

SUPPLEMENTARY MATERIAL

**A new mechanistic insight on the molecular mechanisms of the addition reactions of 2-aryl-3-nitro-2H-chromenes to the pyrazole and cyclopentadiene**

Przemysław Woliński, Ewa Dresler and Radomir Jasiński

# CARTESIAN COORDINATES FOR THE MAJOR PROCESS WITH THE PARTICIPATION OF THE PYRAZOLE

1

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 1                | 0              | 1.929788                | -0.802803 | -0.000061 |
| 2                | 7                | 0              | -0.066916               | -1.197689 | -0.000042 |
| 3                | 6                | 0              | -1.100735               | -0.365653 | 0.000063  |
| 4                | 6                | 0              | 0.690959                | 0.914441  | 0.000053  |
| 5                | 6                | 0              | -0.684695               | 0.980631  | -0.000067 |
| 6                | 1                | 0              | -2.106664               | -0.758955 | -0.000036 |
| 7                | 1                | 0              | 1.449813                | 1.680353  | -0.000122 |
| 8                | 1                | 0              | -1.297199               | 1.867189  | 0.000045  |
| 9                | 7                | 0              | 1.008499                | -0.396924 | 0.000025  |

2a

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.558106               | 0.437719  | 1.009002  |
| 2                | 6                | 0              | -0.071202               | 1.587349  | 0.168867  |
| 3                | 6                | 0              | 1.112523                | 1.567334  | -0.450480 |
| 4                | 1                | 0              | 1.423182                | 2.391310  | -1.081555 |
| 5                | 1                | 0              | -1.087972               | 0.820030  | 1.879879  |
| 6                | 6                | 0              | 1.974741                | 0.422210  | -0.258959 |
| 7                | 6                | 0              | 1.644682                | -0.477905 | 0.765827  |
| 8                | 7                | 0              | -0.969330               | 2.708509  | -0.004240 |
| 9                | 8                | 0              | -0.612673               | 3.654620  | -0.686127 |
| 10               | 8                | 0              | -2.057374               | 2.636811  | 0.547208  |
| 11               | 8                | 0              | 0.574591                | -0.255852 | 1.568443  |
| 12               | 6                | 0              | 3.126573                | 0.200086  | -1.020401 |
| 13               | 6                | 0              | 2.458981                | -1.570161 | 1.034933  |
| 14               | 6                | 0              | 3.932200                | -0.896901 | -0.767183 |
| 15               | 1                | 0              | 4.820457                | -1.070090 | -1.361888 |
| 16               | 6                | 0              | 3.595155                | -1.774671 | 0.264016  |
| 17               | 1                | 0              | 4.225595                | -2.632461 | 0.468452  |
| 18               | 1                | 0              | 3.378674                | 0.899231  | -1.810357 |
| 19               | 1                | 0              | 2.191263                | -2.245442 | 1.838140  |
| 20               | 6                | 0              | -1.460486               | -0.533457 | 0.270835  |
| 21               | 6                | 0              | -1.296931               | -0.811431 | -1.084928 |
| 22               | 6                | 0              | -2.445251               | -1.208144 | 0.991124  |
| 23               | 6                | 0              | -2.104080               | -1.756068 | -1.709279 |
| 24               | 1                | 0              | -0.544938               | -0.288060 | -1.664763 |
| 25               | 6                | 0              | -3.254392               | -2.149476 | 0.368159  |
| 26               | 1                | 0              | -2.581200               | -0.991363 | 2.045806  |
| 27               | 6                | 0              | -3.082815               | -2.426504 | -0.984617 |
| 28               | 1                | 0              | -1.969596               | -1.964827 | -2.764423 |
| 29               | 1                | 0              | -4.021153               | -2.663436 | 0.936430  |
| 30               | 1                | 0              | -3.714911               | -3.158964 | -1.473734 |

