# Supplementary Information

## An Improved Mechanistic Model for the Diastereoselective Addition of Grignard Reagents to *N*-(*tert*-butylsulfinyl)imines

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## 1. Study of the structure of the imine

I performed a study to evaluate the structure of the imine in a solution in $CH_2Cl_2$. The possibility of formation of both *E* and *Z* imines was contemplated and a conformational analysis was done to both of them. The energy profiles for the interconversion of the different forms of the imine are shown in Figure S1.

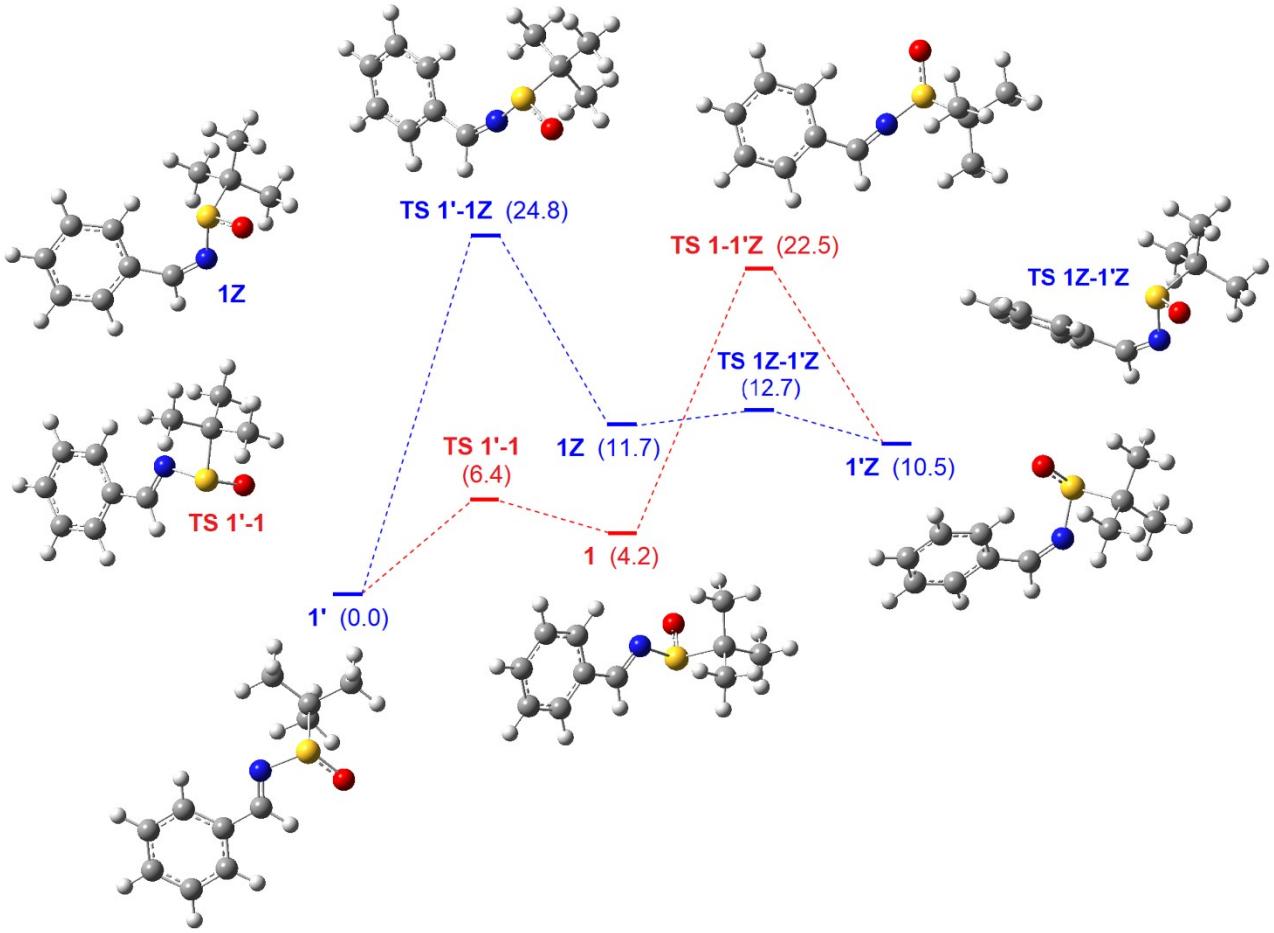



**Figure S1**. Energy profiles for the interconversion of the different forms of the imine, obtained from DFT calculations [geometry optimizations at B3LYP-D3/6-31G(d,p) level and energies by single-point calculations at M062X/6-311G(d,p) level, both in $CH_2Cl_2$ at 298.15 K] (Color of atoms: C, grey; H, white; N, blue; O, red; S, yellow; Mg, green; Br, dark red). Relative Gibbs free energy values are given in brackets (kcal/mol). The *E* imine with *s-cis* conformation, **1'**, was taken as zero-energy.

The most stable structure for the imine is **1'** (*E*, *s-cis*). It could be transformed into structure **1Z** (*Z*, *s-trans*) through **TS 1'-1Z** with an activation barrier of 24.8 kcal/mol. Structure **1Z** could rapidly change its conformation to *s-cis*, giving structure **1'Z**, which is slightly more stable than **1Z**. In an alternative pathway, **1'** could change its conformation to *s-trans*, giving structure **1**, which lies 4.2 kcal/mol above **1'**. Structure **1** could be converted into **1'Z** through **TS 1-1'Z** with a barrier of 18.3

kcal/mol. According to the energy differences between the most stable structure **1'** and the other three structures **1** (4.2 kcal/mol), **1Z** (11.7 kcal/mol) and **1'Z** (10.5 kcal/mol), the (*E*, *s-cis*) imine **1'** should be the only one present in solution, which is in agreement with the experimental results.[1]

Some general trends can be observed in Figure S1. Structures with *E* configuration (**1'** and **1**) are more stable than the ones with *Z* configuration (**1Z** and **1'Z**). For the same configuration in the C=N bond, *s-cis* conformations are more stable than *s-trans* (compare **1'** with **1** and **1'Z** with **1Z**). In the two transition structures for the conversion of an *E* form to a *Z* form (**TS 1'-1Z** and **TS 1-1'Z**), the iminic carbon, the nitrogen and the sulfur atoms show an almost linear arrangement.

## 2. Other reactive complexes between the imine and EtMgBr without a $Et_2O$ molecule

It was indicated in the text that both reactive complexes **R2** and **R3** that were involved in the energy profiles shown in Figure 2 are formed by coordination of the magnesium atom of EtMgBr to the oxygen atom of the sulfinyl group of imine **1** with *s-trans* geometry. Since the DFT calculations discussed in the previous section showed that the *s-cis* conformation **1'** is 4.2 kcal/mol more stable than **1**, two more reactive complexes, **R4** and **R5** (Figure S2), with the *s-cis* conformation in the imine moiety and differing in the spatial orientation of the EtMgBr unit were considered, but their energies were almost the same as the ones of **R2** and **R3**, not leading to any significant variation of the reaction barriers to reach **TS 1-2** and **TS 1-3**.

1) See, for instance: (a) G. Liu, D. A. Cogan, T. D. Owens, T. P. Tang and J. A. Ellman, Synthesis of Enantiomerically Pure N-tert-Butanesulfinyl Imines (tert-Butanesulfinimines) by the Direct Condensation of tert-Butanesulfinamide with Aldehydes and Ketones, *J. Org. Chem.*, 1999, **64**, 1278-1284. (b) J. F. Collados, E. Toledano, D. Guijarro and M. Yus, Microwave-Assisted Solvent-Free Synthesis of Enantiomerically Pure N-(tert-Butylsulfinyl)imines, *J. Org. Chem.*, 2012, **77**, 5744-5750.

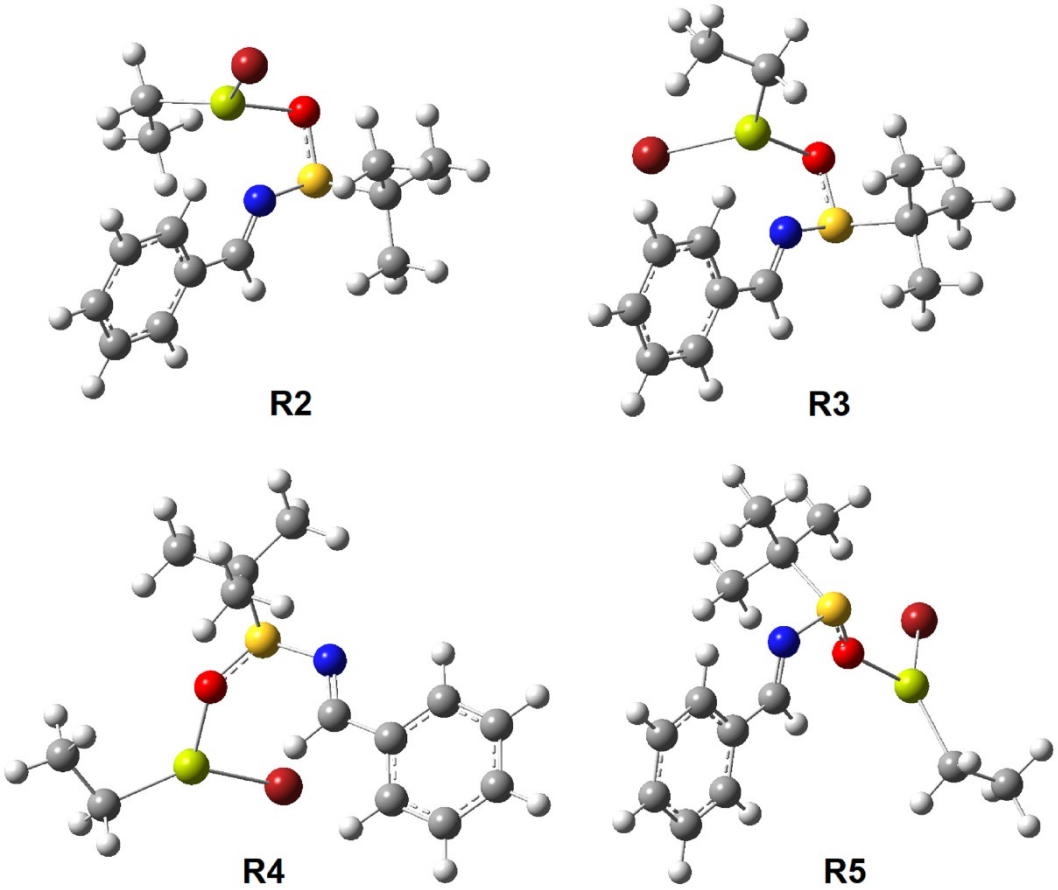
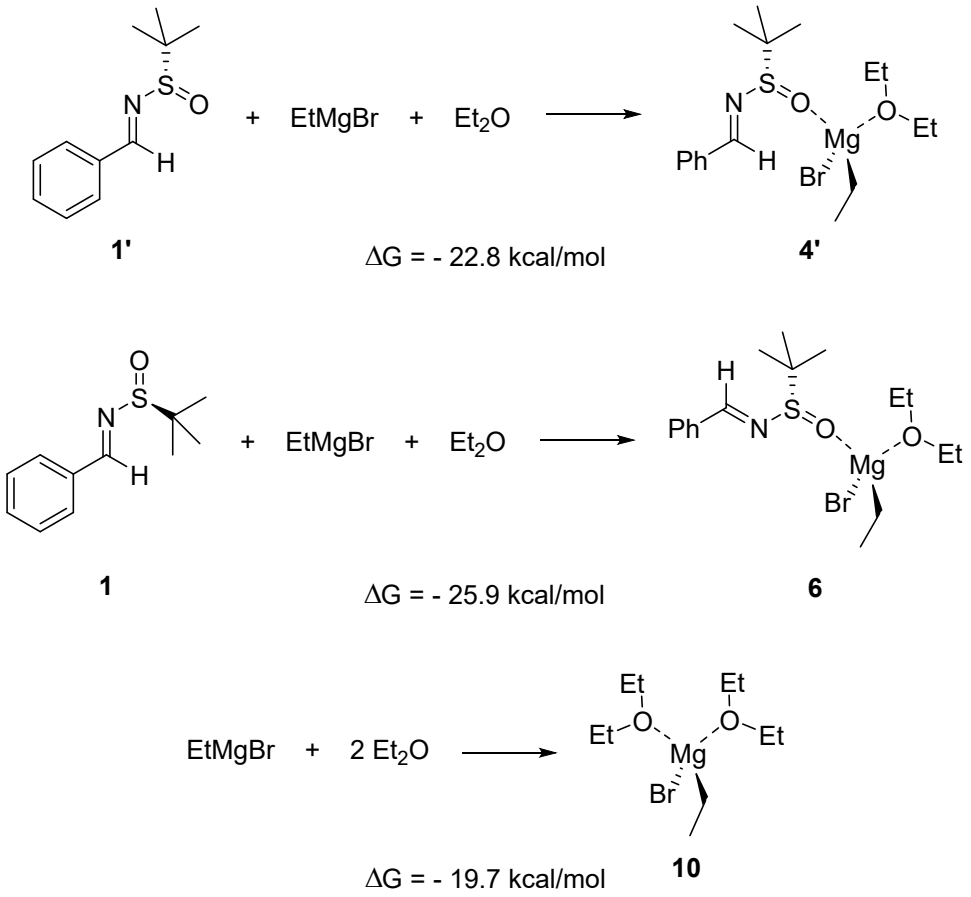



**Figure S2**. Optimized structures of reactive complexes **R2**, **R3**, **R4** and **R5** at the B3LYP-D3/6-31G(d,p) level, in $CH_2Cl_2$ at 298.15 K (Color of atoms: C, grey; H, white; N, blue; O, red; S, yellow; Mg, green; Br, dark red). The relative energies [single-point calculations at M062X/6-311G(d,p) level, in $CH_2Cl_2$ at 298.15 K] in kcal/mol are **R2** (0.0), **R3** (0.2), **R4** (-0.2) and **R5** (0.2).

### 3. Thermodynamic study of the formation of reactive complexes 4' and 6

DFT calculations showed the thermodynamic feasibility of the generation of reactive complexes **4'** and **6** having a molecule of $Et_2O$. Evaluation of the ΔG for the coordination of the imine and one molecule of $Et_2O$ to EtMgBr to give complexes **4'** and **6** led to values of -22.8 kcal/mol for the *s-cis* conformer of the imine and -25.9 kcal/mol for the *s-trans* conformer (Scheme S1), indicating that these two processes are thermodynamically favored.




**Scheme S1**. ΔG values calculated for the generation of the proposed reactive complexes **4'** and **6** and complex **10**.

EtMgBr could also be coordinated to two molecules of $Et_2O$ forming complex **10**. In order to evaluate whether the Grignard reagent would be more stable forming complexes **4'** and **6** or coordinating to two molecules of $Et_2O$, the ΔG value for the latter process was also calculated and gave a value of -19.7 kcal/mol (Scheme S1). Therefore, once all the reagents are together in the reaction flask, the generation of complexes **4'** and **6** would be preferred.

## 4. Calculation of the deformation energies and the interaction energies for transition structures TS 4'-5 and TS 6-7

An estimation of the two components of the activation energy, the deformation energy and the interaction energy, was done for both transition structures **TS 4'-5** and **TS 6-7**. Following recommendations from the literature,[2] since reactive complex **4'** is formed in the system under study, that reactive complex was used as starting point for the analysis. Consequently, structures **4'**,

2) I. Fernández and F. M. Bickelhaupt, The activation strain model and molecular orbital theory: understanding and designing chemical reactions, *Chem. Soc. Rev.*, 2014, **43**, 4953-4967.

