 1                | 0              | -3.624832        | -2.380759        | 0.243338  |
| 25               | 1                | 0              | -3.126563        | 3.008298         | -0.104706 |
| 26               | 1                | 0              | -1.760088        | 1.951213         | -0.089244 |
| 27               | 1                | 0              | -1.555997        | -2.703529        | -0.234124 |
| 28               | 1                | 0              | 1.117642         | 2.163509         | 0.125363  |
| 29               | 1                | 0              | 2.815844         | -1.777271        | -0.091722 |
| 30               | 1                | 0              | 5.378856         | 1.662332         | 0.123771  |
| 31               | 1                | 0              | 3.403550         | 3.119872         | 0.195871  |
| 32               | 1                | 0              | 7.209081         | -1.431809        | -0.037579 |
| 33               | 1                | 0              | 6.768743         | 0.089960         | -0.852020 |
| 34               | 1                | 0              | 6.752389         | -0.009935        | 0.933684  |

## 2B-T-1c3

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.430542        | 1.816912         | -0.073160 |
| 2                | 6                | 0              | -3.126591        | 1.286772         | -0.120799 |
| 3                | 6                | 0              | -5.533119        | 1.004996         | 0.100585  |
| 4                | 6                | 0              | -5.382824        | -0.377330        | 0.237727  |
| 5                | 6                | 0              | -4.110655        | -0.915475        | 0.196972  |
| 6                | 6                | 0              | -2.971108        | -0.117172        | 0.016034  |
| 7                | 7                | 0              | -2.065527        | 2.117231         | -0.340074 |
| 8                | 6                | 0              | -1.651620        | -0.730710        | -0.022334 |
| 9                | 7                | 0              | -0.476631        | -0.108349        | 0.009190  |
| 10               | 7                | 0              | -1.416770        | -2.058578        | -0.089259 |
| 11               | 7                | 0              | -0.101110        | -2.318842        | -0.096125 |
| 12               | 6                | 0              | 0.438152         | -1.112935        | -0.035147 |
| 13               | 6                | 0              | 1.886928         | -0.886946        | -0.019502 |
| 14               | 6                | 0              | 2.780335         | -1.965342        | -0.062692 |
| 15               | 6                | 0              | 2.376920         | 0.412868         | 0.037438  |
| 16               | 6                | 0              | 3.752606         | 0.651077         | 0.051191  |
| 17               | 6                | 0              | 4.644839         | -0.419253        | 0.007467  |
| 18               | 6                | 0              | 4.142776         | -1.719395        | -0.049130 |
| 19               | 8                | 0              | 4.123316         | 1.953064         | 0.108078  |
| 20               | 6                | 0              | 5.508369         | 2.250879         | 0.122276  |
| 21               | 1                | 0              | -4.556138        | 2.890519         | -0.178527 |
| 22               | 1                | 0              | -6.522129        | 1.450935         | 0.134576  |
| 23               | 1                | 0              | -6.244428        | -1.018545        | 0.382428  |
| 24               | 1                | 0              | -3.999312        | -1.987585        | 0.323922  |
| 25               | 1                | 0              | -2.209081        | 3.104552         | -0.206122 |
| 26               | 1                | 0              | -1.140343        | 1.747628         | -0.156846 |
| 27               | 1                | 0              | -2.075828        | -2.818819        | -0.150619 |
| 28               | 1                | 0              | 2.401255         | -2.979480        | -0.106738 |
| 29               | 1                | 0              | 1.695226         | 1.254913         | 0.071462  |
| 30               | 1                | 0              | 5.715417         | -0.257945        | 0.016644  |
| 31               | 1                | 0              | 4.839750         | -2.550588        | -0.082971 |
| 32               | 1                | 0              | 5.581602         | 3.336354         | 0.167981  |
| 33               | 1                | 0              | 5.999469         | 1.817375         | 0.999722  |
| 34               | 1                | 0              | 6.001482         | 1.892260         | -0.787214 |

## 2B-T-1c4

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 5.249363         | 0.376075         | 0.176456  |
| 2                | 6                | 0              | 4.063576         | -0.359846        | 0.267703  |
| 3                | 6                | 0              | 5.233375         | 1.724772         | -0.143167 |
| 4                | 6                | 0              | 4.024447         | 2.380408         | -0.366287 |
| 5                | 6                | 0              | 2.843739         | 1.659989         | -0.295262 |
| 6                | 6                | 0              | 2.842590         | 0.291361         | -0.003816 |
| 7                | 7                | 0              | 4.100729         | -1.724081        | 0.574966  |
| 8                | 6                | 0              | 1.563731         | -0.414681        | -0.040841 |
| 9                | 7                | 0              | 0.362490         | 0.141448         | 0.040953  |
| 10               | 7                | 0              | 1.410286         | -1.740768        | -0.231879 |
| 11               | 7                | 0              | 0.113842         | -2.071043        | -0.287962 |
| 12               | 6                | 0              | -0.490591        | -0.903590        | -0.114335 |
| 13               | 6                | 0              | -1.951030        | -0.766123        | -0.087228 |
| 14               | 6                | 0              | -2.778099        | -1.890175        | -0.211856 |
| 15               | 6                | 0              | -2.518531        | 0.494204         | 0.063172  |
| 16               | 6                | 0              | -3.906029        | 0.647155         | 0.089086  |
| 17               | 6                | 0              | -4.732342        | -0.469048        | -0.034911 |
| 18               | 6                | 0              | -4.152916        | -1.728915        | -0.184832 |
| 19               | 8                | 0              | -4.355103        | 1.917096         | 0.237940  |
| 20               | 6                | 0              | -5.755548        | 2.129671         | 0.261544  |
| 21               | 1                | 0              | 6.192508         | -0.123361        | 0.377845  |
| 22               | 1                | 0              | 6.170180         | 2.269145         | -0.204071 |
| 23               | 1                | 0              | 4.005312         | 3.437872         | -0.604731 |
| 24               | 1                | 0              | 1.891404         | 2.141060         | -0.488793 |
| 25               | 1                | 0              | 5.030220         | -2.047119        | 0.808171  |
| 26               | 1                | 0              | 3.461132         | -1.996690        | 1.312355  |
| 27               | 1                | 0              | 2.139026         | -2.427353        | -0.375249 |
| 28               | 1                | 0              | -2.338343        | -2.873700        | -0.327351 |
| 29               | 1                | 0              | -1.887024        | 1.369774         | 0.160798  |
| 30               | 1                | 0              | -5.810764        | -0.373933        | -0.016979 |
| 31               | 1                | 0              | -4.798429        | -2.596083        | -0.280522 |
| 32               | 1                | 0              | -5.894359        | 3.202961         | 0.382204  |
| 33               | 1                | 0              | -6.222510        | 1.806899         | -0.674842 |
| 34               | 1                | 0              | -6.223375        | 1.607322         | 1.102545  |