## MCA

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.324050                | 1.521320  | -1.175845 |
| 2                | 6                | 0              | 0.117038                | 0.128506  | -1.707276 |
| 3                | 6                | 0              | 0.894527                | -0.896184 | -1.339157 |
| 4                | 1                | 0              | -1.889775               | -2.375795 | -1.160176 |
| 5                | 1                | 0              | 0.708895                | -1.900754 | -1.694476 |
| 6                | 1                | 0              | 0.139186                | 2.248577  | -1.964440 |
| 7                | 6                | 0              | 1.994359                | -0.638598 | -0.439590 |
| 8                | 6                | 0              | 2.355997                | 0.697704  | -0.213042 |
| 9                | 7                | 0              | -0.698003               | -2.877287 | 0.414208  |
| 10               | 6                | 0              | -0.943063               | -2.846664 | 1.718869  |
| 11               | 6                | 0              | -2.803835               | -2.183159 | 0.745920  |
| 12               | 6                | 0              | -2.257436               | -2.418598 | 1.988629  |
| 13               | 1                | 0              | -0.169500               | -3.131092 | 2.416945  |
| 14               | 1                | 0              | -3.777564               | -1.835041 | 0.440987  |
| 15               | 1                | 0              | -2.734974               | -2.297001 | 2.946933  |
| 16               | 7                | 0              | -1.843793               | -2.473780 | -0.154948 |
| 17               | 7                | 0              | -1.019397               | -0.088675 | -2.564791 |
| 18               | 8                | 0              | -1.317376               | -1.235894 | -2.882562 |
| 19               | 8                | 0              | -1.651992               | 0.891366  | -2.920927 |
| 20               | 8                | 0              | 1.714951                | 1.708451  | -0.850841 |
| 21               | 6                | 0              | 2.713765                | -1.660666 | 0.187712  |
| 22               | 6                | 0              | 3.434234                | 1.007433  | 0.605845  |
| 23               | 6                | 0              | 3.777447                | -1.356323 | 1.018961  |
| 24               | 1                | 0              | 4.330080                | -2.147693 | 1.510015  |
| 25               | 6                | 0              | 4.135543                | -0.021780 | 1.218595  |
| 26               | 1                | 0              | 4.970783                | 0.220113  | 1.865948  |
| 27               | 1                | 0              | 2.415155                | -2.689021 | 0.018398  |
| 28               | 1                | 0              | 3.704647                | 2.045116  | 0.757258  |
| 29               | 6                | 0              | -0.551200               | 1.851457  | 0.019189  |
| 30               | 6                | 0              | -0.915546               | 0.885260  | 0.955464  |
| 31               | 6                | 0              | -0.956719               | 3.172288  | 0.207411  |
| 32               | 6                | 0              | -1.670035               | 1.239120  | 2.068398  |
| 33               | 1                | 0              | -0.620929               | -0.150191 | 0.823949  |
| 34               | 6                | 0              | -1.712372               | 3.525977  | 1.317740  |
| 35               | 1                | 0              | -0.681085               | 3.926942  | -0.522285 |
| 36               | 6                | 0              | -2.068858               | 2.558003  | 2.252064  |
| 37               | 1                | 0              | -1.949865               | 0.476151  | 2.785530  |
| 38               | 1                | 0              | -2.027393               | 4.554582  | 1.451516  |
| 39               | 1                | 0              | -2.661348               | 2.831348  | 3.117940  |

# TSA

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.147189                | -0.256657 | -1.800993 |
| 2                | 6                | 0              | -0.042038               | -1.442240 | -0.900523 |
| 3                | 6                | 0              | 0.635197                | -1.473044 | 0.320087  |
| 4                | 1                | 0              | -1.918675               | -2.079746 | 1.352579  |
| 5                | 1                | 0              | 0.655826                | -2.410363 | 0.860575  |
| 6                | 1                | 0              | -0.154378               | -0.513220 | -2.815241 |
| 7                | 6                | 0              | 1.846663                | -0.644033 | 0.388558  |
| 8                | 6                | 0              | 2.252304                | 0.061982  | -0.749684 |
| 9                | 7                | 0              | -0.508051               | -0.653473 | 1.656255  |
| 10               | 6                | 0              | -0.547253               | 0.557197  | 2.196674  |
| 11               | 6                | 0              | -2.557689               | -0.329309 | 2.417548  |
| 12               | 6                | 0              | -1.827163               | 0.805647  | 2.709132  |
| 13               | 1                | 0              | 0.330576                | 1.184636  | 2.183410  |
| 14               | 1                | 0              | -3.585504               | -0.589366 | 2.611669  |
| 15               | 1                | 0              | -2.172605               | 1.693283  | 3.211280  |
| 16               | 7                | 0              | -1.731373               | -1.180191 | 1.787526  |
| 17               | 7                | 0              | -1.007668               | -2.380709 | -1.174064 |
| 18               | 8                | 0              | -1.342155               | -3.197397 | -0.279204 |
| 19               | 8                | 0              | -1.555170               | -2.399522 | -2.286807 |
| 20               | 8                | 0              | 1.538295                | 0.065856  | -1.900876 |
| 21               | 6                | 0              | 2.656793                | -0.619598 | 1.528343  |
| 22               | 6                | 0              | 3.460745                | 0.758388  | -0.749068 |
| 23               | 6                | 0              | 3.843616                | 0.089414  | 1.541722  |
| 24               | 1                | 0              | 4.460801                | 0.105825  | 2.431466  |
| 25               | 6                | 0              | 4.243965                | 0.773796  | 0.391828  |
| 26               | 1                | 0              | 5.176686                | 1.326253  | 0.388309  |
| 27               | 1                | 0              | 2.335247                | -1.169896 | 2.406354  |
| 28               | 1                | 0              | 3.759960                | 1.285680  | -1.646936 |
| 29               | 6                | 0              | -0.657784               | 0.952402  | -1.322226 |
| 30               | 6                | 0              | -2.022603               | 0.796419  | -1.073097 |
| 31               | 6                | 0              | -0.074454               | 2.199913  | -1.123531 |
| 32               | 6                | 0              | -2.785563               | 1.865053  | -0.625253 |
| 33               | 1                | 0              | -2.496319               | -0.166356 | -1.231173 |
| 34               | 6                | 0              | -0.838998               | 3.270313  | -0.665915 |
| 35               | 1                | 0              | 0.979987                | 2.343998  | -1.322928 |
| 36               | 6                | 0              | -2.194486               | 3.107222  | -0.414059 |
| 37               | 1                | 0              | -3.843772               | 1.725909  | -0.434519 |
| 38               | 1                | 0              | -0.368148               | 4.234374  | -0.508127 |
| 39               | 1                | 0              | -2.788432               | 3.940932  | -0.056883 |

