



## Supporting Information

for

### **Mechanistic insights into hydroxy(tosyloxy)iodobenzene-mediated ditosyloxylation of chalcones: a DFT study**

Jai Parkash, Sangeeta Saini, Vaishali Saini, Omkar Bains and Raj Kamal

*Beilstein J. Org. Chem.* **2025**, 21, 2703–2715. doi:10.3762/bjoc.21.208

**Coordinates of all structures reported for the first time**

# COORDINATES OF ALL THE STRUCTURES REPORTED FOR THE FIRST TIME IN THE RESEARCH PAPER

## -SCH<sub>3</sub> group (Formation of β, β-ditosyloxy ketone)

### Reactant

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.247620 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.265439                    |
| Thermal correction to Enthalpy=              | 0.266383                    |
| Thermal correction to Gibbs Free Energy=     | 0.199057                    |
| Sum of electronic and zero-point Energies=   | -1451.471273                |
| Sum of electronic and thermal Energies=      | -1451.453454                |
| Sum of electronic and thermal Enthalpies=    | -1451.452510                |
| Sum of electronic and thermal Free Energies= | -1451.519836                |

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.737186               | -0.404124 | -0.006719 |
| 2                | 6                | 0              | 0.358084                | -1.198746 | -0.014206 |
| 3                | 6                | 0              | -2.094933               | -0.980858 | -0.008626 |
| 4                | 8                | 0              | -2.298951               | -2.207691 | -0.016665 |
| 5                | 6                | 0              | -3.229122               | -0.045553 | -0.000507 |
| 6                | 6                | 0              | -3.257725               | 1.337376  | 0.007174  |
| 7                | 16               | 0              | -4.862428               | -0.691808 | -0.000485 |
| 8                | 6                | 0              | -4.572907               | 1.872163  | 0.013166  |
| 9                | 1                | 0              | -2.367644               | 1.955351  | 0.008289  |
| 10               | 6                | 0              | -5.557545               | 0.906976  | 0.010057  |
| 11               | 1                | 0              | -4.795025               | 2.934033  | 0.019536  |
| 12               | 6                | 0              | -7.041474               | 1.108968  | 0.014523  |
| 13               | 1                | 0              | -7.505742               | 0.652409  | 0.896377  |
| 14               | 1                | 0              | -7.269311               | 2.178634  | 0.021868  |
| 15               | 1                | 0              | -7.509504               | 0.663752  | -0.871151 |
| 16               | 1                | 0              | -0.641874               | 0.675446  | 0.003777  |
| 17               | 1                | 0              | 0.187319                | -2.274499 | -0.018137 |
| 18               | 6                | 0              | 1.755564                | -0.781731 | -0.013611 |
| 19               | 6                | 0              | 2.762270                | -1.770985 | 0.017527  |
| 20               | 6                | 0              | 2.167668                | 0.566408  | -0.041658 |
| 21               | 6                | 0              | 4.110838                | -1.435607 | 0.026348  |
| 22               | 1                | 0              | 2.476532                | -2.819489 | 0.037427  |
| 23               | 6                | 0              | 3.515091                | 0.913283  | -0.034280 |
| 24               | 1                | 0              | 1.430129                | 1.362756  | -0.072928 |
| 25               | 1                | 0              | 4.857931                | -2.224538 | 0.053116  |
| 26               | 1                | 0              | 3.784409                | 1.962540  | -0.058068 |
| 27               | 6                | 0              | 4.506948                | -0.084739 | 0.002005  |

|    |    |   |          |          |           |
|----|----|---|----------|----------|-----------|
| 28 | 16 | 0 | 6.253642 | 0.246744 | 0.017111  |
| 29 | 6  | 0 | 6.357022 | 2.068658 | 0.002914  |
| 30 | 1  | 0 | 7.425382 | 2.299382 | 0.020437  |
| 31 | 1  | 0 | 5.918535 | 2.486530 | -0.906804 |
| 32 | 1  | 0 | 5.885482 | 2.501322 | 0.888916  |

---

### Int1

---

Zero-point correction= 0.352738 (Hartree/Particle)  
 Thermal correction to Energy= 0.380030  
 Thermal correction to Enthalpy= 0.380974  
 Thermal correction to Gibbs Free Energy= 0.292097  
 Sum of electronic and zero-point Energies= -1770.006501  
 Sum of electronic and thermal Energies= -1769.979209  
 Sum of electronic and thermal Enthalpies= -1769.978265  
 Sum of electronic and thermal Free Energies= -1770.067141  
 Standard orientation:

---

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

---

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 0.984457  | -1.204669 | -0.396442 |
| 2  | 6  | 0 | -0.073902 | -1.373387 | -1.255538 |
| 3  | 6  | 0 | 2.381836  | -1.277864 | -0.902341 |
| 4  | 8  | 0 | 2.627803  | -1.346524 | -2.117293 |
| 5  | 6  | 0 | 3.457446  | -1.239153 | 0.086585  |
| 6  | 6  | 0 | 3.399543  | -1.172158 | 1.469170  |
| 7  | 16 | 0 | 5.125345  | -1.271075 | -0.458961 |
| 8  | 6  | 0 | 4.677430  | -1.144217 | 2.081144  |
| 9  | 1  | 0 | 2.472908  | -1.146597 | 2.030275  |
| 10 | 6  | 0 | 5.719470  | -1.190549 | 1.176293  |
| 11 | 1  | 0 | 4.837136  | -1.093543 | 3.152865  |
| 12 | 6  | 0 | 7.187278  | -1.182581 | 1.470899  |
| 13 | 1  | 0 | 7.691165  | -0.343742 | 0.977099  |
| 14 | 1  | 0 | 7.347154  | -1.094263 | 2.548895  |
| 15 | 1  | 0 | 7.668579  | -2.105030 | 1.125119  |
| 16 | 1  | 0 | 0.827126  | -1.182631 | 0.676389  |
| 17 | 1  | 0 | 0.167074  | -1.427899 | -2.316450 |
| 18 | 6  | 0 | -1.470844 | -1.459485 | -0.911501 |
| 19 | 6  | 0 | -2.430809 | -1.424967 | -1.951686 |
| 20 | 6  | 0 | -1.940346 | -1.556583 | 0.418235  |
| 21 | 6  | 0 | -3.788540 | -1.452257 | -1.678064 |
| 22 | 1  | 0 | -2.094705 | -1.362233 | -2.983303 |
| 23 | 6  | 0 | -3.297173 | -1.596571 | 0.700650  |
| 24 | 1  | 0 | -1.238003 | -1.606889 | 1.243592  |
| 25 | 6  | 0 | -4.242771 | -1.530371 | -0.343737 |
| 26 | 1  | 0 | -4.502012 | -1.411911 | -2.496694 |
| 27 | 1  | 0 | -3.616194 | -1.669028 | 1.733256  |
| 28 | 6  | 0 | -6.182882 | -1.656059 | 1.714230  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 29 | 1  | 0 | -5.736029 | -0.796363 | 2.219618  |
| 30 | 1  | 0 | -7.261436 | -1.653198 | 1.892798  |
| 31 | 1  | 0 | -5.761639 | -2.589240 | 2.096377  |
| 32 | 6  | 0 | -3.340021 | 1.865593  | 0.389468  |
| 33 | 6  | 0 | -2.142163 | 1.829710  | -0.326524 |
| 34 | 6  | 0 | -0.946743 | 1.728246  | 0.394756  |
| 35 | 6  | 0 | -0.907318 | 1.645866  | 1.791865  |
| 36 | 6  | 0 | -2.119578 | 1.682514  | 2.484587  |
| 37 | 6  | 0 | -3.327718 | 1.793477  | 1.786449  |
| 38 | 1  | 0 | -4.280201 | 1.938980  | -0.147910 |
| 39 | 1  | 0 | -2.141537 | 1.876761  | -1.409593 |
| 40 | 1  | 0 | 0.034490  | 1.563975  | 2.323150  |
| 41 | 1  | 0 | -2.116140 | 1.624167  | 3.568790  |
| 42 | 1  | 0 | -4.264956 | 1.818565  | 2.334332  |
| 43 | 53 | 0 | 0.864293  | 1.732350  | -0.666198 |
| 44 | 8  | 0 | 1.098067  | 3.738827  | -0.652039 |
| 45 | 1  | 0 | 0.626310  | 4.096373  | -1.429611 |
| 46 | 16 | 0 | -5.991188 | -1.534953 | -0.095217 |

---

### Int2

---

Zero-point correction= 0.485427 (Hartree/Particle)  
 Thermal correction to Energy= 0.524027  
 Thermal correction to Enthalpy= 0.524971  
 Thermal correction to Gibbs Free Energy= 0.407593  
 Sum of electronic and zero-point Energies= -2664.866876  
 Sum of electronic and thermal Energies= -2664.828276  
 Sum of electronic and thermal Enthalpies= -2664.827332  
 Sum of electronic and thermal Free Energies= -2664.944710

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.603764                | 0.478416  | -0.432612 |
| 2                | 6                | 0              | 0.734142                | -0.981240 | -0.847384 |
| 3                | 6                | 0              | 1.617702                | 1.379145  | -1.046837 |
| 4                | 8                | 0              | 2.083537                | 1.150608  | -2.174634 |
| 5                | 6                | 0              | 1.993854                | 2.585746  | -0.300892 |
| 6                | 6                | 0              | 1.624025                | 2.998871  | 0.965793  |
| 7                | 16               | 0              | 3.064833                | 3.760522  | -1.044236 |
| 8                | 6                | 0              | 2.192145                | 4.246390  | 1.335889  |
| 9                | 1                | 0              | 0.962418                | 2.430824  | 1.609383  |
| 10               | 6                | 0              | 2.999177                | 4.791996  | 0.359493  |
| 11               | 1                | 0              | 2.018941                | 4.732011  | 2.290562  |
| 12               | 6                | 0              | 3.756413                | 6.083646  | 0.409713  |
| 13               | 1                | 0              | 3.434229                | 6.768367  | -0.383624 |
| 14               | 1                | 0              | 3.589288                | 6.572585  | 1.373806  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 15 | 1  | 0 | 4.833966  | 5.922432  | 0.287952  |
| 16 | 1  | 0 | 0.538745  | 0.570965  | 0.650062  |
| 17 | 6  | 0 | -2.538335 | 0.790005  | 2.984314  |
| 18 | 6  | 0 | -2.196453 | 0.554525  | 1.648407  |
| 19 | 6  | 0 | -1.958341 | 1.649929  | 0.817549  |
| 20 | 6  | 0 | -2.046589 | 2.965437  | 1.276307  |
| 21 | 6  | 0 | -2.387440 | 3.181652  | 2.616205  |
| 22 | 6  | 0 | -2.632936 | 2.099035  | 3.468178  |
| 23 | 1  | 0 | -2.733623 | -0.054688 | 3.638904  |
| 24 | 1  | 0 | -2.114319 | -0.456317 | 1.269423  |
| 25 | 1  | 0 | -1.858281 | 3.802386  | 0.612841  |
| 26 | 1  | 0 | -2.456919 | 4.199417  | 2.989602  |
| 27 | 1  | 0 | -2.898604 | 2.275899  | 4.506474  |
| 28 | 53 | 0 | -1.452119 | 1.300306  | -1.213810 |
| 29 | 8  | 0 | -3.452814 | 2.085622  | -1.694796 |
| 30 | 1  | 0 | -4.103619 | 1.416830  | -1.423726 |
| 31 | 1  | 0 | 0.585867  | -1.088494 | -1.923913 |
| 32 | 6  | 0 | 2.048132  | -1.605541 | -0.439677 |
| 33 | 6  | 0 | 2.943086  | -2.072251 | -1.410390 |
| 34 | 6  | 0 | 2.406589  | -1.704234 | 0.909887  |
| 35 | 6  | 0 | 4.170405  | -2.621097 | -1.042707 |
| 36 | 1  | 0 | 2.681414  | -2.003787 | -2.462602 |
| 37 | 6  | 0 | 3.629971  | -2.257402 | 1.291253  |
| 38 | 1  | 0 | 1.722600  | -1.353412 | 1.677915  |
| 39 | 6  | 0 | 4.528463  | -2.719106 | 0.314233  |
| 40 | 1  | 0 | 4.848525  | -2.976444 | -1.814455 |
| 41 | 1  | 0 | 3.868743  | -2.320563 | 2.346438  |
| 42 | 6  | 0 | 6.199910  | -3.421068 | 2.500743  |
| 43 | 1  | 0 | 5.400946  | -4.025459 | 2.938753  |
| 44 | 1  | 0 | 7.163942  | -3.869400 | 2.755870  |
| 45 | 1  | 0 | 6.167380  | -2.402192 | 2.895738  |
| 46 | 8  | 0 | -0.374751 | -1.654732 | -0.142480 |
| 47 | 16 | 0 | -1.131859 | -2.940496 | -0.821415 |
| 48 | 8  | 0 | -0.648469 | -4.160245 | -0.165608 |
| 49 | 8  | 0 | -1.038649 | -2.823559 | -2.283334 |
| 50 | 6  | 0 | -2.783130 | -2.572390 | -0.269677 |
| 51 | 6  | 0 | -3.208644 | -3.045086 | 0.973211  |
| 52 | 6  | 0 | -3.592703 | -1.750104 | -1.060712 |
| 53 | 6  | 0 | -4.470600 | -2.667426 | 1.435772  |
| 54 | 1  | 0 | -2.567402 | -3.687357 | 1.567647  |
| 55 | 6  | 0 | -4.848186 | -1.387897 | -0.579936 |
| 56 | 1  | 0 | -3.245657 | -1.401136 | -2.026400 |
| 57 | 6  | 0 | -5.302643 | -1.829775 | 0.676187  |
| 58 | 1  | 0 | -4.810913 | -3.028215 | 2.402338  |
| 59 | 1  | 0 | -5.486249 | -0.751149 | -1.187473 |
| 60 | 6  | 0 | -6.650229 | -1.393214 | 1.191051  |
| 61 | 1  | 0 | -7.426220 | -1.531860 | 0.430230  |
| 62 | 1  | 0 | -6.938436 | -1.950173 | 2.087039  |
| 63 | 1  | 0 | -6.633750 | -0.325971 | 1.445611  |

64 16 0 6.121973 -3.434063 0.678414

---

**Int3**

---

Zero-point correction= 0.473769 (Hartree/Particle)  
Thermal correction to Energy= 0.509978  
Thermal correction to Enthalpy= 0.510922  
Thermal correction to Gibbs Free Energy= 0.398915  
Sum of electronic and zero-point Energies= -2588.904474  
Sum of electronic and thermal Energies= -2588.868265  
Sum of electronic and thermal Enthalpies= -2588.867321  
Sum of electronic and thermal Free Energies= -2588.979328

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.423744               | -0.824208 | -0.470032 |
| 2                | 6                | 0              | -0.244704               | 0.635378  | -0.889447 |
| 3                | 6                | 0              | -1.591438               | -1.483048 | -1.213329 |
| 4                | 8                | 0              | -1.491610               | -1.663196 | -2.430341 |
| 5                | 6                | 0              | -2.771941               | -1.802902 | -0.445657 |
| 6                | 6                | 0              | -3.011739               | -1.669389 | 0.917044  |
| 7                | 16               | 0              | -4.205606               | -2.391199 | -1.272646 |
| 8                | 6                | 0              | -4.322992               | -2.039607 | 1.286605  |
| 9                | 1                | 0              | -2.274347               | -1.306155 | 1.622946  |
| 10               | 6                | 0              | -5.099528               | -2.450727 | 0.217468  |
| 11               | 1                | 0              | -4.701078               | -2.003928 | 2.302208  |
| 12               | 6                | 0              | -6.525231               | -2.902713 | 0.247421  |
| 13               | 1                | 0              | -6.627233               | -3.926807 | -0.129949 |
| 14               | 1                | 0              | -6.900760               | -2.872213 | 1.273571  |
| 15               | 1                | 0              | -7.158786               | -2.258023 | -0.372755 |
| 16               | 1                | 0              | -0.452890               | -0.934778 | 0.613444  |
| 17               | 6                | 0              | 3.695105                | -1.243088 | 2.646289  |
| 18               | 6                | 0              | 3.208436                | -1.207605 | 1.335922  |
| 19               | 6                | 0              | 2.166727                | -2.073720 | 1.001513  |
| 20               | 6                | 0              | 1.598885                | -2.970229 | 1.910644  |
| 21               | 6                | 0              | 2.099227                | -2.981555 | 3.216642  |
| 22               | 6                | 0              | 3.142548                | -2.123386 | 3.581958  |
| 23               | 1                | 0              | 4.504093                | -0.576072 | 2.927704  |
| 24               | 1                | 0              | 3.624414                | -0.523606 | 0.608411  |
| 25               | 1                | 0              | 0.795029                | -3.637726 | 1.620163  |
| 26               | 1                | 0              | 1.672814                | -3.667460 | 3.942574  |
| 27               | 1                | 0              | 3.525855                | -2.142479 | 4.597774  |
| 28               | 53               | 0              | 1.398202                | -2.024497 | -0.974910 |
| 29               | 1                | 0              | -0.089045               | 0.698569  | -1.969644 |
| 30               | 6                | 0              | -1.486762               | 1.392860  | -0.477740 |
| 31               | 6                | 0              | -2.469189               | 1.692958  | -1.431714 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 32 | 6  | 0 | -1.722128 | 1.702693  | 0.866478  |
| 33 | 6  | 0 | -3.669211 | 2.281655  | -1.046361 |
| 34 | 1  | 0 | -2.298626 | 1.457000  | -2.478653 |
| 35 | 6  | 0 | -2.917318 | 2.302475  | 1.261006  |
| 36 | 1  | 0 | -0.964394 | 1.481171  | 1.612520  |
| 37 | 6  | 0 | -3.910797 | 2.587611  | 0.307379  |
| 38 | 1  | 0 | -4.419144 | 2.504334  | -1.800602 |
| 39 | 1  | 0 | -3.063838 | 2.536356  | 2.308737  |
| 40 | 6  | 0 | -5.419005 | 3.566780  | 2.500548  |
| 41 | 1  | 0 | -4.614910 | 4.251840  | 2.782000  |
| 42 | 1  | 0 | -6.378803 | 4.016462  | 2.768593  |
| 43 | 1  | 0 | -5.313277 | 2.614833  | 3.027538  |
| 44 | 8  | 0 | 0.945738  | 1.087834  | -0.194528 |
| 45 | 16 | 0 | 1.692129  | 2.468610  | -0.738186 |
| 46 | 8  | 0 | 1.324383  | 3.558660  | 0.166425  |
| 47 | 8  | 0 | 1.417728  | 2.582903  | -2.175389 |
| 48 | 6  | 0 | 3.380228  | 1.992474  | -0.461179 |
| 49 | 6  | 0 | 3.999341  | 2.338190  | 0.742449  |
| 50 | 6  | 0 | 4.042853  | 1.253853  | -1.447124 |
| 51 | 6  | 0 | 5.314893  | 1.926945  | 0.957141  |
| 52 | 1  | 0 | 3.466459  | 2.911439  | 1.493447  |
| 53 | 6  | 0 | 5.356218  | 0.853997  | -1.209549 |
| 54 | 1  | 0 | 3.544848  | 0.998116  | -2.376268 |
| 55 | 6  | 0 | 6.012266  | 1.182743  | -0.009175 |
| 56 | 1  | 0 | 5.806815  | 2.188317  | 1.889892  |
| 57 | 1  | 0 | 5.881657  | 0.280280  | -1.968026 |
| 58 | 6  | 0 | 7.443082  | 0.769661  | 0.220038  |
| 59 | 1  | 0 | 8.125714  | 1.526576  | -0.187268 |
| 60 | 1  | 0 | 7.664532  | 0.666524  | 1.286548  |
| 61 | 1  | 0 | 7.669357  | -0.177397 | -0.279541 |
| 62 | 16 | 0 | -5.482994 | 3.323525  | 0.694214  |

---

### T.S. 1

---

Zero-point correction= 0.472484 (Hartree/Particle)  
 Thermal correction to Energy= 0.508504  
 Thermal correction to Enthalpy= 0.509448  
 Thermal correction to Gibbs Free Energy= 0.398250  
 Sum of electronic and zero-point Energies= -2588.894990  
 Sum of electronic and thermal Energies= -2588.858970  
 Sum of electronic and thermal Enthalpies= -2588.858026  
 Sum of electronic and thermal Free Energies= -2588.969225

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.892952               | -0.245073 | -0.513007 |