**TS 4'-5** and **TS 6-7** were separated into two interacting subunits: the sulfinyl imine (labelled with **Im**) on one hand and the Grignard reagent coordinated to the $Et_2O$ molecule (labelled with **Gr**) on the other hand. The structures of all of the subunits are depicted in Figure S3.[3]

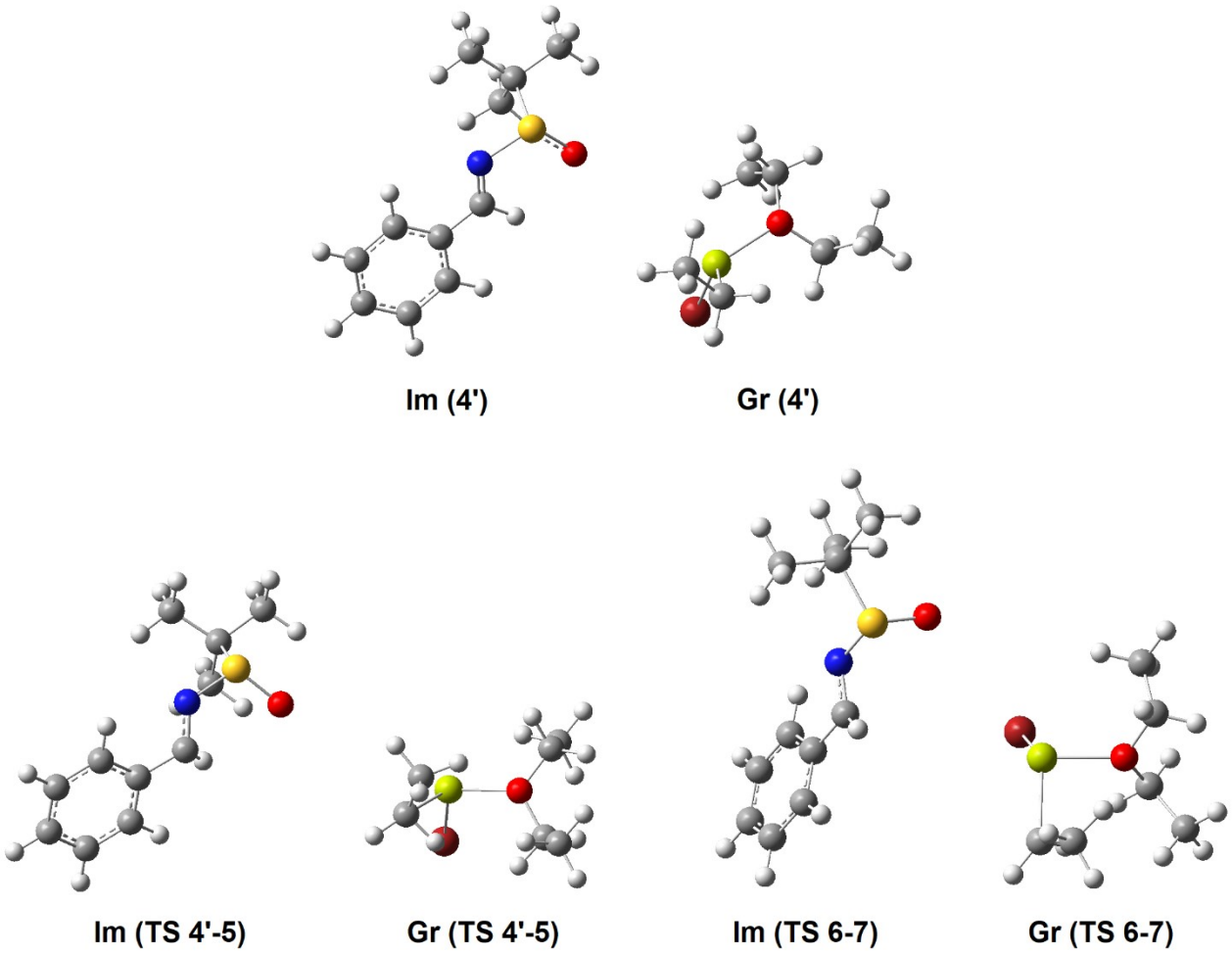



**Figure S3**. Structures of the subunits considered for the determination of the deformation energy and the interaction energy of **4'**, **TS 4'-5** and **TS 6-7**.

Single-point calculations were performed for all the subunits at M062X/6-311G(d,p) level, in $CH_2Cl_2$ at 298.15 K and the corresponding electronic energies are included in Table 1. The activation energies, $\Delta E^{\ddagger}$, and the deformation energies, $\Delta E_{def}$, were calculated according to the following equations:

$$\Delta E^{\ddagger}\,(\textbf{TS i}) = E\,(\textbf{TS i}) - E\,(\textbf{4'})$$

$$\Delta E_{def}\,[\textbf{Im (TS i)}] = E\,[\textbf{Im (TS i)}] - E\,[\textbf{Im (4')}]$$

$$\Delta E_{def}\,[\textbf{Gr (TS i)}] = E\,[\textbf{Gr (TS i)}] - E\,[\textbf{Gr (4')}]$$

$$\Delta E_{def}\,(\textbf{TS i}) = \Delta E_{def}\,[\textbf{Im (TS i)}] + \Delta E_{def}\,[\textbf{Gr (TS i)}]$$

3) The structure of each subunit was obtained from the parent reactive complex or transition structure by deleting the atoms of the partner subunit. For instance, the structure of **Im (4')** was obtained from the structure of reactive complex **4'** by deleting all the atoms belonging to subunit **Gr (4')**.

where **i** could be **4'-5** or **6-7**.

**Table 1**. Electronic energies of structures **4'**, **TS 4'-5**, **TS 6-7** and all the subunits derived from them, activation and deformation energies[a]

| Structure | E[b] | $\Delta E^{\ddagger}$ (TS i) | $\Delta E_{def}$ [Im (TS i)] | $\Delta E_{def}$ [Gr (TS i)] | $\Delta E_{def}$ (TS i) |
|---|---|---|---|---|---|
| **4'** | -4043,439481 | | | | |
| **Im (4')** | -956,2306192 | | | | |
| **Gr (4')** | -3087,159921 | | | | |
| **TS 4'-5** | -4043,418626 | 0,02085505 | | | 0,051446551 |
| **Im (TS 4'-5)** | -956,1974012 | | 0,033217941 | | |
| **Gr (TS 4'-5)** | -3087,141692 | | | 0,01822861 | |
| **TS 6-7** | -4043,421615 | 0,01786554 | | | 0,03762936 |
| **Im (TS 6-7)** | -956,2052672 | | 0,02535199 | | |
| **Gr (TS 6-7)** | -3087,147643 | | | 0,01227737 | |

[a] All energy values are given in hartree. [b] Electronic energy values obtained by single-point calculations at M062X/6-311G(d,p) level, in $CH_2Cl_2$ at 298.15 K.

Table 2 shows the calculated values for the activation energies, the deformation energies and the interaction energies for the two transition structures **TS 4'-5** and **TS 6-7**. As it can be seen, both deformation and interaction energies are higher for **TS 4'-5**, the difference between the latter and **TS 6-7** in the deformation energies (8.7 kcal/mol) being higher (in absolute value) than the difference between the interaction energies (-6.8 kcal/mol). Therefore, although the interaction energy is higher in **TS 4'-5** than in **TS 6-7**, the difference in deformation energies predominates and **TS 6-7** is slightly more stable than **TS 4'-5**.

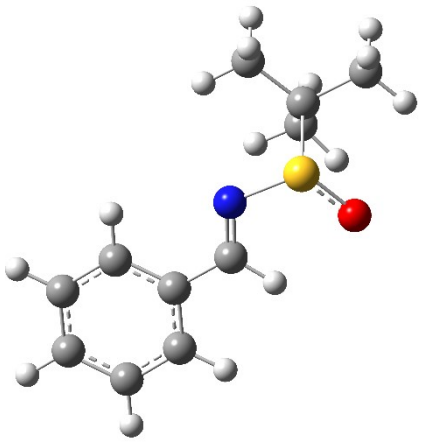
**Table 2**. Decomposition of activation energies into deformation and interaction energies[a]

| Structure | $\Delta E^{\ddagger}$ (TS i) | $\Delta E_{def}$ (TS i) | $\Delta E_{int}$ (TS i)[b] |
|---|---|---|---|
| **TS 4'-5** | 13.1 | 32.3 | -19.2 |
| **TS 6-7** | 11.2 | 23.6 | -12.4 |

[a] All energy values are given in kcal/mol. [b] Calculated as the difference between $\Delta E^{\ddagger}$ (**TS i**) and $\Delta E_{def}$ (**TS i**).

## 5. Cartesian coordinates and energies of the optimized geometries

Gibbs free energies at 298.15 K and at 225.15 K were calculated by the addition of the thermal corrections to Gibbs free energy obtained from the vibrational frequency calculations of the geometries optimized at B3LYP-D3/6-31G(d,p) level with the electronic energies (SCF Done values) obtained from single-point calculations at the M062X/6-311G(d,p) level of the optimized geometries. The effect of the bulk solvent $CH_2Cl_2$ ($\varepsilon = 8.93$) was estimated by using the Solvation Model based on Density (SMD). A correction term [0.003019831 a.u. (corresponding to 1.89 kcal/mol) for calculations at 298.15 K or 0.002080181 a.u. (corresponding to 1.31 kcal/mol) for calculations at 225.15 K] was added to the Gibbs free energies obtained before in order to consider the change in the standard state from 1 atm to 1 M. The energies reported in all this document correspond to the values obtained after adding that correction term. All Gibbs free energy values are given in a.u.

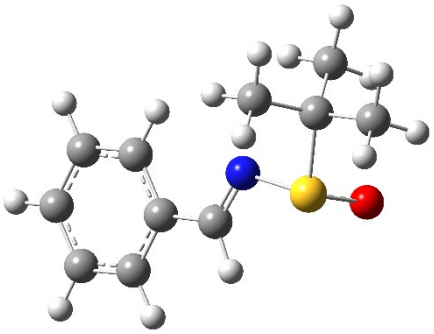


## 1′

Gibbs free energy = -956.0318122
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.63531 | -0.70231 | -0.25547 |
| N | -0.28689 | 0.07184 | -0.70329 |
| S | -1.86564 | -0.64246 | -0.84988 |
| C | -2.74231 | 0.55309 | 0.33306 |
| O | -1.91269 | -2.00440 | -0.18438 |
| C | -4.18962 | 0.04708 | 0.36475 |
| H | -4.24295 | -0.97826 | 0.74117 |
| H | -4.77664 | 0.68856 | 1.03051 |
| H | -4.65338 | 0.08017 | -0.62753 |
| C | -2.65426 | 1.96002 | -0.25952 |
| H | -1.62392 | 2.32109 | -0.29081 |
| H | -3.06932 | 1.99962 | -1.27278 |
| H | -3.24040 | 2.64267 | 0.36617 |
| C | -2.09035 | 0.44562 | 1.70974 |
| H | -1.08350 | 0.87087 | 1.71349 |
| H | -2.69641 | 0.99265 | 2.44016 |

| | | | |
|---|---|---|---|
| H | -2.03239 | -0.60017 | 2.02743 |
| H | 0.41345 | -1.73346 | 0.04631 |
| C | 2.02647 | -0.26256 | -0.10798 |
| C | 2.96955 | -1.17024 | 0.40111 |
| C | 2.43757 | 1.03762 | -0.45500 |
| C | 4.30114 | -0.78803 | 0.56167 |
| H | 2.65293 | -2.17462 | 0.66979 |
| C | 3.76639 | 1.41530 | -0.29455 |
| H | 1.70670 | 1.73699 | -0.84822 |
| C | 4.70090 | 0.50411 | 0.21401 |
| H | 5.02412 | -1.49576 | 0.95603 |
| H | 4.07931 | 2.41966 | -0.56435 |
| H | 5.73761 | 0.80352 | 0.33792 |

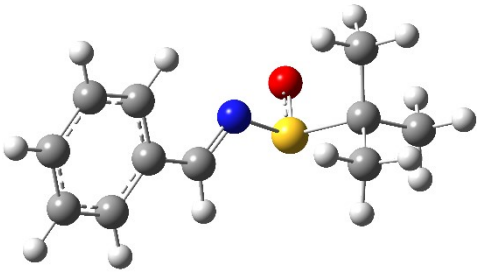


## TS 1′-1

Gibbs free energy = -956.0215535
Temperature = 298.15 K
Only one imaginary frequency = -57.82
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.78021 | -0.81876 | -0.22878 |
| N | -0.25382 | -0.09232 | 0.00847 |
| S | -1.77840 | -0.96327 | -0.17783 |
| C | -2.86804 | 0.56730 | -0.14244 |
| O | -2.05583 | -1.71592 | 1.10770 |
| C | -4.29713 | 0.02517 | -0.27856 |
| H | -4.54596 | -0.64491 | 0.54958 |
| H | -5.00221 | 0.86291 | -0.26531 |
| H | -4.43800 | -0.51736 | -1.22032 |
| C | -2.48704 | 1.44043 | -1.33994 |
| H | -1.46519 | 1.81849 | -1.25253 |
| H | -2.57876 | 0.89397 | -2.28565 |
| H | -3.16715 | 2.29841 | -1.38495 |
| C | -2.67868 | 1.28302 | 1.19470 |
| H | -1.67486 | 1.70505 | 1.28256 |
| H | -3.40757 | 2.09700 | 1.27607 |
| H | -2.84018 | 0.59026 | 2.02603 |
| H | 0.71071 | -1.87126 | -0.53713 |
| C | 2.14561 | -0.29977 | -0.09972 |
| C | 3.22339 | -1.15562 | -0.38011 |
| C | 2.39923 | 1.02800 | 0.29151 |
| C | 4.53493 | -0.69429 | -0.27387 |
| H | 3.02757 | -2.18193 | -0.67918 |
| C | 3.70828 | 1.48493 | 0.39505 |

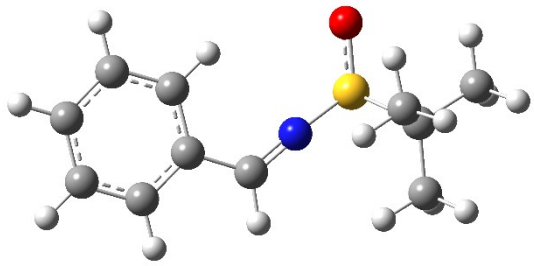
| | | | |
|---|---|---|---|
| H | 1.56289 | 1.68370 | 0.51080 |
| C | 4.77804 | 0.62554 | 0.11269 |
| H | 5.36368 | -1.36111 | -0.49153 |
| H | 3.90114 | 2.51011 | 0.69672 |
| H | 5.79893 | 0.98690 | 0.19597 |



## 1

Gibbs free energy = -956.0251086
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

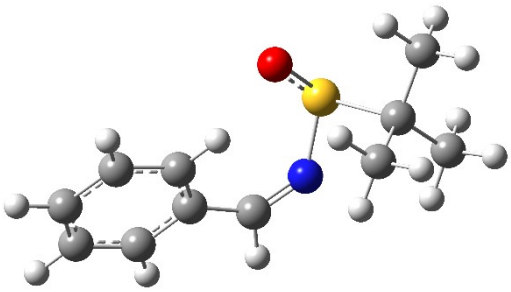
| | | | |
|---|---|---|---|
| C | -0.67842 | -0.77858 | 0.17075 |
| N | 0.27144 | -0.25861 | -0.52407 |
| S | 1.84071 | -0.99397 | -0.23268 |
| C | 2.69089 | 0.56544 | 0.40932 |
| O | 2.43521 | -1.27070 | -1.59395 |
| C | 4.13317 | 0.12114 | 0.68691 |
| H | 4.61511 | -0.24730 | -0.22343 |
| H | 4.70765 | 0.97778 | 1.05528 |
| H | 4.17729 | -0.66582 | 1.44828 |
| C | 1.98383 | 0.99591 | 1.69532 |
| H | 0.96403 | 1.33882 | 1.50266 |
| H | 1.94728 | 0.18371 | 2.43071 |
| H | 2.53974 | 1.82532 | 2.14618 |
| C | 2.64503 | 1.63794 | -0.67810 |
| H | 1.62432 | 1.98578 | -0.85370 |
| H | 3.25650 | 2.49303 | -0.36906 |
| H | 3.04626 | 1.24780 | -1.61817 |
| H | -0.50630 | -1.59741 | 0.88276 |
| C | -2.06546 | -0.31359 | 0.07228 |
| C | -3.04717 | -0.94422 | 0.85402 |
| C | -2.43268 | 0.74445 | -0.77965 |
| C | -4.37622 | -0.52796 | 0.78572 |
| H | -2.76340 | -1.76115 | 1.51244 |
| C | -3.75916 | 1.15607 | -0.84607 |
| H | -1.66962 | 1.22994 | -1.37930 |
| C | -4.73283 | 0.52153 | -0.06396 |
| H | -5.13062 | -1.01995 | 1.39210 |
| H | -4.03975 | 1.97243 | -1.50484 |
| H | -5.76745 | 0.84762 | -0.11827 |



## TS 1-1′Z

Gibbs free energy = -955.9959801
Temperature = 298.15 K
Only one imaginary frequency = -211.56
Cartesian coordinates:

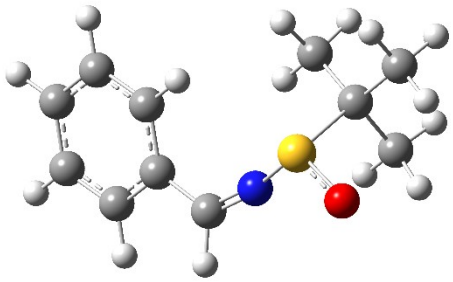
| | | | |
|---|---|---|---|
| C | 0.72077 | 0.96141 | -0.47297 |
| N | -0.31918 | 0.23813 | -0.49475 |
| S | -1.66547 | -0.57881 | -0.83506 |
| C | -2.86168 | 0.34674 | 0.32768 |
| O | -1.63699 | -1.99822 | -0.31592 |
| C | -4.21661 | -0.33509 | 0.11669 |
| H | -4.16556 | -1.39760 | 0.36901 |
| H | -4.96107 | 0.13804 | 0.76639 |
| H | -4.56258 | -0.23755 | -0.91840 |
| C | -2.88918 | 1.81023 | -0.10390 |
| H | -1.91945 | 2.29346 | 0.04408 |
| H | -3.17745 | 1.91743 | -1.15546 |
| H | -3.62943 | 2.34630 | 0.50065 |
| C | -2.36590 | 0.16139 | 1.76056 |
| H | -1.41253 | 0.67227 | 1.92445 |
| H | -3.10215 | 0.57878 | 2.45645 |
| H | -2.23869 | -0.90099 | 1.98793 |
| H | 0.65496 | 2.04320 | -0.66400 |
| C | 2.06981 | 0.44948 | -0.17983 |
| C | 3.15618 | 1.33862 | -0.17488 |
| C | 2.28665 | -0.91304 | 0.09239 |
| C | 4.44316 | 0.87384 | 0.09484 |
| H | 2.98662 | 2.39185 | -0.38435 |
| C | 3.57127 | -1.37359 | 0.36009 |
| H | 1.43649 | -1.58960 | 0.09141 |
| C | 4.65180 | -0.48159 | 0.36171 |
| H | 5.28073 | 1.56509 | 0.09684 |
| H | 3.73667 | -2.42631 | 0.56981 |
| H | 5.65358 | -0.84478 | 0.57246 |