4a

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.049490               | 0.000092  | 1.802886  |
| 2                | 6                | 0              | 0.187443                | -1.255429 | 1.028426  |
| 3                | 6                | 0              | -0.472660               | -1.375534 | -0.296403 |
| 4                | 1                | 0              | 1.790777                | -2.283347 | -0.871553 |
| 5                | 1                | 0              | -0.631827               | -2.426384 | -0.543743 |
| 6                | 1                | 0              | 0.290014                | -0.135083 | 2.828308  |
| 7                | 6                | 0              | -1.787679               | -0.642865 | -0.315510 |
| 8                | 6                | 0              | -2.199212               | 0.108243  | 0.787233  |
| 9                | 7                | 0              | 0.434872                | -0.862339 | -1.376540 |
| 10               | 6                | 0              | 0.418522                | 0.236500  | -2.133715 |
| 11               | 6                | 0              | 2.350983                | -0.805732 | -2.412565 |
| 12               | 6                | 0              | 1.623312                | 0.301547  | -2.823447 |
| 13               | 1                | 0              | -0.433389               | 0.895891  | -2.129750 |
| 14               | 1                | 0              | 3.337404                | -1.146707 | -2.680637 |
| 15               | 1                | 0              | 1.926270                | 1.057946  | -3.526170 |
| 16               | 7                | 0              | 1.605378                | -1.494000 | -1.546943 |
| 17               | 7                | 0              | 1.115485                | -2.129620 | 1.388499  |
| 18               | 8                | 0              | 1.462815                | -3.062287 | 0.550366  |
| 19               | 8                | 0              | 1.701096                | -2.069462 | 2.500869  |
| 20               | 8                | 0              | -1.448733               | 0.278528  | 1.904611  |
| 21               | 6                | 0              | -2.655134               | -0.778078 | -1.402797 |
| 22               | 6                | 0              | -3.459869               | 0.709554  | 0.792145  |
| 23               | 6                | 0              | -3.898482               | -0.171566 | -1.409312 |
| 24               | 1                | 0              | -4.556714               | -0.284906 | -2.261835 |
| 25               | 6                | 0              | -4.298614               | 0.572534  | -0.298752 |
| 26               | 1                | 0              | -5.273086               | 1.047109  | -0.284902 |
| 27               | 1                | 0              | -2.340652               | -1.378178 | -2.251101 |
| 28               | 1                | 0              | -3.755598               | 1.282555  | 1.662877  |
| 29               | 6                | 0              | 0.695706                | 1.174713  | 1.164621  |
| 30               | 6                | 0              | 2.065547                | 1.040891  | 0.926252  |
| 31               | 6                | 0              | 0.055100                | 2.350922  | 0.789054  |
| 32               | 6                | 0              | 2.776640                | 2.060107  | 0.309573  |
| 33               | 1                | 0              | 2.577098                | 0.131927  | 1.226377  |
| 34               | 6                | 0              | 0.768355                | 3.370714  | 0.162616  |
| 35               | 1                | 0              | -1.003882               | 2.476764  | 0.977645  |
| 36               | 6                | 0              | 2.127467                | 3.228065  | -0.082460 |
| 37               | 1                | 0              | 3.839391                | 1.941370  | 0.130511  |
| 38               | 1                | 0              | 0.254503                | 4.278691  | -0.133094 |
| 39               | 1                | 0              | 2.680512                | 4.021775  | -0.571889 |