---

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 2  | 6  | 0 | -0.332688 | 0.978539  | -1.084711 |
| 3  | 6  | 0 | -1.904808 | -1.044882 | -1.278151 |
| 4  | 8  | 0 | -2.018729 | -0.876724 | -2.498405 |
| 5  | 6  | 0 | -2.697510 | -1.988404 | -0.517292 |
| 6  | 6  | 0 | -2.715780 | -2.234197 | 0.850849  |
| 7  | 16 | 0 | -3.840801 | -3.024560 | -1.350282 |
| 8  | 6  | 0 | -3.633746 | -3.241709 | 1.218659  |
| 9  | 1  | 0 | -2.096003 | -1.707845 | 1.566707  |
| 10 | 6  | 0 | -4.323823 | -3.775363 | 0.144088  |
| 11 | 1  | 0 | -3.794152 | -3.575060 | 2.237990  |
| 12 | 6  | 0 | -5.363879 | -4.849408 | 0.171165  |
| 13 | 1  | 0 | -5.070251 | -5.704962 | -0.448121 |
| 14 | 1  | 0 | -5.509700 | -5.197459 | 1.197177  |
| 15 | 1  | 0 | -6.323440 | -4.481218 | -0.210334 |
| 16 | 1  | 0 | -0.737311 | -0.412816 | 0.546474  |
| 17 | 6  | 0 | 2.870398  | -0.875229 | 2.972322  |
| 18 | 6  | 0 | 2.580063  | -1.006783 | 1.610727  |
| 19 | 6  | 0 | 1.729262  | -2.038567 | 1.201318  |
| 20 | 6  | 0 | 1.169755  | -2.937759 | 2.115554  |
| 21 | 6  | 0 | 1.472040  | -2.789751 | 3.474037  |
| 22 | 6  | 0 | 2.317922  | -1.761515 | 3.903420  |
| 23 | 1  | 0 | 3.530303  | -0.076577 | 3.298894  |
| 24 | 1  | 0 | 3.003515  | -0.318361 | 0.890358  |
| 25 | 1  | 0 | 0.515763  | -3.736696 | 1.782404  |
| 26 | 1  | 0 | 1.044681  | -3.483555 | 4.192490  |
| 27 | 1  | 0 | 2.548530  | -1.653488 | 4.959304  |
| 28 | 53 | 0 | 1.251188  | -2.220251 | -0.851125 |
| 29 | 1  | 0 | -0.264645 | 0.990901  | -2.172084 |
| 30 | 6  | 0 | -1.535440 | 1.754448  | -0.556079 |
| 31 | 6  | 0 | -2.633999 | 2.040016  | -1.405598 |
| 32 | 6  | 0 | -1.553549 | 2.211540  | 0.783628  |
| 33 | 6  | 0 | -3.681729 | 2.806295  | -0.943774 |
| 34 | 1  | 0 | -2.637262 | 1.667426  | -2.424263 |
| 35 | 6  | 0 | -2.603337 | 2.984042  | 1.247712  |
| 36 | 1  | 0 | -0.717221 | 1.986079  | 1.437292  |
| 37 | 6  | 0 | -3.681450 | 3.298920  | 0.389214  |
| 38 | 1  | 0 | -4.505785 | 3.043552  | -1.610376 |
| 39 | 1  | 0 | -2.579998 | 3.343019  | 2.269098  |
| 40 | 6  | 0 | -4.697707 | 4.787595  | 2.567884  |
| 41 | 1  | 0 | -3.763943 | 5.352952  | 2.621892  |
| 42 | 1  | 0 | -5.528406 | 5.437328  | 2.854497  |
| 43 | 1  | 0 | -4.669627 | 3.924530  | 3.237421  |
| 44 | 8  | 0 | 0.900090  | 1.295784  | -0.446243 |
| 45 | 16 | 0 | 1.797247  | 2.565664  | -1.053607 |
| 46 | 8  | 0 | 1.507709  | 3.747426  | -0.239745 |
| 47 | 8  | 0 | 1.570207  | 2.603911  | -2.502063 |
| 48 | 6  | 0 | 3.398715  | 1.915313  | -0.660772 |
| 49 | 6  | 0 | 4.029226  | 2.323945  | 0.515874  |
| 50 | 6  | 0 | 3.960547  | 0.952001  | -1.507876 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 51 | 6  | 0 | 5.253823  | 1.743246  | 0.850259  |
| 52 | 1  | 0 | 3.575133  | 3.071967  | 1.156647  |
| 53 | 6  | 0 | 5.180471  | 0.386665  | -1.151048 |
| 54 | 1  | 0 | 3.453221  | 0.647608  | -2.417105 |
| 55 | 6  | 0 | 5.842814  | 0.766966  | 0.031920  |
| 56 | 1  | 0 | 5.755657  | 2.053093  | 1.762419  |
| 57 | 1  | 0 | 5.627853  | -0.363676 | -1.797159 |
| 58 | 6  | 0 | 7.153158  | 0.123121  | 0.403730  |
| 59 | 1  | 0 | 7.017160  | -0.950923 | 0.579882  |
| 60 | 1  | 0 | 7.882169  | 0.226334  | -0.408122 |
| 61 | 1  | 0 | 7.577937  | 0.566687  | 1.308316  |
| 62 | 16 | 0 | -5.053704 | 4.281221  | 0.852968  |

---

#### Int4

---

Zero-point correction= 0.381592 (Hartree/Particle)  
 Thermal correction to Energy= 0.410440  
 Thermal correction to Enthalpy= 0.411384  
 Thermal correction to Gibbs Free Energy= 0.317066  
 Sum of electronic and zero-point Energies= -2345.946836  
 Sum of electronic and thermal Energies= -2345.917989  
 Sum of electronic and thermal Enthalpies= -2345.917045  
 Sum of electronic and thermal Free Energies= -2346.011363

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.938533               | -0.827660 | -0.011283 |
| 2                | 6                | 0              | 0.235819                | -0.389944 | -0.730313 |
| 3                | 6                | 0              | -2.043724               | -1.565493 | -0.744501 |
| 4                | 8                | 0              | -1.958902               | -1.741820 | -1.961985 |
| 5                | 6                | 0              | -3.171747               | -2.011278 | 0.048124  |
| 6                | 6                | 0              | -3.438110               | -1.827653 | 1.397968  |
| 7                | 16               | 0              | -4.475330               | -2.897654 | -0.726177 |
| 8                | 6                | 0              | -4.669717               | -2.392596 | 1.801124  |
| 9                | 1                | 0              | -2.776231               | -1.299838 | 2.075359  |
| 10               | 6                | 0              | -5.353558               | -3.012072 | 0.771647  |
| 11               | 1                | 0              | -5.052853               | -2.353476 | 2.814683  |
| 12               | 6                | 0              | -6.673783               | -3.712204 | 0.843725  |
| 13               | 1                | 0              | -6.586190               | -4.760627 | 0.536618  |
| 14               | 1                | 0              | -7.051903               | -3.682621 | 1.868956  |
| 15               | 1                | 0              | -7.412579               | -3.237337 | 0.187881  |
| 16               | 1                | 0              | -0.791830               | -1.075585 | 1.034381  |
| 17               | 1                | 0              | 0.279513                | -0.474325 | -1.812393 |
| 18               | 6                | 0              | -0.846298               | 0.742786  | -0.249848 |
| 19               | 6                | 0              | -1.597492               | 1.362303  | -1.313993 |
| 20               | 6                | 0              | -0.494720               | 1.549579  | 0.888992  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 21 | 6  | 0 | -1.953266 | 2.678784  | -1.240607 |
| 22 | 1  | 0 | -1.867373 | 0.774892  | -2.185344 |
| 23 | 6  | 0 | -0.862458 | 2.866306  | 0.963691  |
| 24 | 1  | 0 | 0.081316  | 1.103714  | 1.692326  |
| 25 | 6  | 0 | -1.597106 | 3.460832  | -0.100206 |
| 26 | 1  | 0 | -2.505655 | 3.133353  | -2.056934 |
| 27 | 1  | 0 | -0.575160 | 3.446126  | 1.831336  |
| 28 | 6  | 0 | -1.478259 | 5.831503  | 1.432980  |
| 29 | 1  | 0 | -0.387599 | 5.787906  | 1.472366  |
| 30 | 1  | 0 | -1.798092 | 6.875945  | 1.411373  |
| 31 | 1  | 0 | -1.924584 | 5.334139  | 2.296766  |
| 32 | 8  | 0 | 1.437129  | -0.453675 | -0.052725 |
| 33 | 16 | 0 | 2.678904  | 0.587883  | -0.593494 |
| 34 | 8  | 0 | 2.578735  | 1.791446  | 0.231502  |
| 35 | 8  | 0 | 2.549757  | 0.676320  | -2.048840 |
| 36 | 6  | 0 | 4.065741  | -0.398456 | -0.116606 |
| 37 | 6  | 0 | 4.632961  | -0.206013 | 1.147124  |
| 38 | 6  | 0 | 4.546922  | -1.360485 | -1.010547 |
| 39 | 6  | 0 | 5.713708  | -1.003941 | 1.514531  |
| 40 | 1  | 0 | 4.243118  | 0.548041  | 1.822083  |
| 41 | 6  | 0 | 5.629326  | -2.143747 | -0.618225 |
| 42 | 1  | 0 | 4.090401  | -1.491619 | -1.985833 |
| 43 | 6  | 0 | 6.228491  | -1.979489 | 0.643017  |
| 44 | 1  | 0 | 6.166172  | -0.866082 | 2.492380  |
| 45 | 1  | 0 | 6.016606  | -2.893276 | -1.302195 |
| 46 | 6  | 0 | 7.419968  | -2.809632 | 1.042641  |
| 47 | 1  | 0 | 7.437205  | -3.766532 | 0.513092  |
| 48 | 1  | 0 | 8.348880  | -2.278653 | 0.797744  |
| 49 | 1  | 0 | 7.427502  | -3.002453 | 2.119729  |
| 50 | 16 | 0 | -2.099788 | 5.115493  | -0.125616 |

---

### Int5

---

Zero-point correction= 0.380998 (Hartree/Particle)  
 Thermal correction to Energy= 0.410324  
 Thermal correction to Enthalpy= 0.411268  
 Thermal correction to Gibbs Free Energy= 0.316047  
 Sum of electronic and zero-point Energies= -2345.951903  
 Sum of electronic and thermal Energies= -2345.922578  
 Sum of electronic and thermal Enthalpies= -2345.921634  
 Sum of electronic and thermal Free Energies= -2346.016855

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.513506                | 0.450004  | 0.414105  |
| 2                | 6                | 0              | -0.659802               | -0.193759 | -0.230839 |

---

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 3  | 6  | 0 | 0.756922  | 1.819844  | -0.243884 |
| 4  | 8  | 0 | -0.086607 | 2.242007  | -1.041740 |
| 5  | 6  | 0 | 1.944835  | 2.552797  | 0.132370  |
| 6  | 6  | 0 | 2.914798  | 2.225025  | 1.067194  |
| 7  | 16 | 0 | 2.303501  | 4.097509  | -0.622286 |
| 8  | 6  | 0 | 3.930953  | 3.202069  | 1.175608  |
| 9  | 1  | 0 | 2.895074  | 1.311475  | 1.649684  |
| 10 | 6  | 0 | 3.752120  | 4.277357  | 0.325455  |
| 11 | 1  | 0 | 4.776320  | 3.127669  | 1.850495  |
| 12 | 6  | 0 | 4.636181  | 5.474519  | 0.168692  |
| 13 | 1  | 0 | 4.094063  | 6.402756  | 0.382365  |
| 14 | 1  | 0 | 5.481067  | 5.401193  | 0.858372  |
| 15 | 1  | 0 | 5.028438  | 5.548946  | -0.852062 |
| 16 | 1  | 0 | 0.335059  | 0.583681  | 1.484817  |
| 17 | 1  | 0 | -0.693703 | -0.277820 | -1.321912 |
| 18 | 6  | 0 | 1.568909  | -0.633014 | 0.183189  |
| 19 | 6  | 0 | 2.213959  | -0.763272 | -1.060231 |
| 20 | 6  | 0 | 1.873195  | -1.539600 | 1.208712  |
| 21 | 6  | 0 | 3.169373  | -1.751069 | -1.255359 |
| 22 | 1  | 0 | 1.983780  | -0.080134 | -1.872765 |
| 23 | 6  | 0 | 2.832787  | -2.531282 | 1.020412  |
| 24 | 1  | 0 | 1.366228  | -1.460834 | 2.166506  |
| 25 | 6  | 0 | 3.495909  | -2.645953 | -0.215402 |
| 26 | 1  | 0 | 3.666621  | -1.827249 | -2.218053 |
| 27 | 1  | 0 | 3.055726  | -3.205326 | 1.838611  |
| 28 | 6  | 0 | 4.888585  | -4.805608 | 0.983216  |
| 29 | 1  | 0 | 3.952147  | -5.309093 | 1.236217  |
| 30 | 1  | 0 | 5.655832  | -5.559613 | 0.789457  |
| 31 | 1  | 0 | 5.217816  | -4.167081 | 1.806761  |
| 32 | 8  | 0 | -1.561090 | -0.721446 | 0.469092  |
| 33 | 16 | 0 | -2.926288 | -1.803684 | -0.412848 |
| 34 | 8  | 0 | -2.869052 | -2.967477 | 0.451549  |
| 35 | 8  | 0 | -2.478324 | -1.797197 | -1.797315 |
| 36 | 6  | 0 | -4.295615 | -0.768003 | -0.115525 |
| 37 | 6  | 0 | -4.977000 | -0.896552 | 1.103342  |
| 38 | 6  | 0 | -4.643467 | 0.184514  | -1.087887 |
| 39 | 6  | 0 | -6.053910 | -0.048872 | 1.336136  |
| 40 | 1  | 0 | -4.679124 | -1.635530 | 1.838521  |
| 41 | 6  | 0 | -5.723641 | 1.013153  | -0.821784 |
| 42 | 1  | 0 | -4.092557 | 0.265303  | -2.018274 |
| 43 | 6  | 0 | -6.444015 | 0.912188  | 0.385730  |
| 44 | 1  | 0 | -6.602079 | -0.135259 | 2.268976  |
| 45 | 1  | 0 | -6.019209 | 1.751704  | -1.560781 |
| 46 | 6  | 0 | -7.616940 | 1.817817  | 0.634574  |
| 47 | 1  | 0 | -8.011291 | 1.701496  | 1.646860  |
| 48 | 1  | 0 | -7.335040 | 2.865783  | 0.483393  |
| 49 | 1  | 0 | -8.422024 | 1.596561  | -0.076798 |
| 50 | 16 | 0 | 4.737887  | -3.860048 | -0.569868 |

---

### Product

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.515946 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.555665                    |
| Thermal correction to Enthalpy=              | 0.556610                    |
| Thermal correction to Gibbs Free Energy=     | 0.437717                    |
| Sum of electronic and zero-point Energies=   | -3240.877183                |
| Sum of electronic and thermal Energies=      | -3240.837464                |
| Sum of electronic and thermal Enthalpies=    | -3240.836520                |
| Sum of electronic and thermal Free Energies= | -3240.955412                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.025098               | 1.242705  | 0.010731  |
| 2                | 1                | 0              | -0.293983               | 1.182388  | 1.066942  |
| 3                | 6                | 0              | -0.786665               | 0.118752  | -0.699197 |
| 4                | 1                | 0              | -0.623470               | 0.111948  | -1.776228 |
| 5                | 6                | 0              | 1.481067                | 1.089266  | -0.126165 |
| 6                | 6                | 0              | 2.114540                | 1.189282  | -1.374808 |
| 7                | 6                | 0              | 2.268368                | 0.839276  | 1.001911  |
| 8                | 6                | 0              | 3.493025                | 1.037944  | -1.488699 |
| 9                | 1                | 0              | 1.525940                | 1.384407  | -2.265571 |
| 10               | 6                | 0              | 3.653750                | 0.690707  | 0.900279  |
| 11               | 1                | 0              | 1.798677                | 0.748620  | 1.977570  |
| 12               | 6                | 0              | 4.279786                | 0.784031  | -0.350557 |
| 13               | 1                | 0              | 3.955586                | 1.105487  | -2.469854 |
| 14               | 1                | 0              | 4.224925                | 0.490184  | 1.798925  |
| 15               | 8                | 0              | -0.399136               | -1.137672 | -0.124122 |
| 16               | 16               | 0              | 0.246244                | -2.353466 | -1.060006 |
| 17               | 8                | 0              | 0.545070                | -1.825798 | -2.392636 |
| 18               | 8                | 0              | -0.660819               | -3.493553 | -0.902456 |
| 19               | 6                | 0              | 1.751901                | -2.682272 | -0.172136 |
| 20               | 6                | 0              | 2.973429                | -2.396926 | -0.778273 |
| 21               | 6                | 0              | 1.674893                | -3.249543 | 1.105856  |
| 22               | 6                | 0              | 4.148278                | -2.693742 | -0.084167 |
| 23               | 1                | 0              | 3.009732                | -1.947795 | -1.763581 |
| 24               | 6                | 0              | 2.858463                | -3.525702 | 1.781929  |
| 25               | 1                | 0              | 0.714369                | -3.472845 | 1.558610  |
| 26               | 6                | 0              | 4.111289                | -3.257455 | 1.197827  |
| 27               | 1                | 0              | 5.104189                | -2.469613 | -0.547336 |
| 28               | 1                | 0              | 2.813607                | -3.963652 | 2.775479  |
| 29               | 6                | 0              | 5.379313                | -3.563615 | 1.953551  |
| 30               | 1                | 0              | 5.384553                | -4.601753 | 2.304354  |
| 31               | 1                | 0              | 6.265213                | -3.405561 | 1.332923  |
| 32               | 1                | 0              | 5.464901                | -2.924030 | 2.840528  |
| 33               | 8                | 0              | -2.159144               | 0.337405  | -0.381789 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 34 | 16 | 0 | -3.358334 | -0.274332 | -1.368751 |
| 35 | 8  | 0 | -2.705397 | -1.047586 | -2.428924 |
| 36 | 8  | 0 | -4.210867 | 0.868667  | -1.694597 |
| 37 | 6  | 0 | -4.211818 | -1.350200 | -0.239692 |
| 38 | 6  | 0 | -3.752833 | -2.659970 | -0.077992 |
| 39 | 6  | 0 | -5.307265 | -0.857138 | 0.474062  |
| 40 | 6  | 0 | -4.417935 | -3.489960 | 0.822290  |
| 41 | 1  | 0 | -2.894393 | -3.019843 | -0.633462 |
| 42 | 6  | 0 | -5.955676 | -1.707340 | 1.368810  |
| 43 | 1  | 0 | -5.646048 | 0.163209  | 0.331705  |
| 44 | 6  | 0 | -5.526101 | -3.031960 | 1.555419  |
| 45 | 1  | 0 | -4.070250 | -4.510682 | 0.955822  |
| 46 | 1  | 0 | -6.809662 | -1.336087 | 1.928467  |
| 47 | 6  | 0 | -6.258122 | -3.952509 | 2.497804  |
| 48 | 1  | 0 | -7.052458 | -4.489838 | 1.963788  |
| 49 | 1  | 0 | -5.585638 | -4.702248 | 2.925678  |
| 50 | 1  | 0 | -6.728948 | -3.396861 | 3.314426  |
| 51 | 6  | 0 | -0.473004 | 2.589477  | -0.581712 |
| 52 | 8  | 0 | -0.652962 | 2.692368  | -1.797183 |
| 53 | 6  | 0 | -0.623208 | 3.722329  | 0.320895  |
| 54 | 6  | 0 | -0.496169 | 3.785889  | 1.697812  |
| 55 | 16 | 0 | -1.028214 | 5.301303  | -0.335151 |
| 56 | 6  | 0 | -0.719829 | 5.084215  | 2.219556  |
| 57 | 1  | 0 | -0.251964 | 2.930082  | 2.315912  |
| 58 | 6  | 0 | -1.018772 | 6.020723  | 1.250668  |
| 59 | 1  | 0 | -0.666569 | 5.331737  | 3.274195  |
| 60 | 6  | 0 | -1.307117 | 7.477032  | 1.444400  |
| 61 | 1  | 0 | -0.570871 | 8.101986  | 0.925622  |
| 62 | 1  | 0 | -2.297240 | 7.744352  | 1.057883  |
| 63 | 1  | 0 | -1.275666 | 7.721109  | 2.509835  |
| 64 | 6  | 0 | 6.653096  | 0.091686  | 1.034963  |
| 65 | 1  | 0 | 7.720427  | -0.103687 | 0.901543  |
| 66 | 1  | 0 | 6.528681  | 0.895098  | 1.765574  |
| 67 | 1  | 0 | 6.165296  | -0.820649 | 1.385566  |
| 68 | 16 | 0 | 6.032029  | 0.578620  | -0.609457 |