## 2B-T-2c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -5.409964        | -0.315839        | -0.079728 |
| 2                | 6                | 0              | -4.101470        | -0.817354        | 0.049016  |
| 3                | 6                | 0              | -5.651583        | 1.031768         | -0.269387 |
| 4                | 6                | 0              | -4.590970        | 1.937100         | -0.337009 |
| 5                | 6                | 0              | -3.297695        | 1.459275         | -0.218268 |
| 6                | 6                | 0              | -3.022860        | 0.098256         | -0.029553 |
| 7                | 7                | 0              | -3.913825        | -2.153806        | 0.291880  |
| 8                | 6                | 0              | -1.623859        | -0.318328        | 0.063996  |
| 9                | 7                | 0              | -0.586624        | 0.563536         | 0.020171  |
| 10               | 7                | 0              | -1.230479        | -1.583488        | 0.182757  |
| 11               | 7                | 0              | 0.106646         | -1.485440        | 0.208711  |
| 12               | 6                | 0              | 0.489802         | -0.199201        | 0.112693  |
| 13               | 6                | 0              | 1.876356         | 0.266639         | 0.121757  |
| 14               | 6                | 0              | 2.135511         | 1.615470         | 0.392635  |
| 15               | 6                | 0              | 2.930443         | -0.605366        | -0.132903 |
| 16               | 6                | 0              | 4.247964         | -0.143904        | -0.108673 |
| 17               | 6                | 0              | 4.509494         | 1.198437         | 0.165269  |
| 18               | 6                | 0              | 3.445391         | 2.063835         | 0.411584  |
| 19               | 8                | 0              | 5.197679         | -1.070636        | -0.369394 |
| 20               | 6                | 0              | 6.554019         | -0.657506        | -0.362337 |
| 21               | 1                | 0              | -6.239850        | -1.014625        | -0.022807 |
| 22               | 1                | 0              | -6.675297        | 1.380436         | -0.364857 |
| 23               | 1                | 0              | -4.773919        | 2.995633         | -0.484226 |
| 24               | 1                | 0              | -2.455743        | 2.140253         | -0.275301 |
| 25               | 1                | 0              | -4.678151        | -2.771219        | 0.070513  |
| 26               | 1                | 0              | -2.981850        | -2.524882        | 0.164677  |
| 27               | 1                | 0              | 1.310383         | 2.288857         | 0.590011  |
| 28               | 1                | 0              | 2.766416         | -1.650518        | -0.373110 |
| 29               | 1                | 0              | 5.523586         | 1.576900         | 0.186888  |
| 30               | 1                | 0              | 3.653845         | 3.107068         | 0.624637  |
| 31               | 1                | 0              | 7.138796         | -1.547208        | -0.589869 |
| 32               | 1                | 0              | 6.740859         | 0.104444         | -1.125946 |
| 33               | 1                | 0              | 6.846094         | -0.272861        | 0.620074  |
| 34               | 1                | 0              | 0.669883         | -2.312502        | 0.335279  |

## 2B-T-2c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.973603         | 1.198421         | 0.166441  |
| 2                | 6                | 0              | 3.583719         | 1.012307         | 0.043385  |
| 3                | 6                | 0              | 5.844081         | 0.127009         | 0.227021  |
| 4                | 6                | 0              | 5.358694         | -1.180943        | 0.166830  |
| 5                | 6                | 0              | 3.994493         | -1.381093        | 0.053002  |
| 6                | 6                | 0              | 3.088525         | -0.313566        | -0.008957 |
| 7                | 7                | 0              | 2.765093         | 2.108475         | -0.074462 |
| 8                | 6                | 0              | 1.658472         | -0.612260        | -0.116387 |
| 9                | 7                | 0              | 0.665335         | 0.313893         | -0.001647 |
| 10               | 7                | 0              | 1.202912         | -1.844360        | -0.318044 |
| 11               | 7                | 0              | -0.126001        | -1.674787        | -0.321407 |
| 12               | 6                | 0              | -0.453024        | -0.385761        | -0.132864 |
| 13               | 6                | 0              | -1.812646        | 0.148531         | -0.088954 |
| 14               | 6                | 0              | -2.000755        | 1.531486         | -0.201077 |
| 15               | 6                | 0              | -2.912558        | -0.690717        | 0.062411  |
| 16               | 6                | 0              | -4.204104        | -0.161542        | 0.090705  |
| 17               | 6                | 0              | -4.394547        | 1.215440         | -0.024836 |
| 18               | 6                | 0              | -3.285513        | 2.046706         | -0.168218 |
| 19               | 8                | 0              | -5.202272        | -1.061635        | 0.239262  |
| 20               | 6                | 0              | -6.535807        | -0.580893        | 0.272138  |
| 21               | 1                | 0              | 5.357267         | 2.213942         | 0.208832  |
| 22               | 1                | 0              | 6.909648         | 0.311132         | 0.323380  |
| 23               | 1                | 0              | 6.035397         | -2.026691        | 0.215862  |
| 24               | 1                | 0              | 3.595485         | -2.389113        | 0.016904  |
| 25               | 1                | 0              | 3.137694         | 2.987636         | 0.246609  |
| 26               | 1                | 0              | 1.776806         | 1.953220         | 0.083888  |
| 27               | 1                | 0              | -1.141953        | 2.181066         | -0.318380 |
| 28               | 1                | 0              | -2.806204        | -1.764243        | 0.176945  |
| 29               | 1                | 0              | -5.387636        | 1.645871         | -0.002336 |
| 30               | 1                | 0              | -3.437936        | 3.117150         | -0.257804 |
| 31               | 1                | 0              | -7.167358        | -1.459546        | 0.392209  |
| 32               | 1                | 0              | -6.692974        | 0.096837         | 1.117371  |
| 33               | 1                | 0              | -6.796503        | -0.071452        | -0.661082 |
| 34               | 1                | 0              | -0.730718        | -2.464022        | -0.491414 |

## 2B-T-2c3

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.462072        | 1.786951         | -0.188208 |
| 2                | 6                | 0              | -3.157570        | 1.259083         | -0.228068 |
| 3                | 6                | 0              | -5.557057        | 0.989164         | 0.083111  |
| 4                | 6                | 0              | -5.392681        | -0.376012        | 0.326659  |
| 5                | 6                | 0              | -4.116374        | -0.909328        | 0.297653  |
| 6                | 6                | 0              | -2.987657        | -0.123602        | 0.027492  |
| 7                | 7                | 0              | -2.109383        | 2.080193         | -0.562114 |
| 8                | 6                | 0              | -1.670176        | -0.763829        | 0.025610  |
| 9                | 7                | 0              | -0.486155        | -0.093242        | -0.050466 |
| 10               | 7                | 0              | -1.519631        | -2.081571        | 0.111509  |
| 11               | 7                | 0              | -0.188545        | -2.231920        | 0.090592  |
| 12               | 6                | 0              | 0.434247         | -1.046262        | -0.009011 |
| 13               | 6                | 0              | 1.882237         | -0.854505        | -0.058276 |
| 14               | 6                | 0              | 2.755188         | -1.922762        | -0.300654 |
| 15               | 6                | 0              | 2.390173         | 0.425446         | 0.138697  |
| 16               | 6                | 0              | 3.766351         | 0.651519         | 0.104224  |
| 17               | 6                | 0              | 4.639629         | -0.411724        | -0.128601 |
| 18               | 6                | 0              | 4.120157         | -1.688349        | -0.330228 |
| 19               | 8                | 0              | 4.157225         | 1.929674         | 0.309465  |
| 20               | 6                | 0              | 5.545579         | 2.216329         | 0.284454  |
| 21               | 1                | 0              | -4.596856        | 2.847440         | -0.381887 |
| 22               | 1                | 0              | -6.547291        | 1.433563         | 0.106625  |
| 23               | 1                | 0              | -6.246921        | -1.008137        | 0.541858  |
| 24               | 1                | 0              | -3.965129        | -1.965338        | 0.494312  |
| 25               | 1                | 0              | -2.257806        | 3.070862         | -0.456620 |
| 26               | 1                | 0              | -1.179819        | 1.736695         | -0.353248 |
| 27               | 1                | 0              | 2.381885         | -2.924511        | -0.481783 |
| 28               | 1                | 0              | 1.720501         | 1.256783         | 0.325993  |
| 29               | 1                | 0              | 5.711186         | -0.260092        | -0.158155 |
| 30               | 1                | 0              | 4.801585         | -2.510877        | -0.519711 |
| 31               | 1                | 0              | 5.633416         | 3.286029         | 0.467114  |
| 32               | 1                | 0              | 6.077831         | 1.669528         | 1.069413  |
| 33               | 1                | 0              | 5.982443         | 1.977743         | -0.690571 |
| 34               | 1                | 0              | 0.213339         | -3.154023        | 0.165171  |