**TSB**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.113699               | -0.924224 | -1.333838 |
| 2                | 6                | 0              | 0.120236                | -1.529172 | 0.029132  |
| 3                | 6                | 0              | 0.870485                | -0.642838 | 0.993304  |
| 4                | 1                | 0              | -1.140809               | -1.336429 | 0.855813  |
| 5                | 1                | 0              | 1.380922                | -1.258211 | 1.733020  |
| 6                | 1                | 0              | -0.334869               | -1.731706 | -2.027969 |
| 7                | 6                | 0              | 1.851021                | 0.282906  | 0.331067  |
| 8                | 6                | 0              | 1.892287                | 0.378621  | -1.061288 |
| 9                | 7                | 0              | -0.210455               | 0.099293  | 1.730041  |
| 10               | 6                | 0              | -0.301489               | 1.243670  | 2.412049  |
| 11               | 6                | 0              | -2.281636               | 0.252421  | 2.317048  |
| 12               | 6                | 0              | -1.624754               | 1.377000  | 2.815882  |
| 13               | 1                | 0              | 0.551719                | 1.884675  | 2.558656  |
| 14               | 1                | 0              | -3.317012               | -0.040530 | 2.375723  |
| 15               | 1                | 0              | -2.050917               | 2.188600  | 3.381446  |
| 16               | 7                | 0              | -1.392707               | -0.506430 | 1.679807  |
| 17               | 7                | 0              | 0.485630                | -2.901747 | 0.063154  |
| 18               | 8                | 0              | 0.980451                | -3.365436 | 1.095827  |
| 19               | 8                | 0              | 0.225178                | -3.619238 | -0.904235 |
| 20               | 8                | 0              | 1.057219                | -0.296980 | -1.885782 |
| 21               | 6                | 0              | 2.793637                | 0.987323  | 1.083640  |
| 22               | 6                | 0              | 2.852664                | 1.182720  | -1.679466 |
| 23               | 6                | 0              | 3.737937                | 1.798869  | 0.477775  |
| 24               | 1                | 0              | 4.458854                | 2.340453  | 1.077781  |
| 25               | 6                | 0              | 3.761006                | 1.891845  | -0.913646 |
| 26               | 1                | 0              | 4.498834                | 2.516193  | -1.404578 |
| 27               | 1                | 0              | 2.792221                | 0.876629  | 2.163829  |
| 28               | 1                | 0              | 2.863568                | 1.237060  | -2.761477 |
| 29               | 6                | 0              | -1.292749               | 0.039728  | -1.330008 |
| 30               | 6                | 0              | -2.575259               | -0.500564 | -1.428122 |
| 31               | 6                | 0              | -1.150121               | 1.415344  | -1.173744 |
| 32               | 6                | 0              | -3.696250               | 0.314782  | -1.352985 |
| 33               | 1                | 0              | -2.694901               | -1.572485 | -1.555099 |
| 34               | 6                | 0              | -2.273400               | 2.233748  | -1.094845 |
| 35               | 1                | 0              | -0.165028               | 1.861662  | -1.108049 |
| 36               | 6                | 0              | -3.547962               | 1.687793  | -1.179987 |
| 37               | 1                | 0              | -4.685905               | -0.120896 | -1.432914 |
| 38               | 1                | 0              | -2.147444               | 3.303021  | -0.966784 |
| 39               | 1                | 0              | -4.421019               | 2.327548  | -1.118705 |

3a

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.133740               | 0.880567  | -1.413625 |
| 2                | 6                | 0              | -0.414006               | 1.617799  | -0.097863 |
| 3                | 6                | 0              | -0.711468               | 0.661860  | 1.061187  |
| 4                | 1                | 0              | 0.413918                | 2.274357  | 0.162031  |
| 5                | 1                | 0              | -1.265638               | 1.208178  | 1.825507  |
| 6                | 1                | 0              | -0.105116               | 1.619011  | -2.216174 |
| 7                | 6                | 0              | -1.525653               | -0.519271 | 0.604192  |
| 8                | 6                | 0              | -1.737489               | -0.756334 | -0.751409 |
| 9                | 7                | 0              | 0.553606                | 0.259804  | 1.675794  |
| 10               | 6                | 0              | 1.159242                | -0.949557 | 1.690188  |
| 11               | 6                | 0              | 2.379984                | 0.575607  | 2.701072  |
| 12               | 6                | 0              | 2.352481                | -0.787272 | 2.354576  |
| 13               | 1                | 0              | 0.710430                | -1.812464 | 1.227851  |
| 14               | 1                | 0              | 3.142930                | 1.121820  | 3.236200  |
| 15               | 1                | 0              | 3.094759                | -1.542516 | 2.553004  |
| 16               | 7                | 0              | 1.288127                | 1.204742  | 2.287424  |
| 17               | 7                | 0              | -1.573476               | 2.561786  | -0.345191 |
| 18               | 8                | 0              | -2.620280               | 2.375532  | 0.236491  |
| 19               | 8                | 0              | -1.369872               | 3.460129  | -1.135199 |
| 20               | 8                | 0              | -1.230445               | 0.043082  | -1.737946 |
| 21               | 6                | 0              | -2.125901               | -1.368670 | 1.535575  |
| 22               | 6                | 0              | -2.533534               | -1.820986 | -1.170824 |
| 23               | 6                | 0              | -2.907698               | -2.436163 | 1.130302  |
| 24               | 1                | 0              | -3.363470               | -3.087763 | 1.865636  |
| 25               | 6                | 0              | -3.111584               | -2.657004 | -0.232059 |
| 26               | 1                | 0              | -3.726956               | -3.485732 | -0.562665 |
| 27               | 1                | 0              | -1.969788               | -1.177674 | 2.592450  |
| 28               | 1                | 0              | -2.682412               | -1.973486 | -2.233060 |
| 29               | 6                | 0              | 1.191648                | 0.132842  | -1.390825 |
| 30               | 6                | 0              | 2.365882                | 0.816214  | -1.075141 |
| 31               | 6                | 0              | 1.259859                | -1.215964 | -1.725468 |
| 32               | 6                | 0              | 3.584657                | 0.152929  | -1.067366 |
| 33               | 1                | 0              | 2.340658                | 1.872942  | -0.830925 |
| 34               | 6                | 0              | 2.482588                | -1.879415 | -1.718455 |
| 35               | 1                | 0              | 0.360559                | -1.756738 | -1.991635 |
| 36               | 6                | 0              | 3.646538                | -1.200181 | -1.384189 |
| 37               | 1                | 0              | 4.487622                | 0.695089  | -0.811427 |
| 38               | 1                | 0              | 2.520595                | -2.931944 | -1.975397 |
| 39               | 1                | 0              | 4.598047                | -1.719345 | -1.373550 |