---

**Chloride Group (Formation of  $\beta$ ,  $\beta$ -ditosyloxy ketone)**

---

**Reactant**

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.209237 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.224999                    |
| Thermal correction to Enthalpy=              | 0.225943                    |
| Thermal correction to Gibbs Free Energy=     | 0.163570                    |
| Sum of electronic and zero-point Energies=   | -1473.592989                |
| Sum of electronic and thermal Energies=      | -1473.577227                |
| Sum of electronic and thermal Enthalpies=    | -1473.576283                |
| Sum of electronic and thermal Free Energies= | -1473.638656                |

---

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.334076               | 0.280862  | -0.000005 |
| 2                | 6                | 0              | 0.798231                | 1.016987  | -0.000017 |
| 3                | 6                | 0              | -1.662176               | 0.932754  | -0.000010 |
| 4                | 8                | 0              | -1.792657               | 2.168237  | -0.000025 |
| 5                | 6                | 0              | -2.845592               | 0.063876  | 0.000005  |
| 6                | 6                | 0              | -2.952970               | -1.315973 | 0.000021  |
| 7                | 16               | 0              | -4.439532               | 0.802651  | 0.000004  |
| 8                | 6                | 0              | -4.296028               | -1.774135 | 0.000033  |
| 9                | 1                | 0              | -2.100314               | -1.984960 | 0.000024  |
| 10               | 6                | 0              | -5.223851               | -0.753735 | 0.000026  |
| 11               | 1                | 0              | -4.578971               | -2.821368 | 0.000046  |
| 12               | 6                | 0              | -6.716667               | -0.870840 | 0.000036  |
| 13               | 1                | 0              | -7.155848               | -0.393735 | -0.883779 |
| 14               | 1                | 0              | -7.005280               | -1.925624 | 0.000053  |
| 15               | 1                | 0              | -7.155839               | -0.393709 | 0.883843  |
| 16               | 1                | 0              | -0.298063               | -0.802197 | 0.000009  |
| 17               | 1                | 0              | 0.685964                | 2.100163  | -0.000030 |
| 18               | 6                | 0              | 2.176321                | 0.525865  | -0.000014 |
| 19               | 6                | 0              | 3.224663                | 1.467313  | -0.000028 |
| 20               | 6                | 0              | 2.513653                | -0.844276 | 0.000003  |
| 21               | 6                | 0              | 4.561515                | 1.070119  | -0.000026 |
| 22               | 1                | 0              | 2.988889                | 2.527904  | -0.000041 |
| 23               | 6                | 0              | 3.842255                | -1.257423 | 0.000005  |
| 24               | 1                | 0              | 1.736930                | -1.602081 | 0.000015  |
| 25               | 6                | 0              | 4.854998                | -0.293043 | -0.000010 |
| 26               | 1                | 0              | 5.357694                | 1.806898  | -0.000038 |
| 27               | 1                | 0              | 4.090762                | -2.313309 | 0.000018  |
| 28               | 17               | 0              | 6.539188                | -0.816259 | -0.000007 |

### Int1

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.314605 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.339799                    |
| Thermal correction to Enthalpy=              | 0.340743                    |
| Thermal correction to Gibbs Free Energy=     | 0.255717                    |
| Sum of electronic and zero-point Energies=   | -1792.125088                |
| Sum of electronic and thermal Energies=      | -1792.099894                |
| Sum of electronic and thermal Enthalpies=    | -1792.098950                |
| Sum of electronic and thermal Free Energies= | -1792.183976                |

Standard orientation:

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

---

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 1  | 6  | 0 | 0.888378  | -1.193921 | -0.386862 |
| 2  | 6  | 0 | -0.176149 | -1.437591 | -1.204674 |
| 3  | 6  | 0 | 2.274966  | -1.155805 | -0.928697 |
| 4  | 8  | 0 | 2.493501  | -1.169374 | -2.150014 |
| 5  | 6  | 0 | 3.366876  | -1.098733 | 0.039658  |
| 6  | 6  | 0 | 3.334004  | -1.094746 | 1.425670  |
| 7  | 16 | 0 | 5.023945  | -1.040383 | -0.536593 |
| 8  | 6  | 0 | 4.621159  | -1.042073 | 2.014572  |
| 9  | 1  | 0 | 2.419324  | -1.131475 | 2.005647  |
| 10 | 6  | 0 | 5.646265  | -1.008110 | 1.089631  |
| 11 | 1  | 0 | 4.800020  | -1.031833 | 3.084370  |
| 12 | 6  | 0 | 7.117923  | -0.957233 | 1.358722  |
| 13 | 1  | 0 | 7.580577  | -0.078198 | 0.895603  |
| 14 | 1  | 0 | 7.294559  | -0.912746 | 2.436890  |
| 15 | 1  | 0 | 7.626059  | -1.844150 | 0.962123  |
| 16 | 1  | 0 | 0.758398  | -1.142831 | 0.688142  |
| 17 | 1  | 0 | 0.023805  | -1.498465 | -2.273499 |
| 18 | 6  | 0 | -1.560731 | -1.617845 | -0.795359 |
| 19 | 6  | 0 | -2.562210 | -1.626279 | -1.788103 |
| 20 | 6  | 0 | -1.949178 | -1.763194 | 0.553934  |
| 21 | 6  | 0 | -3.909806 | -1.740367 | -1.452907 |
| 22 | 1  | 0 | -2.280672 | -1.529853 | -2.833029 |
| 23 | 6  | 0 | -3.287965 | -1.889317 | 0.902024  |
| 24 | 1  | 0 | -1.203661 | -1.786109 | 1.341193  |
| 25 | 6  | 0 | -4.257437 | -1.863095 | -0.106265 |
| 26 | 1  | 0 | -4.674476 | -1.734793 | -2.222323 |
| 27 | 1  | 0 | -3.579917 | -1.997116 | 1.940598  |
| 28 | 6  | 0 | -3.607936 | 1.563269  | 0.970693  |
| 29 | 6  | 0 | -2.556770 | 1.647275  | 0.056347  |
| 30 | 6  | 0 | -1.248391 | 1.613367  | 0.553312  |
| 31 | 6  | 0 | -0.955637 | 1.479130  | 1.915700  |
| 32 | 6  | 0 | -2.025484 | 1.390097  | 2.808996  |
| 33 | 6  | 0 | -3.343003 | 1.435198  | 2.338598  |
| 34 | 1  | 0 | -4.631374 | 1.585157  | 0.609851  |
| 35 | 1  | 0 | -2.752567 | 1.732856  | -1.006636 |
| 36 | 1  | 0 | 0.069052  | 1.452315  | 2.270063  |
| 37 | 1  | 0 | -1.825728 | 1.288357  | 3.871345  |
| 38 | 1  | 0 | -4.167882 | 1.363323  | 3.041200  |
| 39 | 53 | 0 | 0.338025  | 1.789681  | -0.805116 |
| 40 | 8  | 0 | 0.361769  | 3.792409  | -0.842965 |
| 41 | 1  | 0 | -0.245529 | 4.083807  | -1.551899 |
| 42 | 17 | 0 | -5.953168 | -1.991156 | 0.338287  |

---

## Int2

---

|                                 |                             |
|---------------------------------|-----------------------------|
| Zero-point correction=          | 0.447138 (Hartree/Particle) |
| Thermal correction to Energy=   | 0.483609                    |
| Thermal correction to Enthalpy= | 0.484554                    |

Thermal correction to Gibbs Free Energy= 0.371942  
 Sum of electronic and zero-point Energies= -2686.990191  
 Sum of electronic and thermal Energies= -2686.953720  
 Sum of electronic and thermal Enthalpies= -2686.952776  
 Sum of electronic and thermal Free Energies= -2687.065387

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.844342               | -0.217829 | -0.317816 |
| 2                | 6                | 0              | -0.643177               | 1.254693  | -0.650527 |
| 3                | 6                | 0              | -2.021483               | -0.825986 | -0.997169 |
| 4                | 8                | 0              | -2.397461               | -0.422305 | -2.109923 |
| 5                | 6                | 0              | -2.683945               | -1.959710 | -0.342995 |
| 6                | 6                | 0              | -2.476784               | -2.519694 | 0.904441  |
| 7                | 16               | 0              | -3.959559               | -2.811743 | -1.196387 |
| 8                | 6                | 0              | -3.330821               | -3.621965 | 1.171892  |
| 9                | 1                | 0              | -1.738085               | -2.157550 | 1.609337  |
| 10               | 6                | 0              | -4.194996               | -3.910055 | 0.136183  |
| 11               | 1                | 0              | -3.317652               | -4.188015 | 2.097403  |
| 12               | 6                | 0              | -5.230476               | -4.991107 | 0.077400  |
| 13               | 1                | 0              | -5.046738               | -5.678330 | -0.756744 |
| 14               | 1                | 0              | -5.216497               | -5.567579 | 1.006786  |
| 15               | 1                | 0              | -6.236560               | -4.575632 | -0.053940 |
| 16               | 1                | 0              | -0.823436               | -0.382327 | 0.757593  |
| 17               | 6                | 0              | 2.197022                | -1.372410 | 3.074101  |
| 18               | 6                | 0              | 1.937817                | -1.004211 | 1.749340  |
| 19               | 6                | 0              | 1.399235                | -1.959453 | 0.885700  |
| 20               | 6                | 0              | 1.111484                | -3.260873 | 1.301830  |
| 21               | 6                | 0              | 1.376300                | -3.610061 | 2.630674  |
| 22               | 6                | 0              | 1.916545                | -2.669952 | 3.514854  |
| 23               | 1                | 0              | 2.620376                | -0.639850 | 3.755536  |
| 24               | 1                | 0              | 2.148243                | 0.002133  | 1.408859  |
| 25               | 1                | 0              | 0.694176                | -3.987327 | 0.613069  |
| 26               | 1                | 0              | 1.155808                | -4.618288 | 2.969765  |
| 27               | 1                | 0              | 2.119593                | -2.948790 | 4.544861  |
| 28               | 53               | 0              | 1.005253                | -1.421295 | -1.127988 |
| 29               | 8                | 0              | 2.785144                | -2.604386 | -1.642574 |
| 30               | 1                | 0              | 3.566449                | -2.077464 | -1.405395 |
| 31               | 1                | 0              | -0.508713               | 1.385601  | -1.726078 |
| 32               | 6                | 0              | -1.767747               | 2.137465  | -0.153438 |
| 33               | 6                | 0              | -2.572694               | 2.831170  | -1.062457 |
| 34               | 6                | 0              | -2.024667               | 2.254051  | 1.220156  |
| 35               | 6                | 0              | -3.628094               | 3.631881  | -0.616016 |
| 36               | 1                | 0              | -2.379182               | 2.748990  | -2.127792 |
| 37               | 6                | 0              | -3.068866               | 3.053045  | 1.684444  |
| 38               | 1                | 0              | -1.401001               | 1.726632  | 1.936024  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 39 | 6  | 0 | -3.861218 | 3.731448  | 0.754751  |
| 40 | 1  | 0 | -4.251363 | 4.168804  | -1.323169 |
| 41 | 1  | 0 | -3.263776 | 3.147293  | 2.747529  |
| 42 | 8  | 0 | 0.605923  | 1.619514  | 0.035896  |
| 43 | 16 | 0 | 1.571236  | 2.798726  | -0.574988 |
| 44 | 8  | 0 | 1.436936  | 3.980263  | 0.283093  |
| 45 | 8  | 0 | 1.312334  | 2.917085  | -2.016220 |
| 46 | 6  | 0 | 3.146074  | 2.021377  | -0.287328 |
| 47 | 6  | 0 | 3.782936  | 2.207183  | 0.941082  |
| 48 | 6  | 0 | 3.678201  | 1.181699  | -1.272063 |
| 49 | 6  | 0 | 4.973951  | 1.521714  | 1.188348  |
| 50 | 1  | 0 | 3.355280  | 2.865677  | 1.689671  |
| 51 | 6  | 0 | 4.868768  | 0.510589  | -1.004656 |
| 52 | 1  | 0 | 3.171971  | 1.055564  | -2.222615 |
| 53 | 6  | 0 | 5.530148  | 0.662059  | 0.228015  |
| 54 | 1  | 0 | 5.474614  | 1.655690  | 2.143161  |
| 55 | 1  | 0 | 5.291821  | -0.143298 | -1.763002 |
| 56 | 6  | 0 | 6.816474  | -0.078091 | 0.491344  |
| 57 | 1  | 0 | 7.613333  | 0.287716  | -0.167764 |
| 58 | 1  | 0 | 7.147642  | 0.045860  | 1.525983  |
| 59 | 1  | 0 | 6.698708  | -1.149138 | 0.290930  |
| 60 | 17 | 0 | -5.188066 | 4.744546  | 1.333685  |

---

### Int3

---

Zero-point correction= 0.435397 (Hartree/Particle)  
 Thermal correction to Energy= 0.469499  
 Thermal correction to Enthalpy= 0.470443  
 Thermal correction to Gibbs Free Energy= 0.363346  
 Sum of electronic and zero-point Energies= -2611.026078  
 Sum of electronic and thermal Energies= -2610.991976  
 Sum of electronic and thermal Enthalpies= -2610.991032  
 Sum of electronic and thermal Free Energies= -2611.098129

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.629711               | -0.518895 | -0.485046 |
| 2                | 6                | 0              | -0.401261               | 0.973855  | -0.730406 |
| 3                | 6                | 0              | -1.870385               | -1.029653 | -1.223817 |
| 4                | 8                | 0              | -1.894200               | -0.954037 | -2.455194 |
| 5                | 6                | 0              | -2.967639               | -1.527279 | -0.427764 |
| 6                | 6                | 0              | -3.069480               | -1.698075 | 0.948146  |
| 7                | 16               | 0              | -4.469156               | -1.977268 | -1.220639 |
| 8                | 6                | 0              | -4.330679               | -2.185758 | 1.353219  |
| 9                | 1                | 0              | -2.266479               | -1.479743 | 1.641839  |
| 10               | 6                | 0              | -5.205205               | -2.388656 | 0.299864  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 11 | 1  | 0 | -4.603525 | -2.383059 | 2.383948  |
| 12 | 6  | 0 | -6.610112 | -2.897492 | 0.367620  |
| 13 | 1  | 0 | -6.716045 | -3.843246 | -0.176722 |
| 14 | 1  | 0 | -6.892558 | -3.064792 | 1.410337  |
| 15 | 1  | 0 | -7.314647 | -2.182910 | -0.073025 |
| 16 | 1  | 0 | -0.596497 | -0.754864 | 0.577410  |
| 17 | 6  | 0 | 3.303510  | -1.957919 | 2.488165  |
| 18 | 6  | 0 | 2.840855  | -1.548355 | 1.233960  |
| 19 | 6  | 0 | 1.834501  | -2.304790 | 0.630231  |
| 20 | 6  | 0 | 1.275832  | -3.441792 | 1.219949  |
| 21 | 6  | 0 | 1.752677  | -3.826890 | 2.477086  |
| 22 | 6  | 0 | 2.761793  | -3.089691 | 3.106574  |
| 23 | 1  | 0 | 4.086264  | -1.385514 | 2.976577  |
| 24 | 1  | 0 | 3.248102  | -0.667725 | 0.753758  |
| 25 | 1  | 0 | 0.496717  | -4.010161 | 0.723466  |
| 26 | 1  | 0 | 1.333723  | -4.705924 | 2.957595  |
| 27 | 1  | 0 | 3.127691  | -3.399330 | 4.081007  |
| 28 | 53 | 0 | 1.103091  | -1.699550 | -1.263418 |
| 29 | 1  | 0 | -0.302285 | 1.165131  | -1.801746 |
| 30 | 6  | 0 | -1.568552 | 1.747644  | -0.152404 |
| 31 | 6  | 0 | -2.552182 | 2.263495  | -1.003286 |
| 32 | 6  | 0 | -1.701718 | 1.892867  | 1.235259  |
| 33 | 6  | 0 | -3.669244 | 2.916827  | -0.478619 |
| 34 | 1  | 0 | -2.451561 | 2.157316  | -2.079520 |
| 35 | 6  | 0 | -2.808242 | 2.547201  | 1.773313  |
| 36 | 1  | 0 | -0.935295 | 1.505162  | 1.899349  |
| 37 | 6  | 0 | -3.783551 | 3.046152  | 0.905719  |
| 38 | 1  | 0 | -4.431771 | 3.320334  | -1.135988 |
| 39 | 1  | 0 | -2.912961 | 2.666955  | 2.846270  |
| 40 | 8  | 0 | 0.839587  | 1.286520  | -0.051569 |
| 41 | 16 | 0 | 1.737480  | 2.579903  | -0.584489 |
| 42 | 8  | 0 | 1.467529  | 3.706176  | 0.310184  |
| 43 | 8  | 0 | 1.503616  | 2.717489  | -2.026777 |
| 44 | 6  | 0 | 3.354009  | 1.917545  | -0.268292 |
| 45 | 6  | 0 | 3.933548  | 2.111264  | 0.987773  |
| 46 | 6  | 0 | 3.993008  | 1.180759  | -1.271717 |
| 47 | 6  | 0 | 5.182849  | 1.543104  | 1.239515  |
| 48 | 1  | 0 | 3.422270  | 2.689269  | 1.750177  |
| 49 | 6  | 0 | 5.241114  | 0.626429  | -0.997557 |
| 50 | 1  | 0 | 3.527730  | 1.048278  | -2.242431 |
| 51 | 6  | 0 | 5.853599  | 0.795086  | 0.257964  |
| 52 | 1  | 0 | 5.643280  | 1.685174  | 2.213128  |
| 53 | 1  | 0 | 5.749258  | 0.054305  | -1.769068 |
| 54 | 6  | 0 | 7.213349  | 0.204317  | 0.527482  |
| 55 | 1  | 0 | 7.993206  | 0.812252  | 0.051570  |
| 56 | 1  | 0 | 7.428475  | 0.164038  | 1.598938  |
| 57 | 1  | 0 | 7.294520  | -0.807026 | 0.115389  |
| 58 | 17 | 0 | -5.191353 | 3.864298  | 1.579422  |