## 2B-T-2c4

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -5.272045        | 0.431942         | 0.031567  |
| 2                | 6                | 0              | -4.118245        | -0.369306        | 0.114191  |
| 3                | 6                | 0              | -5.190613        | 1.799283         | -0.153181 |
| 4                | 6                | 0              | -3.947043        | 2.424372         | -0.261903 |
| 5                | 6                | 0              | -2.802690        | 1.649697         | -0.189594 |
| 6                | 6                | 0              | -2.855241        | 0.261304         | -0.007011 |
| 7                | 7                | 0              | -4.248609        | -1.713112        | 0.354053  |
| 8                | 6                | 0              | -1.594368        | -0.478749        | 0.032860  |
| 9                | 7                | 0              | -0.378883        | 0.128664         | -0.060674 |
| 10               | 7                | 0              | -1.511040        | -1.801785        | 0.144237  |
| 11               | 7                | 0              | -0.189595        | -2.026995        | 0.114535  |
| 12               | 6                | 0              | 0.486388         | -0.870112        | -0.007761 |
| 13               | 6                | 0              | 1.943510         | -0.756120        | -0.065861 |
| 14               | 6                | 0              | 2.757456         | -1.871754        | -0.298942 |
| 15               | 6                | 0              | 2.519005         | 0.497456         | 0.112965  |
| 16               | 6                | 0              | 3.904917         | 0.650211         | 0.068173  |
| 17               | 6                | 0              | 4.719650         | -0.460491        | -0.155738 |
| 18               | 6                | 0              | 4.132777         | -1.710395        | -0.338345 |
| 19               | 8                | 0              | 4.364342         | 1.908407         | 0.254561  |
| 20               | 6                | 0              | 5.765488         | 2.121058         | 0.213759  |
| 21               | 1                | 0              | -6.242366        | -0.048254        | 0.120774  |
| 22               | 1                | 0              | -6.103746        | 2.383487         | -0.212649 |
| 23               | 1                | 0              | -3.875941        | 3.496728         | -0.405549 |
| 24               | 1                | 0              | -1.824821        | 2.109375         | -0.280779 |
| 25               | 1                | 0              | -5.147065        | -2.127018        | 0.164569  |
| 26               | 1                | 0              | -3.439055        | -2.297305        | 0.193563  |
| 27               | 1                | 0              | 2.331226         | -2.854674        | -0.465412 |
| 28               | 1                | 0              | 1.893525         | 1.364162         | 0.292241  |
| 29               | 1                | 0              | 5.797565         | -0.365991        | -0.192776 |
| 30               | 1                | 0              | 4.768894         | -2.570060        | -0.520373 |
| 31               | 1                | 0              | 5.911267         | 3.186962         | 0.380918  |
| 32               | 1                | 0              | 6.275714         | 1.557406         | 1.001430  |
| 33               | 1                | 0              | 6.179998         | 1.846722         | -0.761664 |
| 34               | 1                | 0              | 0.163279         | -2.966563        | 0.213104  |

## 2B-T-3c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -5.417397        | -0.424910        | -0.003653 |
| 2                | 6                | 0              | -4.083462        | -0.870792        | 0.062100  |
| 3                | 6                | 0              | -5.725363        | 0.913364         | -0.144926 |
| 4                | 6                | 0              | -4.710163        | 1.869134         | -0.228151 |
| 5                | 6                | 0              | -3.394047        | 1.449925         | -0.170380 |
| 6                | 6                | 0              | -3.048436        | 0.097752         | -0.026567 |
| 7                | 7                | 0              | -3.821264        | -2.196151        | 0.248104  |
| 8                | 6                | 0              | -1.649833        | -0.299555        | 0.018211  |
| 9                | 7                | 0              | -0.589194        | 0.557153         | 0.028111  |
| 10               | 7                | 0              | -1.179821        | -1.535502        | 0.044760  |
| 11               | 7                | 0              | 0.177318         | -1.482394        | 0.067290  |
| 12               | 6                | 0              | 0.530535         | -0.217226        | 0.056617  |
| 13               | 6                | 0              | 1.901683         | 0.287135         | 0.074901  |
| 14               | 6                | 0              | 2.181141         | 1.649354         | 0.240690  |
| 15               | 6                | 0              | 2.948263         | -0.618980        | -0.074117 |
| 16               | 6                | 0              | 4.271023         | -0.179355        | -0.058584 |
| 17               | 6                | 0              | 4.552476         | 1.178508         | 0.103580  |
| 18               | 6                | 0              | 3.499476         | 2.076963         | 0.251699  |
| 19               | 8                | 0              | 5.211525         | -1.139887        | -0.210664 |
| 20               | 6                | 0              | 6.574045         | -0.748836        | -0.199263 |
| 21               | 1                | 0              | -6.211417        | -1.162907        | 0.062512  |
| 22               | 1                | 0              | -6.766082        | 1.218085         | -0.192278 |
| 23               | 1                | 0              | -4.944564        | 2.921105         | -0.341940 |
| 24               | 1                | 0              | -2.613503        | 2.199797         | -0.250302 |
| 25               | 1                | 0              | -4.568209        | -2.852065        | 0.090347  |
| 26               | 1                | 0              | -2.867916        | -2.512792        | 0.110701  |
| 27               | 1                | 0              | 1.387419         | 2.376326         | 0.371385  |
| 28               | 1                | 0              | 2.742220         | -1.674687        | -0.206175 |
| 29               | 1                | 0              | 5.572005         | 1.542474         | 0.116166  |
| 30               | 1                | 0              | 3.719679         | 3.131325         | 0.381010  |
| 31               | 1                | 0              | 7.149066         | -1.663793        | -0.331966 |
| 32               | 1                | 0              | 6.796396         | -0.058994        | -1.019771 |
| 33               | 1                | 0              | 6.845830         | -0.285000        | 0.754435  |
| 34               | 1                | 0              | -0.622039        | 1.563592         | 0.010394  |