**MCD\_endo**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.702935                | 4.017181  | -0.351295 |
| 2                | 6                | 0              | 0.205675                | 2.946818  | -1.082592 |
| 3                | 6                | 0              | 0.219311                | 1.675883  | -0.521531 |
| 4                | 6                | 0              | 0.745797                | 1.470053  | 0.762380  |
| 5                | 6                | 0              | 1.246297                | 2.560751  | 1.478985  |
| 6                | 6                | 0              | 1.220535                | 3.832189  | 0.930959  |
| 7                | 1                | 0              | 0.684289                | 5.009592  | -0.787003 |
| 8                | 1                | 0              | -0.195712               | 3.081169  | -2.079529 |
| 9                | 1                | 0              | 1.659621                | 2.393629  | 2.467663  |
| 10               | 1                | 0              | 1.605336                | 4.675450  | 1.490880  |
| 11               | 6                | 0              | 0.797817                | 0.113432  | 1.261074  |
| 12               | 1                | 0              | 1.371110                | -0.122106 | 2.148428  |
| 13               | 6                | 0              | 0.146101                | -0.839660 | 0.591501  |
| 14               | 6                | 0              | -0.687720               | -0.551822 | -0.627611 |
| 15               | 1                | 0              | -0.533134               | -1.339484 | -1.363590 |
| 16               | 8                | 0              | -0.203466               | 0.637139  | -1.282151 |
| 17               | 6                | 0              | -2.172046               | -0.424487 | -0.343504 |
| 18               | 6                | 0              | -3.081270               | -0.875775 | -1.298533 |
| 19               | 6                | 0              | -2.647625               | 0.179653  | 0.819250  |
| 20               | 6                | 0              | -4.447621               | -0.723668 | -1.098522 |
| 21               | 1                | 0              | -2.716737               | -1.353141 | -2.202459 |
| 22               | 6                | 0              | -4.014480               | 0.336940  | 1.018684  |
| 23               | 1                | 0              | -1.954902               | 0.525383  | 1.578653  |
| 24               | 6                | 0              | -4.916159               | -0.114271 | 0.061012  |
| 25               | 1                | 0              | -5.146317               | -1.084117 | -1.844831 |
| 26               | 1                | 0              | -4.375045               | 0.808198  | 1.925856  |
| 27               | 1                | 0              | -5.982001               | 0.003559  | 0.220363  |
| 28               | 7                | 0              | 0.192110                | -2.211340 | 1.046036  |
| 29               | 8                | 0              | -0.405556               | -3.039027 | 0.373623  |
| 30               | 8                | 0              | 0.810275                | -2.480486 | 2.061677  |
| 31               | 6                | 0              | 3.508349                | -1.818251 | 0.061505  |
| 32               | 6                | 0              | 2.793593                | -2.204120 | -1.089318 |
| 33               | 6                | 0              | 2.570643                | -1.024699 | -1.765793 |
| 34               | 1                | 0              | 3.875444                | -2.439512 | 0.864755  |
| 35               | 1                | 0              | 2.485461                | -3.194569 | -1.381115 |
| 36               | 1                | 0              | 2.060578                | -0.807635 | -2.690229 |
| 37               | 7                | 0              | 3.135993                | -0.049399 | -1.026565 |
| 38               | 1                | 0              | 3.138528                | 0.939217  | -1.218448 |
| 39               | 7                | 0              | 3.710849                | -0.506907 | 0.095601  |