## 1′Z

Gibbs free energy = -956.015129
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

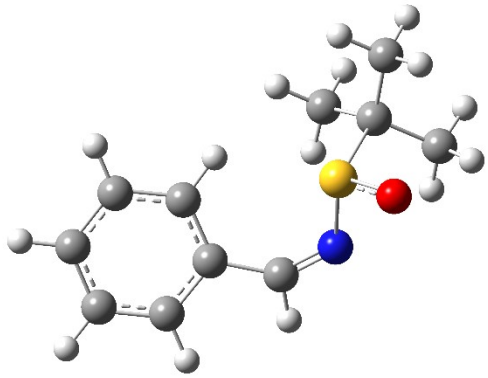
| | | | |
|---|---|---|---|
| C | 0.69184 | 1.49450 | -0.01414 |
| N | -0.55171 | 1.33181 | -0.29729 |
| S | -1.40779 | 0.03933 | -1.00701 |
| C | -2.73737 | -0.06311 | 0.35238 |
| O | -0.76440 | -1.33332 | -1.04162 |
| C | -3.68122 | -1.16657 | -0.13974 |
| H | -3.15197 | -2.11463 | -0.26668 |
| H | -4.47389 | -1.31107 | 0.60195 |
| H | -4.15527 | -0.89980 | -1.09090 |
| C | -3.45896 | 1.28106 | 0.44899 |
| H | -2.80030 | 2.06787 | 0.82150 |
| H | -3.86154 | 1.59437 | -0.52046 |
| H | -4.30197 | 1.17724 | 1.14178 |
| C | -2.05966 | -0.46416 | 1.66116 |
| H | -1.38390 | 0.31685 | 2.02084 |
| H | -2.82549 | -0.63135 | 2.42674 |
| H | -1.49528 | -1.39311 | 1.53709 |
| H | 0.93595 | 2.53285 | 0.23935 |
| C | 1.86609 | 0.60640 | 0.04679 |
| C | 3.12293 | 1.23868 | -0.03820 |
| C | 1.81827 | -0.78568 | 0.24723 |
| C | 4.30012 | 0.49836 | 0.02698 |
| H | 3.16956 | 2.31680 | -0.16747 |
| C | 3.00010 | -1.51984 | 0.32489 |
| H | 0.86137 | -1.28269 | 0.33147 |
| C | 4.24049 | -0.88597 | 0.20878 |
| H | 5.26017 | 0.99911 | -0.05464 |
| H | 2.95215 | -2.59324 | 0.48341 |
| H | 5.15643 | -1.46646 | 0.27149 |



## TS 1′-1Z

Gibbs free energy = -955.9922512
Temperature = 298.15 K
Only one imaginary frequency = -259.11
Cartesian coordinates:

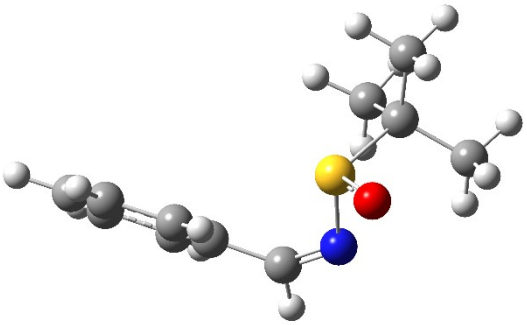
| | | | |
|---|---|---|---|
| C | 0.75207 | -1.43710 | 0.21979 |
| N | -0.43863 | -1.09085 | -0.04935 |
| S | -1.78704 | -0.63137 | -0.82723 |
| C | -2.32208 | 0.75654 | 0.37390 |
| O | -2.89359 | -1.65390 | -0.72801 |
| C | -3.62557 | 1.29043 | -0.22928 |
| H | -4.37637 | 0.50021 | -0.31086 |
| H | -4.02251 | 2.07704 | 0.42160 |
| H | -3.46447 | 1.72423 | -1.22248 |
| C | -1.24195 | 1.83287 | 0.41547 |
| H | -0.32214 | 1.46459 | 0.87438 |
| H | -1.00946 | 2.21513 | -0.58437 |
| H | -1.60674 | 2.67511 | 1.01460 |
| C | -2.56741 | 0.12090 | 1.74142 |
| H | -1.63520 | -0.23271 | 2.19126 |
| H | -3.01087 | 0.86615 | 2.41116 |
| H | -3.25896 | -0.72200 | 1.65538 |
| H | 0.94071 | -2.44720 | 0.61406 |
| C | 1.95765 | -0.60260 | 0.07907 |
| C | 3.16270 | -1.05675 | 0.64109 |
| C | 1.94407 | 0.60808 | -0.63504 |
| C | 4.32862 | -0.30371 | 0.51206 |
| H | 3.17686 | -2.00012 | 1.18124 |
| C | 3.11115 | 1.35327 | -0.77186 |
| H | 1.01855 | 0.94656 | -1.08736 |
| C | 4.30391 | 0.90241 | -0.19344 |
| H | 5.25458 | -0.65675 | 0.95605 |
| H | 3.09653 | 2.28456 | -1.33034 |
| H | 5.21244 | 1.48833 | -0.29830 |



## 1z

Gibbs free energy = -956.0132322
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

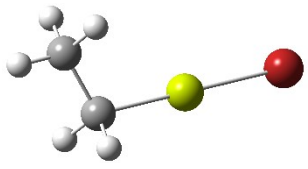
| | | | |
|---|---|---|---|
| C | 0.70477 | -1.41798 | 0.55122 |
| N | -0.54770 | -1.43453 | 0.25665 |
| S | -1.28413 | -0.28644 | -0.85166 |
| C | -2.42558 | 0.52416 | 0.42552 |
| O | -2.16988 | -1.15056 | -1.71816 |
| C | -3.25696 | 1.51552 | -0.39851 |
| H | -3.82810 | 1.00028 | -1.17635 |
| H | -3.96420 | 2.02749 | 0.26287 |
| H | -2.62842 | 2.27714 | -0.87350 |
| C | -1.57103 | 1.24522 | 1.46846 |
| H | -0.93605 | 0.55112 | 2.02561 |
| H | -0.93983 | 2.01910 | 1.01976 |
| H | -2.23564 | 1.73964 | 2.18573 |
| C | -3.31396 | -0.55493 | 1.04357 |
| H | -2.73923 | -1.23037 | 1.68125 |
| H | -4.09032 | -0.07638 | 1.65078 |
| H | -3.80105 | -1.14517 | 0.26193 |
| H | 1.01011 | -2.28384 | 1.15017 |
| C | 1.83665 | -0.52058 | 0.24797 |
| C | 3.11941 | -1.06318 | 0.46410 |
| C | 1.73776 | 0.80335 | -0.22261 |
| C | 4.26657 | -0.32418 | 0.18839 |
| H | 3.20917 | -2.07818 | 0.84176 |
| C | 2.88741 | 1.54264 | -0.49077 |
| H | 0.77269 | 1.26788 | -0.36753 |
| C | 4.15244 | 0.98240 | -0.29229 |
| H | 5.24578 | -0.76330 | 0.35303 |
| H | 2.79490 | 2.56355 | -0.84855 |
| H | 5.04421 | 1.56569 | -0.50195 |



## TS 1Z-1′Z

Gibbs free energy = -956.0116294
Temperature = 298.15 K
Only one imaginary frequency = -19.00
Cartesian coordinates:

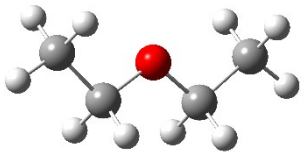
| | | | |
|---|---|---|---|
| C | 0.63238 | 0.34417 | 1.57320 |
| N | -0.60492 | 0.01411 | 1.48464 |
| S | -1.18463 | -0.82066 | 0.02993 |
| C | -2.39381 | 0.53606 | -0.47878 |
| O | -2.01591 | -1.97095 | 0.55331 |
| C | -3.08266 | -0.03729 | -1.72508 |
| H | -3.60727 | -0.96896 | -1.49346 |
| H | -3.81743 | 0.68674 | -2.09306 |
| H | -2.36744 | -0.23049 | -2.53254 |
| C | -1.58223 | 1.78707 | -0.82056 |
| H | -1.10811 | 2.21732 | 0.06527 |
| H | -0.80618 | 1.57757 | -1.56567 |
| H | -2.25382 | 2.54182 | -1.24426 |
| C | -3.40058 | 0.76895 | 0.64611 |
| H | -2.92642 | 1.21629 | 1.52246 |
| H | -4.18795 | 1.44371 | 0.29210 |
| H | -3.86431 | -0.17563 | 0.94613 |
| H | 0.87527 | 0.91051 | 2.48031 |
| C | 1.79349 | 0.13171 | 0.67534 |
| C | 2.70360 | 1.19218 | 0.53160 |
| C | 2.04997 | -1.08638 | 0.02306 |
| C | 3.81857 | 1.05871 | -0.29451 |
| H | 2.52428 | 2.12559 | 1.05841 |
| C | 3.17899 | -1.22369 | -0.78199 |
| H | 1.39221 | -1.93531 | 0.17270 |
| C | 4.05718 | -0.14961 | -0.95381 |
| H | 4.50568 | 1.89101 | -0.41365 |
| H | 3.37595 | -2.17226 | -1.27234 |
| H | 4.93198 | -0.25969 | -1.58787 |



## EtMgBr

Gibbs free energy = -2853.483129
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

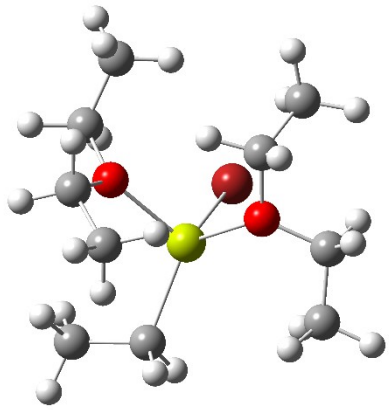
| | | | |
|---|---|---|---|
| C | -2.69958 | -0.63030 | -0.00000 |
| H | -2.96560 | -1.24342 | -0.87452 |
| H | -2.96560 | -1.24342 | 0.87452 |
| Mg | -0.61093 | -0.29573 | 0.00000 |
| Br | 1.77030 | 0.08045 | -0.00000 |
| C | -3.53783 | 0.66088 | 0.00000 |
| H | -3.32536 | 1.28214 | -0.87945 |
| H | -4.62301 | 0.47188 | 0.00000 |
| H | -3.32536 | 1.28214 | 0.87944 |



## $Et_2O$

Gibbs free energy = -233.5037989
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 1.18598 | 0.52271 | 0.00000 |
| O | -0.00000 | -0.26112 | -0.00001 |
| C | 2.37954 | -0.41548 | 0.00000 |
| C | -1.18598 | 0.52271 | -0.00000 |
| C | -2.37954 | -0.41548 | 0.00001 |
| H | 1.21094 | 1.17949 | 0.88647 |
| H | 1.21096 | 1.17950 | -0.88645 |
| H | 3.31396 | 0.15515 | 0.00001 |
| H | 2.36477 | -1.05650 | -0.88747 |
| H | 2.36476 | -1.05652 | 0.88747 |
| H | -1.21094 | 1.17949 | 0.88646 |
| H | -1.21096 | 1.17950 | -0.88646 |
| H | -3.31396 | 0.15515 | 0.00001 |
| H | -2.36477 | -1.05651 | -0.88747 |
| H | -2.36476 | -1.05651 | 0.88748 |

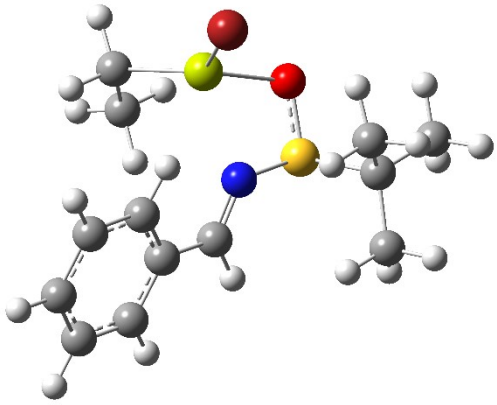


## 10

Gibbs free energy = -3320.52207
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -0.90138 | 2.56255 | 0.95790 |
| Mg | -0.12760 | 0.66914 | 0.34476 |
| Br | 1.25126 | -0.69081 | 1.87591 |
| C | -2.28221 | 2.40290 | 1.62536 |
| H | -2.23227 | 1.71625 | 2.48269 |
| H | -2.72752 | 3.33982 | 2.00302 |
| H | -3.01764 | 1.96865 | 0.93324 |
| C | -2.72911 | -0.27240 | -1.21739 |
| O | -1.71577 | -0.56842 | -0.22143 |
| C | -1.97935 | -1.78614 | 0.53161 |
| H | -2.81895 | -1.13460 | -1.88741 |
| H | -3.68456 | -0.13759 | -0.69675 |
| H | -1.48673 | -1.64748 | 1.49578 |
| H | -3.05977 | -1.85569 | 0.69860 |
| C | 2.31637 | 1.14130 | -1.51506 |
| O | 1.03159 | 0.47735 | -1.40078 |
| C | 0.92756 | -0.74409 | -2.18119 |
| H | 3.07606 | 0.54036 | -1.00504 |
| H | 2.56960 | 1.19679 | -2.58075 |
| H | -0.09195 | -1.09044 | -2.01129 |
| H | 1.03105 | -0.47516 | -3.23966 |
| C | 1.92635 | -1.81675 | -1.77809 |
| H | 2.95150 | -1.55020 | -2.04971 |
| H | 1.88268 | -1.98981 | -0.69952 |
| H | 1.67390 | -2.74631 | -2.29944 |
| C | 2.23455 | 2.52539 | -0.90326 |
| H | 1.43325 | 3.11265 | -1.36054 |
| H | 2.06374 | 2.47793 | 0.17683 |
| H | 3.18507 | 3.04292 | -1.06769 |
| C | -2.35624 | 0.97569 | -1.99161 |
| H | -2.28949 | 1.84417 | -1.33202 |
| H | -1.39986 | 0.85754 | -2.50818 |
| H | -3.12868 | 1.17021 | -2.74215 |
| C | -1.43048 | -3.00904 | -0.17879 |
| H | -1.88071 | -3.14250 | -1.16728 |
| H | -0.34629 | -2.92645 | -0.29042 |
| H | -1.64683 | -3.90374 | 0.41484 |
| H | -0.22417 | 3.00819 | 1.65625 |

| | | | |
|---|---|---|---|
| H | -1.00941 | 3.18378 | 0.09343 |

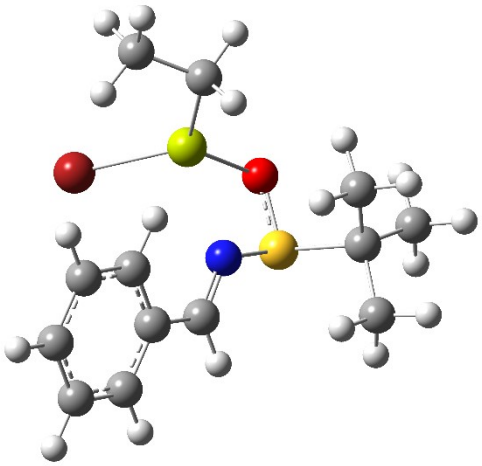


## R2

Gibbs free energy = -3809.54168
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.58261 | 1.64803 | 2.75192 |
| C | 0.91184 | -1.60249 | 0.26537 |
| H | 1.64809 | 1.84873 | 2.55105 |
| Mg | -0.52654 | 1.36941 | 0.95124 |
| H | 0.23312 | 2.52728 | 3.31848 |
| N | -0.08478 | -0.78021 | 0.31873 |
| S | -1.64319 | -1.28920 | 0.87806 |
| C | -2.47585 | -1.73553 | -0.75810 |
| O | -2.17934 | 0.11167 | 1.25469 |
| C | -2.26030 | -0.61068 | -1.76511 |
| H | -1.21087 | -0.51838 | -2.05237 |
| H | -2.84579 | -0.83707 | -2.66264 |
| H | -2.59429 | 0.35068 | -1.36925 |
| C | -1.86012 | -3.06126 | -1.20757 |
| H | -1.95997 | -3.84382 | -0.44766 |
| H | -2.39308 | -3.39721 | -2.10296 |
| H | -0.80485 | -2.95454 | -1.47533 |
| C | -3.95513 | -1.88790 | -0.38264 |
| H | -4.50882 | -2.17609 | -1.28205 |
| H | -4.11181 | -2.66691 | 0.37142 |
| H | -4.36972 | -0.94591 | -0.01385 |
| C | 2.22976 | -1.16750 | -0.16421 |
| C | 3.31194 | -2.05133 | 0.00146 |
| C | 2.44448 | 0.10701 | -0.72922 |
| C | 4.59575 | -1.65975 | -0.36877 |
| H | 3.14026 | -3.03474 | 0.43027 |
| C | 3.72849 | 0.48870 | -1.09729 |
| H | 1.60772 | 0.77909 | -0.89757 |
| C | 4.80412 | -0.39030 | -0.91466 |
| H | 5.43042 | -2.34037 | -0.23431 |
| H | 3.89385 | 1.46855 | -1.53399 |
| H | 5.80486 | -0.08572 | -1.20643 |
| Br | -0.67287 | 2.74893 | -1.05717 |
| C | 0.46667 | 0.40089 | 3.64891 |

| | | | |
|---|---|---|---|
| H | 1.02255 | 0.46548 | 4.60000 |
| H | -0.58034 | 0.19639 | 3.91167 |
| H | 0.83675 | -0.49955 | 3.13757 |
| H | 0.76797 | -2.58858 | 0.53362 |