---

### T.S.1

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.433366 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.467604                    |
| Thermal correction to Enthalpy=              | 0.468548                    |
| Thermal correction to Gibbs Free Energy=     | 0.360694                    |
| Sum of electronic and zero-point Energies=   | -2611.008794                |
| Sum of electronic and thermal Energies=      | -2610.974557                |
| Sum of electronic and thermal Enthalpies=    | -2610.973613                |
| Sum of electronic and thermal Free Energies= | -2611.081467                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.069939               | 0.218905  | -0.432330 |
| 2                | 6                | 0              | -0.270333               | 1.301493  | -0.967336 |
| 3                | 6                | 0              | -2.218120               | -0.383447 | -1.195979 |
| 4                | 8                | 0              | -2.388158               | -0.078236 | -2.381061 |
| 5                | 6                | 0              | -3.049937               | -1.312558 | -0.465207 |
| 6                | 6                | 0              | -2.984038               | -1.706844 | 0.868640  |
| 7                | 16               | 0              | -4.355737               | -2.138632 | -1.293902 |
| 8                | 6                | 0              | -3.969805               | -2.654357 | 1.212727  |
| 9                | 1                | 0              | -2.254304               | -1.330825 | 1.575003  |
| 10               | 6                | 0              | -4.795083               | -2.997859 | 0.154604  |
| 11               | 1                | 0              | -4.083664               | -3.080572 | 2.203209  |
| 12               | 6                | 0              | -5.936674               | -3.962733 | 0.167599  |
| 13               | 1                | 0              | -5.778350               | -4.777217 | -0.548848 |
| 14               | 1                | 0              | -6.044567               | -4.393999 | 1.166263  |
| 15               | 1                | 0              | -6.877163               | -3.467312 | -0.100474 |
| 16               | 1                | 0              | -0.854904               | -0.098856 | 0.581965  |
| 17               | 6                | 0              | 2.251374                | -1.360009 | 2.909828  |
| 18               | 6                | 0              | 2.031965                | -1.327420 | 1.528946  |
| 19               | 6                | 0              | 1.150280                | -2.254330 | 0.962795  |
| 20               | 6                | 0              | 0.488506                | -3.207074 | 1.744861  |
| 21               | 6                | 0              | 0.720317                | -3.224666 | 3.125463  |
| 22               | 6                | 0              | 1.597248                | -2.304157 | 3.708871  |
| 23               | 1                | 0              | 2.936830                | -0.644161 | 3.354840  |
| 24               | 1                | 0              | 2.532697                | -0.592057 | 0.911552  |
| 25               | 1                | 0              | -0.193140               | -3.920295 | 1.293718  |
| 26               | 1                | 0              | 0.212282                | -3.962391 | 3.740260  |
| 27               | 1                | 0              | 1.772940                | -2.324454 | 4.780520  |
| 28               | 53               | 0              | 0.775181                | -2.173958 | -1.119452 |
| 29               | 1                | 0              | -0.265216               | 1.415152  | -2.050322 |
| 30               | 6                | 0              | -1.324793               | 2.188400  | -0.274923 |
| 31               | 6                | 0              | -2.398920               | 2.728215  | -1.027149 |
| 32               | 6                | 0              | -1.175648               | 2.523083  | 1.094529  |
| 33               | 6                | 0              | -3.281307               | 3.611201  | -0.432247 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 34 | 1  | 0 | -2.522805 | 2.452925  | -2.068380 |
| 35 | 6  | 0 | -2.061630 | 3.403598  | 1.692777  |
| 36 | 1  | 0 | -0.347679 | 2.114339  | 1.663435  |
| 37 | 6  | 0 | -3.106767 | 3.936455  | 0.924193  |
| 38 | 1  | 0 | -4.095440 | 4.047100  | -1.000378 |
| 39 | 1  | 0 | -1.949011 | 3.680272  | 2.734980  |
| 40 | 8  | 0 | 1.011354  | 1.329580  | -0.374528 |
| 41 | 16 | 0 | 2.131113  | 2.430749  | -0.970888 |
| 42 | 8  | 0 | 2.017395  | 3.652802  | -0.174562 |
| 43 | 8  | 0 | 1.943526  | 2.482765  | -2.423583 |
| 44 | 6  | 0 | 3.579660  | 1.515791  | -0.527980 |
| 45 | 6  | 0 | 4.210778  | 1.790624  | 0.687157  |
| 46 | 6  | 0 | 4.012855  | 0.490744  | -1.377897 |
| 47 | 6  | 0 | 5.307448  | 1.010162  | 1.055637  |
| 48 | 1  | 0 | 3.855024  | 2.590283  | 1.327898  |
| 49 | 6  | 0 | 5.106062  | -0.274327 | -0.985456 |
| 50 | 1  | 0 | 3.504691  | 0.295526  | -2.316203 |
| 51 | 6  | 0 | 5.766522  | -0.031703 | 0.234081  |
| 52 | 1  | 0 | 5.811318  | 1.213429  | 1.996118  |
| 53 | 1  | 0 | 5.454555  | -1.074765 | -1.632361 |
| 54 | 6  | 0 | 6.943153  | -0.882441 | 0.635481  |
| 55 | 1  | 0 | 7.343484  | -0.584296 | 1.608046  |
| 56 | 1  | 0 | 6.654853  | -1.938856 | 0.689636  |
| 57 | 1  | 0 | 7.746657  | -0.805657 | -0.106511 |
| 58 | 17 | 0 | -4.227157 | 5.036991  | 1.674318  |

---

**Int5 [In electron-withdrawing no Int4 structure]**

---

Zero-point correction= 0.342765 (Hartree/Particle)  
Thermal correction to Energy= 0.370110  
Thermal correction to Enthalpy= 0.371054  
Thermal correction to Gibbs Free Energy= 0.280193  
Sum of electronic and zero-point Energies= -2368.071235  
Sum of electronic and thermal Energies= -2368.043890  
Sum of electronic and thermal Enthalpies= -2368.042946  
Sum of electronic and thermal Free Energies= -2368.133807

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.801664               | 0.166029  | -0.170715 |
| 2                | 6                | 0              | 0.443215                | -0.357847 | 0.445477  |
| 3                | 6                | 0              | -1.397440               | 1.306252  | 0.682235  |
| 4                | 8                | 0              | -1.081982               | 1.401254  | 1.870419  |
| 5                | 6                | 0              | -2.343995               | 2.186326  | 0.032589  |
| 6                | 6                | 0              | -2.801842               | 2.180941  | -1.276846 |
| 7                | 16               | 0              | -3.116046               | 3.466552  | 0.955671  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 8  | 6  | 0 | -3.755824 | 3.191776  | -1.533475 |
| 9  | 1  | 0 | -2.467589 | 1.471852  | -2.025229 |
| 10 | 6  | 0 | -4.036565 | 3.975669  | -0.429967 |
| 11 | 1  | 0 | -4.230353 | 3.349024  | -2.495643 |
| 12 | 6  | 0 | -4.986495 | 5.128728  | -0.348735 |
| 13 | 1  | 0 | -4.465148 | 6.055587  | -0.083002 |
| 14 | 1  | 0 | -5.475249 | 5.272213  | -1.315934 |
| 15 | 1  | 0 | -5.760092 | 4.956990  | 0.408354  |
| 16 | 1  | 0 | -0.600092 | 0.481841  | -1.195531 |
| 17 | 1  | 0 | 0.490414  | -0.500470 | 1.531453  |
| 18 | 6  | 0 | -1.702252 | -1.084912 | -0.180476 |
| 19 | 6  | 0 | -2.386384 | -1.495587 | 0.973060  |
| 20 | 6  | 0 | -1.806071 | -1.838335 | -1.358610 |
| 21 | 6  | 0 | -3.194297 | -2.632287 | 0.943918  |
| 22 | 1  | 0 | -2.303988 | -0.928456 | 1.894896  |
| 23 | 6  | 0 | -2.610800 | -2.975081 | -1.398311 |
| 24 | 1  | 0 | -1.266167 | -1.533491 | -2.250089 |
| 25 | 6  | 0 | -3.297741 | -3.358085 | -0.243356 |
| 26 | 1  | 0 | -3.732634 | -2.944904 | 1.831789  |
| 27 | 1  | 0 | -2.702849 | -3.551445 | -2.312212 |
| 28 | 8  | 0 | 1.406694  | -0.697395 | -0.275793 |
| 29 | 16 | 0 | 2.956341  | -1.601374 | 0.581032  |
| 30 | 8  | 0 | 2.967185  | -2.807963 | -0.223746 |
| 31 | 8  | 0 | 2.572888  | -1.559800 | 1.983742  |
| 32 | 6  | 0 | 4.176320  | -0.441566 | 0.145508  |
| 33 | 6  | 0 | 4.813415  | -0.578339 | -1.097315 |
| 34 | 6  | 0 | 4.449816  | 0.613586  | 1.033293  |
| 35 | 6  | 0 | 5.769863  | 0.369089  | -1.441509 |
| 36 | 1  | 0 | 4.575485  | -1.399166 | -1.764383 |
| 37 | 6  | 0 | 5.409392  | 1.540435  | 0.655483  |
| 38 | 1  | 0 | 3.935806  | 0.696220  | 1.984498  |
| 39 | 6  | 0 | 6.082143  | 1.436607  | -0.579619 |
| 40 | 1  | 0 | 6.283737  | 0.278754  | -2.393228 |
| 41 | 1  | 0 | 5.646929  | 2.360279  | 1.326533  |
| 42 | 6  | 0 | 7.124031  | 2.453095  | -0.949795 |
| 43 | 1  | 0 | 7.476053  | 2.318892  | -1.975362 |
| 44 | 1  | 0 | 6.728620  | 3.469107  | -0.841095 |
| 45 | 1  | 0 | 7.985412  | 2.370978  | -0.275445 |
| 46 | 17 | 0 | -4.315426 | -4.792610 | -0.287741 |

---

**Product**

---

|                                            |                             |
|--------------------------------------------|-----------------------------|
| Zero-point correction=                     | 0.477394 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.515206                    |
| Thermal correction to Enthalpy=            | 0.516150                    |
| Thermal correction to Gibbs Free Energy=   | 0.400975                    |
| Sum of electronic and zero-point Energies= | -3262.998749                |
| Sum of electronic and thermal Energies=    | -3262.960937                |
| Sum of electronic and thermal Enthalpies=  | -3262.959992                |

Sum of electronic and thermal Free Energies= -3263.075167

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.235878                | 1.199999  | 0.021177  |
| 2                | 1                | 0              | -0.069012               | 1.174399  | 1.069281  |
| 3                | 6                | 0              | -0.632650               | 0.171393  | -0.709831 |
| 4                | 1                | 0              | -0.446874               | 0.143501  | -1.783139 |
| 5                | 6                | 0              | 1.718442                | 0.871694  | -0.070683 |
| 6                | 6                | 0              | 2.388830                | 0.894646  | -1.301239 |
| 7                | 6                | 0              | 2.436231                | 0.551448  | 1.088238  |
| 8                | 6                | 0              | 3.753138                | 0.610516  | -1.376872 |
| 9                | 1                | 0              | 1.848531                | 1.141098  | -2.209518 |
| 10               | 6                | 0              | 3.801419                | 0.266453  | 1.031820  |
| 11               | 1                | 0              | 1.926394                | 0.518463  | 2.046664  |
| 12               | 6                | 0              | 4.443087                | 0.302212  | -0.205115 |
| 13               | 1                | 0              | 4.266738                | 0.625394  | -2.332036 |
| 14               | 1                | 0              | 4.350205                | 0.011564  | 1.931844  |
| 15               | 8                | 0              | -0.406470               | -1.119220 | -0.124209 |
| 16               | 16               | 0              | 0.128892                | -2.406020 | -1.033508 |
| 17               | 8                | 0              | 0.488686                | -1.932921 | -2.371561 |
| 18               | 8                | 0              | -0.885483               | -3.449198 | -0.864518 |
| 19               | 6                | 0              | 1.590460                | -2.858704 | -0.127346 |
| 20               | 6                | 0              | 2.832429                | -2.743626 | -0.748367 |
| 21               | 6                | 0              | 1.458831                | -3.346125 | 1.178770  |
| 22               | 6                | 0              | 3.971158                | -3.129525 | -0.038930 |
| 23               | 1                | 0              | 2.911146                | -2.353939 | -1.756196 |
| 24               | 6                | 0              | 2.609252                | -3.711597 | 1.869803  |
| 25               | 1                | 0              | 0.482597                | -3.435374 | 1.644151  |
| 26               | 6                | 0              | 3.880970                | -3.611482 | 1.273485  |
| 27               | 1                | 0              | 4.943973                | -3.037272 | -0.511648 |
| 28               | 1                | 0              | 2.522789                | -4.083683 | 2.887144  |
| 29               | 6                | 0              | 5.112211                | -4.020861 | 2.040309  |
| 30               | 1                | 0              | 5.097777                | -5.097094 | 2.250862  |
| 31               | 1                | 0              | 6.025089                | -3.794775 | 1.482606  |
| 32               | 1                | 0              | 5.160480                | -3.504108 | 3.005686  |
| 33               | 8                | 0              | -1.975677               | 0.548586  | -0.422681 |
| 34               | 16               | 0              | -3.224368               | 0.040235  | -1.408493 |
| 35               | 8                | 0              | -2.647246               | -0.810995 | -2.452251 |
| 36               | 8                | 0              | -3.955858               | 1.258455  | -1.754634 |
| 37               | 6                | 0              | -4.184762               | -0.926131 | -0.266706 |
| 38               | 6                | 0              | -3.898832               | -2.285644 | -0.121792 |
| 39               | 6                | 0              | -5.185294               | -0.296685 | 0.479716  |
| 40               | 6                | 0              | -4.641885               | -3.025760 | 0.796831  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 41 | 1  | 0 | -3.111901 | -2.752671 | -0.702682 |
| 42 | 6  | 0 | -5.913176 | -1.058216 | 1.391991  |
| 43 | 1  | 0 | -5.391366 | 0.760079  | 0.348652  |
| 44 | 6  | 0 | -5.656592 | -2.429456 | 1.563750  |
| 45 | 1  | 0 | -4.428796 | -4.084192 | 0.918346  |
| 46 | 1  | 0 | -6.694083 | -0.580984 | 1.977597  |
| 47 | 6  | 0 | -6.476633 | -3.247227 | 2.528254  |
| 48 | 1  | 0 | -7.398593 | -3.594062 | 2.044047  |
| 49 | 1  | 0 | -5.929542 | -4.131389 | 2.868531  |
| 50 | 1  | 0 | -6.768760 | -2.657402 | 3.402759  |
| 51 | 6  | 0 | -0.022939 | 2.592740  | -0.580833 |
| 52 | 8  | 0 | -0.209419 | 2.709362  | -1.793606 |
| 53 | 6  | 0 | 0.021139  | 3.740767  | 0.312620  |
| 54 | 6  | 0 | 0.214799  | 3.791974  | 1.682372  |
| 55 | 16 | 0 | -0.167108 | 5.358699  | -0.345913 |
| 56 | 6  | 0 | 0.213265  | 5.112150  | 2.196696  |
| 57 | 1  | 0 | 0.357394  | 2.912502  | 2.299108  |
| 58 | 6  | 0 | 0.018075  | 6.077376  | 1.229162  |
| 59 | 1  | 0 | 0.349834  | 5.355217  | 3.244811  |
| 60 | 6  | 0 | -0.042344 | 7.561582  | 1.415962  |
| 61 | 1  | 0 | 0.732539  | 8.069831  | 0.830664  |
| 62 | 1  | 0 | -1.011543 | 7.964742  | 1.100308  |
| 63 | 1  | 0 | 0.105843  | 7.807752  | 2.471027  |
| 64 | 17 | 0 | 6.166776  | -0.071779 | -0.292589 |

---

**Nitro group (Formation of  $\beta$ ,  $\beta$ -ditosyloxy ketone)**

---

**Reactant**

---

Zero-point correction= 0.221266 (Hartree/Particle)  
Thermal correction to Energy= 0.238376  
Thermal correction to Enthalpy= 0.239320  
Thermal correction to Gibbs Free Energy= 0.173345  
Sum of electronic and zero-point Energies= -1218.499463  
Sum of electronic and thermal Energies= -1218.482353  
Sum of electronic and thermal Enthalpies= -1218.481409  
Sum of electronic and thermal Free Energies= -1218.547384

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.625625                | -0.318223 | -0.000012 |
| 2                | 6                | 0              | -0.493191               | -1.071921 | -0.000013 |
| 3                | 6                | 0              | 1.967322                | -0.953094 | -0.000013 |
| 4                | 8                | 0              | 2.107295                | -2.186187 | -0.000024 |
| 5                | 6                | 0              | 3.135005                | -0.068342 | -0.000000 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 6  | 6  | 0 | 3.218998  | 1.314142  | 0.000016  |
| 7  | 16 | 0 | 4.740776  | -0.780699 | -0.000006 |
| 8  | 6  | 0 | 4.553341  | 1.793986  | 0.000023  |
| 9  | 1  | 0 | 2.355705  | 1.969209  | 0.000024  |
| 10 | 6  | 0 | 5.498168  | 0.788442  | 0.000012  |
| 11 | 1  | 0 | 4.819072  | 2.845610  | 0.000036  |
| 12 | 6  | 0 | 6.988518  | 0.930301  | 0.000016  |
| 13 | 1  | 0 | 7.435022  | 0.460020  | -0.883737 |
| 14 | 1  | 0 | 7.259833  | 1.989610  | 0.000022  |
| 15 | 1  | 0 | 7.435018  | 0.460010  | 0.883766  |
| 16 | 1  | 0 | 0.574085  | 0.763981  | -0.000009 |
| 17 | 1  | 0 | -0.368795 | -2.153334 | -0.000013 |
| 18 | 6  | 0 | -1.876653 | -0.592179 | -0.000012 |
| 19 | 6  | 0 | -2.913799 | -1.548461 | 0.000020  |
| 20 | 6  | 0 | -2.223612 | 0.777214  | -0.000039 |
| 21 | 6  | 0 | -4.250560 | -1.165589 | 0.000028  |
| 22 | 1  | 0 | -2.664111 | -2.605106 | 0.000040  |
| 23 | 6  | 0 | -3.552668 | 1.176313  | -0.000033 |
| 24 | 1  | 0 | -1.453190 | 1.540375  | -0.000068 |
| 25 | 6  | 0 | -4.553294 | 0.197463  | 0.000002  |
| 26 | 1  | 0 | -5.042920 | -1.903802 | 0.000055  |
| 27 | 1  | 0 | -3.816968 | 2.226441  | -0.000055 |
| 28 | 7  | 0 | -5.955638 | 0.614957  | 0.000009  |
| 29 | 8  | 0 | -6.207729 | 1.825589  | -0.000013 |
| 30 | 8  | 0 | -6.828929 | -0.260258 | 0.000037  |

---

### Int1

---

Zero-point correction= 0.326650 (Hartree/Particle)  
 Thermal correction to Energy= 0.353219  
 Thermal correction to Enthalpy= 0.354163  
 Thermal correction to Gibbs Free Energy= 0.265983  
 Sum of electronic and zero-point Energies= -1537.028391  
 Sum of electronic and thermal Energies= -1537.001822  
 Sum of electronic and thermal Enthalpies= -1537.000877  
 Sum of electronic and thermal Free Energies= -1537.089057

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.047759                | -1.214754 | -0.449739 |
| 2                | 6                | 0              | -0.008458               | -1.351985 | -1.293358 |
| 3                | 6                | 0              | 2.438492                | -1.129460 | -0.985349 |
| 4                | 8                | 0              | 2.651698                | -1.056308 | -2.204766 |
| 5                | 6                | 0              | 3.528665                | -1.129928 | -0.017665 |
| 6                | 6                | 0              | 3.496482                | -1.212601 | 1.366624  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 7  | 16 | 0 | 5.184692  | -1.033498 | -0.591313 |
| 8  | 6  | 0 | 4.783852  | -1.197613 | 1.955612  |
| 9  | 1  | 0 | 2.582039  | -1.284995 | 1.943492  |
| 10 | 6  | 0 | 5.807951  | -1.104131 | 1.032707  |
| 11 | 1  | 0 | 4.964584  | -1.255717 | 3.023484  |
| 12 | 6  | 0 | 7.279642  | -1.063028 | 1.301502  |
| 13 | 1  | 0 | 7.726620  | -0.131855 | 0.934089  |
| 14 | 1  | 0 | 7.460951  | -1.132003 | 2.377435  |
| 15 | 1  | 0 | 7.798541  | -1.893584 | 0.809081  |
| 16 | 1  | 0 | 0.907900  | -1.233159 | 0.625172  |
| 17 | 1  | 0 | 0.198269  | -1.328707 | -2.361932 |
| 18 | 6  | 0 | -1.409778 | -1.502816 | -0.907465 |
| 19 | 6  | 0 | -2.397567 | -1.306566 | -1.894272 |
| 20 | 6  | 0 | -1.810061 | -1.802392 | 0.411513  |
| 21 | 6  | 0 | -3.750041 | -1.364985 | -1.574238 |
| 22 | 1  | 0 | -2.099366 | -1.091001 | -2.915930 |
| 23 | 6  | 0 | -3.155560 | -1.873977 | 0.743755  |
| 24 | 1  | 0 | -1.069423 | -1.982902 | 1.182285  |
| 25 | 6  | 0 | -4.107703 | -1.640900 | -0.253368 |
| 26 | 1  | 0 | -4.510891 | -1.197133 | -2.326483 |
| 27 | 1  | 0 | -3.467614 | -2.094169 | 1.756764  |
| 28 | 6  | 0 | -3.400228 | 1.505551  | 1.223635  |
| 29 | 6  | 0 | -2.404647 | 1.676608  | 0.260863  |
| 30 | 6  | 0 | -1.068893 | 1.599063  | 0.675720  |
| 31 | 6  | 0 | -0.698070 | 1.345353  | 2.002412  |
| 32 | 6  | 0 | -1.714339 | 1.166869  | 2.943553  |
| 33 | 6  | 0 | -3.056735 | 1.248179  | 2.555661  |
| 34 | 1  | 0 | -4.443286 | 1.559612  | 0.927850  |
| 35 | 1  | 0 | -2.661474 | 1.857789  | -0.776815 |
| 36 | 1  | 0 | 0.345454  | 1.290145  | 2.293236  |
| 37 | 1  | 0 | -1.454105 | 0.966763  | 3.978461  |
| 38 | 1  | 0 | -3.839902 | 1.103869  | 3.293866  |
| 39 | 53 | 0 | 0.443968  | 1.855510  | -0.752071 |
| 40 | 8  | 0 | 0.482921  | 3.848489  | -0.726179 |
| 41 | 1  | 0 | -0.172164 | 4.168649  | -1.378446 |
| 42 | 7  | 0 | -5.529526 | -1.664407 | 0.107461  |
| 43 | 8  | 0 | -5.829103 | -1.884537 | 1.285430  |
| 44 | 8  | 0 | -6.361696 | -1.452112 | -0.780199 |