## 2B-T-3c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.989254        | 1.138284         | -0.154063 |
| 2                | 6                | 0              | -3.630945        | 0.952519         | 0.122500  |
| 3                | 6                | 0              | -5.810827        | 0.065757         | -0.464226 |
| 4                | 6                | 0              | -5.295304        | -1.228270        | -0.494759 |
| 5                | 6                | 0              | -3.947501        | -1.424174        | -0.242939 |
| 6                | 6                | 0              | -3.098148        | -0.351070        | 0.049207  |
| 7                | 7                | 0              | -2.812600        | 2.050252         | 0.413618  |
| 8                | 6                | 0              | -1.674442        | -0.624738        | 0.225937  |
| 9                | 7                | 0              | -0.671752        | 0.268441         | 0.001269  |
| 10               | 7                | 0              | -1.145772        | -1.785000        | 0.559421  |
| 11               | 7                | 0              | 0.206966         | -1.648755        | 0.543505  |
| 12               | 6                | 0              | 0.489824         | -0.409866        | 0.201744  |
| 13               | 6                | 0              | 1.827927         | 0.160354         | 0.067809  |
| 14               | 6                | 0              | 2.025893         | 1.544403         | -0.015326 |
| 15               | 6                | 0              | 2.923165         | -0.697925        | 0.027253  |
| 16               | 6                | 0              | 4.215354         | -0.188359        | -0.094256 |
| 17               | 6                | 0              | 4.415779         | 1.190516         | -0.181350 |
| 18               | 6                | 0              | 3.313893         | 2.040675         | -0.140381 |
| 19               | 8                | 0              | 5.208990         | -1.106281        | -0.123888 |
| 20               | 6                | 0              | 6.542726         | -0.642888        | -0.249322 |
| 21               | 1                | 0              | -5.400716        | 2.142314         | -0.106213 |
| 22               | 1                | 0              | -6.861479        | 0.241147         | -0.671554 |
| 23               | 1                | 0              | -5.934843        | -2.072048        | -0.728357 |
| 24               | 1                | 0              | -3.517885        | -2.418538        | -0.291905 |
| 25               | 1                | 0              | -3.333096        | 2.912888         | 0.500324  |
| 26               | 1                | 0              | -2.235953        | 1.927533         | 1.237728  |
| 27               | 1                | 0              | 1.190926         | 2.234742         | 0.032150  |
| 28               | 1                | 0              | 2.779626         | -1.770601        | 0.085442  |
| 29               | 1                | 0              | 5.410137         | 1.607409         | -0.278969 |
| 30               | 1                | 0              | 3.471902         | 3.112193         | -0.202540 |
| 31               | 1                | 0              | 7.169892         | -1.532892        | -0.251936 |
| 32               | 1                | 0              | 6.686456         | -0.095301        | -1.186394 |
| 33               | 1                | 0              | 6.822346         | -0.004768        | 0.595186  |
| 34               | 1                | 0              | -0.805974        | 1.220300         | -0.313525 |

## 2B-T-3c3

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.480006        | 1.757420         | 0.058889  |
| 2                | 6                | 0              | -3.209712        | 1.229754         | -0.192772 |
| 3                | 6                | 0              | -5.539687        | 0.936828         | 0.412840  |
| 4                | 6                | 0              | -5.357952        | -0.440803        | 0.513674  |
| 5                | 6                | 0              | -4.099819        | -0.974525        | 0.288148  |
| 6                | 6                | 0              | -3.012954        | -0.158929        | -0.046610 |
| 7                | 7                | 0              | -2.147170        | 2.076567         | -0.531587 |
| 8                | 6                | 0              | -1.698734        | -0.780101        | -0.187865 |
| 9                | 7                | 0              | -0.509500        | -0.143248        | -0.004655 |
| 10               | 7                | 0              | -1.467085        | -2.052797        | -0.439996 |
| 11               | 7                | 0              | -0.121836        | -2.246807        | -0.412372 |
| 12               | 6                | 0              | 0.453222         | -1.093485        | -0.144745 |
| 13               | 6                | 0              | 1.890662         | -0.862795        | -0.027421 |
| 14               | 6                | 0              | 2.752823         | -1.961660        | 0.087422  |
| 15               | 6                | 0              | 2.413468         | 0.426887         | -0.030503 |
| 16               | 6                | 0              | 3.790344         | 0.632427         | 0.082154  |
| 17               | 6                | 0              | 4.649825         | -0.459173        | 0.195964  |
| 18               | 6                | 0              | 4.115652         | -1.747167        | 0.195801  |
| 19               | 8                | 0              | 4.191983         | 1.924275         | 0.065015  |
| 20               | 6                | 0              | 5.581011         | 2.192372         | 0.155999  |
| 21               | 1                | 0              | -4.632004        | 2.827957         | -0.043663 |
| 22               | 1                | 0              | -6.514845        | 1.375087         | 0.598822  |
| 23               | 1                | 0              | -6.185118        | -1.088693        | 0.781247  |
| 24               | 1                | 0              | -3.927586        | -2.040117        | 0.391775  |
| 25               | 1                | 0              | -2.439540        | 3.036142         | -0.659661 |
| 26               | 1                | 0              | -1.628153        | 1.777856         | -1.349144 |
| 27               | 1                | 0              | 2.343873         | -2.964580        | 0.095016  |
| 28               | 1                | 0              | 1.781114         | 1.302145         | -0.135601 |
| 29               | 1                | 0              | 5.720176         | -0.322214        | 0.283495  |
| 30               | 1                | 0              | 4.786928         | -2.594741        | 0.287350  |
| 31               | 1                | 0              | 5.679886         | 3.275919         | 0.116599  |
| 32               | 1                | 0              | 5.995505         | 1.824457         | 1.100115  |
| 33               | 1                | 0              | 6.126340         | 1.747412         | -0.682549 |
| 34               | 1                | 0              | -0.412159        | 0.830872         | 0.250504  |

## 2B-T-3c4

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 5.314657         | 0.325196         | 0.008300  |
| 2                | 6                | 0              | 4.127151         | -0.431332        | 0.030234  |
| 3                | 6                | 0              | 5.291357         | 1.705054         | -0.022064 |
| 4                | 6                | 0              | 4.075780         | 2.393209         | -0.030654 |
| 5                | 6                | 0              | 2.899283         | 1.667619         | -0.016266 |
| 6                | 6                | 0              | 2.889150         | 0.264734         | 0.009995  |
| 7                | 7                | 0              | 4.192250         | -1.791076        | 0.108183  |
| 8                | 6                | 0              | 1.627184         | -0.458116        | 0.000220  |
| 9                | 7                | 0              | 0.391876         | 0.118645         | 0.014534  |
| 10               | 7                | 0              | 1.467221         | -1.770609        | -0.035717 |
| 11               | 7                | 0              | 0.137187         | -2.044431        | -0.047256 |
| 12               | 6                | 0              | -0.510004        | -0.901369        | -0.015436 |
| 13               | 6                | 0              | -1.963124        | -0.750475        | -0.009718 |
| 14               | 6                | 0              | -2.765444        | -1.900125        | -0.012805 |
| 15               | 6                | 0              | -2.561538        | 0.505838         | -0.000721 |
| 16               | 6                | 0              | -3.952955        | 0.627874         | 0.005232  |
| 17               | 6                | 0              | -4.751795        | -0.514192        | 0.001713  |
| 18               | 6                | 0              | -4.142506        | -1.768453        | -0.007390 |
| 19               | 8                | 0              | -4.428018        | 1.894412         | 0.013881  |
| 20               | 6                | 0              | -5.833436        | 2.079743         | 0.021041  |
| 21               | 1                | 0              | 6.262995         | -0.203960        | 0.020498  |
| 22               | 1                | 0              | 6.228092         | 2.253148         | -0.038635 |
| 23               | 1                | 0              | 4.049996         | 3.476424         | -0.053120 |
| 24               | 1                | 0              | 1.961456         | 2.213666         | -0.032996 |
| 25               | 1                | 0              | 5.070485         | -2.235763        | -0.101456 |
| 26               | 1                | 0              | 3.338266         | -2.315108        | -0.047761 |
| 27               | 1                | 0              | -2.299218        | -2.877581        | -0.018748 |
| 28               | 1                | 0              | -1.982348        | 1.422973         | 0.001114  |
| 29               | 1                | 0              | -5.832072        | -0.442597        | 0.006183  |
| 30               | 1                | 0              | -4.766528        | -2.656096        | -0.009519 |
| 31               | 1                | 0              | -5.993083        | 3.156698         | 0.027561  |
| 32               | 1                | 0              | -6.294897        | 1.649995         | -0.873839 |
| 33               | 1                | 0              | -6.287030        | 1.640295         | 0.915251  |
| 34               | 1                | 0              | 0.185747         | 1.103670         | 0.046123  |