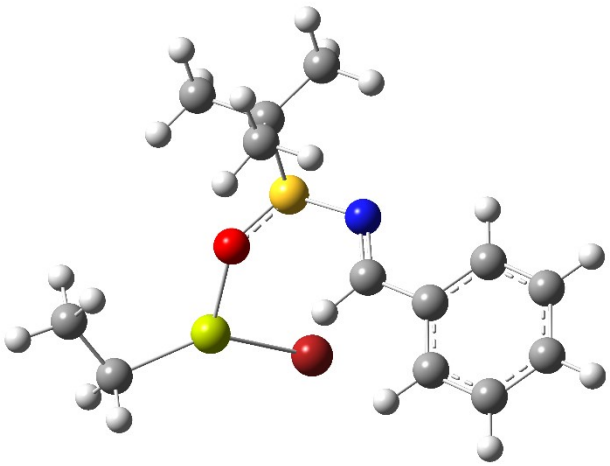


## R3

Gibbs free energy = -3809.541409
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.21005 | 2.02114 | 2.38552 |
| C | -0.20161 | -1.60330 | -0.71260 |
| H | 0.30355 | 1.08748 | 2.96752 |
| Mg | 0.38976 | 1.59962 | 0.30241 |
| N | 0.53441 | -0.62084 | -0.30736 |
| S | 2.09844 | -0.34115 | -0.99623 |
| C | 3.19257 | -1.17445 | 0.29874 |
| O | 2.18213 | 1.17365 | -0.69461 |
| H | 0.15344 | -2.31130 | -1.46675 |
| C | 2.96614 | -2.68059 | 0.15948 |
| H | 1.95863 | -2.97445 | 0.46661 |
| H | 3.67506 | -3.19455 | 0.81658 |
| H | 3.14627 | -3.03275 | -0.86212 |
| C | 2.82937 | -0.64686 | 1.68433 |
| H | 1.81217 | -0.92454 | 1.97036 |
| H | 2.92375 | 0.44130 | 1.73186 |
| H | 3.52299 | -1.08108 | 2.41167 |
| C | 4.61487 | -0.77022 | -0.10923 |
| H | 5.31762 | -1.22583 | 0.59580 |
| H | 4.74820 | 0.31438 | -0.06919 |
| H | 4.87023 | -1.12393 | -1.11384 |
| C | -1.54413 | -1.81548 | -0.19934 |
| C | -2.34358 | -2.79908 | -0.80964 |
| C | -2.06296 | -1.05603 | 0.86926 |
| C | -3.64925 | -3.00789 | -0.37260 |
| H | -1.93909 | -3.38514 | -1.63021 |
| C | -3.36548 | -1.26987 | 1.30011 |
| H | -1.44009 | -0.31736 | 1.36222 |
| C | -4.16016 | -2.24254 | 0.67881 |

| | | | |
|---|---|---|---|
| H | -4.26661 | -3.76302 | -0.84865 |
| H | -3.76476 | -0.68437 | 2.12220 |
| H | -5.17811 | -2.40515 | 1.02044 |
| Br | -1.25309 | 2.30601 | -1.37095 |
| H | 1.02549 | 2.66042 | 2.76495 |
| C | -1.14002 | 2.68393 | 2.72262 |
| H | -1.24309 | 3.65514 | 2.22064 |
| H | -1.98609 | 2.07695 | 2.37085 |
| H | -1.30645 | 2.86456 | 3.79879 |

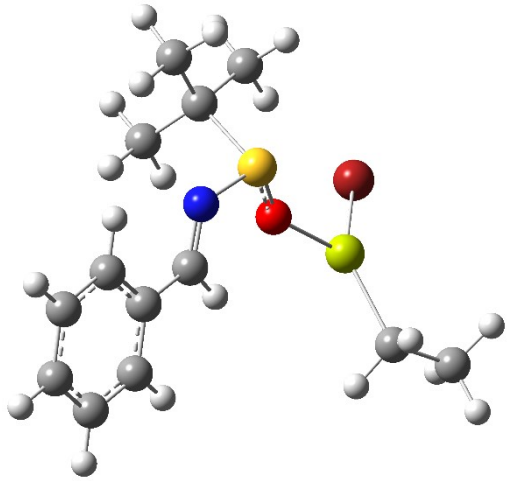


**R4**

Gibbs free energy = -3809.541947
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -3.48891 | -2.11104 | 1.81003 |
| C | 1.26256 | 0.17808 | 0.21662 |
| H | -4.23339 | -2.81976 | 1.41338 |
| Mg | -2.08154 | -1.53479 | 0.32784 |
| H | -3.01006 | -2.64495 | 2.64656 |
| N | 0.80900 | 1.08929 | -0.57051 |
| S | -0.87600 | 1.21064 | -0.77014 |
| C | -1.10075 | 2.99451 | -0.19236 |
| O | -1.61600 | 0.40538 | 0.33832 |
| H | 0.59365 | -0.46341 | 0.79800 |
| C | -0.56856 | 3.12408 | 1.23249 |
| H | 0.51432 | 2.98214 | 1.27282 |
| H | -0.79502 | 4.13192 | 1.59595 |
| H | -1.04880 | 2.40402 | 1.90064 |
| C | -0.35162 | 3.88401 | -1.18738 |
| H | -0.70855 | 3.73939 | -2.21266 |
| H | -0.53378 | 4.92901 | -0.91526 |
| H | 0.72542 | 3.70443 | -1.15967 |
| C | -2.61556 | 3.22262 | -0.25595 |
| H | -2.82062 | 4.25676 | 0.03823 |
| H | -3.00782 | 3.07880 | -1.26858 |
| H | -3.14958 | 2.55912 | 0.42910 |
| C | 2.69200 | -0.05425 | 0.40512 |
| C | 3.09039 | -1.10412 | 1.24974 |

| | | | |
|---|---|---|---|
| C | 3.66767 | 0.74016 | -0.22541 |
| C | 4.44414 | -1.35939 | 1.46109 |
| H | 2.33442 | -1.72021 | 1.72954 |
| C | 5.01656 | 0.48313 | -0.00964 |
| H | 3.35495 | 1.54944 | -0.87732 |
| C | 5.40685 | -0.56557 | 0.83349 |
| H | 4.74712 | -2.17359 | 2.11207 |
| H | 5.76886 | 1.09698 | -0.49563 |
| H | 6.46220 | -0.76202 | 0.99861 |
| Br | -0.71828 | -2.44311 | -1.48487 |
| C | -4.21685 | -0.86536 | 2.35517 |
| H | -4.96587 | -1.08767 | 3.13342 |
| H | -3.51186 | -0.14609 | 2.79285 |
| H | -4.74412 | -0.32758 | 1.55540 |

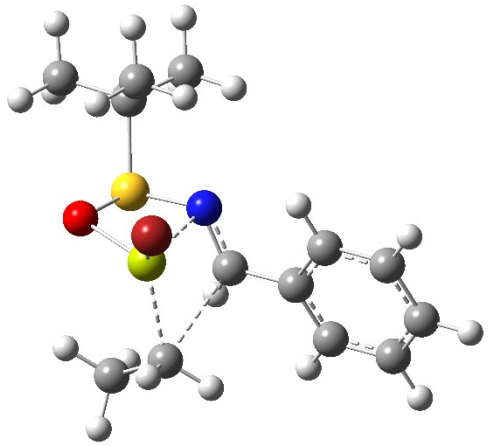


## R5

Gibbs free energy = -3809.541402
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -1.95211 | 3.26501 | 0.72287 |
| C | 2.12063 | 0.29740 | 0.19873 |
| H | -1.42767 | 3.30983 | 1.69248 |
| Mg | -2.25586 | 1.23327 | 0.17164 |
| H | -1.26187 | 3.75278 | 0.01411 |
| N | 1.75340 | -0.79044 | 0.78316 |
| S | 0.08645 | -1.03668 | 1.02666 |
| C | -0.11508 | -2.63838 | 0.04141 |
| O | -0.69921 | 0.00733 | 0.19832 |
| H | 1.38771 | 1.03136 | -0.15268 |
| C | 0.26088 | -2.36623 | -1.41233 |
| H | 1.32140 | -2.12319 | -1.51788 |
| H | 0.05784 | -3.27045 | -1.99544 |
| H | -0.33779 | -1.55154 | -1.82840 |
| C | 0.78045 | -3.68945 | 0.70042 |
| H | 0.54708 | -3.81728 | 1.76290 |
| H | 0.59932 | -4.64834 | 0.20332 |
| H | 1.83934 | -3.44260 | 0.59829 |

| | | | |
|---|---|---|---|
| C | -1.60141 | -2.98343 | 0.19125 |
| H | -1.79219 | -3.91405 | -0.35307 |
| H | -1.87508 | -3.14825 | 1.23927 |
| H | -2.24946 | -2.20626 | -0.22371 |
| C | 3.52606 | 0.61575 | -0.04041 |
| C | 3.83472 | 1.82544 | -0.68562 |
| C | 4.56551 | -0.25142 | 0.34598 |
| C | 5.16193 | 2.16530 | -0.94217 |
| H | 3.03057 | 2.49315 | -0.98304 |
| C | 5.88740 | 0.09232 | 0.08838 |
| H | 4.32296 | -1.18469 | 0.84389 |
| C | 6.18776 | 1.29978 | -0.55588 |
| H | 5.39524 | 3.10066 | -1.44141 |
| H | 6.68859 | -0.57700 | 0.38668 |
| H | 7.22242 | 1.56282 | -0.75549 |
| Br | -4.17390 | -0.03904 | -0.63806 |
| C | -3.24867 | 4.09189 | 0.81207 |
| H | -3.09199 | 5.14459 | 1.10188 |
| H | -3.78336 | 4.10684 | -0.14697 |
| H | -3.94779 | 3.66605 | 1.54430 |

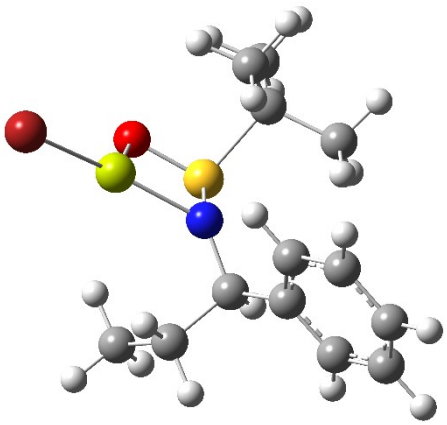


## TS 1-2

Gibbs free energy = -3809.515146
Temperature = 298.15 K
Only one imaginary frequency = -268.54
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 1.11686 | 0.39159 | 2.37350 |
| C | 0.78371 | -1.25048 | 0.56078 |
| H | 2.13108 | -0.00325 | 2.35295 |
| Mg | -0.24021 | 1.05318 | 0.74535 |
| H | 1.24003 | 1.49090 | 2.46924 |
| N | -0.31324 | -0.98765 | -0.18110 |
| S | -1.78387 | -1.21872 | 0.64044 |
| C | -2.93139 | -1.32304 | -0.83779 |
| O | -2.02101 | 0.22262 | 1.22787 |
| H | 0.73345 | -1.90117 | 1.43392 |
| C | -2.77237 | -0.07201 | -1.69887 |
| H | -1.76691 | 0.00608 | -2.11775 |
| H | -3.48786 | -0.12816 | -2.52588 |

| | | | |
|---|---|---|---|
| H | -2.98702 | 0.83232 | -1.12338 |
| C | -2.55039 | -2.60417 | -1.58459 |
| H | -2.61157 | -3.48808 | -0.93994 |
| H | -3.25513 | -2.74611 | -2.41058 |
| H | -1.54145 | -2.53944 | -1.99998 |
| C | -4.33760 | -1.41183 | -0.23103 |
| H | -5.06470 | -1.49240 | -1.04531 |
| H | -4.45217 | -2.29251 | 0.41010 |
| H | -4.57744 | -0.51718 | 0.35088 |
| C | 2.10213 | -1.14531 | -0.08682 |
| C | 3.21889 | -1.71531 | 0.54721 |
| C | 2.26468 | -0.51152 | -1.33136 |
| C | 4.47731 | -1.64502 | -0.04608 |
| H | 3.09332 | -2.21248 | 1.50503 |
| C | 3.52604 | -0.43641 | -1.91645 |
| H | 1.40243 | -0.08499 | -1.83299 |
| C | 4.63457 | -1.00138 | -1.27681 |
| H | 5.33388 | -2.09125 | 0.45007 |
| H | 3.64552 | 0.05868 | -2.87546 |
| H | 5.61609 | -0.94268 | -1.73783 |
| Br | -0.08312 | 3.09010 | -0.50887 |
| C | 0.30178 | -0.14512 | 3.54769 |
| H | 0.76054 | 0.07760 | 4.52302 |
| H | -0.71289 | 0.27094 | 3.56553 |
| H | 0.18975 | -1.23620 | 3.49580 |

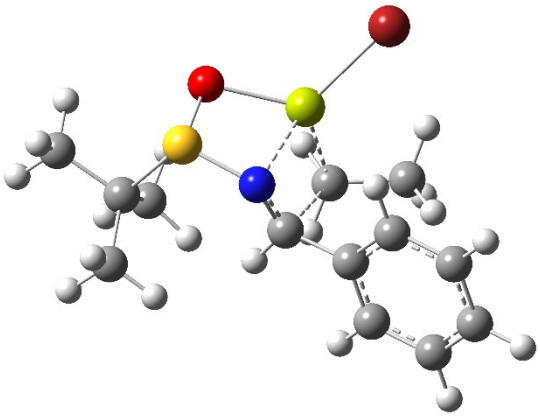


## 2

Gibbs free energy = -3809.588739
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.94676 | 1.56012 | 2.03752 |
| C | 1.36999 | 0.34204 | 1.18301 |
| H | 1.84466 | 2.06800 | 2.40859 |
| Mg | -1.69499 | 0.43777 | 0.13017 |
| H | 0.43575 | 2.27186 | 1.37191 |
| N | 0.19613 | -0.22045 | 0.50294 |
| S | -0.36432 | -1.69558 | 0.97793 |
| C | -0.08576 | -2.82891 | -0.50682 |
| O | -1.92670 | -1.41599 | 0.87512 |

| | | | |
|---|---|---|---|
| H | 1.80577 | -0.40129 | 1.86648 |
| C | -0.69658 | -2.18689 | -1.74904 |
| H | -0.23036 | -1.21920 | -1.96127 |
| H | -0.52910 | -2.83739 | -2.61368 |
| H | -1.77590 | -2.04741 | -1.63320 |
| C | 1.43299 | -2.97221 | -0.62790 |
| H | 1.87796 | -3.38340 | 0.28567 |
| H | 1.66589 | -3.65901 | -1.44872 |
| H | 1.90604 | -2.00975 | -0.84463 |
| C | -0.76387 | -4.15674 | -0.15895 |
| H | -0.60026 | -4.87167 | -0.97284 |
| H | -0.35191 | -4.59450 | 0.75737 |
| H | -1.84198 | -4.02595 | -0.02934 |
| C | 2.45777 | 0.73717 | 0.18968 |
| C | 3.79190 | 0.81222 | 0.61444 |
| C | 2.15681 | 1.07853 | -1.13456 |
| C | 4.80068 | 1.21879 | -0.26030 |
| H | 4.04065 | 0.54600 | 1.63939 |
| C | 3.16327 | 1.48852 | -2.01284 |
| H | 1.12961 | 1.00881 | -1.47755 |
| C | 4.48889 | 1.56019 | -1.57938 |
| H | 5.82985 | 1.26349 | 0.08545 |
| H | 2.91065 | 1.74846 | -3.03732 |
| H | 5.27250 | 1.87457 | -2.26291 |
| Br | -3.46380 | 1.79211 | -0.73325 |
| C | 0.04179 | 1.18579 | 3.21197 |
| H | -0.26637 | 2.07506 | 3.77125 |
| H | -0.86800 | 0.67131 | 2.88103 |
| H | 0.55940 | 0.51357 | 3.90645 |