---

## Int2

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.459547 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.497229                    |
| Thermal correction to Enthalpy=              | 0.498173                    |
| Thermal correction to Gibbs Free Energy=     | 0.383479                    |
| Sum of electronic and zero-point Energies=   | -2431.896387                |
| Sum of electronic and thermal Energies=      | -2431.858706                |
| Sum of electronic and thermal Enthalpies=    | -2431.857762                |
| Sum of electronic and thermal Free Energies= | -2431.972455                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.721957               | -0.406827 | -0.354684 |
| 2                | 6                | 0              | -0.726734               | 1.062946  | -0.760204 |
| 3                | 6                | 0              | -1.797788               | -1.216535 | -0.987820 |
| 4                | 8                | 0              | -2.259058               | -0.912302 | -2.100392 |
| 5                | 6                | 0              | -2.241782               | -2.426511 | -0.288556 |
| 6                | 6                | 0              | -1.885771               | -2.916145 | 0.954656  |
| 7                | 16               | 0              | -3.388927               | -3.500834 | -1.069758 |
| 8                | 6                | 0              | -2.525384               | -4.141788 | 1.277010  |
| 9                | 1                | 0              | -1.184512               | -2.418423 | 1.614049  |
| 10               | 6                | 0              | -3.372576               | -4.594713 | 0.287188  |
| 11               | 1                | 0              | -2.373551               | -4.678449 | 2.207637  |
| 12               | 6                | 0              | -4.207084               | -5.838708 | 0.292558  |
| 13               | 1                | 0              | -3.948674               | -6.499583 | -0.543060 |
| 14               | 1                | 0              | -4.046676               | -6.385972 | 1.225825  |
| 15               | 1                | 0              | -5.275130               | -5.605449 | 0.209551  |
| 16               | 1                | 0              | -0.667658               | -0.514006 | 0.728057  |
| 17               | 6                | 0              | 2.448728                | -0.922033 | 3.023130  |
| 18               | 6                | 0              | 2.106560                | -0.666406 | 1.691019  |
| 19               | 6                | 0              | 1.778270                | -1.744718 | 0.868438  |
| 20               | 6                | 0              | 1.779788                | -3.061751 | 1.330927  |
| 21               | 6                | 0              | 2.123190                | -3.297932 | 2.666734  |
| 22               | 6                | 0              | 2.456550                | -2.233029 | 3.510938  |
| 23               | 1                | 0              | 2.711762                | -0.091470 | 3.672082  |
| 24               | 1                | 0              | 2.093584                | 0.347039  | 1.310044  |
| 25               | 1                | 0              | 1.523471                | -3.885335 | 0.673530  |
| 26               | 1                | 0              | 2.125893                | -4.317042 | 3.042740  |
| 27               | 1                | 0              | 2.722769                | -2.425097 | 4.546349  |
| 28               | 53               | 0              | 1.272415                | -1.373711 | -1.159028 |
| 29               | 8                | 0              | 3.191797                | -2.296641 | -1.671602 |
| 30               | 1                | 0              | 3.890851                | -1.661102 | -1.443700 |
| 31               | 1                | 0              | -0.638095               | 1.158957  | -1.844418 |
| 32               | 6                | 0              | -1.961524               | 1.790955  | -0.268952 |
| 33               | 6                | 0              | -2.993022               | 2.100079  | -1.164981 |
| 34               | 6                | 0              | -2.095063               | 2.119941  | 1.089095  |
| 35               | 6                | 0              | -4.152367               | 2.730227  | -0.717538 |
| 36               | 1                | 0              | -2.891124               | 1.843234  | -2.213940 |
| 37               | 6                | 0              | -3.242959               | 2.752891  | 1.552721  |
| 38               | 1                | 0              | -1.292345               | 1.890306  | 1.782048  |
| 39               | 6                | 0              | -4.259775               | 3.047244  | 0.638266  |
| 40               | 1                | 0              | -4.954037               | 2.974880  | -1.403460 |
| 41               | 1                | 0              | -3.352667               | 3.015919  | 2.597574  |
| 42               | 8                | 0              | 0.461206                | 1.633924  | -0.122674 |
| 43               | 16               | 0              | 1.287800                | 2.855832  | -0.855460 |

|    |   |   |           |          |           |
|----|---|---|-----------|----------|-----------|
| 44 | 8 | 0 | 0.921120  | 4.112402 | -0.194763 |
| 45 | 8 | 0 | 1.115436  | 2.726028 | -2.308183 |
| 46 | 6 | 0 | 2.926978  | 2.369639 | -0.368704 |
| 47 | 6 | 0 | 3.423299  | 2.799514 | 0.865599  |
| 48 | 6 | 0 | 3.654347  | 1.509436 | -1.195431 |
| 49 | 6 | 0 | 4.673707  | 2.342116 | 1.277666  |
| 50 | 1 | 0 | 2.842165  | 3.469049 | 1.490884  |
| 51 | 6 | 0 | 4.905293  | 1.068752 | -0.764129 |
| 52 | 1 | 0 | 3.252680  | 1.190284 | -2.150386 |
| 53 | 6 | 0 | 5.430619  | 1.470097 | 0.475688  |
| 54 | 1 | 0 | 5.067207  | 2.664768 | 2.237801  |
| 55 | 1 | 0 | 5.480021  | 0.400309 | -1.399583 |
| 56 | 6 | 0 | 6.790357  | 1.002775 | 0.927621  |
| 57 | 1 | 0 | 7.546843  | 1.769016 | 0.714771  |
| 58 | 1 | 0 | 6.807490  | 0.818854 | 2.006755  |
| 59 | 1 | 0 | 7.090764  | 0.086348 | 0.411455  |
| 60 | 7 | 0 | -5.473461 | 3.713403 | 1.117655  |
| 61 | 8 | 0 | -5.559625 | 3.981388 | 2.321600  |
| 62 | 8 | 0 | -6.360896 | 3.978799 | 0.299294  |

---

### Int3

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.447680 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.482973                    |
| Thermal correction to Enthalpy=              | 0.483918                    |
| Thermal correction to Gibbs Free Energy=     | 0.374490                    |
| Sum of electronic and zero-point Energies=   | -2355.930232                |
| Sum of electronic and thermal Energies=      | -2355.894939                |
| Sum of electronic and thermal Enthalpies=    | -2355.893995                |
| Sum of electronic and thermal Free Energies= | -2356.003422                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.442247               | -0.572895 | -0.513738 |
| 2                | 6                | 0              | -0.348340               | 0.938146  | -0.758621 |
| 3                | 6                | 0              | -1.634713               | -1.196282 | -1.247339 |
| 4                | 8                | 0              | -1.678087               | -1.118031 | -2.478167 |
| 5                | 6                | 0              | -2.676163               | -1.788142 | -0.441282 |
| 6                | 6                | 0              | -2.746302               | -1.977020 | 0.935065  |
| 7                | 16               | 0              | -4.149530               | -2.344876 | -1.219040 |
| 8                | 6                | 0              | -3.961603               | -2.562027 | 1.350988  |
| 9                | 1                | 0              | -1.954506               | -1.704400 | 1.623036  |
| 10               | 6                | 0              | -4.832747               | -2.820901 | 0.306893  |
| 11               | 1                | 0              | -4.205064               | -2.787840 | 2.383191  |
| 12               | 6                | 0              | -6.196729               | -3.428935 | 0.387985  |
| 13               | 1                | 0              | -6.246621               | -4.368056 | -0.175243 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 14 | 1  | 0 | -6.447678 | -3.636613 | 1.431418  |
| 15 | 1  | 0 | -6.956836 | -2.756157 | -0.025619 |
| 16 | 1  | 0 | -0.386792 | -0.797957 | 0.550326  |
| 17 | 6  | 0 | 3.444749  | -1.881848 | 2.552048  |
| 18 | 6  | 0 | 2.992651  | -1.430009 | 1.308681  |
| 19 | 6  | 0 | 2.105782  | -2.245138 | 0.601428  |
| 20 | 6  | 0 | 1.659071  | -3.481486 | 1.075705  |
| 21 | 6  | 0 | 2.124925  | -3.908260 | 2.323482  |
| 22 | 6  | 0 | 3.012859  | -3.113197 | 3.056569  |
| 23 | 1  | 0 | 4.133899  | -1.264950 | 3.120861  |
| 24 | 1  | 0 | 3.316623  | -0.475415 | 0.914137  |
| 25 | 1  | 0 | 0.972955  | -4.092579 | 0.499485  |
| 26 | 1  | 0 | 1.792145  | -4.864567 | 2.715700  |
| 27 | 1  | 0 | 3.370506  | -3.455568 | 4.023048  |
| 28 | 53 | 0 | 1.394537  | -1.581786 | -1.280689 |
| 29 | 1  | 0 | -0.223492 | 1.136798  | -1.825931 |
| 30 | 6  | 0 | -1.614775 | 1.596735  | -0.239557 |
| 31 | 6  | 0 | -2.649570 | 1.905880  | -1.131787 |
| 32 | 6  | 0 | -1.776176 | 1.826411  | 1.134004  |
| 33 | 6  | 0 | -3.851543 | 2.427551  | -0.658819 |
| 34 | 1  | 0 | -2.520657 | 1.732852  | -2.195580 |
| 35 | 6  | 0 | -2.967661 | 2.354133  | 1.621175  |
| 36 | 1  | 0 | -0.968396 | 1.599489  | 1.821388  |
| 37 | 6  | 0 | -3.991678 | 2.637914  | 0.713938  |
| 38 | 1  | 0 | -4.660241 | 2.667452  | -1.337974 |
| 39 | 1  | 0 | -3.104985 | 2.537761  | 2.679558  |
| 40 | 8  | 0 | 0.812764  | 1.377920  | -0.023929 |
| 41 | 16 | 0 | 1.686039  | 2.682020  | -0.585880 |
| 42 | 8  | 0 | 1.357874  | 3.820471  | 0.271972  |
| 43 | 8  | 0 | 1.472861  | 2.765195  | -2.035252 |
| 44 | 6  | 0 | 3.318378  | 2.087413  | -0.223152 |
| 45 | 6  | 0 | 3.868569  | 2.333090  | 1.037425  |
| 46 | 6  | 0 | 4.002860  | 1.354909  | -1.199232 |
| 47 | 6  | 0 | 5.134749  | 1.820897  | 1.322086  |
| 48 | 1  | 0 | 3.323064  | 2.908540  | 1.777833  |
| 49 | 6  | 0 | 5.267355  | 0.857632  | -0.892457 |
| 50 | 1  | 0 | 3.558766  | 1.182293  | -2.173234 |
| 51 | 6  | 0 | 5.851096  | 1.078544  | 0.368548  |
| 52 | 1  | 0 | 5.572565  | 2.003074  | 2.299405  |
| 53 | 1  | 0 | 5.810848  | 0.289612  | -1.642522 |
| 54 | 6  | 0 | 7.228190  | 0.549399  | 0.674574  |
| 55 | 1  | 0 | 7.992003  | 1.191357  | 0.217537  |
| 56 | 1  | 0 | 7.417457  | 0.521042  | 1.751372  |
| 57 | 1  | 0 | 7.364968  | -0.457781 | 0.267266  |
| 58 | 7  | 0 | -5.261375 | 3.174668  | 1.223560  |
| 59 | 8  | 0 | -6.169763 | 3.391436  | 0.416380  |
| 60 | 8  | 0 | -5.363334 | 3.379787  | 2.436900  |

---

**T.S. 1**

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.445628 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.481096                    |
| Thermal correction to Enthalpy=              | 0.482040                    |
| Thermal correction to Gibbs Free Energy=     | 0.371211                    |
| Sum of electronic and zero-point Energies=   | -2355.904074                |
| Sum of electronic and thermal Energies=      | -2355.868606                |
| Sum of electronic and thermal Enthalpies=    | -2355.867662                |
| Sum of electronic and thermal Free Energies= | -2355.978491                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.037800               | -0.073104 | -0.589731 |
| 2                | 6                | 0              | -0.203623               | 0.884423  | -1.258390 |
| 3                | 6                | 0              | -2.174455               | -0.769856 | -1.299185 |
| 4                | 8                | 0              | -2.279582               | -0.646873 | -2.522722 |
| 5                | 6                | 0              | -3.052816               | -1.558599 | -0.471497 |
| 6                | 6                | 0              | -3.077052               | -1.697843 | 0.914578  |
| 7                | 16               | 0              | -4.323867               | -2.510234 | -1.215942 |
| 8                | 6                | 0              | -4.101918               | -2.554406 | 1.363037  |
| 9                | 1                | 0              | -2.384226               | -1.201263 | 1.583284  |
| 10               | 6                | 0              | -4.867021               | -3.081605 | 0.334637  |
| 11               | 1                | 0              | -4.285867               | -2.789596 | 2.405321  |
| 12               | 6                | 0              | -6.022907               | -4.021403 | 0.450178  |
| 13               | 1                | 0              | -5.836522               | -4.948476 | -0.104156 |
| 14               | 1                | 0              | -6.193535               | -4.271736 | 1.500239  |
| 15               | 1                | 0              | -6.938384               | -3.574323 | 0.045167  |
| 16               | 1                | 0              | -0.795624               | -0.328170 | 0.434287  |
| 17               | 6                | 0              | 2.587328                | -0.800665 | 2.852798  |
| 18               | 6                | 0              | 2.401267                | -1.242331 | 1.538586  |
| 19               | 6                | 0              | 1.279188                | -2.021745 | 1.239977  |
| 20               | 6                | 0              | 0.344827                | -2.362843 | 2.225062  |
| 21               | 6                | 0              | 0.546246                | -1.910921 | 3.534677  |
| 22               | 6                | 0              | 1.663961                | -1.131130 | 3.850445  |
| 23               | 1                | 0              | 3.457318                | -0.194195 | 3.087455  |
| 24               | 1                | 0              | 3.112402                | -0.973441 | 0.766743  |
| 25               | 1                | 0              | -0.522470               | -2.967441 | 1.981309  |
| 26               | 1                | 0              | -0.173018               | -2.174819 | 4.305062  |
| 27               | 1                | 0              | 1.814862                | -0.784074 | 4.868544  |
| 28               | 53               | 0              | 0.936548                | -2.628580 | -0.763605 |
| 29               | 1                | 0              | -0.261933               | 0.940947  | -2.344690 |
| 30               | 6                | 0              | -1.271895               | 1.811013  | -0.564276 |
| 31               | 6                | 0              | -2.375752               | 2.290922  | -1.311275 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 32 | 6  | 0 | -1.015748 | 2.291496  | 0.743671  |
| 33 | 6  | 0 | -3.196822 | 3.264670  | -0.765817 |
| 34 | 1  | 0 | -2.574906 | 1.900763  | -2.303272 |
| 35 | 6  | 0 | -1.840837 | 3.262153  | 1.290676  |
| 36 | 1  | 0 | -0.166692 | 1.915026  | 1.302721  |
| 37 | 6  | 0 | -2.911692 | 3.726332  | 0.523370  |
| 38 | 1  | 0 | -4.038035 | 3.659984  | -1.321214 |
| 39 | 1  | 0 | -1.661486 | 3.652544  | 2.284335  |
| 40 | 8  | 0 | 1.082626  | 0.962135  | -0.718309 |
| 41 | 16 | 0 | 2.113359  | 2.166286  | -1.310970 |
| 42 | 8  | 0 | 1.794828  | 3.398278  | -0.588899 |
| 43 | 8  | 0 | 2.011357  | 2.124153  | -2.770813 |
| 44 | 6  | 0 | 3.616898  | 1.446299  | -0.725166 |
| 45 | 6  | 0 | 4.109532  | 1.835358  | 0.525077  |
| 46 | 6  | 0 | 4.233181  | 0.453432  | -1.492828 |
| 47 | 6  | 0 | 5.251647  | 1.204508  | 1.010018  |
| 48 | 1  | 0 | 3.610516  | 2.605178  | 1.103453  |
| 49 | 6  | 0 | 5.375469  | -0.161631 | -0.983968 |
| 50 | 1  | 0 | 3.829108  | 0.162000  | -2.456432 |
| 51 | 6  | 0 | 5.898653  | 0.198487  | 0.269949  |
| 52 | 1  | 0 | 5.646363  | 1.493358  | 1.980145  |
| 53 | 1  | 0 | 5.864291  | -0.936753 | -1.566911 |
| 54 | 6  | 0 | 7.137989  | -0.463026 | 0.812592  |
| 55 | 1  | 0 | 7.991638  | 0.224172  | 0.757664  |
| 56 | 1  | 0 | 7.008820  | -0.734553 | 1.865877  |
| 57 | 1  | 0 | 7.393048  | -1.363651 | 0.247492  |
| 58 | 7  | 0 | -3.797341 | 4.761553  | 1.110690  |
| 59 | 8  | 0 | -4.777334 | 5.115069  | 0.456443  |
| 60 | 8  | 0 | -3.501678 | 5.205693  | 2.219454  |

---

**Int5 [In electron-withdrawing no Int4 structure]**

---

Zero-point correction= 0.354498 (Hartree/Particle)  
Thermal correction to Energy= 0.383212  
Thermal correction to Enthalpy= 0.384156  
Thermal correction to Gibbs Free Energy= 0.289274  
Sum of electronic and zero-point Energies= -2112.975907  
Sum of electronic and thermal Energies= -2112.947193  
Sum of electronic and thermal Enthalpies= -2112.946249  
Sum of electronic and thermal Free Energies= -2113.041131

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.621162                | 0.048342  | -0.663739 |
| 2                | 6                | 0              | -0.508304               | 0.846220  | -0.059900 |
| 3                | 6                | 0              | 0.413574                | -1.336696 | -0.023874 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 4  | 8  | 0 | -0.637025 | -1.465527 | 0.626486  |
| 5  | 6  | 0 | 1.371130  | -2.390140 | -0.223801 |
| 6  | 6  | 0 | 2.531056  | -2.389692 | -0.986566 |
| 7  | 16 | 0 | 1.123725  | -3.956700 | 0.533958  |
| 8  | 6  | 0 | 3.207852  | -3.628499 | -0.962496 |
| 9  | 1  | 0 | 2.878574  | -1.526024 | -1.540508 |
| 10 | 6  | 0 | 2.578737  | -4.583243 | -0.183564 |
| 11 | 1  | 0 | 4.130834  | -3.827475 | -1.495350 |
| 12 | 6  | 0 | 3.016735  | -5.991558 | 0.064941  |
| 13 | 1  | 0 | 2.265430  | -6.708116 | -0.286216 |
| 14 | 1  | 0 | 3.953616  | -6.185834 | -0.463462 |
| 15 | 1  | 0 | 3.175856  | -6.176589 | 1.133373  |
| 16 | 1  | 0 | 0.461680  | -0.040119 | -1.742879 |
| 17 | 1  | 0 | -0.473404 | 1.096808  | 1.006580  |
| 18 | 6  | 0 | 1.927808  | 0.774678  | -0.377394 |
| 19 | 6  | 0 | 2.447401  | 0.821406  | 0.925462  |
| 20 | 6  | 0 | 2.599878  | 1.421697  | -1.423306 |
| 21 | 6  | 0 | 3.639530  | 1.491533  | 1.182949  |
| 22 | 1  | 0 | 1.930334  | 0.325461  | 1.741647  |
| 23 | 6  | 0 | 3.795366  | 2.093813  | -1.181821 |
| 24 | 1  | 0 | 2.193550  | 1.393034  | -2.429308 |
| 25 | 6  | 0 | 4.295898  | 2.115498  | 0.120581  |
| 26 | 1  | 0 | 4.052774  | 1.527829  | 2.183017  |
| 27 | 1  | 0 | 4.326874  | 2.590367  | -1.983903 |
| 28 | 8  | 0 | -1.429312 | 1.277150  | -0.775909 |
| 29 | 16 | 0 | -2.880226 | 2.380634  | 0.083674  |
| 30 | 8  | 0 | -3.009365 | 3.377498  | -0.960725 |
| 31 | 8  | 0 | -2.292572 | 2.634660  | 1.389744  |
| 32 | 6  | 0 | -4.130920 | 1.176067  | 0.089144  |
| 33 | 6  | 0 | -4.961719 | 1.070259  | -1.037881 |
| 34 | 6  | 0 | -4.235225 | 0.320774  | 1.200839  |
| 35 | 6  | 0 | -5.943884 | 0.088268  | -1.025283 |
| 36 | 1  | 0 | -4.849176 | 1.737210  | -1.885326 |
| 37 | 6  | 0 | -5.226355 | -0.647868 | 1.176036  |
| 38 | 1  | 0 | -3.568121 | 0.414737  | 2.050497  |
| 39 | 6  | 0 | -6.094113 | -0.780038 | 0.072166  |
| 40 | 1  | 0 | -6.606544 | -0.006374 | -1.879584 |
| 41 | 1  | 0 | -5.333437 | -1.317221 | 2.024098  |
| 42 | 6  | 0 | -7.170399 | -1.826820 | 0.087200  |
| 43 | 1  | 0 | -7.644686 | -1.934094 | -0.891167 |
| 44 | 1  | 0 | -6.765505 | -2.796544 | 0.395798  |
| 45 | 1  | 0 | -7.944894 | -1.555454 | 0.815702  |
| 46 | 7  | 0 | 5.557750  | 2.824346  | 0.384265  |
| 47 | 8  | 0 | 6.125874  | 3.373989  | -0.563210 |
| 48 | 8  | 0 | 5.987996  | 2.836107  | 1.540723  |