## 2C-T-1c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.269646         | -4.943141        | 0.062755  |
| 2                | 6                | 0              | 4.248083         | -3.548954        | -0.046350 |
| 3                | 6                | 0              | 5.464704         | -5.634493        | 0.185918  |
| 4                | 6                | 0              | 6.677023         | -4.947881        | 0.188722  |
| 5                | 6                | 0              | 6.669326         | -3.565815        | 0.097660  |
| 6                | 6                | 0              | 5.471372         | -2.848909        | 0.002268  |
| 7                | 7                | 0              | 3.030512         | -2.869306        | -0.151633 |
| 8                | 6                | 0              | 5.544908         | -1.389198        | 0.003232  |
| 9                | 7                | 0              | 6.614093         | -0.661559        | -0.291832 |
| 10               | 7                | 0              | 4.548948         | -0.559632        | 0.372045  |
| 11               | 7                | 0              | 4.950753         | 0.719107         | 0.336352  |
| 12               | 6                | 0              | 6.207885         | 0.617212         | -0.075139 |
| 13               | 6                | 0              | 7.070580         | 1.781867         | -0.280857 |
| 14               | 6                | 0              | 8.391155         | 1.621081         | -0.694766 |
| 15               | 6                | 0              | 6.593073         | 3.081830         | -0.066267 |
| 16               | 6                | 0              | 7.411663         | 4.177485         | -0.258745 |
| 17               | 6                | 0              | 8.737004         | 4.004088         | -0.674294 |
| 18               | 6                | 0              | 9.225945         | 2.716199         | -0.892684 |
| 19               | 1                | 0              | 3.328876         | -5.484925        | 0.033167  |
| 20               | 1                | 0              | 5.448753         | -6.716600        | 0.266297  |
| 21               | 1                | 0              | 7.615463         | -5.484255        | 0.273038  |
| 22               | 1                | 0              | 7.597854         | -3.006317        | 0.122384  |
| 23               | 1                | 0              | 2.240790         | -3.493454        | -0.249020 |
| 24               | 1                | 0              | 3.004356         | -2.182327        | -0.896074 |
| 25               | 1                | 0              | 8.774311         | 0.620954         | -0.865066 |
| 26               | 1                | 0              | 5.567517         | 3.227792         | 0.255054  |
| 27               | 8                | 0              | 9.461002         | 5.135049         | -0.836191 |
| 28               | 1                | 0              | 10.247018        | 2.552769         | -1.214007 |
| 29               | 1                | 0              | 7.043461         | 5.184318         | -0.092908 |
| 30               | 6                | 0              | 10.809507        | 5.010748         | -1.254525 |
| 31               | 1                | 0              | 11.197289        | 6.025859         | -1.323024 |
| 32               | 1                | 0              | 11.400203        | 4.445093         | -0.526673 |
| 33               | 1                | 0              | 10.877962        | 4.529192         | -2.235350 |
| 34               | 1                | 0              | 3.626604         | -0.815201        | 0.698102  |

## 2C-T-1c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -4.714758        | 1.703631         | -0.032613 |
| 2                | 6                | 0              | -3.378491        | 1.261776         | -0.085638 |
| 3                | 6                | 0              | -5.763149        | 0.816311         | 0.104010  |
| 4                | 6                | 0              | -5.523282        | -0.557062        | 0.196420  |
| 5                | 6                | 0              | -4.218154        | -1.008803        | 0.151760  |
| 6                | 6                | 0              | -3.131567        | -0.132764        | 0.009332  |
| 7                | 7                | 0              | -2.372632        | 2.166206         | -0.269784 |
| 8                | 6                | 0              | -1.774018        | -0.657918        | -0.029738 |
| 9                | 7                | 0              | -0.643038        | 0.041607         | 0.012735  |
| 10               | 7                | 0              | -1.451788        | -1.965841        | -0.106420 |
| 11               | 7                | 0              | -0.119696        | -2.138253        | -0.109670 |
| 12               | 6                | 0              | 0.338420         | -0.899340        | -0.036061 |
| 13               | 6                | 0              | 1.765024         | -0.575499        | -0.013054 |
| 14               | 6                | 0              | 2.189350         | 0.750143         | 0.044925  |
| 15               | 6                | 0              | 2.736066         | -1.585266        | -0.051860 |
| 16               | 6                | 0              | 4.081430         | -1.274042        | -0.034319 |
| 17               | 6                | 0              | 4.496631         | 0.061551         | 0.023491  |
| 18               | 6                | 0              | 3.541424         | 1.077092         | 0.063516  |
| 19               | 1                | 0              | -4.909548        | 2.769576         | -0.104920 |
| 20               | 1                | 0              | -6.779473        | 1.195488         | 0.142675  |
| 21               | 1                | 0              | -6.341959        | -1.258039        | 0.310058  |
| 22               | 1                | 0              | -4.038756        | -2.075131        | 0.243331  |
| 23               | 1                | 0              | -2.579552        | 3.137396         | -0.104280 |
| 24               | 1                | 0              | -1.425868        | 1.849180         | -0.096900 |
| 25               | 1                | 0              | 1.450712         | 1.543563         | 0.075515  |
| 26               | 1                | 0              | 2.425745         | -2.623539        | -0.096651 |
| 27               | 8                | 0              | 5.833154         | 0.266648         | 0.036512  |
| 28               | 1                | 0              | 3.833462         | 2.118870         | 0.108508  |
| 29               | 1                | 0              | 4.834236         | -2.054477        | -0.064499 |
| 30               | 6                | 0              | 6.304379         | 1.602073         | 0.097238  |
| 31               | 1                | 0              | 7.391233         | 1.536857         | 0.098174  |
| 32               | 1                | 0              | 5.976362         | 2.178672         | -0.773690 |
| 33               | 1                | 0              | 5.970019         | 2.099363         | 1.013438  |
| 34               | 1                | 0              | -2.057586        | -2.768286        | -0.175334 |

## 2C-T-2c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 5.447763         | 0.255283         | 0.002903  |
| 2                | 6                | 0              | 4.244883         | -0.474217        | 0.031969  |
| 3                | 6                | 0              | 5.454219         | 1.637027         | -0.034703 |
| 4                | 6                | 0              | 4.253288         | 2.348767         | -0.043589 |
| 5                | 6                | 0              | 3.061301         | 1.645846         | -0.021837 |
| 6                | 6                | 0              | 3.024347         | 0.245522         | 0.012164  |
| 7                | 7                | 0              | 4.289354         | -1.841622        | 0.125198  |
| 8                | 6                | 0              | 1.717749         | -0.412756        | 0.009037  |
| 9                | 7                | 0              | 0.544001         | 0.277649         | 0.014310  |
| 10               | 7                | 0              | 1.550846         | -1.731352        | -0.012928 |
| 11               | 7                | 0              | 0.214754         | -1.867825        | -0.025356 |
| 12               | 6                | 0              | -0.387377        | -0.663470        | -0.006965 |
| 13               | 6                | 0              | -1.829095        | -0.442713        | -0.008273 |
| 14               | 6                | 0              | -2.318407        | 0.863132         | 0.029544  |
| 15               | 6                | 0              | -2.749601        | -1.498934        | -0.045976 |
| 16               | 6                | 0              | -4.108196        | -1.252234        | -0.044457 |
| 17               | 6                | 0              | -4.587552        | 0.061963         | -0.005392 |
| 18               | 6                | 0              | -3.681822        | 1.124004         | 0.031191  |
| 19               | 1                | 0              | 6.385513         | -0.293007        | 0.015587  |
| 20               | 1                | 0              | 6.402991         | 2.164332         | -0.056710 |
| 21               | 1                | 0              | 4.251085         | 3.432702         | -0.071534 |
| 22               | 1                | 0              | 2.114586         | 2.174395         | -0.036554 |
| 23               | 1                | 0              | 5.152841         | -2.290609        | -0.134123 |
| 24               | 1                | 0              | 3.437683         | -2.350195        | -0.071731 |
| 25               | 1                | 0              | -1.615163        | 1.687730         | 0.058686  |
| 26               | 1                | 0              | -2.416777        | -2.531335        | -0.078073 |
| 27               | 8                | 0              | -5.928788        | 0.202523         | -0.006444 |
| 28               | 1                | 0              | -4.024489        | 2.150549         | 0.061216  |
| 29               | 1                | 0              | -4.820852        | -2.068968        | -0.073624 |
| 30               | 6                | 0              | -6.467869        | 1.514420         | 0.033611  |
| 31               | 1                | 0              | -7.549644        | 1.392877         | 0.028369  |
| 32               | 1                | 0              | -6.165428        | 2.038686         | 0.945511  |
| 33               | 1                | 0              | -6.163086        | 2.094260         | -0.843226 |
| 34               | 1                | 0              | -0.193412        | -2.789392        | -0.036169 |