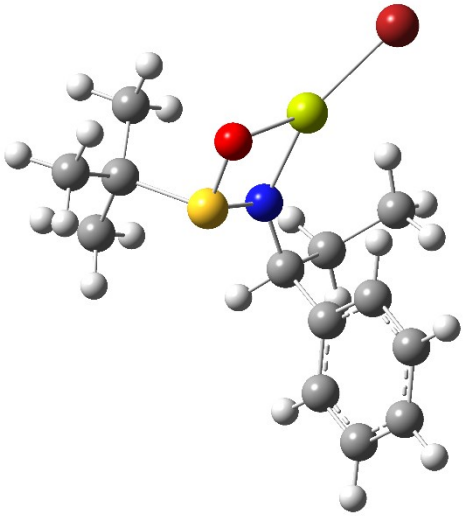


## TS 1-3

Gibbs free energy = -3809.503552
Temperature = 298.15 K
Only one imaginary frequency = -221.19
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -0.37620 | -0.11255 | 2.04295 |
| C | 0.11704 | -1.19341 | -0.09678 |
| H | -0.04171 | -1.09838 | 2.36122 |
| Mg | 0.03778 | 1.26381 | 0.36528 |
| N | 0.64378 | -0.39272 | -1.05518 |

| | | | |
|---|---|---|---|
| S | 2.20194 | 0.24685 | -0.98157 |
| C | 3.42053 | -0.81560 | 0.01597 |
| O | 1.98097 | 1.50739 | -0.05129 |
| H | 0.74920 | -1.82745 | 0.51197 |
| C | 3.44286 | -2.20662 | -0.62195 |
| H | 2.51192 | -2.75610 | -0.46491 |
| H | 4.25425 | -2.78428 | -0.16613 |
| H | 3.63901 | -2.15605 | -1.69851 |
| C | 3.08888 | -0.82091 | 1.50800 |
| H | 2.25084 | -1.47238 | 1.75676 |
| H | 2.86258 | 0.18886 | 1.86088 |
| H | 3.96563 | -1.18303 | 2.05561 |
| C | 4.75082 | -0.08070 | -0.22766 |
| H | 5.55009 | -0.64237 | 0.26705 |
| H | 4.73400 | 0.92864 | 0.19354 |
| H | 4.99655 | -0.01566 | -1.29261 |
| C | -1.25432 | -1.68952 | -0.29543 |
| C | -1.69134 | -2.78956 | 0.46000 |
| C | -2.13629 | -1.08784 | -1.20961 |
| C | -2.98623 | -3.28110 | 0.30498 |
| H | -1.01172 | -3.25373 | 1.16925 |
| C | -3.43195 | -1.57676 | -1.35531 |
| H | -1.79940 | -0.24413 | -1.80255 |
| C | -3.86050 | -2.67400 | -0.60072 |
| H | -3.31327 | -4.13505 | 0.89055 |
| H | -4.10833 | -1.10428 | -2.06132 |
| H | -4.87110 | -3.05360 | -0.71893 |
| Br | -1.52624 | 2.97995 | -0.22008 |
| H | 0.28812 | 0.59971 | 2.57375 |
| C | -1.84372 | 0.12053 | 2.39596 |
| H | -2.14638 | 1.16263 | 2.24378 |
| H | -2.50383 | -0.49623 | 1.77520 |
| H | -2.06402 | -0.13266 | 3.44410 |

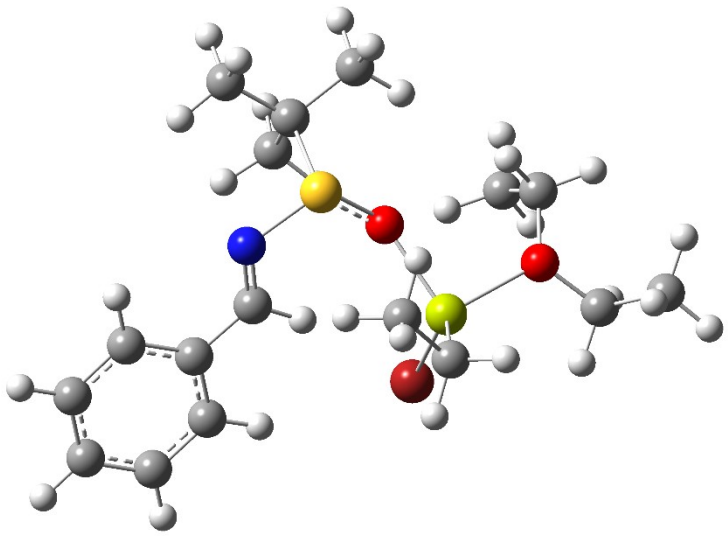


## 3

Gibbs free energy = -3809.584962
Temperature = 298.15 K

No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -1.23937 | 0.49514 | 2.46805 |
| C | -1.41198 | -0.28190 | 1.13984 |
| H | -2.23358 | 0.58632 | 2.92094 |
| Mg | 1.57440 | 0.48276 | -0.06085 |
| N | -0.07820 | -0.53265 | 0.57267 |
| S | 0.01785 | -1.56576 | -0.72486 |
| C | 0.74437 | -3.16567 | -0.03440 |
| O | 1.28370 | -0.92820 | -1.44505 |
| H | -1.87789 | -1.23472 | 1.42462 |
| C | -0.33792 | -3.75886 | 0.87142 |
| H | -0.51390 | -3.12834 | 1.74784 |
| H | -0.01036 | -4.74265 | 1.22470 |
| H | -1.28686 | -3.89708 | 0.34046 |
| C | 2.01915 | -2.84536 | 0.73852 |
| H | 1.81410 | -2.15981 | 1.56723 |
| H | 2.77525 | -2.40035 | 0.08459 |
| H | 2.43198 | -3.76933 | 1.15672 |
| C | 1.01997 | -4.05430 | -1.25089 |
| H | 1.41767 | -5.01748 | -0.91267 |
| H | 1.75588 | -3.59414 | -1.91640 |
| H | 0.10653 | -4.25267 | -1.82290 |
| C | -2.40090 | 0.41772 | 0.20339 |
| C | -3.77017 | 0.14509 | 0.33620 |
| C | -2.00279 | 1.35372 | -0.75950 |
| C | -4.71479 | 0.78971 | -0.46385 |
| H | -4.09742 | -0.58470 | 1.07357 |
| C | -2.94340 | 2.00208 | -1.56368 |
| H | -0.95116 | 1.58532 | -0.88765 |
| C | -4.30369 | 1.72289 | -1.41936 |
| H | -5.77003 | 0.55846 | -0.34671 |
| H | -2.60990 | 2.72469 | -2.30340 |
| H | -5.03534 | 2.22326 | -2.04729 |
| Br | 3.05322 | 2.36177 | -0.20949 |
| H | -0.63687 | -0.12967 | 3.13856 |
| C | -0.61010 | 1.88519 | 2.35816 |
| H | 0.44178 | 1.84493 | 2.05104 |
| H | -1.14507 | 2.51872 | 1.64400 |
| H | -0.62847 | 2.38776 | 3.33077 |



**4′**

Gibbs free energy = -4043.055128
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

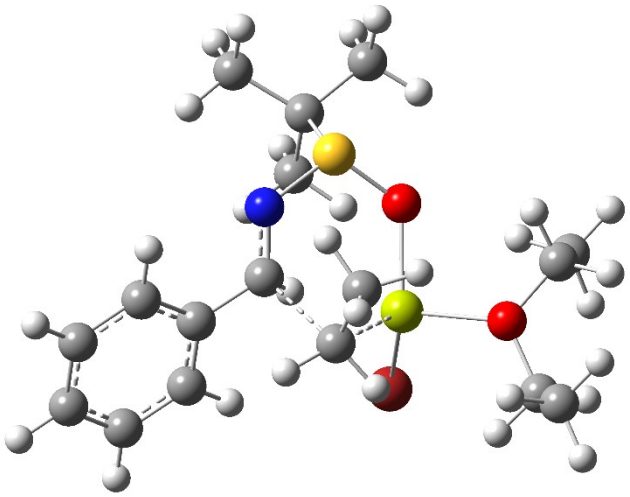
| | | | |
|---|---|---|---|
| C | -1.22217 | -1.39024 | -2.74867 |
| C | 1.99141 | 0.13017 | -0.22828 |
| Mg | -1.46140 | -0.83181 | -0.69544 |
| N | 1.88189 | 1.30814 | -0.73945 |
| S | 0.31155 | 1.97683 | -0.85656 |
| C | 0.46868 | 3.28414 | 0.50726 |
| O | -0.74691 | 1.01604 | -0.26615 |
| H | 1.12407 | -0.41419 | 0.15745 |
| C | 1.52528 | 4.29121 | 0.05031 |
| H | 2.51044 | 3.82820 | -0.04289 |
| H | 1.58941 | 5.08694 | 0.80017 |
| H | 1.26018 | 4.75421 | -0.90610 |
| C | 0.84049 | 2.58507 | 1.81290 |
| H | 1.87252 | 2.22711 | 1.80118 |
| H | 0.17543 | 1.74002 | 2.01341 |
| H | 0.73846 | 3.30314 | 2.63325 |
| C | -0.92605 | 3.91539 | 0.58342 |
| H | -0.89860 | 4.72608 | 1.31859 |
| H | -1.67440 | 3.18700 | 0.90425 |
| H | -1.23508 | 4.34425 | -0.37606 |
| C | 3.26827 | -0.56483 | -0.09916 |
| C | 3.25764 | -1.84061 | 0.49294 |
| C | 4.48265 | -0.00516 | -0.53716 |
| C | 4.44919 | -2.54750 | 0.64594 |
| H | 2.31195 | -2.26065 | 0.82782 |
| C | 5.66691 | -0.71617 | -0.38163 |
| H | 4.48114 | 0.97883 | -0.99522 |
| C | 5.65189 | -1.98685 | 0.20952 |
| H | 4.43958 | -3.53233 | 1.10277 |
| H | 6.60510 | -0.28673 | -0.71988 |
| H | 6.58054 | -2.53768 | 0.32769 |
| Br | -0.67857 | -2.17433 | 1.25010 |
| C | -0.47159 | -0.30206 | -3.54344 |
| H | -1.00023 | 0.66072 | -3.50403 |

| | | | |
|---|---|---|---|
| H | 0.53062 | -0.11840 | -3.13049 |
| H | -0.32430 | -0.53025 | -4.61365 |
| C | -3.73380 | 0.84009 | 0.55106 |
| O | -3.41542 | -0.37699 | -0.17346 |
| C | -3.17091 | 0.81877 | 1.96083 |
| C | -4.32866 | -1.48616 | 0.02931 |
| C | -5.53303 | -1.38068 | -0.88791 |
| H | -4.81987 | 0.97577 | 0.54552 |
| H | -3.28459 | 1.64285 | -0.03676 |
| H | -3.42360 | 1.75501 | 2.47068 |
| H | -2.08433 | 0.71364 | 1.92788 |
| H | -3.58006 | -0.01039 | 2.54555 |
| H | -3.75241 | -2.38973 | -0.19106 |
| H | -4.61301 | -1.52733 | 1.08581 |
| H | -6.18609 | -2.24712 | -0.73789 |
| H | -6.11757 | -0.47790 | -0.68585 |
| H | -5.21343 | -1.36343 | -1.93441 |
| H | -0.66685 | -2.30348 | -2.79875 |
| H | -2.19369 | -1.51282 | -3.17997 |

Gibbs free energy = -4043.034289
Temperature = 225.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -1.22219 | -1.39024 | -2.74867 |
| C | 1.99141 | 0.13017 | -0.22828 |
| H | -0.68351 | -2.34571 | -2.86622 |
| Mg | -1.46141 | -0.83181 | -0.69544 |
| N | 1.88190 | 1.30814 | -0.73945 |
| S | 0.31156 | 1.97683 | -0.85657 |
| C | 0.46869 | 3.28414 | 0.50726 |
| O | -0.74690 | 1.01603 | -0.26615 |
| H | 1.12407 | -0.41420 | 0.15744 |
| C | 1.52529 | 4.29121 | 0.05031 |
| H | 2.51045 | 3.82819 | -0.04289 |
| H | 1.58942 | 5.08694 | 0.80017 |
| H | 1.26019 | 4.75421 | -0.90610 |
| C | 0.84050 | 2.58506 | 1.81290 |
| H | 1.87253 | 2.22710 | 1.80118 |
| H | 0.17544 | 1.74001 | 2.01340 |
| H | 0.73846 | 3.30314 | 2.63325 |
| C | -0.92604 | 3.91539 | 0.58341 |
| H | -0.89860 | 4.72607 | 1.31859 |
| H | -1.67439 | 3.18699 | 0.90424 |
| H | -1.23507 | 4.34425 | -0.37606 |
| C | 3.26828 | -0.56483 | -0.09917 |
| C | 3.25764 | -1.84062 | 0.49293 |
| C | 4.48265 | -0.00516 | -0.53715 |
| C | 4.44919 | -2.54751 | 0.64594 |
| H | 2.31195 | -2.26065 | 0.82781 |
| C | 5.66692 | -0.71617 | -0.38161 |
| H | 4.48115 | 0.97883 | -0.99521 |
| C | 5.65189 | -1.98685 | 0.20953 |
| H | 4.43958 | -3.53233 | 1.10277 |
| H | 6.60511 | -0.28673 | -0.71986 |
| H | 6.58055 | -2.53769 | 0.32770 |
| Br | -0.67858 | -2.17432 | 1.25009 |

| | | | |
|---|---|---|---|
| H | -2.19823 | -1.56501 | -3.23525 |
| C | -0.47160 | -0.30206 | -3.54344 |
| H | -1.00024 | 0.66072 | -3.50403 |
| H | 0.53061 | -0.11841 | -3.13049 |
| H | -0.32431 | -0.53025 | -4.61365 |
| C | -3.73380 | 0.84010 | 0.55106 |
| O | -3.41543 | -0.37698 | -0.17346 |
| C | -3.17091 | 0.81878 | 1.96083 |
| C | -4.32867 | -1.48615 | 0.02933 |
| C | -5.53305 | -1.38068 | -0.88789 |
| H | -4.81987 | 0.97579 | 0.54553 |
| H | -3.28458 | 1.64286 | -0.03676 |
| H | -3.42359 | 1.75503 | 2.47068 |
| H | -2.08433 | 0.71364 | 1.92788 |
| H | -3.58006 | -0.01038 | 2.54556 |
| H | -3.75243 | -2.38973 | -0.19103 |
| H | -4.61302 | -1.52732 | 1.08583 |
| H | -6.18610 | -2.24711 | -0.73786 |
| H | -6.11758 | -0.47789 | -0.68583 |
| H | -5.21345 | -1.36343 | -1.93439 |



## TS 4′-5

Gibbs free energy = -4043.031028
Temperature = 298.15 K
Only one imaginary frequency = -298.62
Cartesian coordinates:

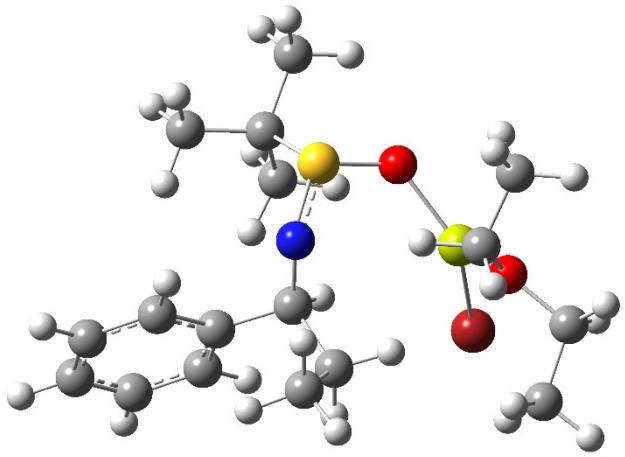
| | | | |
|---|---|---|---|
| C | 0.22742 | -1.55123 | -1.47140 |
| C | 1.47651 | 0.00765 | -0.36518 |
| H | 1.13307 | -2.14568 | -1.53252 |
| Mg | -1.06646 | -0.44911 | -0.01175 |
| N | 1.53626 | 1.08853 | -1.16696 |
| S | 0.27363 | 2.16440 | -1.07023 |
| C | 0.73832 | 3.36132 | 0.33009 |
| O | -1.00338 | 1.46022 | -0.46171 |
| H | 0.93998 | 0.05223 | 0.58680 |
| C | 2.06897 | 3.99904 | -0.07128 |
| H | 2.86724 | 3.25378 | -0.12372 |
| H | 2.34495 | 4.74786 | 0.67928 |

| | | | |
|---|---|---|---|
| H | 2.00173 | 4.50697 | -1.04003 |
| C | 0.83079 | 2.61218 | 1.65587 |
| H | 1.66903 | 1.91055 | 1.67155 |
| H | -0.09578 | 2.07097 | 1.86774 |
| H | 0.99158 | 3.33718 | 2.46185 |
| C | -0.40287 | 4.38419 | 0.35080 |
| H | -0.18819 | 5.14330 | 1.11078 |
| H | -1.35485 | 3.90858 | 0.60354 |
| H | -0.50971 | 4.89551 | -0.61230 |
| C | 2.69432 | -0.82726 | -0.22923 |
| C | 2.78215 | -1.72605 | 0.84594 |
| C | 3.75842 | -0.73334 | -1.13664 |
| C | 3.91860 | -2.51552 | 1.01194 |
| H | 1.94935 | -1.80176 | 1.54165 |
| C | 4.89331 | -1.52733 | -0.96898 |
| H | 3.68902 | -0.03445 | -1.96363 |
| C | 4.97790 | -2.41964 | 0.10374 |
| H | 3.97843 | -3.20521 | 1.84914 |
| H | 5.71479 | -1.44802 | -1.67564 |
| H | 5.86358 | -3.03530 | 0.23223 |
| Br | -1.01187 | -1.21370 | 2.29164 |
| H | -0.54108 | -2.26770 | -1.11232 |
| C | -0.14764 | -0.93097 | -2.80503 |
| H | -1.18609 | -0.57869 | -2.83084 |
| H | 0.50015 | -0.06470 | -3.00538 |
| H | -0.02171 | -1.62393 | -3.64817 |
| C | -3.85620 | 0.33642 | -0.82613 |
| O | -2.93312 | -0.78632 | -0.71802 |
| C | -4.15325 | 0.92463 | 0.54121 |
| C | -3.54774 | -2.09669 | -0.58329 |
| C | -3.82481 | -2.69884 | -1.94696 |
| H | -4.76102 | -0.01409 | -1.33089 |
| H | -3.35430 | 1.06197 | -1.46790 |
| H | -4.86937 | 1.74716 | 0.44087 |
| H | -3.23947 | 1.32063 | 0.99590 |
| H | -4.57912 | 0.17328 | 1.21323 |
| H | -2.83631 | -2.70550 | -0.01830 |
| H | -4.45371 | -1.99797 | 0.02308 |
| H | -4.27125 | -3.69179 | -1.82844 |
| H | -4.51870 | -2.07863 | -2.52278 |
| H | -2.89437 | -2.80054 | -2.51381 |

Gibbs free energy = -4043.011148
Temperature = 225.15 K
Only one imaginary frequency = -298.61
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.22742 | -1.55123 | -1.47140 |
| C | 1.47652 | 0.00765 | -0.36518 |
| H | 1.13306 | -2.14569 | -1.53250 |
| Mg | -1.06646 | -0.44910 | -0.01176 |
| N | 1.53628 | 1.08853 | -1.16695 |
| S | 0.27365 | 2.16441 | -1.07023 |
| C | 0.73834 | 3.36132 | 0.33010 |
| O | -1.00337 | 1.46023 | -0.46171 |
| H | 0.93998 | 0.05223 | 0.58681 |
| C | 2.06900 | 3.99902 | -0.07126 |
| H | 2.86726 | 3.25375 | -0.12368 |

| | | | |
|---|---|---|---|
| H | 2.34498 | 4.74785 | 0.67929 |
| H | 2.00178 | 4.50695 | -1.04002 |
| C | 0.83078 | 2.61219 | 1.65588 |
| H | 1.66901 | 1.91055 | 1.67157 |
| H | -0.09581 | 2.07099 | 1.86773 |
| H | 0.99156 | 3.33719 | 2.46185 |
| C | -0.40284 | 4.38421 | 0.35079 |
| H | -0.18817 | 5.14331 | 1.11077 |
| H | -1.35483 | 3.90861 | 0.60350 |
| H | -0.50965 | 4.89553 | -0.61231 |
| C | 2.69432 | -0.82727 | -0.22922 |
| C | 2.78214 | -1.72606 | 0.84594 |
| C | 3.75842 | -0.73335 | -1.13663 |
| C | 3.91859 | -2.51554 | 1.01195 |
| H | 1.94934 | -1.80177 | 1.54165 |
| C | 4.89330 | -1.52735 | -0.96897 |
| H | 3.68903 | -0.03446 | -1.96361 |
| C | 4.97788 | -2.41966 | 0.10375 |
| H | 3.97841 | -3.20523 | 1.84914 |
| H | 5.71479 | -1.44804 | -1.67562 |
| H | 5.86357 | -3.03533 | 0.23224 |
| Br | -1.01190 | -1.21370 | 2.29163 |
| H | -0.54109 | -2.26769 | -1.11231 |
| C | -0.14763 | -0.93097 | -2.80502 |
| H | -1.18608 | -0.57869 | -2.83084 |
| H | 0.50016 | -0.06470 | -3.00537 |
| H | -0.02170 | -1.62393 | -3.64817 |
| C | -3.85620 | 0.33642 | -0.82614 |
| O | -2.93312 | -0.78632 | -0.71802 |
| C | -4.15326 | 0.92465 | 0.54119 |
| C | -3.54773 | -2.09668 | -0.58329 |
| C | -3.82480 | -2.69884 | -1.94696 |
| H | -4.76101 | -0.01409 | -1.33091 |
| H | -3.35429 | 1.06197 | -1.46792 |
| H | -4.86937 | 1.74717 | 0.44083 |
| H | -3.23947 | 1.32065 | 0.99587 |
| H | -4.57913 | 0.17330 | 1.21321 |
| H | -2.83630 | -2.70549 | -0.01829 |
| H | -4.45370 | -1.99797 | 0.02307 |
| H | -4.27123 | -3.69179 | -1.82844 |
| H | -4.51869 | -2.07863 | -2.52278 |
| H | -2.89435 | -2.80054 | -2.51381 |



## 9

Gibbs free energy = -4043.078955
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

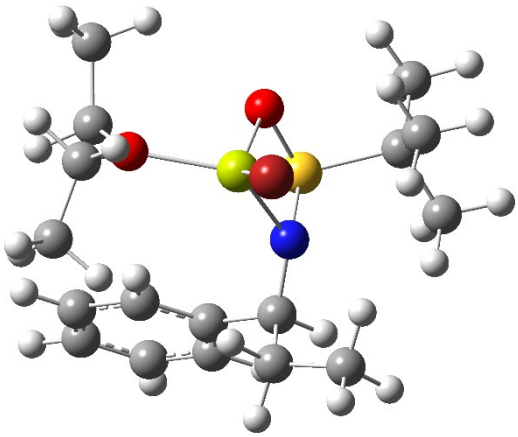
| | | | |
|---|---|---|---|
| C | 0.06487 | -1.82057 | -0.98825 |
| C | 0.95759 | -0.66389 | -0.45820 |
| H | 0.14422 | -2.66602 | -0.29347 |
| Mg | -1.92483 | 0.56795 | 0.65143 |
| N | 0.80639 | 0.50588 | -1.34118 |
| S | 0.51240 | 1.96190 | -0.78222 |
| C | 1.74856 | 2.57204 | 0.54948 |
| O | -0.81433 | 2.00571 | 0.16509 |
| H | 0.60703 | -0.46552 | 0.56667 |
| C | 3.13326 | 2.53457 | -0.09799 |
| H | 3.44406 | 1.51317 | -0.32665 |
| H | 3.86794 | 2.96808 | 0.59088 |
| H | 3.16216 | 3.11988 | -1.02448 |
| C | 1.68947 | 1.73492 | 1.82632 |
| H | 2.12334 | 0.74286 | 1.68785 |
| H | 0.65901 | 1.62895 | 2.17784 |
| H | 2.26289 | 2.23827 | 2.61460 |
| C | 1.31914 | 4.01728 | 0.83610 |
| H | 2.03923 | 4.47971 | 1.52162 |
| H | 0.33068 | 4.04992 | 1.30130 |
| H | 1.29321 | 4.62319 | -0.07690 |
| C | 2.40371 | -1.13377 | -0.32914 |
| C | 2.80831 | -1.82778 | 0.81983 |
| C | 3.33878 | -0.92951 | -1.35226 |
| C | 4.11578 | -2.30160 | 0.94881 |
| H | 2.09253 | -1.98732 | 1.62338 |
| C | 4.64647 | -1.40460 | -1.22849 |
| H | 3.03455 | -0.37623 | -2.23439 |
| C | 5.04057 | -2.09203 | -0.07741 |
| H | 4.41298 | -2.82818 | 1.85177 |
| H | 5.35951 | -1.23387 | -2.03078 |
| H | 6.05954 | -2.45580 | 0.02124 |
| Br | -1.94077 | -0.93544 | 2.50451 |
| H | -0.98008 | -1.48937 | -0.94813 |
| C | 0.37988 | -2.27368 | -2.41337 |
| H | 0.31002 | -1.43378 | -3.11081 |
| H | 1.39015 | -2.68887 | -2.48827 |

| | | | |
|---|---|---|---|
| H | -0.32515 | -3.04710 | -2.73741 |
| C | -2.80594 | 0.46312 | -2.21095 |
| O | -3.10131 | 0.00289 | -0.85269 |
| C | -3.43380 | 1.82077 | -2.44673 |
| C | -4.24815 | -0.88577 | -0.70951 |
| C | -3.85890 | -2.32663 | -0.97570 |
| H | -3.17067 | -0.29389 | -2.90988 |
| H | -1.71565 | 0.49814 | -2.27984 |
| H | -3.20125 | 2.16339 | -3.46046 |
| H | -3.03301 | 2.55009 | -1.73558 |
| H | -4.52212 | 1.77883 | -2.33762 |
| H | -4.59677 | -0.74906 | 0.31746 |
| H | -5.03276 | -0.53365 | -1.38613 |
| H | -4.73757 | -2.96916 | -0.85601 |
| H | -3.47848 | -2.45530 | -1.99358 |
| H | -3.09030 | -2.65414 | -0.26989 |

Gibbs free energy = -4043.059156
Temperature = 225.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.06481 | -1.82053 | -0.98818 |
| C | 0.95757 | -0.66387 | -0.45817 |
| H | 0.14414 | -2.66597 | -0.29338 |
| Mg | -1.92483 | 0.56797 | 0.65144 |
| N | 0.80637 | 0.50590 | -1.34116 |
| S | 0.51241 | 1.96192 | -0.78218 |
| C | 1.74862 | 2.57205 | 0.54948 |
| O | -0.81429 | 2.00571 | 0.16518 |
| H | 0.60705 | -0.46548 | 0.56671 |
| C | 3.13330 | 2.53456 | -0.09803 |
| H | 3.44408 | 1.51315 | -0.32670 |
| H | 3.86800 | 2.96807 | 0.59081 |
| H | 3.16217 | 3.11986 | -1.02452 |
| C | 1.68956 | 1.73492 | 1.82632 |
| H | 2.12342 | 0.74287 | 1.68784 |
| H | 0.65910 | 1.62895 | 2.17786 |
| H | 2.26300 | 2.23828 | 2.61459 |
| C | 1.31922 | 4.01729 | 0.83611 |
| H | 2.03933 | 4.47972 | 1.52161 |
| H | 0.33077 | 4.04994 | 1.30133 |
| H | 1.29327 | 4.62320 | -0.07690 |
| C | 2.40369 | -1.13379 | -0.32915 |
| C | 2.80831 | -1.82780 | 0.81981 |
| C | 3.33873 | -0.92956 | -1.35230 |
| C | 4.11578 | -2.30164 | 0.94875 |
| H | 2.09256 | -1.98732 | 1.62338 |
| C | 4.64641 | -1.40467 | -1.22857 |
| H | 3.03449 | -0.37627 | -2.23443 |
| C | 5.04054 | -2.09210 | -0.07750 |
| H | 4.41299 | -2.82822 | 1.85171 |
| H | 5.35943 | -1.23396 | -2.03088 |
| H | 6.05950 | -2.45589 | 0.02112 |
| Br | -1.94074 | -0.93545 | 2.50449 |
| H | -0.98013 | -1.48930 | -0.94806 |
| C | 0.37978 | -2.27369 | -2.41330 |
| H | 0.30994 | -1.43380 | -3.11076 |

| | | | |
|---|---|---|---|
| H | 1.39002 | -2.68892 | -2.48820 |
| H | -0.32529 | -3.04709 | -2.73731 |
| C | -2.80593 | 0.46313 | -2.21095 |
| O | -3.10129 | 0.00291 | -0.85269 |
| C | -3.43382 | 1.82077 | -2.44676 |
| C | -4.24818 | -0.88569 | -0.70949 |
| C | -3.85899 | -2.32657 | -0.97566 |
| H | -3.17064 | -0.29390 | -2.90987 |
| H | -1.71564 | 0.49818 | -2.27983 |
| H | -3.20128 | 2.16337 | -3.46050 |
| H | -3.03305 | 2.55010 | -1.73562 |
| H | -4.52214 | 1.77880 | -2.33766 |
| H | -4.59679 | -0.74894 | 0.31748 |
| H | -5.03277 | -0.53354 | -1.38611 |
| H | -4.73769 | -2.96906 | -0.85594 |
| H | -3.47859 | -2.45528 | -1.99354 |
| H | -3.09040 | -2.65410 | -0.26986 |



## 5

Gibbs free energy = -4043.113151
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

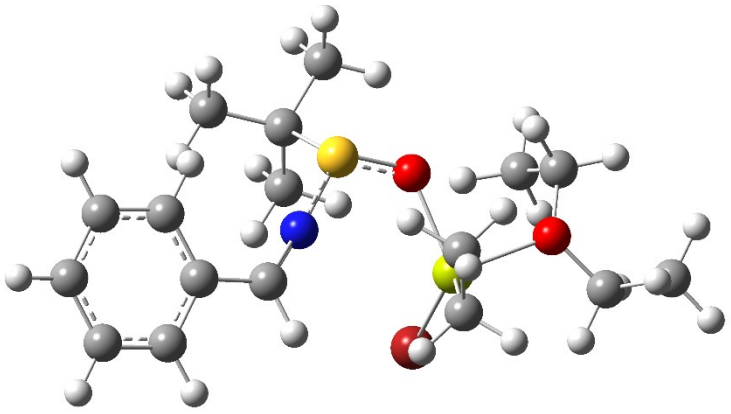
| | | | |
|---|---|---|---|
| C | -0.84257 | 0.29538 | -2.72186 |
| C | -1.42023 | 0.83662 | -1.39763 |
| H | -0.32455 | -0.65006 | -2.50701 |
| Mg | 1.18587 | -0.30405 | 0.22018 |
| N | -0.28452 | 0.96499 | -0.47238 |
| S | -0.52644 | 1.60701 | 1.02931 |
| C | 0.28373 | 3.31049 | 0.96576 |
| O | 0.55553 | 0.76295 | 1.82761 |
| H | -1.85824 | 1.82198 | -1.61432 |
| C | -0.57691 | 4.13829 | 0.00768 |
| H | -0.52616 | 3.74241 | -1.01073 |
| H | -0.20800 | 5.16965 | -0.01151 |
| H | -1.62703 | 4.16780 | 0.32172 |
| C | 1.71558 | 3.16802 | 0.45928 |
| H | 1.73736 | 2.71312 | -0.53504 |
| H | 2.31608 | 2.55393 | 1.13654 |
| H | 2.17817 | 4.15886 | 0.39452 |

| | | | |
|---|---|---|---|
| C | 0.23419 | 3.85808 | 2.39459 |
| H | 0.66585 | 4.86511 | 2.41514 |
| H | 0.80912 | 3.22592 | 3.07762 |
| H | -0.79435 | 3.92838 | 2.76671 |
| C | -2.54012 | -0.05727 | -0.87464 |
| C | -3.85244 | 0.41825 | -0.77615 |
| C | -2.27596 | -1.37890 | -0.48581 |
| C | -4.87955 | -0.40298 | -0.30040 |
| H | -4.07146 | 1.44181 | -1.07160 |
| C | -3.29647 | -2.20342 | -0.01367 |
| H | -1.26118 | -1.75903 | -0.54776 |
| C | -4.60478 | -1.71698 | 0.08179 |
| H | -5.89144 | -0.01400 | -0.22557 |
| H | -3.07382 | -3.22558 | 0.28061 |
| H | -5.40029 | -2.35689 | 0.45303 |
| Br | 3.23353 | -0.53827 | -1.04704 |
| H | -1.67589 | 0.05575 | -3.39304 |
| C | 0.12324 | 1.26558 | -3.40308 |
| H | -0.37864 | 2.20777 | -3.65500 |
| H | 0.96937 | 1.49364 | -2.75004 |
| H | 0.51636 | 0.83777 | -4.33191 |
| C | -0.12710 | -2.32686 | 2.07364 |
| O | 0.81081 | -2.15385 | 0.97311 |
| C | 0.58818 | -2.24918 | 3.40719 |
| C | 1.44733 | -3.37083 | 0.49044 |
| C | 0.65929 | -3.96238 | -0.66171 |
| H | -0.64726 | -3.27932 | 1.93164 |
| H | -0.85358 | -1.51980 | 1.97248 |
| H | -0.13214 | -2.39227 | 4.22001 |
| H | 1.05020 | -1.26456 | 3.52216 |
| H | 1.35992 | -3.02045 | 3.49453 |
| H | 2.44728 | -3.07099 | 0.17217 |
| H | 1.53998 | -4.06724 | 1.32890 |
| H | 1.15214 | -4.87308 | -1.01849 |
| H | -0.35993 | -4.22143 | -0.35816 |
| H | 0.60960 | -3.25257 | -1.49386 |