---

**Product**

---

Zero-point correction= 0.489043 (Hartree/Particle)  
Thermal correction to Energy= 0.528182  
Thermal correction to Enthalpy= 0.529127  
Thermal correction to Gibbs Free Energy= 0.410569  
Sum of electronic and zero-point Energies= -3007.908979  
Sum of electronic and thermal Energies= -3007.869840  
Sum of electronic and thermal Enthalpies= -3007.868895  
Sum of electronic and thermal Free Energies= -3007.987454

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.448619                | 1.378645  | 0.290580  |
| 2                | 1                | 0              | 0.273275                | 1.560632  | 1.351813  |
| 3                | 6                | 0              | -0.711575               | 0.496160  | -0.192742 |
| 4                | 1                | 0              | -0.645559               | 0.250563  | -1.254024 |
| 5                | 6                | 0              | 1.779356                | 0.661841  | 0.129892  |
| 6                | 6                | 0              | 2.361014                | 0.480720  | -1.134904 |
| 7                | 6                | 0              | 2.416262                | 0.135504  | 1.262679  |
| 8                | 6                | 0              | 3.558176                | -0.214694 | -1.270627 |
| 9                | 1                | 0              | 1.874387                | 0.880558  | -2.017707 |
| 10               | 6                | 0              | 3.612418                | -0.565003 | 1.145427  |
| 11               | 1                | 0              | 1.964738                | 0.258995  | 2.241730  |
| 12               | 6                | 0              | 4.167064                | -0.728620 | -0.124668 |
| 13               | 1                | 0              | 4.007521                | -0.364684 | -2.244371 |
| 14               | 1                | 0              | 4.099286                | -0.988417 | 2.014839  |
| 15               | 8                | 0              | -0.701452               | -0.678346 | 0.623490  |
| 16               | 16               | 0              | -0.982180               | -2.192345 | -0.013885 |
| 17               | 8                | 0              | -1.374582               | -2.024513 | -1.415212 |
| 18               | 8                | 0              | -1.876221               | -2.822427 | 0.954737  |
| 19               | 6                | 0              | 0.618022                | -2.963834 | 0.078766  |
| 20               | 6                | 0              | 1.412108                | -3.025046 | -1.066845 |
| 21               | 6                | 0              | 1.032490                | -3.523715 | 1.293019  |
| 22               | 6                | 0              | 2.646713                | -3.670299 | -0.989551 |
| 23               | 1                | 0              | 1.072154                | -2.588916 | -1.999314 |
| 24               | 6                | 0              | 2.270234                | -4.157358 | 1.346439  |
| 25               | 1                | 0              | 0.396675                | -3.473119 | 2.170484  |
| 26               | 6                | 0              | 3.094360                | -4.244339 | 0.209279  |
| 27               | 1                | 0              | 3.270971                | -3.724656 | -1.876500 |
| 28               | 1                | 0              | 2.601708                | -4.597891 | 2.282767  |
| 29               | 6                | 0              | 4.438004                | -4.921978 | 0.293407  |
| 30               | 1                | 0              | 4.355268                | -5.898062 | 0.783711  |
| 31               | 1                | 0              | 4.877388                | -5.066407 | -0.697173 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 32 | 1  | 0 | 5.135376  | -4.317831 | 0.885862  |
| 33 | 8  | 0 | -1.901351 | 1.229838  | 0.088708  |
| 34 | 16 | 0 | -3.229864 | 1.159725  | -0.916021 |
| 35 | 8  | 0 | -2.777804 | 0.876386  | -2.278168 |
| 36 | 8  | 0 | -3.916270 | 2.411557  | -0.596535 |
| 37 | 6  | 0 | -4.154861 | -0.219509 | -0.281972 |
| 38 | 6  | 0 | -4.411876 | -1.309062 | -1.113944 |
| 39 | 6  | 0 | -4.638976 | -0.161502 | 1.030208  |
| 40 | 6  | 0 | -5.173023 | -2.365197 | -0.612388 |
| 41 | 1  | 0 | -4.020011 | -1.335195 | -2.123283 |
| 42 | 6  | 0 | -5.388393 | -1.230383 | 1.510435  |
| 43 | 1  | 0 | -4.435513 | 0.697766  | 1.660941  |
| 44 | 6  | 0 | -5.666674 | -2.346862 | 0.699919  |
| 45 | 1  | 0 | -5.379056 | -3.218402 | -1.252361 |
| 46 | 1  | 0 | -5.766781 | -1.199410 | 2.528429  |
| 47 | 6  | 0 | -6.455147 | -3.507932 | 1.248814  |
| 48 | 1  | 0 | -7.280640 | -3.163956 | 1.880517  |
| 49 | 1  | 0 | -6.863679 | -4.130390 | 0.447599  |
| 50 | 1  | 0 | -5.811485 | -4.143539 | 1.870386  |
| 51 | 6  | 0 | 0.440875  | 2.705053  | -0.489158 |
| 52 | 8  | 0 | 0.225485  | 2.697388  | -1.702598 |
| 53 | 6  | 0 | 0.738161  | 3.926376  | 0.241020  |
| 54 | 6  | 0 | 0.988449  | 4.119037  | 1.589771  |
| 55 | 16 | 0 | 0.829052  | 5.450677  | -0.628211 |
| 56 | 6  | 0 | 1.251540  | 5.470650  | 1.919895  |
| 57 | 1  | 0 | 0.981651  | 3.319414  | 2.321052  |
| 58 | 6  | 0 | 1.202927  | 6.320653  | 0.832810  |
| 59 | 1  | 0 | 1.467915  | 5.818798  | 2.923977  |
| 60 | 6  | 0 | 1.424331  | 7.801116  | 0.819954  |
| 61 | 1  | 0 | 2.262788  | 8.074201  | 0.168897  |
| 62 | 1  | 0 | 0.537878  | 8.334257  | 0.457347  |
| 63 | 1  | 0 | 1.645690  | 8.150080  | 1.832264  |
| 64 | 7  | 0 | 5.406880  | -1.496248 | -0.259370 |
| 65 | 8  | 0 | 5.991317  | -1.851166 | 0.770454  |
| 66 | 8  | 0 | 5.812647  | -1.762726 | -1.395563 |

---

**Transition state and product for  $\alpha$ ,  $\beta$ -ditosyloxy ketone**  
**[Rest all Structures Int1, Int2, Int3 before transition state are the same]**

---

**-OCH<sub>3</sub> (T. S. 1)**

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.608167 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.654769                    |
| Thermal correction to Enthalpy=              | 0.655713                    |
| Thermal correction to Gibbs Free Energy=     | 0.522865                    |
| Sum of electronic and zero-point Energies=   | -3160.775859                |
| Sum of electronic and thermal Energies=      | -3160.729256                |
| Sum of electronic and thermal Enthalpies=    | -3160.728312                |
| Sum of electronic and thermal Free Energies= | -3160.861160                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.126629                | 0.351882  | -0.716469 |
| 2                | 6                | 0              | 1.053970                | 1.528797  | -0.873712 |
| 3                | 6                | 0              | -1.043330               | 0.170699  | -1.647488 |
| 4                | 8                | 0              | -1.152286               | 0.915862  | -2.625942 |
| 5                | 6                | 0              | -1.941877               | -0.934451 | -1.372934 |
| 6                | 6                | 0              | -1.927936               | -1.848007 | -0.330347 |
| 7                | 16               | 0              | -3.223305               | -1.307347 | -2.510595 |
| 8                | 6                | 0              | -2.928939               | -2.838133 | -0.449849 |
| 9                | 1                | 0              | -1.236511               | -1.800014 | 0.499530  |
| 10               | 6                | 0              | -3.721594               | -2.684766 | -1.570049 |
| 11               | 1                | 0              | -3.086692               | -3.629738 | 0.273565  |
| 12               | 6                | 0              | -4.901888               | -3.512470 | -1.969055 |
| 13               | 1                | 0              | -4.815395               | -3.876371 | -2.999079 |
| 14               | 1                | 0              | -4.989925               | -4.374311 | -1.301911 |
| 15               | 1                | 0              | -5.828625               | -2.930428 | -1.900287 |
| 16               | 1                | 0              | 0.212525                | -0.238981 | 0.180757  |
| 17               | 6                | 0              | 1.806186                | -3.025247 | 2.265030  |
| 18               | 6                | 0              | 1.980823                | -2.278933 | 1.095779  |
| 19               | 6                | 0              | 1.450615                | -2.775764 | -0.099204 |
| 20               | 6                | 0              | 0.764538                | -3.992651 | -0.158102 |
| 21               | 6                | 0              | 0.609228                | -4.728375 | 1.021383  |
| 22               | 6                | 0              | 1.124058                | -4.246386 | 2.229489  |
| 23               | 1                | 0              | 2.208216                | -2.646229 | 3.199998  |
| 24               | 1                | 0              | 2.509906                | -1.333508 | 1.120018  |
| 25               | 1                | 0              | 0.350855                | -4.355604 | -1.092525 |
| 26               | 1                | 0              | 0.076065                | -5.674200 | 0.991142  |
| 27               | 1                | 0              | 0.992589                | -4.820329 | 3.142108  |
| 28               | 53               | 0              | 1.652412                | -1.618056 | -1.853905 |
| 29               | 1                | 0              | 1.452620                | 1.511239  | -1.892515 |
| 30               | 6                | 0              | 0.447124                | 2.899324  | -0.627646 |
| 31               | 6                | 0              | 0.028059                | 3.675445  | -1.716876 |
| 32               | 6                | 0              | 0.339597                | 3.418708  | 0.663514  |
| 33               | 6                | 0              | -0.499414               | 4.945588  | -1.515531 |
| 34               | 1                | 0              | 0.103893                | 3.279431  | -2.724303 |
| 35               | 6                | 0              | -0.172940               | 4.697994  | 0.879849  |
| 36               | 1                | 0              | 0.656519                | 2.824047  | 1.511177  |
| 37               | 6                | 0              | -0.606606               | 5.463338  | -0.213492 |
| 38               | 1                | 0              | -0.829834               | 5.552524  | -2.352886 |
| 39               | 1                | 0              | -0.248124               | 5.072297  | 1.893350  |
| 40               | 8                | 0              | -1.134768               | 6.715536  | -0.114758 |
| 41               | 6                | 0              | -1.320677               | 7.279941  | 1.188202  |
| 42               | 1                | 0              | -0.362576               | 7.405706  | 1.707313  |
| 43               | 1                | 0              | -1.774844               | 8.258639  | 1.023687  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 44 | 1  | 0 | -1.993098 | 6.661928  | 1.794970  |
| 45 | 8  | 0 | 2.121498  | 1.244241  | 0.077858  |
| 46 | 16 | 0 | 3.654161  | 1.765470  | -0.244826 |
| 47 | 8  | 0 | 3.896342  | 2.984132  | 0.530486  |
| 48 | 8  | 0 | 3.832655  | 1.783277  | -1.702815 |
| 49 | 6  | 0 | 4.530014  | 0.400312  | 0.481208  |
| 50 | 6  | 0 | 4.679498  | 0.356880  | 1.871076  |
| 51 | 6  | 0 | 4.999119  | -0.625027 | -0.342654 |
| 52 | 6  | 0 | 5.301043  | -0.753137 | 2.439905  |
| 53 | 1  | 0 | 4.314902  | 1.168155  | 2.492545  |
| 54 | 6  | 0 | 5.623932  | -1.722549 | 0.248927  |
| 55 | 1  | 0 | 4.876525  | -0.566756 | -1.417858 |
| 56 | 6  | 0 | 5.774597  | -1.810178 | 1.642690  |
| 57 | 1  | 0 | 5.420779  | -0.799730 | 3.518825  |
| 58 | 1  | 0 | 5.995131  | -2.525218 | -0.382263 |
| 59 | 6  | 0 | 6.398268  | -3.027206 | 2.275756  |
| 60 | 1  | 0 | 5.618355  | -3.748112 | 2.554403  |
| 61 | 1  | 0 | 7.083373  | -3.530855 | 1.587382  |
| 62 | 1  | 0 | 6.945053  | -2.767398 | 3.187542  |
| 63 | 16 | 0 | -2.620929 | 1.609460  | 1.300355  |
| 64 | 8  | 0 | -3.034230 | 2.388503  | 0.106965  |
| 65 | 8  | 0 | -2.688617 | 2.343449  | 2.596986  |
| 66 | 8  | 0 | -1.262600 | 0.947112  | 1.136833  |
| 67 | 6  | 0 | -3.802609 | 0.247948  | 1.444681  |
| 68 | 6  | 0 | -4.831215 | 0.117738  | 0.513829  |
| 69 | 6  | 0 | -5.740196 | -0.938811 | 0.634292  |
| 70 | 6  | 0 | -5.636860 | -1.870017 | 1.675293  |
| 71 | 6  | 0 | -4.596129 | -1.711821 | 2.609210  |
| 72 | 6  | 0 | -3.684493 | -0.663046 | 2.501368  |
| 73 | 1  | 0 | -4.910876 | 0.827943  | -0.301704 |
| 74 | 1  | 0 | -6.533405 | -1.042968 | -0.101724 |
| 75 | 1  | 0 | -4.499316 | -2.421999 | 3.427538  |
| 76 | 1  | 0 | -2.885310 | -0.555711 | 3.228798  |
| 77 | 6  | 0 | -6.592439 | -3.033505 | 1.784523  |
| 78 | 1  | 0 | -7.394754 | -2.963789 | 1.043933  |
| 79 | 1  | 0 | -6.068788 | -3.984870 | 1.625820  |
| 80 | 1  | 0 | -7.048770 | -3.080735 | 2.780186  |

---

### Product

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.519322 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.558376                    |
| Thermal correction to Enthalpy=              | 0.559320                    |
| Thermal correction to Gibbs Free Energy=     | 0.441800                    |
| Sum of electronic and zero-point Energies=   | -2917.877692                |
| Sum of electronic and thermal Energies=      | -2917.838638                |
| Sum of electronic and thermal Enthalpies=    | -2917.837693                |
| Sum of electronic and thermal Free Energies= | -2917.955214                |

---

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.068929               | -0.199116 | 0.756802  |
| 2                | 6                | 0              | -1.365966               | 0.583140  | 1.011464  |
| 3                | 6                | 0              | 1.029625                | 0.032484  | 1.815590  |
| 4                | 8                | 0              | 0.844367                | 0.803569  | 2.753873  |
| 5                | 6                | 0              | 2.217274                | -0.799263 | 1.687389  |
| 6                | 6                | 0              | 2.422005                | -1.896596 | 0.869141  |
| 7                | 16               | 0              | 3.614036                | -0.516902 | 2.710376  |
| 8                | 6                | 0              | 3.684836                | -2.505428 | 1.063049  |
| 9                | 1                | 0              | 1.691209                | -2.251277 | 0.154807  |
| 10               | 6                | 0              | 4.457837                | -1.872594 | 2.015165  |
| 11               | 1                | 0              | 4.029508                | -3.373771 | 0.513058  |
| 12               | 6                | 0              | 5.851579                | -2.219445 | 2.438175  |
| 13               | 1                | 0              | 5.912358                | -2.406608 | 3.516319  |
| 14               | 1                | 0              | 6.182900                | -3.119101 | 1.912098  |
| 15               | 1                | 0              | 6.550420                | -1.407426 | 2.204101  |
| 16               | 1                | 0              | -0.335936               | -1.254588 | 0.844165  |
| 17               | 1                | 0              | -1.602377               | 0.450226  | 2.070806  |
| 18               | 6                | 0              | -1.391875               | 2.045304  | 0.643369  |
| 19               | 6                | 0              | -1.096978               | 3.017980  | 1.611249  |
| 20               | 6                | 0              | -1.690883               | 2.457959  | -0.656182 |
| 21               | 6                | 0              | -1.084815               | 4.367878  | 1.279667  |
| 22               | 1                | 0              | -0.860379               | 2.710817  | 2.624364  |
| 23               | 6                | 0              | -1.687847               | 3.811625  | -1.005113 |
| 24               | 1                | 0              | -1.933202               | 1.720244  | -1.412108 |
| 25               | 6                | 0              | -1.375860               | 4.773113  | -0.034184 |
| 26               | 1                | 0              | -0.854982               | 5.124025  | 2.024436  |
| 27               | 1                | 0              | -1.921338               | 4.095645  | -2.024070 |
| 28               | 8                | 0              | -1.338307               | 6.118325  | -0.263245 |
| 29               | 6                | 0              | -1.621754               | 6.594179  | -1.582614 |
| 30               | 1                | 0              | -2.640187               | 6.327880  | -1.891207 |
| 31               | 1                | 0              | -1.531142               | 7.680679  | -1.531451 |
| 32               | 1                | 0              | -0.900825               | 6.201970  | -2.310399 |
| 33               | 8                | 0              | -2.341482               | -0.176932 | 0.218918  |
| 34               | 16               | 0              | -3.918923               | -0.193213 | 0.674094  |
| 35               | 8                | 0              | -4.644638               | 0.810815  | -0.110934 |
| 36               | 8                | 0              | -3.983926               | -0.142498 | 2.141149  |
| 37               | 6                | 0              | -4.316292               | -1.823105 | 0.082697  |
| 38               | 6                | 0              | -4.464750               | -2.023019 | -1.294247 |
| 39               | 6                | 0              | -4.419986               | -2.875127 | 0.993330  |
| 40               | 6                | 0              | -4.707551               | -3.313343 | -1.758272 |
| 41               | 1                | 0              | -4.387574               | -1.190629 | -1.986171 |
| 42               | 6                | 0              | -4.672257               | -4.158507 | 0.505869  |
| 43               | 1                | 0              | -4.298345               | -2.698304 | 2.055577  |
| 44               | 6                | 0              | -4.809635               | -4.399573 | -0.869673 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 45 | 1  | 0 | -4.820620 | -3.481910 | -2.825868 |
| 46 | 1  | 0 | -4.754097 | -4.984034 | 1.207291  |
| 47 | 6  | 0 | -5.032819 | -5.795227 | -1.393843 |
| 48 | 1  | 0 | -4.086110 | -6.223438 | -1.747967 |
| 49 | 1  | 0 | -5.427211 | -6.457131 | -0.617390 |
| 50 | 1  | 0 | -5.727447 | -5.796028 | -2.240181 |
| 51 | 16 | 0 | 1.382556  | 1.052184  | -1.215690 |
| 52 | 8  | 0 | 1.671038  | 2.033949  | -0.168111 |
| 53 | 8  | 0 | 0.763699  | 1.454809  | -2.479937 |
| 54 | 8  | 0 | 0.368307  | -0.111542 | -0.623564 |
| 55 | 6  | 0 | 2.855885  | 0.115522  | -1.573253 |
| 56 | 6  | 0 | 4.051370  | 0.471506  | -0.948954 |
| 57 | 6  | 0 | 5.202137  | -0.260725 | -1.242777 |
| 58 | 6  | 0 | 5.168022  | -1.341137 | -2.137363 |
| 59 | 6  | 0 | 3.946376  | -1.667191 | -2.753520 |
| 60 | 6  | 0 | 2.787315  | -0.943316 | -2.483521 |
| 61 | 1  | 0 | 4.079428  | 1.292904  | -0.242178 |
| 62 | 1  | 0 | 6.137557  | 0.006664  | -0.759034 |
| 63 | 1  | 0 | 3.903575  | -2.497255 | -3.453669 |
| 64 | 1  | 0 | 1.849985  | -1.204042 | -2.963896 |
| 65 | 6  | 0 | 6.403995  | -2.162637 | -2.402357 |
| 66 | 1  | 0 | 7.315121  | -1.576834 | -2.247292 |
| 67 | 1  | 0 | 6.443012  | -3.021119 | -1.718763 |
| 68 | 1  | 0 | 6.411168  | -2.556670 | -3.423543 |