**TSD\_endo**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.884258               | 3.905924  | -0.134481 |
| 2                | 6                | 0              | -0.933534               | 2.835634  | -1.017993 |
| 3                | 6                | 0              | -0.233595               | 1.677136  | -0.713545 |
| 4                | 6                | 0              | 0.518099                | 1.569051  | 0.455038  |
| 5                | 6                | 0              | 0.544348                | 2.646773  | 1.336738  |
| 6                | 6                | 0              | -0.152198               | 3.811778  | 1.046959  |
| 7                | 1                | 0              | -1.430108               | 4.813748  | -0.364022 |
| 8                | 1                | 0              | -1.510844               | 2.880726  | -1.933454 |
| 9                | 1                | 0              | 1.123272                | 2.567834  | 2.250795  |
| 10               | 1                | 0              | -0.125546               | 4.645134  | 1.738734  |
| 11               | 6                | 0              | 1.280334                | 0.316841  | 0.713210  |
| 12               | 1                | 0              | 1.463507                | 0.136858  | 1.766136  |
| 13               | 6                | 0              | 0.814569                | -0.844515 | -0.040227 |
| 14               | 6                | 0              | -0.360506               | -0.667198 | -0.995888 |
| 15               | 1                | 0              | -0.271496               | -1.356372 | -1.834107 |
| 16               | 8                | 0              | -0.257037               | 0.633740  | -1.605747 |
| 17               | 6                | 0              | -1.741955               | -0.839047 | -0.384471 |
| 18               | 6                | 0              | -2.787637               | -1.208456 | -1.229623 |
| 19               | 6                | 0              | -2.016106               | -0.582915 | 0.957142  |
| 20               | 6                | 0              | -4.084998               | -1.317595 | -0.746589 |
| 21               | 1                | 0              | -2.582353               | -1.414451 | -2.275401 |
| 22               | 6                | 0              | -3.314099               | -0.693512 | 1.444425  |
| 23               | 1                | 0              | -1.221202               | -0.299289 | 1.637633  |
| 24               | 6                | 0              | -4.351123               | -1.058223 | 0.594352  |
| 25               | 1                | 0              | -4.887293               | -1.609646 | -1.414675 |
| 26               | 1                | 0              | -3.512800               | -0.494061 | 2.491238  |
| 27               | 1                | 0              | -5.362190               | -1.145838 | 0.975677  |
| 28               | 7                | 0              | 0.793715                | -2.101196 | 0.650995  |
| 29               | 8                | 0              | 0.226310                | -3.041703 | 0.099610  |
| 30               | 8                | 0              | 1.376786                | -2.211893 | 1.723479  |
| 31               | 6                | 0              | 3.603305                | -0.480434 | 0.536833  |
| 32               | 6                | 0              | 3.421441                | -1.514770 | -0.309866 |
| 33               | 6                | 0              | 2.499820                | -0.996901 | -1.290768 |
| 34               | 1                | 0              | 4.083436                | -0.454706 | 1.503055  |
| 35               | 1                | 0              | 3.751849                | -2.534983 | -0.205887 |
| 36               | 1                | 0              | 2.188084                | -1.483475 | -2.206042 |
| 37               | 7                | 0              | 2.685168                | 0.362656  | -1.251382 |
| 38               | 1                | 0              | 2.006414                | 0.964871  | -1.698698 |
| 39               | 7                | 0              | 2.890738                | 0.650692  | 0.100787  |

**5\_endo**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.426347               | 4.026711  | -0.182208 |
| 2                | 6                | 0              | -0.602654               | 2.967680  | -1.061467 |
| 3                | 6                | 0              | -0.013736               | 1.744101  | -0.772687 |
| 4                | 6                | 0              | 0.747427                | 1.557897  | 0.376568  |
| 5                | 6                | 0              | 0.900382                | 2.627327  | 1.255444  |
| 6                | 6                | 0              | 0.320368                | 3.857767  | 0.981619  |
| 7                | 1                | 0              | -0.883845               | 4.984758  | -0.400364 |
| 8                | 1                | 0              | -1.192864               | 3.070521  | -1.963893 |
| 9                | 1                | 0              | 1.488188                | 2.489120  | 2.156831  |
| 10               | 1                | 0              | 0.447683                | 4.682825  | 1.672120  |
| 11               | 6                | 0              | 1.418085                | 0.237075  | 0.642533  |
| 12               | 1                | 0              | 1.387924                | 0.012404  | 1.706967  |
| 13               | 6                | 0              | 0.840060                | -0.928646 | -0.203155 |
| 14               | 6                | 0              | -0.389867               | -0.568188 | -1.076163 |
| 15               | 1                | 0              | -0.398918               | -1.251015 | -1.924844 |
| 16               | 8                | 0              | -0.171180               | 0.715137  | -1.669226 |
| 17               | 6                | 0              | -1.749239               | -0.639657 | -0.407590 |
| 18               | 6                | 0              | -2.812312               | -1.131722 | -1.165457 |
| 19               | 6                | 0              | -1.996997               | -0.195516 | 0.892281  |
| 20               | 6                | 0              | -4.098038               | -1.175958 | -0.642969 |
| 21               | 1                | 0              | -2.630232               | -1.485804 | -2.174901 |
| 22               | 6                | 0              | -3.283616               | -0.239722 | 1.416800  |
| 23               | 1                | 0              | -1.195442               | 0.184770  | 1.512703  |
| 24               | 6                | 0              | -4.336200               | -0.727230 | 0.651580  |
| 25               | 1                | 0              | -4.911826               | -1.563869 | -1.244688 |
| 26               | 1                | 0              | -3.460445               | 0.106784  | 2.428394  |
| 27               | 1                | 0              | -5.337970               | -0.762476 | 1.064334  |
| 28               | 7                | 0              | 0.448656                | -2.142321 | 0.612563  |
| 29               | 8                | 0              | 0.153518                | -3.128574 | -0.036052 |
| 30               | 8                | 0              | 0.441288                | -2.089406 | 1.821802  |
| 31               | 6                | 0              | 3.478924                | -0.926186 | 0.669633  |
| 32               | 6                | 0              | 3.084524                | -1.937919 | -0.094234 |
| 33               | 6                | 0              | 2.111995                | -1.301171 | -1.071415 |
| 34               | 1                | 0              | 4.091081                | -0.906965 | 1.558991  |
| 35               | 1                | 0              | 3.309716                | -2.989369 | -0.004355 |
| 36               | 1                | 0              | 1.891305                | -1.823912 | -1.997646 |
| 37               | 7                | 0              | 2.772572                | -0.009183 | -1.223070 |
| 38               | 1                | 0              | 2.182161                | 0.689460  | -1.667190 |
| 39               | 7                | 0              | 2.874189                | 0.309456  | 0.194889  |