## 2C-T-2c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.726667         | 1.693452         | -0.017048 |
| 2                | 6                | 0              | 3.391468         | 1.252211         | -0.083012 |
| 3                | 6                | 0              | 5.776641         | 0.804654         | 0.113272  |
| 4                | 6                | 0              | 5.533702         | -0.568717        | 0.183056  |
| 5                | 6                | 0              | 4.226367         | -1.018028        | 0.127960  |
| 6                | 6                | 0              | 3.141911         | -0.139656        | -0.001374 |
| 7                | 7                | 0              | 2.387471         | 2.168931         | -0.275817 |
| 8                | 6                | 0              | 1.787525         | -0.697878        | -0.037675 |
| 9                | 7                | 0              | 0.645162         | 0.044487         | 0.000021  |
| 10               | 7                | 0              | 1.560873         | -2.005034        | -0.094555 |
| 11               | 7                | 0              | 0.220611         | -2.075759        | -0.086817 |
| 12               | 6                | 0              | -0.333006        | -0.852138        | -0.032117 |
| 13               | 6                | 0              | -1.761553        | -0.564220        | -0.013707 |
| 14               | 6                | 0              | -2.189815        | 0.762451         | 0.040939  |
| 15               | 6                | 0              | -2.730560        | -1.576384        | -0.050533 |
| 16               | 6                | 0              | -4.076098        | -1.267460        | -0.032571 |
| 17               | 6                | 0              | -4.493957        | 0.066998         | 0.022927  |
| 18               | 6                | 0              | -3.539731        | 1.085679         | 0.059588  |
| 19               | 1                | 0              | 4.921788         | 2.760500         | -0.076524 |
| 20               | 1                | 0              | 6.792774         | 1.183821         | 0.161770  |
| 21               | 1                | 0              | 6.352160         | -1.272398        | 0.286190  |
| 22               | 1                | 0              | 4.014880         | -2.080009        | 0.191973  |
| 23               | 1                | 0              | 2.596740         | 3.126368         | -0.042668 |
| 24               | 1                | 0              | 1.444655         | 1.851825         | -0.084003 |
| 25               | 1                | 0              | -1.450959        | 1.555359         | 0.069318  |
| 26               | 1                | 0              | -2.445846        | -2.622521        | -0.093929 |
| 27               | 8                | 0              | -5.827211        | 0.268750         | 0.037199  |
| 28               | 1                | 0              | -3.833653        | 2.126829         | 0.102397  |
| 29               | 1                | 0              | -4.825790        | -2.050348        | -0.060908 |
| 30               | 6                | 0              | -6.305194        | 1.603420         | 0.094942  |
| 31               | 1                | 0              | -7.391417        | 1.531624         | 0.096626  |
| 32               | 1                | 0              | -5.972597        | 2.103155         | 1.010072  |
| 33               | 1                | 0              | -5.980326        | 2.178053         | -0.778054 |
| 34               | 1                | 0              | -0.229748        | -2.976950        | -0.127562 |

## 2C-T-3c1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | -5.485852        | 0.121422         | 0.019756  |
| 2                | 6                | 0              | -4.244803        | -0.543218        | 0.036447  |
| 3                | 6                | 0              | -5.566962        | 1.499305         | -0.015246 |
| 4                | 6                | 0              | -4.406860        | 2.276725         | -0.034180 |
| 5                | 6                | 0              | -3.178817        | 1.641408         | -0.024412 |
| 6                | 6                | 0              | -3.062684        | 0.243784         | 0.007192  |
| 7                | 7                | 0              | -4.205625        | -1.904299        | 0.119206  |
| 8                | 6                | 0              | -1.749483        | -0.382026        | -0.005069 |
| 9                | 7                | 0              | -0.560215        | 0.287407         | 0.013131  |
| 10               | 7                | 0              | -1.491539        | -1.676965        | -0.046549 |
| 11               | 7                | 0              | -0.142778        | -1.850482        | -0.058073 |
| 12               | 6                | 0              | 0.417253         | -0.661408        | -0.020414 |
| 13               | 6                | 0              | 1.851568         | -0.401227        | -0.011955 |
| 14               | 6                | 0              | 2.379004         | 0.889240         | 0.006420  |
| 15               | 6                | 0              | 2.744145         | -1.483937        | -0.022152 |
| 16               | 6                | 0              | 4.107605         | -1.277635        | -0.014730 |
| 17               | 6                | 0              | 4.626023         | 0.023214         | 0.003847  |
| 18               | 6                | 0              | 3.752004         | 1.109734         | 0.014407  |
| 19               | 1                | 0              | -6.392026        | -0.476819        | 0.039917  |
| 20               | 1                | 0              | -6.542457        | 1.975148         | -0.027533 |
| 21               | 1                | 0              | -4.462597        | 3.358757         | -0.061027 |
| 22               | 1                | 0              | -2.284483        | 2.255491         | -0.049976 |
| 23               | 1                | 0              | -5.047809        | -2.414894        | -0.088616 |
| 24               | 1                | 0              | -3.314991        | -2.360613        | -0.045657 |
| 25               | 1                | 0              | 1.729804         | 1.758616         | 0.014079  |
| 26               | 1                | 0              | 2.350224         | -2.493769        | -0.035375 |
| 27               | 8                | 0              | 5.971572         | 0.125608         | 0.010454  |
| 28               | 1                | 0              | 4.122521         | 2.126712         | 0.028394  |
| 29               | 1                | 0              | -0.430218        | 1.285192         | 0.050173  |
| 30               | 1                | 0              | 4.796900         | -2.115005        | -0.022288 |
| 31               | 6                | 0              | 6.545573         | 1.422574         | 0.029575  |
| 32               | 1                | 0              | 7.623800         | 1.272479         | 0.032828  |
| 33               | 1                | 0              | 6.261080         | 1.994525         | -0.859354 |
| 34               | 1                | 0              | 6.252504         | 1.971949         | 0.929868  |