---

**Transition state and product for  $\alpha$ ,  $\beta$ -ditosyloxy ketone  
-SCH<sub>3</sub> Group (T. S. 1)**

---

Zero-point correction= 0.603662 (Hartree/Particle)  
Thermal correction to Energy= 0.651309  
Thermal correction to Enthalpy= 0.652254  
Thermal correction to Gibbs Free Energy= 0.515419  
Sum of electronic and zero-point Energies= -3483.756576  
Sum of electronic and thermal Energies= -3483.708928  
Sum of electronic and thermal Enthalpies= -3483.707984  
Sum of electronic and thermal Free Energies= -3483.844818  
Input orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.103854                | 0.346219  | -0.670619 |
| 2                | 6                | 0              | 0.951637                | 1.588060  | -0.802697 |
| 3                | 6                | 0              | -1.034427               | 0.106044  | -1.628285 |
| 4                | 8                | 0              | -1.151540               | 0.844376  | -2.610832 |
| 5                | 6                | 0              | -1.892892               | -1.034840 | -1.375213 |
| 6                | 6                | 0              | -1.857720               | -1.960986 | -0.345217 |
| 7                | 16               | 0              | -3.155296               | -1.430704 | -2.526460 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 8  | 6  | 0 | -2.824140 | -2.982725 | -0.487018 |
| 9  | 1  | 0 | -1.172896 | -1.902117 | 0.489401  |
| 10 | 6  | 0 | -3.613195 | -2.839148 | -1.611046 |
| 11 | 1  | 0 | -2.960030 | -3.790070 | 0.223346  |
| 12 | 6  | 0 | -4.755329 | -3.705301 | -2.039335 |
| 13 | 1  | 0 | -4.620239 | -4.078944 | -3.060821 |
| 14 | 1  | 0 | -4.841585 | -4.561716 | -1.364948 |
| 15 | 1  | 0 | -5.701101 | -3.151128 | -2.013133 |
| 16 | 1  | 0 | 0.229836  | -0.259739 | 0.211452  |
| 17 | 6  | 0 | 2.029483  | -3.134411 | 2.191428  |
| 18 | 6  | 0 | 2.167749  | -2.308999 | 1.071277  |
| 19 | 6  | 0 | 1.627297  | -2.738676 | -0.144682 |
| 20 | 6  | 0 | 0.962216  | -3.962424 | -0.271392 |
| 21 | 6  | 0 | 0.842381  | -4.776764 | 0.859358  |
| 22 | 6  | 0 | 1.370739  | -4.364429 | 2.087347  |
| 23 | 1  | 0 | 2.441020  | -2.809454 | 3.142541  |
| 24 | 1  | 0 | 2.679972  | -1.357361 | 1.150505  |
| 25 | 1  | 0 | 0.538400  | -4.270888 | -1.220744 |
| 26 | 1  | 0 | 0.327346  | -5.729396 | 0.775785  |
| 27 | 1  | 0 | 1.268647  | -5.000038 | 2.962061  |
| 28 | 53 | 0 | 1.773910  | -1.472637 | -1.826294 |
| 29 | 1  | 0 | 1.356559  | 1.613353  | -1.818992 |
| 30 | 6  | 0 | 0.259690  | 2.916624  | -0.545571 |
| 31 | 6  | 0 | -0.192318 | 3.680706  | -1.627620 |
| 32 | 6  | 0 | 0.107094  | 3.410135  | 0.751504  |
| 33 | 6  | 0 | -0.807039 | 4.911385  | -1.413975 |
| 34 | 1  | 0 | -0.080420 | 3.306156  | -2.639842 |
| 35 | 6  | 0 | -0.495989 | 4.646768  | 0.974539  |
| 36 | 1  | 0 | 0.452479  | 2.826501  | 1.595614  |
| 37 | 6  | 0 | -0.970846 | 5.405775  | -0.106770 |
| 38 | 1  | 0 | -1.161514 | 5.485391  | -2.266090 |
| 39 | 1  | 0 | -0.604048 | 4.995240  | 1.994540  |
| 40 | 8  | 0 | 2.029899  | 1.365304  | 0.150710  |
| 41 | 16 | 0 | 3.532139  | 1.969221  | -0.171984 |
| 42 | 8  | 0 | 3.707640  | 3.191753  | 0.614795  |
| 43 | 8  | 0 | 3.704967  | 2.011235  | -1.630092 |
| 44 | 6  | 0 | 4.483696  | 0.645304  | 0.535499  |
| 45 | 6  | 0 | 4.599601  | 0.566546  | 1.926931  |
| 46 | 6  | 0 | 5.048853  | -0.314757 | -0.306658 |
| 47 | 6  | 0 | 5.283188  | -0.515638 | 2.478006  |
| 48 | 1  | 0 | 4.161453  | 1.328175  | 2.563677  |
| 49 | 6  | 0 | 5.735443  | -1.384228 | 0.267861  |
| 50 | 1  | 0 | 4.951997  | -0.229151 | -1.382665 |
| 51 | 6  | 0 | 5.852703  | -1.508970 | 1.661902  |
| 52 | 1  | 0 | 5.376073  | -0.590656 | 3.557960  |
| 53 | 1  | 0 | 6.181131  | -2.136007 | -0.377611 |
| 54 | 6  | 0 | 6.542699  | -2.701015 | 2.273464  |
| 55 | 1  | 0 | 5.811227  | -3.492241 | 2.484494  |
| 56 | 1  | 0 | 7.294594  | -3.119158 | 1.597516  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 57 | 1  | 0 | 7.027157  | -2.441038 | 3.219682  |
| 58 | 16 | 0 | -2.706192 | 1.427472  | 1.286837  |
| 59 | 8  | 0 | -3.169067 | 2.137061  | 0.069654  |
| 60 | 8  | 0 | -2.815888 | 2.196238  | 2.559430  |
| 61 | 8  | 0 | -1.306531 | 0.847052  | 1.139869  |
| 62 | 6  | 0 | -3.794319 | -0.002180 | 1.485932  |
| 63 | 6  | 0 | -4.872492 | -0.185715 | 0.621844  |
| 64 | 6  | 0 | -5.720146 | -1.283713 | 0.802227  |
| 65 | 6  | 0 | -5.504921 | -2.204982 | 1.835949  |
| 66 | 6  | 0 | -4.414404 | -1.994328 | 2.699369  |
| 67 | 6  | 0 | -3.563607 | -0.902742 | 2.532169  |
| 68 | 1  | 0 | -5.039662 | 0.518159  | -0.185986 |
| 69 | 1  | 0 | -6.556595 | -1.426063 | 0.122501  |
| 70 | 1  | 0 | -4.232384 | -2.694848 | 3.511275  |
| 71 | 1  | 0 | -2.726423 | -0.753257 | 3.207490  |
| 72 | 6  | 0 | -6.392582 | -3.414439 | 2.002410  |
| 73 | 1  | 0 | -7.342949 | -3.290480 | 1.474141  |
| 74 | 1  | 0 | -5.904055 | -4.311954 | 1.600432  |
| 75 | 1  | 0 | -6.608132 | -3.609367 | 3.058617  |
| 76 | 16 | 0 | -1.768659 | 6.990469  | 0.062481  |
| 77 | 6  | 0 | -1.970596 | 7.182424  | 1.865570  |
| 78 | 1  | 0 | -2.559228 | 6.362100  | 2.284603  |
| 79 | 1  | 0 | -1.005469 | 7.256682  | 2.373610  |
| 80 | 1  | 0 | -2.516178 | 8.120086  | 2.002252  |

---

**Product**

---

Zero-point correction= 0.516022 (Hartree/Particle)  
Thermal correction to Energy= 0.554808  
Thermal correction to Enthalpy= 0.555752  
Thermal correction to Gibbs Free Energy= 0.440966  
Sum of electronic and zero-point Energies= -3240.864510  
Sum of electronic and thermal Energies= -3240.825725  
Sum of electronic and thermal Enthalpies= -3240.824781  
Sum of electronic and thermal Free Energies= -3240.939566

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -0.149952               | -0.673145 | -0.067247 |
| 2                | 6                | 0              | -1.516297               | -1.343057 | 0.177046  |
| 3                | 6                | 0              | 0.596345                | -0.312670 | 1.238978  |
| 4                | 8                | 0              | 0.069422                | -0.496714 | 2.333476  |
| 5                | 6                | 0              | 1.970628                | 0.137209  | 1.083518  |
| 6                | 6                | 0              | 2.761320                | 0.143832  | -0.052836 |
| 7                | 16               | 0              | 2.875647                | 0.710671  | 2.472370  |
| 8                | 6                | 0              | 4.077194                | 0.603824  | 0.188319  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 9  | 1  | 0 | 2.404532  | -0.165065 | -1.027563 |
| 10 | 6  | 0 | 4.300032  | 0.961541  | 1.502947  |
| 11 | 1  | 0 | 4.839882  | 0.689087  | -0.577583 |
| 12 | 6  | 0 | 5.554896  | 1.522798  | 2.094947  |
| 13 | 1  | 0 | 5.908441  | 0.921237  | 2.939802  |
| 14 | 1  | 0 | 6.340809  | 1.547684  | 1.335110  |
| 15 | 1  | 0 | 5.397577  | 2.544628  | 2.460052  |
| 16 | 1  | 0 | 0.476213  | -1.417630 | -0.565135 |
| 17 | 1  | 0 | -1.404682 | -1.978899 | 1.057628  |
| 18 | 6  | 0 | -2.704652 | -0.438612 | 0.373164  |
| 19 | 6  | 0 | -3.093286 | -0.075754 | 1.669969  |
| 20 | 6  | 0 | -3.417800 | 0.072122  | -0.713489 |
| 21 | 6  | 0 | -4.162423 | 0.789892  | 1.873766  |
| 22 | 1  | 0 | -2.539813 | -0.456451 | 2.522129  |
| 23 | 6  | 0 | -4.496252 | 0.938370  | -0.519437 |
| 24 | 1  | 0 | -3.135162 | -0.201110 | -1.724031 |
| 25 | 6  | 0 | -4.873939 | 1.312977  | 0.777603  |
| 26 | 1  | 0 | -4.441704 | 1.062819  | 2.888106  |
| 27 | 1  | 0 | -5.021313 | 1.318327  | -1.387627 |
| 28 | 6  | 0 | -6.827171 | 2.930454  | -0.499601 |
| 29 | 1  | 0 | -7.222357 | 2.080306  | -1.061712 |
| 30 | 1  | 0 | -7.638988 | 3.637413  | -0.308777 |
| 31 | 1  | 0 | -6.043929 | 3.434154  | -1.072215 |
| 32 | 8  | 0 | -1.766931 | -2.190501 | -1.000721 |
| 33 | 16 | 0 | -1.590572 | -3.812903 | -0.827167 |
| 34 | 8  | 0 | -1.945523 | -4.333981 | -2.147277 |
| 35 | 8  | 0 | -2.324062 | -4.241178 | 0.368892  |
| 36 | 6  | 0 | 0.157977  | -3.998185 | -0.535102 |
| 37 | 6  | 0 | 1.035776  | -3.937341 | -1.622716 |
| 38 | 6  | 0 | 0.626180  | -4.087109 | 0.778715  |
| 39 | 6  | 0 | 2.407114  | -3.960492 | -1.377568 |
| 40 | 1  | 0 | 0.654170  | -3.869905 | -2.636176 |
| 41 | 6  | 0 | 2.003018  | -4.105744 | 1.000360  |
| 42 | 1  | 0 | -0.068466 | -4.135623 | 1.610163  |
| 43 | 6  | 0 | 2.912218  | -4.033925 | -0.067068 |
| 44 | 1  | 0 | 3.096831  | -3.918704 | -2.216068 |
| 45 | 1  | 0 | 2.374083  | -4.171288 | 2.019194  |
| 46 | 6  | 0 | 4.396939  | -4.000838 | 0.187702  |
| 47 | 1  | 0 | 4.738506  | -2.963228 | 0.296064  |
| 48 | 1  | 0 | 4.655998  | -4.529764 | 1.109698  |
| 49 | 1  | 0 | 4.954864  | -4.446736 | -0.641201 |
| 50 | 16 | 0 | -0.518409 | 1.975097  | -0.728670 |
| 51 | 8  | 0 | -0.895886 | 2.111008  | 0.679058  |
| 52 | 8  | 0 | -1.423270 | 2.385375  | -1.802361 |
| 53 | 8  | 0 | -0.203068 | 0.379658  | -1.063426 |
| 54 | 6  | 0 | 1.069790  | 2.742776  | -0.990470 |
| 55 | 6  | 0 | 1.693314  | 3.387282  | 0.079187  |
| 56 | 6  | 0 | 2.935588  | 3.982582  | -0.132311 |
| 57 | 6  | 0 | 3.562101  | 3.933617  | -1.387572 |

|    |    |   |           |          |           |
|----|----|---|-----------|----------|-----------|
| 58 | 6  | 0 | 2.899449  | 3.287582 | -2.445111 |
| 59 | 6  | 0 | 1.651854  | 2.694124 | -2.259359 |
| 60 | 1  | 0 | 1.223249  | 3.413200 | 1.055322  |
| 61 | 1  | 0 | 3.430025  | 4.483389 | 0.695449  |
| 62 | 1  | 0 | 3.364708  | 3.249115 | -3.426133 |
| 63 | 1  | 0 | 1.148787  | 2.198497 | -3.083315 |
| 64 | 6  | 0 | 4.934079  | 4.527638 | -1.578768 |
| 65 | 1  | 0 | 5.045881  | 5.460027 | -1.016259 |
| 66 | 1  | 0 | 5.701423  | 3.832620 | -1.213403 |
| 67 | 1  | 0 | 5.142446  | 4.728785 | -2.633512 |
| 68 | 16 | 0 | -6.222396 | 2.422966 | 1.145683  |

---

**Transition state and product for  $\alpha$ ,  $\beta$ -ditosyloxy ketone  
Chloride Group (T.S.1)**

---

Zero-point correction= 0.565231 (Hartree/Particle)  
Thermal correction to Energy= 0.610845  
Thermal correction to Enthalpy= 0.611789  
Thermal correction to Gibbs Free Energy= 0.478119  
Sum of electronic and zero-point Energies= -3505.879578  
Sum of electronic and thermal Energies= -3505.833964  
Sum of electronic and thermal Enthalpies= -3505.833020  
Sum of electronic and thermal Free Energies= -3505.966689

---

Input orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.131769                | 0.303663  | -0.671734 |
| 2                | 6                | 0              | 0.957967                | 1.561377  | -0.815504 |
| 3                | 6                | 0              | -1.005256               | 0.039521  | -1.624636 |
| 4                | 8                | 0              | -1.116699               | 0.751625  | -2.626768 |
| 5                | 6                | 0              | -1.864543               | -1.093923 | -1.345347 |
| 6                | 6                | 0              | -1.844523               | -1.982231 | -0.282240 |
| 7                | 16               | 0              | -3.109541               | -1.532383 | -2.500210 |
| 8                | 6                | 0              | -2.809421               | -3.008303 | -0.400658 |
| 9                | 1                | 0              | -1.172783               | -1.892310 | 0.560354  |
| 10               | 6                | 0              | -3.581636               | -2.906087 | -1.540683 |
| 11               | 1                | 0              | -2.956444               | -3.789185 | 0.336615  |
| 12               | 6                | 0              | -4.719855               | -3.785790 | -1.951222 |
| 13               | 1                | 0              | -4.582196               | -4.182975 | -2.963382 |
| 14               | 1                | 0              | -4.805399               | -4.626028 | -1.256688 |
| 15               | 1                | 0              | -5.666939               | -3.233318 | -1.939026 |
| 16               | 1                | 0              | 0.255156                | -0.275293 | 0.228598  |
| 17               | 6                | 0              | 2.084214                | -3.154920 | 2.227049  |
| 18               | 6                | 0              | 2.216149                | -2.330992 | 1.105162  |
| 19               | 6                | 0              | 1.654020                | -2.755252 | -0.102853 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 20 | 6  | 0 | 0.974181  | -3.971620 | -0.221249 |
| 21 | 6  | 0 | 0.861379  | -4.784583 | 0.911217  |
| 22 | 6  | 0 | 1.411008  | -4.377828 | 2.131689  |
| 23 | 1  | 0 | 2.511975  | -2.834501 | 3.172513  |
| 24 | 1  | 0 | 2.739471  | -1.384937 | 1.177189  |
| 25 | 1  | 0 | 0.534159  | -4.275198 | -1.164737 |
| 26 | 1  | 0 | 0.335067  | -5.731612 | 0.835052  |
| 27 | 1  | 0 | 1.314220  | -5.012434 | 3.007721  |
| 28 | 53 | 0 | 1.794201  | -1.491995 | -1.787242 |
| 29 | 1  | 0 | 1.377628  | 1.577522  | -1.826043 |
| 30 | 6  | 0 | 0.243401  | 2.889007  | -0.593018 |
| 31 | 6  | 0 | -0.266854 | 3.586677  | -1.690981 |
| 32 | 6  | 0 | 0.150264  | 3.442560  | 0.686816  |
| 33 | 6  | 0 | -0.878406 | 4.829762  | -1.518546 |
| 34 | 1  | 0 | -0.199138 | 3.159252  | -2.685323 |
| 35 | 6  | 0 | -0.451073 | 4.685860  | 0.875079  |
| 36 | 1  | 0 | 0.542416  | 2.904957  | 1.540597  |
| 37 | 6  | 0 | -0.962335 | 5.362223  | -0.232748 |
| 38 | 1  | 0 | -1.277320 | 5.371030  | -2.369659 |
| 39 | 1  | 0 | -0.531277 | 5.112356  | 1.868909  |
| 40 | 8  | 0 | 2.024754  | 1.378204  | 0.154327  |
| 41 | 16 | 0 | 3.526880  | 1.990361  | -0.164402 |
| 42 | 8  | 0 | 3.681488  | 3.225925  | 0.605658  |
| 43 | 8  | 0 | 3.710826  | 2.011925  | -1.621300 |
| 44 | 6  | 0 | 4.483383  | 0.686582  | 0.571485  |
| 45 | 6  | 0 | 4.590551  | 0.632955  | 1.964827  |
| 46 | 6  | 0 | 5.062760  | -0.282142 | -0.250951 |
| 47 | 6  | 0 | 5.282051  | -0.432349 | 2.538402  |
| 48 | 1  | 0 | 4.140708  | 1.400786  | 2.585705  |
| 49 | 6  | 0 | 5.756930  | -1.334137 | 0.346193  |
| 50 | 1  | 0 | 4.971455  | -0.215991 | -1.328879 |
| 51 | 6  | 0 | 5.867608  | -1.433056 | 1.742852  |
| 52 | 1  | 0 | 5.369126  | -0.487674 | 3.620007  |
| 53 | 1  | 0 | 6.214561  | -2.092236 | -0.283305 |
| 54 | 6  | 0 | 6.568610  | -2.605533 | 2.379145  |
| 55 | 1  | 0 | 5.844564  | -3.398528 | 2.608284  |
| 56 | 1  | 0 | 7.323681  | -3.031316 | 1.711619  |
| 57 | 1  | 0 | 7.051493  | -2.320911 | 3.319076  |
| 58 | 16 | 0 | -2.677410 | 1.478757  | 1.198062  |
| 59 | 8  | 0 | -3.073259 | 2.162435  | -0.056697 |
| 60 | 8  | 0 | -2.812905 | 2.286569  | 2.443072  |
| 61 | 8  | 0 | -1.287067 | 0.862351  | 1.117110  |
| 62 | 6  | 0 | -3.808991 | 0.083089  | 1.395133  |
| 63 | 6  | 0 | -4.841169 | -0.112252 | 0.479474  |
| 64 | 6  | 0 | -5.720311 | -1.186634 | 0.651841  |
| 65 | 6  | 0 | -5.582805 | -2.071537 | 1.729108  |
| 66 | 6  | 0 | -4.538571 | -1.848112 | 2.645424  |
| 67 | 6  | 0 | -3.656586 | -0.780661 | 2.486181  |
| 68 | 1  | 0 | -4.947857 | 0.563128  | -0.362114 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 69 | 1  | 0 | -6.518881 | -1.340127 | -0.069648 |
| 70 | 1  | 0 | -4.416937 | -2.521067 | 3.491276  |
| 71 | 1  | 0 | -2.854530 | -0.622324 | 3.200992  |
| 72 | 6  | 0 | -6.503866 | -3.256259 | 1.892113  |
| 73 | 1  | 0 | -7.370183 | -3.185445 | 1.227356  |
| 74 | 1  | 0 | -5.978435 | -4.191343 | 1.657974  |
| 75 | 1  | 0 | -6.867072 | -3.340077 | 2.922615  |
| 76 | 17 | 0 | -1.729228 | 6.937332  | -0.001116 |