**MCD\_exo**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.781422               | 4.018051  | 0.348701  |
| 2                | 6                | 0              | -0.251815               | 2.963797  | 1.079514  |
| 3                | 6                | 0              | -0.240084               | 1.689665  | 0.524746  |
| 4                | 6                | 0              | -0.772768               | 1.466935  | -0.753387 |
| 5                | 6                | 0              | -1.306047               | 2.542101  | -1.470411 |
| 6                | 6                | 0              | -1.306144               | 3.815768  | -0.928623 |
| 7                | 1                | 0              | -0.783659               | 5.012346  | 0.780649  |
| 8                | 1                | 0              | 0.153644                | 3.112029  | 2.072794  |
| 9                | 1                | 0              | -1.725341               | 2.360221  | -2.454017 |
| 10               | 1                | 0              | -1.716711               | 4.647194  | -1.487956 |
| 11               | 6                | 0              | -0.802446               | 0.108490  | -1.243251 |
| 12               | 1                | 0              | -1.373083               | -0.141416 | -2.128483 |
| 13               | 6                | 0              | -0.131008               | -0.831045 | -0.571810 |
| 14               | 6                | 0              | 0.704674                | -0.523674 | 0.641532  |
| 15               | 1                | 0              | 0.558174                | -1.304270 | 1.386907  |
| 16               | 8                | 0              | 0.219183                | 0.669050  | 1.285316  |
| 17               | 6                | 0              | 2.186988                | -0.389781 | 0.348045  |
| 18               | 6                | 0              | 3.106130                | -0.846164 | 1.290733  |
| 19               | 6                | 0              | 2.650157                | 0.226739  | -0.813339 |
| 20               | 6                | 0              | 4.470282                | -0.687744 | 1.079737  |
| 21               | 1                | 0              | 2.751213                | -1.332397 | 2.193742  |
| 22               | 6                | 0              | 4.014505                | 0.390412  | -1.023782 |
| 23               | 1                | 0              | 1.949163                | 0.577655  | -1.562820 |
| 24               | 6                | 0              | 4.926386                | -0.066432 | -0.078315 |
| 25               | 1                | 0              | 5.176839                | -1.052105 | 1.816719  |
| 26               | 1                | 0              | 4.365338                | 0.871473  | -1.929649 |
| 27               | 1                | 0              | 5.990350                | 0.056700  | -0.246073 |
| 28               | 7                | 0              | -0.156981               | -2.202702 | -1.019243 |
| 29               | 8                | 0              | 0.479203                | -3.014479 | -0.362169 |
| 30               | 8                | 0              | -0.801911               | -2.494809 | -2.014273 |
| 31               | 6                | 0              | -3.275238               | -0.052769 | 1.035470  |
| 32               | 6                | 0              | -2.645708               | -1.024821 | 1.835329  |
| 33               | 6                | 0              | -2.696522               | -2.176535 | 1.080995  |
| 34               | 1                | 0              | -3.436380               | 0.993632  | 1.249072  |
| 35               | 1                | 0              | -2.212449               | -0.901906 | 2.813938  |
| 36               | 1                | 0              | -2.345317               | -3.178751 | 1.268521  |
| 37               | 7                | 0              | -3.681074               | -0.559746 | -0.122701 |
| 38               | 7                | 0              | -3.321845               | -1.849901 | -0.069266 |
| 39               | 1                | 0              | -3.503792               | -2.450029 | -0.857162 |