## 2C-T-3c2

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates<br>X | (Angstroms)<br>Y | Z         |
|------------------|------------------|----------------|------------------|------------------|-----------|
| 1                | 6                | 0              | 4.778950         | 1.615953         | 0.040528  |
| 2                | 6                | 0              | 3.475404         | 1.180212         | -0.218292 |
| 3                | 6                | 0              | 5.762238         | 0.730075         | 0.453022  |
| 4                | 6                | 0              | 5.468372         | -0.622969        | 0.608188  |
| 5                | 6                | 0              | 4.176308         | -1.064235        | 0.374601  |
| 6                | 6                | 0              | 3.165429         | -0.181089        | -0.021004 |
| 7                | 7                | 0              | 2.491238         | 2.092370         | -0.615048 |
| 8                | 6                | 0              | 1.811135         | -0.706040        | -0.177259 |
| 9                | 7                | 0              | 0.666436         | 0.017527         | -0.021616 |
| 10               | 7                | 0              | 1.493586         | -1.960485        | -0.418764 |
| 11               | 7                | 0              | 0.135969         | -2.058164        | -0.413028 |
| 12               | 6                | 0              | -0.360638        | -0.863307        | -0.167893 |
| 13               | 6                | 0              | -1.776968        | -0.532950        | -0.072648 |
| 14               | 6                | 0              | -2.229943        | 0.783609         | -0.000518 |
| 15               | 6                | 0              | -2.726109        | -1.565643        | -0.052947 |
| 16               | 6                | 0              | -4.073989        | -1.285958        | 0.035230  |
| 17               | 6                | 0              | -4.517678        | 0.040025         | 0.110156  |
| 18               | 6                | 0              | -3.586085        | 1.077777         | 0.091594  |
| 19               | 1                | 0              | 5.018144         | 2.665655         | -0.103065 |
| 20               | 1                | 0              | 6.765506         | 1.097495         | 0.643061  |
| 21               | 1                | 0              | 6.235049         | -1.322096        | 0.922801  |
| 22               | 1                | 0              | 3.917310         | -2.107451        | 0.517538  |
| 23               | 1                | 0              | 2.863060         | 3.015444         | -0.794350 |
| 24               | 1                | 0              | 1.948916         | 1.791120         | -1.416007 |
| 25               | 1                | 0              | -1.531208        | 1.613708         | -0.024233 |
| 26               | 1                | 0              | -2.389295        | -2.594823        | -0.104788 |
| 27               | 8                | 0              | -5.853621        | 0.213464         | 0.197235  |
| 28               | 1                | 0              | -3.898757        | 2.112945         | 0.143679  |
| 29               | 1                | 0              | 0.632797         | 1.000626         | 0.212577  |
| 30               | 1                | 0              | -4.807866        | -2.084408        | 0.052439  |
| 31               | 6                | 0              | -6.354213        | 1.537466         | 0.284946  |
| 32               | 1                | 0              | -7.436878        | 1.444246         | 0.350941  |
| 33               | 1                | 0              | -5.978120        | 2.044181         | 1.179362  |
| 34               | 1                | 0              | -6.093576        | 2.119343         | -0.604864 |

STO<sup>##</sup>-3G<sub>el</sub> basis set

H 0

S 3 1.00 0.000000000000  
0.3425250914D+01 0.1543289673D+00  
0.6239137298D+00 0.5353281423D+00  
0.1688554040D+00 0.4446345422D+00  
P 3 1.00 0.000000000000  
0.3798226486D+00 0.1639453352D+00  
0.6918516958D-01 0.5686848896D+00  
0.1872420689D-01 0.4723400949D+00

\*\*\*\*

C 0

S 3 1.00 0.000000000000  
0.7161683735D+02 0.1543289673D+00  
0.1304509632D+02 0.5353281423D+00  
0.3530512160D+01 0.4446345422D+00  
S 3 1.00 0.000000000000  
0.7353123388D+00 0.1484327036D+00  
0.1708707741D+00 0.5785164971D+00  
0.5557247898D-01 0.3731444683D+00  
SP 3 1.00 0.000000000000  
0.2941249355D+01 -0.9996722919D-01 0.1559162750D+00  
0.6834830964D+00 0.3995128261D+00 0.6076837186D+00  
0.2222899159D+00 0.7001154689D+00 0.3919573931D+00  
P 3 1.00 0.000000000000  
0.7941519477D+01 0.1639453352D+00  
0.1446557686D+01 0.5686848896D+00  
0.3914949629D+00 0.4723400949D+00  
P 3 1.00 0.000000000000  
0.7353123388D+00 -0.1012509754D+00  
0.1708707741D+00 0.4046432382D+00  
0.5557247898D-01 0.7091061211D+00  
D 3 1.00 0.000000000000  
0.7353123388D+00 0.1624749562D+00  
0.1708707741D+00 0.6332461802D+00  
0.5557247898D-01 0.4084452395D+00

\*\*\*\*

N 0

S 3 1.00 0.000000000000  
0.9910616896D+02 0.1543289673D+00  
0.1805231239D+02 0.5353281423D+00  
0.4885660238D+01 0.4446345422D+00  
S 3 1.00 0.000000000000  
0.9451139698D+00 0.1484327036D+00  
0.2196241612D+00 0.5785164971D+00  
0.7142859360D-01 0.3731444683D+00  
SP 3 1.00 0.000000000000  
0.3780455879D+01 -0.9996722919D-01 0.1559162750D+00  
0.8784966449D+00 0.3995128261D+00 0.6076837186D+00  
0.2857143744D+00 0.7001154689D+00 0.3919573931D+00  
P 3 1.00 0.000000000000  
0.1098978397D+02 0.1639453352D+00  
0.2001802869D+01 0.5686848896D+00  
0.5417659781D+00 0.4723400949D+00  
P 3 1.00 0.000000000000

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0.9451139698D+00 -0.1012509754D+00
0.2196241612D+00 0.4046432382D+00
0.7142859360D-01 0.7091061211D+00
D 3 1.00 0.0000000000000
0.9451139698D+00 0.1624749562D+00
0.2196241612D+00 0.6332461802D+00
0.7142859360D-01 0.4084452395D+00
****
O 0
S 3 1.00 0.0000000000000
0.1307093214D+03 0.1543289673D+00
0.2380886605D+02 0.5353281423D+00
0.6443608313D+01 0.4446345422D+00
S 3 1.00 0.0000000000000
0.1258287830D+01 0.1484327036D+00
0.2923990313D+00 0.5785164971D+00
0.9509724000D-01 0.3731444683D+00
SP 3 1.00 0.0000000000000
0.5033151319D+01 -0.9996722919D-01 0.1559162750D+00
0.1169596125D+01 0.3995128261D+00 0.6076837186D+00
0.3803889600D+00 0.7001154689D+00 0.3919573931D+00
P 3 1.00 0.0000000000000
0.1449422594D+02 0.1639453352D+00
0.2640141347D+01 0.5686848896D+00
0.7145252822D+00 0.4723400949D+00
P 3 1.00 0.0000000000000
0.1258287830D+01 -0.1012509754D+00
0.2923990313D+00 0.4046432382D+00
0.9509724000D-01 0.7091061211D+00
D 3 1.00 0.0000000000000
0.1258287830D+01 0.1624749562D+00
0.2923990313D+00 0.6332461802D+00
0.9509724000D-01 0.4084452395D+00
****
F 0
S 3 1.00 0.0000000000000
0.1666791340D+03 0.1543289673D+00
0.3036081233D+02 0.5353281423D+00
0.8216820672D+01 0.4446345422D+00
S 3 1.00 0.0000000000000
0.1616200812D+01 0.1484327036D+00
0.3755703113D+00 0.5785164971D+00
0.1221471216D+00 0.3731444683D+00
SP 3 1.00 0.0000000000000
0.6464803249D+01 -0.9996722919D-01 0.1559162750D+00
0.1502281245D+01 0.3995128261D+00 0.6076837186D+00
0.4885884864D+00 0.7001154689D+00 0.3919573931D+00
P 3 1.00 0.0000000000000
0.1848288249D+02 0.1639453352D+00
0.3366680118D+01 0.5686848896D+00
0.9111550275D+00 0.4723400949D+00
P 3 1.00 0.0000000000000
0.1616200812D+01 -0.1012509754D+00
0.3755703113D+00 0.4046432382D+00
0.1221471216D+00 0.7091061212D+00