Gibbs free energy = --4043.093502
Temperature = 225.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -0.84256 | 0.29538 | -2.72186 |
| C | -1.42022 | 0.83662 | -1.39763 |
| H | -0.32455 | -0.65006 | -2.50701 |
| Mg | 1.18588 | -0.30405 | 0.22018 |
| N | -0.28452 | 0.96499 | -0.47238 |
| S | -0.52643 | 1.60700 | 1.02931 |
| C | 0.28373 | 3.31049 | 0.96576 |
| O | 0.55553 | 0.76295 | 1.82762 |
| H | -1.85824 | 1.82198 | -1.61432 |
| C | -0.57692 | 4.13828 | 0.00768 |
| H | -0.52616 | 3.74241 | -1.01073 |
| H | -0.20801 | 5.16965 | -0.01151 |
| H | -1.62703 | 4.16779 | 0.32173 |
| C | 1.71558 | 3.16802 | 0.45928 |
| H | 1.73736 | 2.71312 | -0.53504 |
| H | 2.31608 | 2.55393 | 1.13653 |

| | | | |
|---|---|---|---|
| H | 2.17816 | 4.15886 | 0.39451 |
| C | 0.23420 | 3.85808 | 2.39459 |
| H | 0.66585 | 4.86511 | 2.41514 |
| H | 0.80912 | 3.22592 | 3.07762 |
| H | -0.79435 | 3.92837 | 2.76671 |
| C | -2.54012 | -0.05727 | -0.87464 |
| C | -3.85244 | 0.41826 | -0.77616 |
| C | -2.27596 | -1.37890 | -0.48582 |
| C | -4.87955 | -0.40297 | -0.30040 |
| H | -4.07145 | 1.44181 | -1.07161 |
| C | -3.29648 | -2.20341 | -0.01368 |
| H | -1.26119 | -1.75903 | -0.54776 |
| C | -4.60478 | -1.71698 | 0.08178 |
| H | -5.89144 | -0.01399 | -0.22558 |
| H | -3.07383 | -3.22558 | 0.28060 |
| H | -5.40030 | -2.35688 | 0.45302 |
| Br | 3.23353 | -0.53827 | -1.04704 |
| H | -1.67589 | 0.05576 | -3.39304 |
| C | 0.12324 | 1.26559 | -3.40308 |
| H | -0.37863 | 2.20778 | -3.65499 |
| H | 0.96938 | 1.49364 | -2.75004 |
| H | 0.51636 | 0.83778 | -4.33191 |
| C | -0.12712 | -2.32686 | 2.07364 |
| O | 0.81080 | -2.15385 | 0.97311 |
| C | 0.58817 | -2.24917 | 3.40719 |
| C | 1.44733 | -3.37082 | 0.49044 |
| C | 0.65929 | -3.96238 | -0.66170 |
| H | -0.64728 | -3.27931 | 1.93164 |
| H | -0.85359 | -1.51980 | 1.97248 |
| H | -0.13216 | -2.39226 | 4.22001 |
| H | 1.05018 | -1.26456 | 3.52216 |
| H | 1.35990 | -3.02044 | 3.49453 |
| H | 2.44728 | -3.07098 | 0.17218 |
| H | 1.53996 | -4.06724 | 1.32891 |
| H | 1.15215 | -4.87308 | -1.01848 |
| H | -0.35993 | -4.22143 | -0.35816 |
| H | 0.60961 | -3.25257 | -1.49385 |



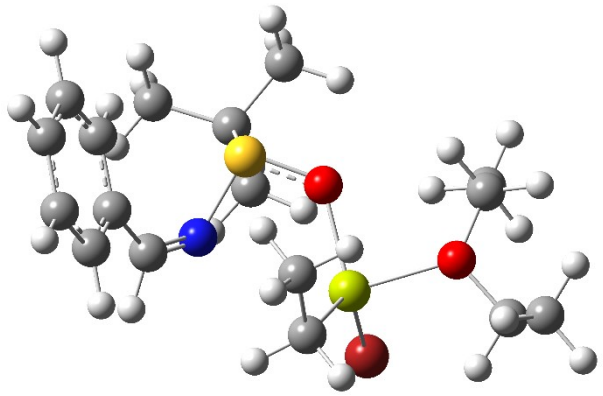
**TS 4′-4Z**

Gibbs free energy = -4043.023191

Temperature = 298.15 K

Only one imaginary frequency = -253.46
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.90582 | -2.57030 | 1.16012 |
| C | -2.18962 | -0.89811 | -0.13117 |
| H | 0.10072 | -3.09969 | 0.62164 |
| Mg | 1.57920 | -0.81103 | 0.13271 |
| N | -1.42787 | 0.04464 | 0.25500 |
| S | -0.64488 | 1.14638 | 1.09232 |
| C | -0.92429 | 2.69685 | 0.01484 |
| O | 0.88197 | 0.91586 | 0.94327 |
| H | -1.72119 | -1.78415 | -0.57666 |
| C | -2.41002 | 3.04101 | 0.07886 |
| H | -3.01949 | 2.28635 | -0.42256 |
| H | -2.56346 | 3.99541 | -0.43619 |
| H | -2.76278 | 3.15965 | 1.10896 |
| C | -0.45538 | 2.38478 | -1.40230 |
| H | -1.09276 | 1.63731 | -1.88104 |
| H | 0.57127 | 2.01391 | -1.41493 |
| H | -0.50245 | 3.30634 | -1.99301 |
| C | -0.05663 | 3.77203 | 0.67612 |
| H | -0.17339 | 4.70282 | 0.11136 |
| H | 0.99942 | 3.49251 | 0.66361 |
| H | -0.36110 | 3.96580 | 1.71039 |
| C | -3.65186 | -0.92046 | -0.06049 |
| C | -4.33567 | -1.95082 | -0.72927 |
| C | -4.37924 | 0.02663 | 0.68270 |
| C | -5.72609 | -2.02001 | -0.67518 |
| H | -3.77030 | -2.68984 | -1.29079 |
| C | -5.76617 | -0.05119 | 0.74262 |
| H | -3.84962 | 0.80661 | 1.21840 |
| C | -6.44156 | -1.07016 | 0.05896 |
| H | -6.25076 | -2.81294 | -1.19911 |
| H | -6.32507 | 0.67743 | 1.32192 |
| H | -7.52524 | -1.12544 | 0.10498 |
| Br | 1.72747 | -0.65016 | -2.32587 |
| H | 1.71212 | -3.32106 | 1.24482 |
| C | 0.40658 | -2.23606 | 2.57943 |
| H | 1.18668 | -1.73642 | 3.17164 |
| H | -0.44610 | -1.54250 | 2.55313 |
| H | 0.07418 | -3.10560 | 3.17406 |
| C | 3.92346 | 1.00968 | 1.04233 |
| O | 3.52432 | -0.34815 | 0.72516 |
| C | 3.83719 | 1.91630 | -0.17268 |
| C | 4.58417 | -1.21546 | 0.25321 |
| C | 5.32531 | -1.85220 | 1.41493 |
| H | 4.93365 | 0.98679 | 1.46375 |
| H | 3.23214 | 1.33804 | 1.82062 |
| H | 4.15824 | 2.92794 | 0.10008 |
| H | 2.80754 | 1.95816 | -0.53490 |
| H | 4.47419 | 1.55924 | -0.98738 |
| H | 4.09580 | -1.97788 | -0.36040 |
| H | 5.25115 | -0.64416 | -0.40160 |
| H | 6.09744 | -2.53013 | 1.03529 |
| H | 5.81295 | -1.10029 | 2.04335 |
| H | 4.63140 | -2.42752 | 2.03565 |

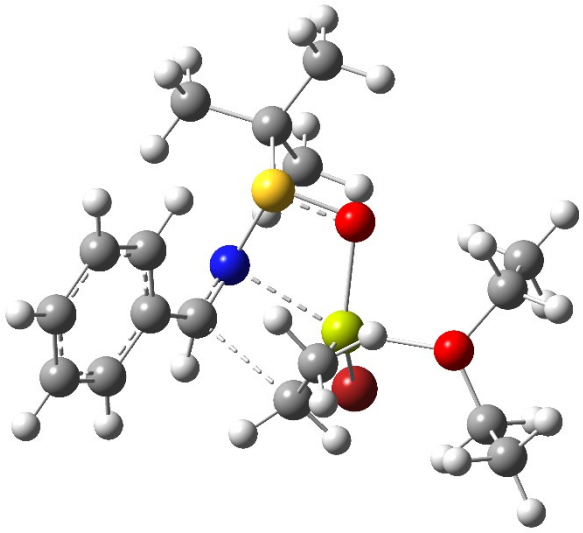


**4Z**

Gibbs free energy = -4043.042841
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -0.31936 | -2.53639 | 0.83591 |
| C | 2.29767 | -0.15762 | 1.34918 |
| H | 0.30738 | -2.43955 | 1.73983 |
| Mg | -1.37550 | -0.71678 | 0.41168 |
| N | 1.28648 | 0.55252 | 0.97944 |
| S | 1.05204 | 1.00421 | -0.68236 |
| C | 0.83277 | 2.85939 | -0.44655 |
| O | -0.38275 | 0.48153 | -0.90793 |
| H | 2.19811 | -0.53169 | 2.37214 |
| C | 2.20945 | 3.43685 | -0.11243 |
| H | 2.60968 | 3.02054 | 0.81695 |
| H | 2.10512 | 4.51814 | 0.02500 |
| H | 2.93059 | 3.27555 | -0.92051 |
| C | -0.19451 | 3.11573 | 0.65363 |
| H | 0.18837 | 2.83876 | 1.63736 |
| H | -1.11745 | 2.55756 | 0.48102 |
| H | -0.43067 | 4.18544 | 0.65941 |
| C | 0.32459 | 3.34765 | -1.80916 |
| H | 0.19684 | 4.43391 | -1.76235 |
| H | -0.64246 | 2.89953 | -2.05304 |
| H | 1.03175 | 3.12685 | -2.61611 |
| C | 3.51374 | -0.59811 | 0.65426 |
| C | 4.02725 | -1.85661 | 1.02236 |
| C | 4.17443 | 0.15269 | -0.33442 |
| C | 5.14265 | -2.37774 | 0.37327 |
| H | 3.52946 | -2.42869 | 1.79997 |
| C | 5.30310 | -0.36479 | -0.96546 |
| H | 3.84135 | 1.15396 | -0.57729 |
| C | 5.78064 | -1.63297 | -0.62307 |
| H | 5.51945 | -3.35780 | 0.64859 |
| H | 5.81535 | 0.22544 | -1.71886 |
| H | 6.65836 | -2.03367 | -1.12132 |
| Br | -2.81259 | 0.55349 | 1.96900 |
| H | -0.98445 | -3.39044 | 1.05335 |
| C | 0.58244 | -2.91872 | -0.35412 |
| H | -0.01230 | -3.10348 | -1.25988 |
| H | 1.28075 | -2.11109 | -0.61324 |

| | | | |
|---|---|---|---|
| H | 1.20439 | -3.81865 | -0.20012 |
| C | -2.98084 | -0.29651 | -2.23883 |
| O | -2.77560 | -1.15733 | -1.09098 |
| C | -3.49399 | 1.07379 | -1.83160 |
| C | -3.92872 | -1.93244 | -0.68358 |
| C | -4.02809 | -3.22284 | -1.47720 |
| H | -3.66459 | -0.79664 | -2.93261 |
| H | -2.00312 | -0.21683 | -2.71743 |
| H | -3.64480 | 1.68900 | -2.72596 |
| H | -2.76919 | 1.56825 | -1.18068 |
| H | -4.44479 | 1.00482 | -1.29493 |
| H | -3.78849 | -2.14233 | 0.38050 |
| H | -4.82900 | -1.31561 | -0.77896 |
| H | -4.89029 | -3.80427 | -1.13289 |
| H | -4.15466 | -3.03046 | -2.54731 |
| H | -3.12461 | -3.82402 | -1.33587 |

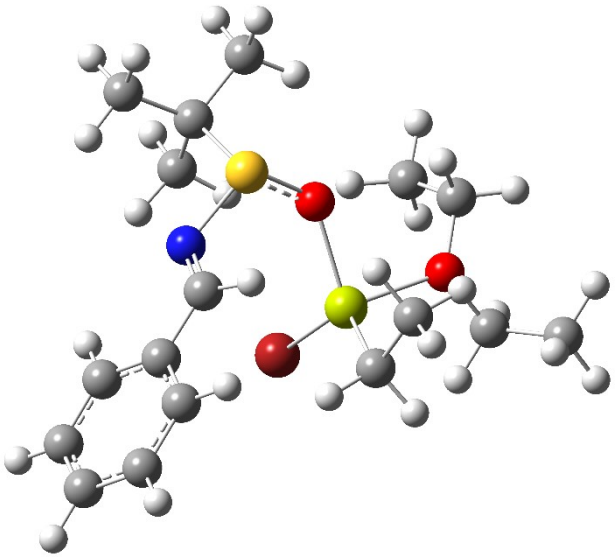


## TS 4Z-5

Gibbs free energy = -4043.021862
Temperature = 298.15 K
Only one imaginary frequency = -237.44
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.44265 | -2.22744 | 0.07881 |
| C | 1.63970 | -0.20257 | 1.00342 |
| H | 1.17397 | -2.70058 | 0.73200 |
| Mg | -0.91084 | -0.43140 | 0.22731 |
| N | 0.94364 | 0.91966 | 0.77696 |
| S | 0.83606 | 1.59522 | -0.77229 |
| C | 0.34960 | 3.33573 | -0.28503 |
| O | -0.49345 | 0.91784 | -1.25415 |
| H | 1.38920 | -0.61936 | 1.97687 |
| C | 1.59969 | 3.96491 | 0.33696 |
| H | 1.88600 | 3.45171 | 1.25926 |
| H | 1.38275 | 5.01043 | 0.57992 |
| H | 2.45079 | 3.95290 | -0.35324 |
| C | -0.82785 | 3.29861 | 0.68591 |
| H | -0.55888 | 2.81940 | 1.62796 |

| | | | |
|---|---|---|---|
| H | -1.67711 | 2.76019 | 0.25744 |
| H | -1.14253 | 4.32804 | 0.88862 |
| C | -0.03502 | 4.01306 | -1.60650 |
| H | -0.30875 | 5.05318 | -1.40227 |
| H | -0.89438 | 3.51812 | -2.06825 |
| H | 0.79496 | 4.01866 | -2.32162 |
| C | 2.94726 | -0.66466 | 0.50026 |
| C | 3.58066 | -1.68524 | 1.23806 |
| C | 3.61069 | -0.14722 | -0.62804 |
| C | 4.82528 | -2.17853 | 0.86071 |
| H | 3.08534 | -2.08845 | 2.11686 |
| C | 4.85836 | -0.64341 | -1.00442 |
| H | 3.16629 | 0.64401 | -1.21620 |
| C | 5.46863 | -1.66002 | -0.26696 |
| H | 5.29483 | -2.96365 | 1.44563 |
| H | 5.35443 | -0.23137 | -1.87806 |
| H | 6.44006 | -2.04275 | -0.56571 |
| Br | -2.31873 | -0.15736 | 2.21904 |
| H | -0.51017 | -2.74145 | 0.30583 |
| C | 0.79869 | -2.39916 | -1.39462 |
| H | -0.00649 | -2.03805 | -2.04502 |
| H | 1.70258 | -1.83414 | -1.65680 |
| H | 0.99271 | -3.44591 | -1.68047 |
| C | -2.98245 | -0.48253 | -2.08874 |
| O | -2.35889 | -1.27990 | -1.04949 |
| C | -3.80268 | 0.64916 | -1.49536 |
| C | -3.15814 | -2.39544 | -0.58354 |
| C | -2.92313 | -3.62764 | -1.43847 |
| H | -3.59290 | -1.14220 | -2.71386 |
| H | -2.16183 | -0.09483 | -2.69356 |
| H | -4.27112 | 1.22864 | -2.29845 |
| H | -3.15890 | 1.31580 | -0.91569 |
| H | -4.58931 | 0.27187 | -0.83509 |
| H | -2.85971 | -2.56665 | 0.45310 |
| H | -4.21225 | -2.09787 | -0.57172 |
| H | -3.52950 | -4.45906 | -1.06280 |
| H | -3.19941 | -3.45070 | -2.48280 |
| H | -1.87024 | -3.92186 | -1.40348 |