---

**Product**

---

|                                              |                             |
|----------------------------------------------|-----------------------------|
| Zero-point correction=                       | 0.477251 (Hartree/Particle) |
| Thermal correction to Energy=                | 0.514864                    |
| Thermal correction to Enthalpy=              | 0.515808                    |
| Thermal correction to Gibbs Free Energy=     | 0.402175                    |
| Sum of electronic and zero-point Energies=   | -3262.988915                |
| Sum of electronic and thermal Energies=      | -3262.951302                |
| Sum of electronic and thermal Enthalpies=    | -3262.950358                |
| Sum of electronic and thermal Free Energies= | -3263.063990                |

---

Standard orientation:

---

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.574216                | -1.286906 | 0.062128  |
| 2                | 6                | 0              | -0.927590               | -1.311404 | 0.384168  |
| 3                | 6                | 0              | 1.463874                | -1.172127 | 1.323212  |
| 4                | 8                | 0              | 0.955530                | -1.080518 | 2.437726  |
| 5                | 6                | 0              | 2.898187                | -1.276002 | 1.106966  |
| 6                | 6                | 0              | 3.579021                | -1.671693 | -0.031459 |
| 7                | 16               | 0              | 4.018133                | -0.941651 | 2.415182  |
| 8                | 6                | 0              | 4.982538                | -1.706172 | 0.144058  |
| 9                | 1                | 0              | 3.084935                | -1.918937 | -0.963001 |
| 10               | 6                | 0              | 5.385535                | -1.326976 | 1.408580  |
| 11               | 1                | 0              | 5.684250                | -1.983770 | -0.634317 |
| 12               | 6                | 0              | 6.785864                | -1.206933 | 1.923063  |
| 13               | 1                | 0              | 6.936432                | -1.802835 | 2.830122  |
| 14               | 1                | 0              | 7.489199                | -1.553813 | 1.161226  |
| 15               | 1                | 0              | 7.029207                | -0.166163 | 2.167521  |
| 16               | 1                | 0              | 0.801384                | -2.258858 | -0.387999 |
| 17               | 1                | 0              | -1.043541               | -2.002102 | 1.222749  |
| 18               | 6                | 0              | -1.605163               | 0.002346  | 0.698390  |
| 19               | 6                | 0              | -1.832661               | 0.366362  | 2.029599  |
| 20               | 6                | 0              | -2.050531               | 0.840864  | -0.328376 |
| 21               | 6                | 0              | -2.494270               | 1.555056  | 2.339972  |
| 22               | 1                | 0              | -1.489553               | -0.278958 | 2.830760  |
| 23               | 6                | 0              | -2.715937               | 2.030854  | -0.037461 |
| 24               | 1                | 0              | -1.895434               | 0.561440  | -1.363111 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 25 | 6  | 0 | -2.931438 | 2.371090  | 1.296953  |
| 26 | 1  | 0 | -2.675354 | 1.833055  | 3.372563  |
| 27 | 1  | 0 | -3.067182 | 2.674886  | -0.836060 |
| 28 | 8  | 0 | -1.519890 | -1.926568 | -0.809018 |
| 29 | 16 | 0 | -2.904165 | -2.806696 | -0.659957 |
| 30 | 8  | 0 | -2.882613 | -3.482383 | 0.643278  |
| 31 | 8  | 0 | -2.935018 | -3.580050 | -1.902499 |
| 32 | 6  | 0 | -4.205481 | -1.593334 | -0.678057 |
| 33 | 6  | 0 | -4.752400 | -1.158582 | 0.531598  |
| 34 | 6  | 0 | -4.597849 | -1.044409 | -1.901192 |
| 35 | 6  | 0 | -5.703998 | -0.141798 | 0.507055  |
| 36 | 1  | 0 | -4.430345 | -1.595151 | 1.469924  |
| 37 | 6  | 0 | -5.552747 | -0.029116 | -1.901993 |
| 38 | 1  | 0 | -4.163438 | -1.397845 | -2.830237 |
| 39 | 6  | 0 | -6.111043 | 0.444618  | -0.702983 |
| 40 | 1  | 0 | -6.128256 | 0.209954  | 1.443178  |
| 41 | 1  | 0 | -5.864138 | 0.405671  | -2.847618 |
| 42 | 6  | 0 | -7.095027 | 1.585767  | -0.705592 |
| 43 | 1  | 0 | -6.576712 | 2.529271  | -0.491040 |
| 44 | 1  | 0 | -7.587748 | 1.690521  | -1.676519 |
| 45 | 1  | 0 | -7.861883 | 1.453711  | 0.064292  |
| 46 | 16 | 0 | 1.275240  | 1.237382  | -0.794549 |
| 47 | 8  | 0 | 1.075381  | 1.595207  | 0.611105  |
| 48 | 8  | 0 | 0.531344  | 1.911736  | -1.859425 |
| 49 | 8  | 0 | 0.908433  | -0.367818 | -1.011102 |
| 50 | 6  | 0 | 3.014288  | 1.298926  | -1.178790 |
| 51 | 6  | 0 | 3.903164  | 1.743212  | -0.199625 |
| 52 | 6  | 0 | 5.260663  | 1.811648  | -0.511516 |
| 53 | 6  | 0 | 5.736072  | 1.434566  | -1.776561 |
| 54 | 6  | 0 | 4.809888  | 1.000071  | -2.741543 |
| 55 | 6  | 0 | 3.448174  | 0.934055  | -2.456405 |
| 56 | 1  | 0 | 3.543621  | 2.020727  | 0.784347  |
| 57 | 1  | 0 | 5.960284  | 2.156051  | 0.244776  |
| 58 | 1  | 0 | 5.159930  | 0.712301  | -3.729079 |
| 59 | 1  | 0 | 2.742197  | 0.599828  | -3.209618 |
| 60 | 6  | 0 | 7.211616  | 1.454959  | -2.083312 |
| 61 | 1  | 0 | 7.736249  | 2.200316  | -1.478092 |
| 62 | 1  | 0 | 7.657968  | 0.476610  | -1.861976 |
| 63 | 1  | 0 | 7.397763  | 1.668669  | -3.140277 |
| 64 | 17 | 0 | -3.799664 | 3.864139  | 1.675347  |

---

**Transition state and product for  $\alpha$ ,  $\beta$ -ditosyloxy ketone**  
**T.S. 1 (Nitro group)**

---

Zero-point correction= 0.578137 (Hartree/Particle)  
Thermal correction to Energy= 0.624749  
Thermal correction to Enthalpy= 0.625693  
Thermal correction to Gibbs Free Energy= 0.492090

Sum of electronic and zero-point Energies= -3250.785765  
Sum of electronic and thermal Energies= -3250.739153  
Sum of electronic and thermal Enthalpies= -3250.738209  
Sum of electronic and thermal Free Energies= -3250.871812

-----  
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.156510                | 0.194052  | -0.676414 |
| 2                | 6                | 0              | 0.852848                | 1.533023  | -0.797784 |
| 3                | 6                | 0              | -0.977712               | -0.170632 | -1.599102 |
| 4                | 8                | 0              | -1.187078               | 0.527301  | -2.595681 |
| 5                | 6                | 0              | -1.717684               | -1.379550 | -1.292251 |
| 6                | 6                | 0              | -1.601126               | -2.239694 | -0.211485 |
| 7                | 16               | 0              | -2.938473               | -1.950757 | -2.414147 |
| 8                | 6                | 0              | -2.476294               | -3.346647 | -0.289360 |
| 9                | 1                | 0              | -0.928908               | -2.068948 | 0.618775  |
| 10               | 6                | 0              | -3.274555               | -3.336996 | -1.416057 |
| 11               | 1                | 0              | -2.543571               | -4.119339 | 0.468043  |
| 12               | 6                | 0              | -4.345847               | -4.315395 | -1.780847 |
| 13               | 1                | 0              | -4.231990               | -4.682261 | -2.807006 |
| 14               | 1                | 0              | -4.313285               | -5.170617 | -1.100170 |
| 15               | 1                | 0              | -5.337336               | -3.853476 | -1.702242 |
| 16               | 1                | 0              | 0.350150                | -0.381758 | 0.214072  |
| 17               | 6                | 0              | 2.445863                | -3.133837 | 2.099483  |
| 18               | 6                | 0              | 2.500937                | -2.274633 | 0.997980  |
| 19               | 6                | 0              | 1.941528                | -2.703733 | -0.209685 |
| 20               | 6                | 0              | 1.339709                | -3.958261 | -0.348146 |
| 21               | 6                | 0              | 1.304091                | -4.805801 | 0.763788  |
| 22               | 6                | 0              | 1.850765                | -4.395036 | 1.984136  |
| 23               | 1                | 0              | 2.871558                | -2.810427 | 3.044861  |
| 24               | 1                | 0              | 2.964959                | -1.299919 | 1.085063  |
| 25               | 1                | 0              | 0.899621                | -4.264995 | -1.290537 |
| 26               | 1                | 0              | 0.838786                | -5.782896 | 0.672099  |
| 27               | 1                | 0              | 1.812892                | -5.056607 | 2.844659  |
| 28               | 53               | 0              | 1.952337                | -1.386573 | -1.857902 |
| 29               | 1                | 0              | 1.248255                | 1.625157  | -1.813331 |
| 30               | 6                | 0              | 0.010706                | 2.775282  | -0.524414 |
| 31               | 6                | 0              | -0.656653               | 3.394230  | -1.586143 |
| 32               | 6                | 0              | -0.044522               | 3.325652  | 0.760384  |
| 33               | 6                | 0              | -1.395329               | 4.553207  | -1.369614 |
| 34               | 1                | 0              | -0.612798               | 2.963122  | -2.579179 |
| 35               | 6                | 0              | -0.772520               | 4.486864  | 0.992261  |
| 36               | 1                | 0              | 0.472026                | 2.844025  | 1.579884  |
| 37               | 6                | 0              | -1.441175               | 5.083351  | -0.079267 |
| 38               | 1                | 0              | -1.920885               | 5.038385  | -2.182524 |
| 39               | 1                | 0              | -0.833475               | 4.914255  | 1.985036  |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 40 | 8  | 0 | 1.947347  | 1.436646  | 0.148573  |
| 41 | 16 | 0 | 3.391092  | 2.172652  | -0.197280 |
| 42 | 8  | 0 | 3.449175  | 3.416485  | 0.572299  |
| 43 | 8  | 0 | 3.542898  | 2.210211  | -1.657254 |
| 44 | 6  | 0 | 4.466678  | 0.954334  | 0.518244  |
| 45 | 6  | 0 | 4.591772  | 0.900255  | 1.910633  |
| 46 | 6  | 0 | 5.122899  | 0.047738  | -0.317361 |
| 47 | 6  | 0 | 5.381233  | -0.102683 | 2.468792  |
| 48 | 1  | 0 | 4.082043  | 1.620304  | 2.542450  |
| 49 | 6  | 0 | 5.913525  | -0.942951 | 0.265250  |
| 50 | 1  | 0 | 5.019036  | 0.114448  | -1.394142 |
| 51 | 6  | 0 | 6.046549  | -1.041323 | 1.659594  |
| 52 | 1  | 0 | 5.484157  | -0.157234 | 3.549032  |
| 53 | 1  | 0 | 6.430876  | -1.652390 | -0.374564 |
| 54 | 6  | 0 | 6.858170  | -2.147003 | 2.283616  |
| 55 | 1  | 0 | 6.200152  | -2.968762 | 2.595296  |
| 56 | 1  | 0 | 7.588562  | -2.555664 | 1.579345  |
| 57 | 1  | 0 | 7.388103  | -1.797257 | 3.175316  |
| 58 | 16 | 0 | -2.712615 | 1.183758  | 1.225142  |
| 59 | 8  | 0 | -3.151316 | 1.870755  | -0.014176 |
| 60 | 8  | 0 | -2.878413 | 1.960121  | 2.485779  |
| 61 | 8  | 0 | -1.291308 | 0.643835  | 1.120733  |
| 62 | 6  | 0 | -3.765311 | -0.272548 | 1.404200  |
| 63 | 6  | 0 | -4.736827 | -0.553736 | 0.445643  |
| 64 | 6  | 0 | -5.552035 | -1.679391 | 0.601750  |
| 65 | 6  | 0 | -5.410201 | -2.531147 | 1.704876  |
| 66 | 6  | 0 | -4.428980 | -2.220771 | 2.664320  |
| 67 | 6  | 0 | -3.610616 | -1.101503 | 2.521666  |
| 68 | 1  | 0 | -4.847621 | 0.096478  | -0.414909 |
| 69 | 1  | 0 | -6.304533 | -1.898244 | -0.151621 |
| 70 | 1  | 0 | -4.307065 | -2.865500 | 3.531756  |
| 71 | 1  | 0 | -2.859062 | -0.874066 | 3.271735  |
| 72 | 6  | 0 | -6.258237 | -3.771093 | 1.851028  |
| 73 | 1  | 0 | -7.111800 | -3.757035 | 1.166534  |
| 74 | 1  | 0 | -5.669167 | -4.671201 | 1.631810  |
| 75 | 1  | 0 | -6.638748 | -3.875827 | 2.873232  |
| 76 | 7  | 0 | -2.213457 | 6.305063  | 0.157926  |
| 77 | 8  | 0 | -2.223780 | 6.782879  | 1.297993  |
| 78 | 8  | 0 | -2.822481 | 6.810392  | -0.792411 |

---

**Product (Nitro group)**

---

|                                            |                             |
|--------------------------------------------|-----------------------------|
| Zero-point correction=                     | 0.489474 (Hartree/Particle) |
| Thermal correction to Energy=              | 0.528247                    |
| Thermal correction to Enthalpy=            | 0.529191                    |
| Thermal correction to Gibbs Free Energy=   | 0.413894                    |
| Sum of electronic and zero-point Energies= | -3007.896202                |
| Sum of electronic and thermal Energies=    | -3007.857429                |
| Sum of electronic and thermal Enthalpies=  | -3007.856485                |

Sum of electronic and thermal Free Energies= -3007.971783

-----  
Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 0.667420                | -1.341940 | 0.091626  |
| 2                | 6                | 0              | -0.839669               | -1.372624 | 0.397068  |
| 3                | 6                | 0              | 1.541677                | -1.144314 | 1.353065  |
| 4                | 8                | 0              | 1.018585                | -1.001784 | 2.455851  |
| 5                | 6                | 0              | 2.978280                | -1.235755 | 1.156242  |
| 6                | 6                | 0              | 3.676853                | -1.669904 | 0.042261  |
| 7                | 16               | 0              | 4.079234                | -0.826438 | 2.459309  |
| 8                | 6                | 0              | 5.078452                | -1.673322 | 0.232525  |
| 9                | 1                | 0              | 3.195996                | -1.964438 | -0.882529 |
| 10               | 6                | 0              | 5.462422                | -1.232734 | 1.483360  |
| 11               | 1                | 0              | 5.792639                | -1.973801 | -0.525698 |
| 12               | 6                | 0              | 6.855235                | -1.069222 | 2.006036  |
| 13               | 1                | 0              | 7.007436                | -1.631786 | 2.933911  |
| 14               | 1                | 0              | 7.572234                | -1.428194 | 1.262775  |
| 15               | 1                | 0              | 7.076989                | -0.016599 | 2.218000  |
| 16               | 1                | 0              | 0.910610                | -2.335534 | -0.298851 |
| 17               | 1                | 0              | -0.957953               | -1.992983 | 1.288724  |
| 18               | 6                | 0              | -1.534390               | -0.042970 | 0.596563  |
| 19               | 6                | 0              | -1.707698               | 0.462378  | 1.891713  |
| 20               | 6                | 0              | -2.032242               | 0.668113  | -0.501634 |
| 21               | 6                | 0              | -2.372649               | 1.666610  | 2.095309  |
| 22               | 1                | 0              | -1.316196               | -0.087098 | 2.739578  |
| 23               | 6                | 0              | -2.705868               | 1.870110  | -0.316775 |
| 24               | 1                | 0              | -1.910634               | 0.274380  | -1.502544 |
| 25               | 6                | 0              | -2.868124               | 2.351754  | 0.983092  |
| 26               | 1                | 0              | -2.517366               | 2.062048  | 3.092887  |
| 27               | 1                | 0              | -3.100003               | 2.422189  | -1.160395 |
| 28               | 8                | 0              | -1.410178               | -2.080797 | -0.747702 |
| 29               | 16               | 0              | -2.753536               | -3.016714 | -0.530620 |
| 30               | 8                | 0              | -2.672237               | -3.630974 | 0.799803  |
| 31               | 8                | 0              | -2.771692               | -3.841954 | -1.738418 |
| 32               | 6                | 0              | -4.100430               | -1.856097 | -0.569617 |
| 33               | 6                | 0              | -4.631457               | -1.384220 | 0.633314  |
| 34               | 6                | 0              | -4.539637               | -1.375590 | -1.806046 |
| 35               | 6                | 0              | -5.613622               | -0.397051 | 0.587633  |
| 36               | 1                | 0              | -4.277463               | -1.771760 | 1.581832  |
| 37               | 6                | 0              | -5.522567               | -0.388332 | -1.827337 |
| 38               | 1                | 0              | -4.117889               | -1.758251 | -2.729302 |
| 39               | 6                | 0              | -6.064369               | 0.124552  | -0.636414 |
| 40               | 1                | 0              | -6.028750               | -0.018735 | 1.517512  |
| 41               | 1                | 0              | -5.869598               | -0.005531 | -2.782893 |
| 42               | 6                | 0              | -7.077870               | 1.238893  | -0.666244 |

|    |    |   |           |           |           |
|----|----|---|-----------|-----------|-----------|
| 43 | 1  | 0 | -6.575185 | 2.207032  | -0.543915 |
| 44 | 1  | 0 | -7.619487 | 1.264780  | -1.616230 |
| 45 | 1  | 0 | -7.802476 | 1.142202  | 0.148287  |
| 46 | 16 | 0 | 1.318827  | 1.144063  | -0.898002 |
| 47 | 8  | 0 | 1.069137  | 1.571048  | 0.480520  |
| 48 | 8  | 0 | 0.581419  | 1.732877  | -2.016221 |
| 49 | 8  | 0 | 0.998571  | -0.482385 | -1.029049 |
| 50 | 6  | 0 | 3.064304  | 1.236285  | -1.240263 |
| 51 | 6  | 0 | 3.914967  | 1.745954  | -0.258390 |
| 52 | 6  | 0 | 5.277467  | 1.837957  | -0.538670 |
| 53 | 6  | 0 | 5.795714  | 1.421097  | -1.774401 |
| 54 | 6  | 0 | 4.907492  | 0.920656  | -2.742710 |
| 55 | 6  | 0 | 3.540698  | 0.829582  | -2.489634 |
| 56 | 1  | 0 | 3.522497  | 2.056853  | 0.702742  |
| 57 | 1  | 0 | 5.948076  | 2.232666  | 0.219344  |
| 58 | 1  | 0 | 5.291033  | 0.601275  | -3.707754 |
| 59 | 1  | 0 | 2.863740  | 0.445442  | -3.245629 |
| 60 | 6  | 0 | 7.277991  | 1.470791  | -2.042200 |
| 61 | 1  | 0 | 7.755714  | 2.290499  | -1.496992 |
| 62 | 1  | 0 | 7.753458  | 0.536998  | -1.714426 |
| 63 | 1  | 0 | 7.488766  | 1.590508  | -3.109149 |
| 64 | 7  | 0 | -3.598169 | 3.605505  | 1.188025  |
| 65 | 8  | 0 | -4.094559 | 4.164168  | 0.203286  |
| 66 | 8  | 0 | -3.691756 | 4.049904  | 2.337768  |

-----  
-----**End of File**-----  
-----