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D 3 1.00 0.000000000000
0.1616200812D+01 0.1624749562D+00
0.3755703113D+00 0.6332461802D+00
0.1221471216D+00 0.4084452395D+00
****
S 0
S 3 1.00 0.000000000000
0.5331257359D+03 0.1543289673D+00
0.9710951830D+02 0.5353281423D+00
0.2628162542D+02 0.4446345422D+00
S 3 1.00 0.000000000000
0.8332437933D+01 0.1484327036D+00
0.1936279380D+01 0.5785164971D+00
0.6297381498D+00 0.3731444683D+00
S 3 1.00 0.000000000000
0.7305099386D+00 0.1032896585D-01
0.2038104186D+00 0.5806280160D+00
0.7977001651D-01 0.4507150574D+00
SP 3 1.00 0.000000000000
0.3332975173D+02 -0.9996722919D-01 0.1559162750D+00
0.7745117521D+01 0.3995128261D+00 0.6076837186D+00
0.2518952599D+01 0.7001154689D+00 0.3919573931D+00
SP 3 1.00 0.000000000000
0.2029194274D+01 -0.2196203690D+00 0.1058760429D-01
0.5661400518D+00 0.2255954336D+00 0.5951670053D+00
0.2215833792D+00 0.9003984260D+00 0.4620010120D+00
P 3 1.00 0.000000000000
0.5911777973D+02 0.1639453352D+00
0.1076837737D+02 0.5686848896D+00
0.2914343161D+01 0.4723400949D+00
P 3 1.00 0.000000000000
0.8332437933D+01 -0.1012509754D+00
0.1936279380D+01 0.4046432382D+00
0.6297381498D+00 0.7091061211D+00
P 3 1.00 0.000000000000
0.7305099386D+00 -0.2141682022D+00
0.2038104186D+00 0.2199949334D+00
0.7977001651D-01 0.8780456615D+00
D 3 1.00 0.000000000000
0.8332437933D+01 0.1624749562D+00
0.1936279380D+01 0.6332461802D+00
0.6297381498D+00 0.4084452395D+00
D 3 1.00 0.000000000000
0.7305099386D+00 0.1083376326D-01
0.2038104186D+00 0.6090044793D+00
0.7977001651D-01 0.4727424122D+00
****
Si 0
S 3 1.00 0.000000000000
0.4077975514D+03 0.1543289673D+00
0.7428083305D+02 0.5353281423D+00
0.2010329229D+02 0.4446345422D+00
S 3 1.00 0.000000000000
0.5798414015D+01 0.1484327036D+00
0.1347426718D+01 0.5785164971D+00

```

0.4382249880D+00 0.3731444683D+00  
 S 3 1.00 0.000000000000  
 0.5323466239D+00 0.1032896585D-01  
 0.1485233568D+00 0.5806280160D+00  
 0.5813103524D-01 0.4507150574D+00  
 SP 3 1.00 0.000000000000  
 0.2319365606D+02 -0.9996722919D-01 0.1559162750D+00  
 0.5389706871D+01 0.3995128261D+00 0.6076837186D+00  
 0.1752899952D+01 0.7001154689D+00 0.3919573931D+00  
 SP 3 1.00 0.000000000000  
 0.1478740622D+01 -0.2196203690D+00 0.1058760429D-01  
 0.4125648801D+00 0.2255954336D+00 0.5951670053D+00  
 0.1614750979D+00 0.9003984260D+00 0.4620010120D+00  
 P 3 1.00 0.000000000000  
 0.4522026268D+02 0.1639453352D+00  
 0.8236927296D+01 0.5686848896D+00  
 0.2229233979D+01 0.4723400949D+00  
 P 3 1.00 0.000000000000  
 0.5798414015D+01 -0.1012509754D+00  
 0.1347426718D+01 0.4046432382D+00  
 0.4382249880D+00 0.7091061211D+00  
 P 3 1.00 0.000000000000  
 0.5323466239D+00 -0.2141682022D+00  
 0.1485233568D+00 0.2199949334D+00  
 0.5813103524D-01 0.8780456615D+00  
 D 3 1.00 0.000000000000  
 0.5798414015D+01 0.1624749562D+00  
 0.1347426718D+01 0.6332461802D+00  
 0.4382249880D+00 0.4084452395D+00  
 D 3 1.00 0.000000000000  
 0.5323466239D+00 0.1083376326D-01  
 0.1485233568D+00 0.6090044793D+00  
 0.5813103524D-01 0.4727424122D+00

\*\*\*\*

Cl 0

S 3 1.00 0.000000000000  
 0.6013456136D+03 0.1543289673D+00  
 0.1095358542D+03 0.5353281423D+00  
 0.2964467686D+02 0.4446345422D+00  
 S 3 1.00 0.000000000000  
 0.9740104722D+01 0.1484327036D+00  
 0.2263390869D+01 0.5785164971D+00  
 0.7361249585D+00 0.3731444683D+00  
 S 3 1.00 0.000000000000  
 0.7665791382D+00 0.1032896585D-01  
 0.2138736339D+00 0.5806280160D+00  
 0.8370869076D-01 0.4507150574D+00  
 SP 3 1.00 0.000000000000  
 0.3896041889D+02 -0.9996722919D-01 0.1559162750D+00  
 0.9053563477D+01 0.3995128261D+00 0.6076837186D+00  
 0.2944499834D+01 0.7001154689D+00 0.3919573931D+00  
 SP 3 1.00 0.000000000000  
 0.2129386495D+01 -0.2196203690D+00 0.1058760429D-01  
 0.5940934274D+00 0.2255954336D+00 0.5951670053D+00  
 0.2325241410D+00 0.9003984260D+00 0.4620010120D+00

P 3 1.00 0.000000000000  
 0.6668261375D+02 0.1639453352D+00  
 0.1214632134D+02 0.5686848896D+00  
 0.3287268572D+01 0.4723400949D+00  
 P 3 1.00 0.000000000000  
 0.9740104722D+01 -0.1012509754D+00  
 0.2263390869D+01 0.4046432382D+00  
 0.7361249585D+00 0.7091061211D+00  
 P 3 1.00 0.000000000000  
 0.7665791382D+00 -0.2141682022D+00  
 0.2138736339D+00 0.2199949334D+00  
 0.8370869076D-01 0.8780456616D+00  
 D 3 1.00 0.000000000000  
 0.9740104722D+01 0.1624749562D+00  
 0.2263390869D+01 0.6332461802D+00  
 0.7361249585D+00 0.4084452395D+00  
 D 3 1.00 0.000000000000  
 0.7665791382D+00 0.1083376326D-01  
 0.2138736339D+00 0.6090044793D+00  
 0.8370869076D-01 0.4727424122D+00  
 \*\*\*\*  
 Br 0  
 S 3 1.00 0.000000000000  
 0.2629997471D+04 0.1543289673D+00  
 0.4790573224D+03 0.5353281423D+00  
 0.1296516070D+03 0.4446345422D+00  
 S 3 1.00 0.000000000000  
 0.5495875638D+02 0.1484327036D+00  
 0.1277123306D+02 0.5785164971D+00  
 0.4153601365D+01 0.3731444683D+00  
 S 3 1.00 0.000000000000  
 0.7020623192D+01 0.4830334660D-02  
 0.2141513848D+01 0.5636270047D+00  
 0.8262626184D+00 0.4727854740D+00  
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 P 3 1.00 0.000000000000

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