**TSD\_exo**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.168577               | 3.974709  | 0.089924  |
| 2                | 6                | 0              | 0.145018                | 2.942979  | 0.965720  |
| 3                | 6                | 0              | -0.213230               | 1.641878  | 0.640305  |
| 4                | 6                | 0              | -0.883546               | 1.360173  | -0.550324 |
| 5                | 6                | 0              | -1.173569               | 2.402549  | -1.426089 |
| 6                | 6                | 0              | -0.821169               | 3.708319  | -1.110854 |
| 7                | 1                | 0              | 0.110934                | 4.991352  | 0.341688  |
| 8                | 1                | 0              | 0.668625                | 3.129270  | 1.895644  |
| 9                | 1                | 0              | -1.689851               | 2.182715  | -2.354667 |
| 10               | 1                | 0              | -1.052946               | 4.514065  | -1.796913 |
| 11               | 6                | 0              | -1.306572               | -0.039845 | -0.829113 |
| 12               | 1                | 0              | -1.352857               | -0.262097 | -1.890716 |
| 13               | 6                | 0              | -0.591848               | -1.058985 | -0.048888 |
| 14               | 6                | 0              | 0.458262                | -0.611209 | 0.958532  |
| 15               | 1                | 0              | 0.471598                | -1.293278 | 1.808538  |
| 16               | 8                | 0              | 0.066553                | 0.646291  | 1.531094  |
| 17               | 6                | 0              | 1.875356                | -0.488493 | 0.417320  |
| 18               | 6                | 0              | 2.934726                | -0.687184 | 1.300744  |
| 19               | 6                | 0              | 2.152417                | -0.114050 | -0.895951 |
| 20               | 6                | 0              | 4.248323                | -0.514894 | 0.883558  |
| 21               | 1                | 0              | 2.728548                | -0.983077 | 2.324522  |
| 22               | 6                | 0              | 3.466488                | 0.059010  | -1.316756 |
| 23               | 1                | 0              | 1.348232                | 0.040070  | -1.606834 |
| 24               | 6                | 0              | 4.517194                | -0.139272 | -0.428738 |
| 25               | 1                | 0              | 5.062071                | -0.678160 | 1.581120  |
| 26               | 1                | 0              | 3.667651                | 0.347690  | -2.342145 |
| 27               | 1                | 0              | 5.541366                | -0.006780 | -0.758687 |
| 28               | 7                | 0              | -0.240940               | -2.258892 | -0.740748 |
| 29               | 8                | 0              | 0.607266                | -2.991443 | -0.241681 |
| 30               | 8                | 0              | -0.853522               | -2.559352 | -1.771146 |
| 31               | 6                | 0              | -2.997282               | 0.224702  | 0.922873  |
| 32               | 6                | 0              | -2.611328               | -0.771950 | 1.739573  |
| 33               | 6                | 0              | -2.322129               | -1.868619 | 0.840950  |
| 34               | 1                | 0              | -3.182424               | 1.264921  | 1.139826  |
| 35               | 1                | 0              | -2.438007               | -0.746394 | 2.802354  |
| 36               | 1                | 0              | -2.105221               | -2.892116 | 1.121248  |
| 37               | 7                | 0              | -2.967287               | -0.202756 | -0.425484 |
| 38               | 7                | 0              | -3.044481               | -1.594868 | -0.288776 |
| 39               | 1                | 0              | -2.822339               | -2.095437 | -1.142780 |

**5\_exo**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.009401               | 3.867790  | 0.125736  |
| 2                | 6                | 0              | -0.504384               | 2.918732  | 1.003484  |
| 3                | 6                | 0              | -0.593983               | 1.571403  | 0.676698  |
| 4                | 6                | 0              | -1.183475               | 1.160994  | -0.516978 |
| 5                | 6                | 0              | -1.665674               | 2.127502  | -1.396372 |
| 6                | 6                | 0              | -1.585775               | 3.476585  | -1.080295 |
| 7                | 1                | 0              | -0.940086               | 4.919467  | 0.379060  |
| 8                | 1                | 0              | -0.036107               | 3.204032  | 1.937761  |
| 9                | 1                | 0              | -2.116957               | 1.810114  | -2.330595 |
| 10               | 1                | 0              | -1.967903               | 4.219635  | -1.769869 |
| 11               | 6                | 0              | -1.335969               | -0.300631 | -0.819737 |
| 12               | 1                | 0              | -1.124212               | -0.495871 | -1.869785 |
| 13               | 6                | 0              | -0.475769               | -1.221682 | 0.078424  |
| 14               | 6                | 0              | 0.503570                | -0.503451 | 1.036560  |
| 15               | 1                | 0              | 0.662775                | -1.143318 | 1.904058  |
| 16               | 8                | 0              | -0.119808               | 0.661628  | 1.579238  |
| 17               | 6                | 0              | 1.858926                | -0.144573 | 0.453814  |
| 18               | 6                | 0              | 2.972086                | -0.243922 | 1.287610  |
| 19               | 6                | 0              | 2.029823                | 0.335990  | -0.844914 |
| 20               | 6                | 0              | 4.231776                | 0.129628  | 0.838416  |
| 21               | 1                | 0              | 2.851246                | -0.621236 | 2.297832  |
| 22               | 6                | 0              | 3.290736                | 0.709498  | -1.296687 |
| 23               | 1                | 0              | 1.188892                | 0.425714  | -1.522000 |
| 24               | 6                | 0              | 4.393362                | 0.609080  | -0.457210 |
| 25               | 1                | 0              | 5.087300                | 0.042590  | 1.498331  |
| 26               | 1                | 0              | 3.408282                | 1.079189  | -2.308731 |
| 27               | 1                | 0              | 5.375700                | 0.899006  | -0.812263 |
| 28               | 7                | 0              | 0.341028                | -2.233182 | -0.719864 |
| 29               | 8                | 0              | 1.082715                | -2.940209 | -0.069504 |
| 30               | 8                | 0              | 0.190310                | -2.322413 | -1.921020 |
| 31               | 6                | 0              | -3.077463               | -0.377908 | 0.797245  |
| 32               | 6                | 0              | -2.403461               | -1.146404 | 1.642528  |
| 33               | 6                | 0              | -1.617102               | -2.086739 | 0.751257  |
| 34               | 1                | 0              | -3.719704               | 0.471444  | 0.971498  |
| 35               | 1                | 0              | -2.355091               | -1.098861 | 2.718637  |
| 36               | 1                | 0              | -1.271814               | -3.024247 | 1.179440  |
| 37               | 7                | 0              | -2.768800               | -0.784263 | -0.571872 |
| 38               | 7                | 0              | -2.579069               | -2.205562 | -0.346349 |
| 39               | 1                | 0              | -2.187128               | -2.609995 | -1.193959 |