## 8

Gibbs free energy = -4043.050017
Temperature = 298.15 K
Only one imaginary frequency = -22.70
Cartesian coordinates:

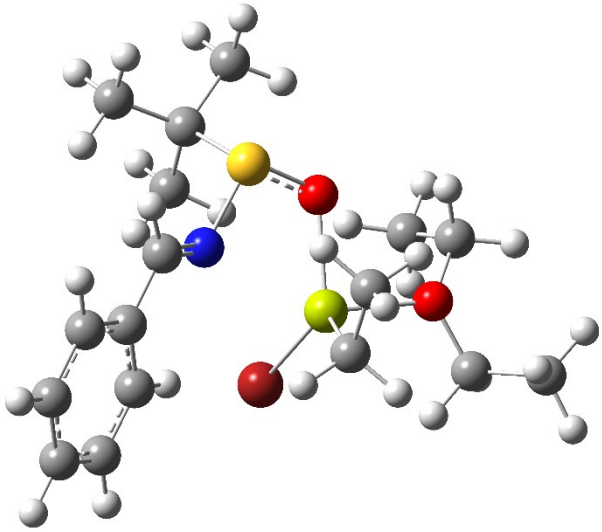
| | | | |
|---|---|---|---|
| C | -3.58748 | -2.34459 | 0.19989 |
| O | -2.98192 | -1.16925 | -0.39306 |
| C | -4.15885 | -3.25739 | -0.86940 |
| C | -3.87942 | -0.05586 | -0.62757 |
| C | -3.97929 | 0.84329 | 0.59151 |
| H | -4.34557 | -2.02951 | 0.92476 |
| H | -2.79079 | -2.84615 | 0.75662 |
| H | -4.59157 | -4.14955 | -0.40385 |
| H | -3.36945 | -3.57271 | -1.55849 |
| H | -4.94539 | -2.75828 | -1.44426 |
| H | -3.45281 | 0.48352 | -1.47553 |
| H | -4.85574 | -0.45172 | -0.92618 |
| H | -4.67511 | 1.66525 | 0.38970 |
| H | -4.33748 | 0.29414 | 1.46754 |
| H | -2.99798 | 1.26005 | 0.82763 |
| C | 0.01851 | -2.39956 | -1.35181 |
| C | 2.15989 | 0.29650 | -1.03045 |
| H | 1.10660 | -2.48117 | -1.20005 |
| Mg | -0.93312 | -0.92780 | -0.11535 |
| H | -0.36519 | -3.40841 | -1.11631 |
| N | 1.58691 | 1.29914 | -0.44769 |
| S | 0.18699 | 1.89080 | -1.27801 |
| C | -0.12571 | 3.38948 | -0.20261 |
| O | -0.97565 | 0.92334 | -0.94826 |
| H | 1.81399 | -0.11023 | -1.98709 |
| C | -0.23836 | 2.96216 | 1.25907 |
| H | 0.71824 | 2.60932 | 1.64766 |
| H | -0.55804 | 3.82836 | 1.84869 |
| H | -0.96917 | 2.16158 | 1.38992 |
| C | 1.04578 | 4.34513 | -0.44749 |
| H | 1.13408 | 4.62451 | -1.50311 |
| H | 0.86917 | 5.26078 | 0.12646 |
| H | 1.99327 | 3.91292 | -0.11447 |

| | | | |
|---|---|---|---|
| C | -1.44817 | 3.96604 | -0.72479 |
| H | -1.67714 | 4.87671 | -0.16260 |
| H | -1.38925 | 4.23272 | -1.78585 |
| H | -2.27113 | 3.26054 | -0.58316 |
| C | 3.30727 | -0.38229 | -0.43905 |
| C | 3.91892 | -1.41907 | -1.16562 |
| C | 3.79933 | -0.03714 | 0.83413 |
| C | 5.01455 | -2.09518 | -0.63305 |
| H | 3.52867 | -1.69024 | -2.14269 |
| C | 4.89121 | -0.71638 | 1.36097 |
| H | 3.31245 | 0.75270 | 1.39599 |
| C | 5.50062 | -1.74378 | 0.62861 |
| H | 5.48469 | -2.89523 | -1.19623 |
| H | 5.26896 | -0.45340 | 2.34425 |
| H | 6.35174 | -2.27299 | 1.04709 |
| Br | -0.74376 | -0.73477 | 2.33169 |
| C | -0.26305 | -2.11330 | -2.83973 |
| H | 0.16680 | -2.84620 | -3.54529 |
| H | -1.34323 | -2.08517 | -3.04175 |
| H | 0.12153 | -1.12950 | -3.14729 |

Gibbs free energy = -4043.029559
Temperature = 225.15 K
Only one imaginary frequency = -22.70
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -3.58748 | -2.34459 | 0.19989 |
| O | -2.98192 | -1.16925 | -0.39306 |
| C | -4.15885 | -3.25739 | -0.86940 |
| C | -3.87942 | -0.05586 | -0.62757 |
| C | -3.97929 | 0.84329 | 0.59151 |
| H | -4.34557 | -2.02951 | 0.92476 |
| H | -2.79079 | -2.84615 | 0.75662 |
| H | -4.59157 | -4.14955 | -0.40385 |
| H | -3.36945 | -3.57271 | -1.55849 |
| H | -4.94539 | -2.75828 | -1.44426 |
| H | -3.45281 | 0.48352 | -1.47553 |
| H | -4.85574 | -0.45172 | -0.92618 |
| H | -4.67511 | 1.66525 | 0.38970 |
| H | -4.33748 | 0.29414 | 1.46754 |
| H | -2.99798 | 1.26005 | 0.82763 |
| C | 0.01851 | -2.39956 | -1.35181 |
| C | 2.15989 | 0.29650 | -1.03045 |
| H | 1.10660 | -2.48117 | -1.20005 |
| Mg | -0.93312 | -0.92780 | -0.11535 |
| H | -0.36519 | -3.40841 | -1.11631 |
| N | 1.58691 | 1.29914 | -0.44769 |
| S | 0.18699 | 1.89080 | -1.27801 |
| C | -0.12571 | 3.38948 | -0.20261 |
| O | -0.97565 | 0.92334 | -0.94826 |
| H | 1.81399 | -0.11023 | -1.98709 |
| C | -0.23836 | 2.96216 | 1.25907 |
| H | 0.71824 | 2.60932 | 1.64766 |
| H | -0.55804 | 3.82836 | 1.84869 |
| H | -0.96917 | 2.16158 | 1.38992 |
| C | 1.04578 | 4.34513 | -0.44749 |
| H | 1.13408 | 4.62451 | -1.50311 |
| H | 0.86917 | 5.26078 | 0.12646 |

| | | | |
|---|---|---|---|
| H | 1.99327 | 3.91292 | -0.11447 |
| C | -1.44817 | 3.96604 | -0.72479 |
| H | -1.67714 | 4.87671 | -0.16260 |
| H | -1.38925 | 4.23272 | -1.78585 |
| H | -2.27113 | 3.26054 | -0.58316 |
| C | 3.30727 | -0.38229 | -0.43905 |
| C | 3.91892 | -1.41907 | -1.16562 |
| C | 3.79933 | -0.03714 | 0.83413 |
| C | 5.01455 | -2.09518 | -0.63305 |
| H | 3.52867 | -1.69024 | -2.14269 |
| C | 4.89121 | -0.71638 | 1.36097 |
| H | 3.31245 | 0.75270 | 1.39599 |
| C | 5.50062 | -1.74378 | 0.62861 |
| H | 5.48469 | -2.89523 | -1.19623 |
| H | 5.26896 | -0.45340 | 2.34425 |
| H | 6.35174 | -2.27299 | 1.04709 |
| Br | -0.74376 | -0.73477 | 2.33169 |
| C | -0.26305 | -2.11330 | -2.83973 |
| H | 0.16680 | -2.84620 | -3.54529 |
| H | -1.34323 | -2.08517 | -3.04175 |
| H | 0.12153 | -1.12950 | -3.14729 |



## 6

Gibbs free energy = -4043.05329
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

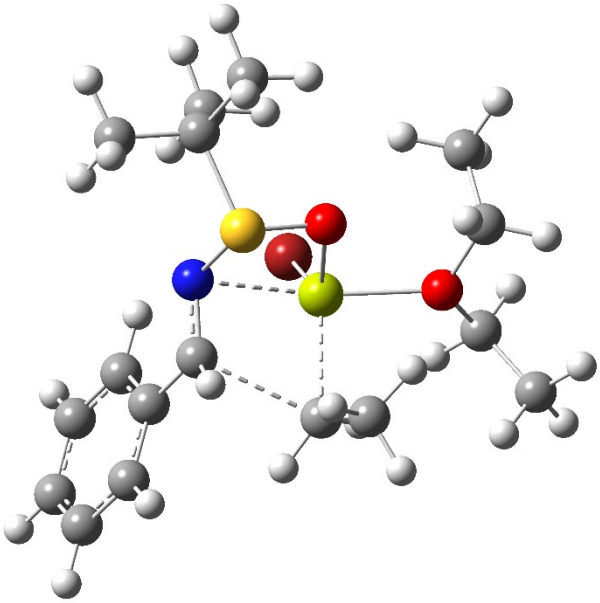
| | | | |
|---|---|---|---|
| C | -3.55189 | -2.23510 | -0.20890 |
| O | -3.01842 | -0.94096 | -0.57554 |
| C | -4.21466 | -2.91160 | -1.39580 |
| C | -3.96532 | 0.15394 | -0.53314 |
| C | -3.98947 | 0.81861 | 0.83174 |
| H | -4.23852 | -2.11625 | 0.63688 |
| H | -2.69865 | -2.82097 | 0.14283 |
| H | -4.57382 | -3.90447 | -1.10363 |
| H | -3.49623 | -3.02794 | -2.21319 |
| H | -5.07052 | -2.33702 | -1.76406 |

| | | | |
|---|---|---|---|
| H | -3.63236 | 0.85630 | -1.29952 |
| H | -4.95264 | -0.22393 | -0.81854 |
| H | -4.72327 | 1.63249 | 0.83407 |
| H | -4.25514 | 0.10899 | 1.62071 |
| H | -3.00487 | 1.23219 | 1.06089 |
| C | -0.06823 | -1.98166 | -1.78057 |
| C | 2.41639 | 0.72911 | -0.86764 |
| H | 0.93685 | -2.33627 | -1.49686 |
| Mg | -0.93792 | -0.69031 | -0.29709 |
| H | -0.66352 | -2.90432 | -1.90294 |
| N | 1.20323 | 0.83079 | -0.43913 |
| S | 0.15379 | 2.01021 | -1.11420 |
| C | 0.20743 | 3.31238 | 0.24837 |
| O | -1.19273 | 1.27765 | -0.91790 |
| H | 2.83042 | 1.39942 | -1.62794 |
| C | 0.01154 | 2.63947 | 1.60379 |
| H | 0.85531 | 1.99793 | 1.86417 |
| H | -0.08380 | 3.41940 | 2.36698 |
| H | -0.89338 | 2.02888 | 1.61863 |
| C | 1.56318 | 4.00976 | 0.12601 |
| H | 1.71644 | 4.44270 | -0.86846 |
| H | 1.59717 | 4.82676 | 0.85412 |
| H | 2.39197 | 3.33206 | 0.35093 |
| C | -0.95513 | 4.25326 | -0.09086 |
| H | -0.97813 | 5.05752 | 0.65159 |
| H | -0.83912 | 4.71175 | -1.07905 |
| H | -1.91230 | 3.72602 | -0.05502 |
| C | 3.30232 | -0.30500 | -0.35029 |
| C | 4.59185 | -0.42738 | -0.89616 |
| C | 2.88334 | -1.18353 | 0.67012 |
| C | 5.45440 | -1.41955 | -0.43517 |
| H | 4.90764 | 0.25210 | -1.68321 |
| C | 3.75020 | -2.17158 | 1.12191 |
| H | 1.88921 | -1.08297 | 1.09724 |
| C | 5.03334 | -2.29174 | 0.57214 |
| H | 6.44930 | -1.51432 | -0.85904 |
| H | 3.42922 | -2.85067 | 1.90594 |
| H | 5.70495 | -3.06573 | 0.93223 |
| Br | -0.79274 | -1.09213 | 2.14346 |
| C | 0.02617 | -1.28440 | -3.15044 |
| H | 0.44619 | -1.90372 | -3.96333 |
| H | -0.96080 | -0.94645 | -3.49808 |
| H | 0.65641 | -0.38375 | -3.10225 |

Gibbs free energy = -4043.032601
Temperature = 225.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -3.55189 | -2.23511 | -0.20890 |
| O | -3.01842 | -0.94097 | -0.57554 |
| C | -4.21465 | -2.91162 | -1.39579 |
| C | -3.96532 | 0.15393 | -0.53315 |
| C | -3.98947 | 0.81861 | 0.83173 |
| H | -4.23852 | -2.11625 | 0.63688 |
| H | -2.69864 | -2.82097 | 0.14283 |
| H | -4.57382 | -3.90448 | -1.10361 |
| H | -3.49624 | -3.02796 | -2.21318 |

| | | | |
|---|---|---|---|
| H | -5.07052 | -2.33703 | -1.76406 |
| H | -3.63236 | 0.85629 | -1.29953 |
| H | -4.95263 | -0.22394 | -0.81855 |
| H | -4.72328 | 1.63248 | 0.83406 |
| H | -4.25514 | 0.10899 | 1.62070 |
| H | -3.00487 | 1.23219 | 1.06088 |
| C | -0.06822 | -1.98166 | -1.78056 |
| C | 2.41640 | 0.72911 | -0.86764 |
| H | 0.93686 | -2.33627 | -1.49685 |
| Mg | -0.93792 | -0.69031 | -0.29710 |
| H | -0.66350 | -2.90432 | -1.90294 |
| N | 1.20323 | 0.83080 | -0.43913 |
| S | 0.15380 | 2.01021 | -1.11421 |
| C | 0.20742 | 3.31238 | 0.24836 |
| O | -1.19272 | 1.27765 | -0.91790 |
| H | 2.83042 | 1.39942 | -1.62795 |
| C | 0.01154 | 2.63947 | 1.60379 |
| H | 0.85530 | 1.99793 | 1.86417 |
| H | -0.08381 | 3.41940 | 2.36698 |
| H | -0.89338 | 2.02888 | 1.61863 |
| C | 1.56317 | 4.00976 | 0.12601 |
| H | 1.71644 | 4.44271 | -0.86846 |
| H | 1.59716 | 4.82676 | 0.85412 |
| H | 2.39196 | 3.33207 | 0.35094 |
| C | -0.95514 | 4.25326 | -0.09087 |
| H | -0.97814 | 5.05752 | 0.65159 |
| H | -0.83912 | 4.71175 | -1.07906 |
| H | -1.91230 | 3.72602 | -0.05502 |
| C | 3.30232 | -0.30499 | -0.35029 |
| C | 4.59185 | -0.42738 | -0.89616 |
| C | 2.88335 | -1.18353 | 0.67013 |
| C | 5.45440 | -1.41955 | -0.43517 |
| H | 4.90764 | 0.25209 | -1.68321 |
| C | 3.75020 | -2.17157 | 1.12192 |
| H | 1.88921 | -1.08296 | 1.09725 |
| C | 5.03334 | -2.29174 | 0.57215 |
| H | 6.44929 | -1.51434 | -0.85904 |
| H | 3.42922 | -2.85066 | 1.90595 |
| H | 5.70494 | -3.06574 | 0.93223 |
| Br | -0.79274 | -1.09212 | 2.14346 |
| C | 0.02619 | -1.28440 | -3.15044 |
| H | 0.44622 | -1.90372 | -3.96332 |
| H | -0.96078 | -0.94646 | -3.49808 |
| H | 0.65643 | -0.38375 | -3.10224 |



**TS 6-7**

Gibbs free energy = -4043.033116
Temperature = 298.15 K
Only one imaginary frequency = -257.19
Cartesian coordinates:

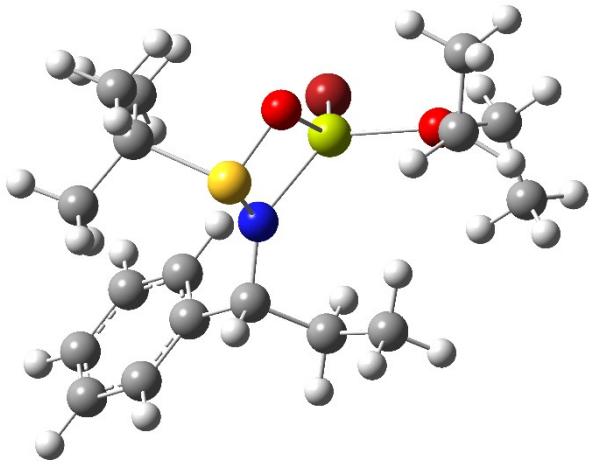
| | | | |
|---|---|---|---|
| C | -2.47750 | -2.98120 | -0.01970 |
| O | -2.38940 | -1.59530 | -0.43410 |
| C | -2.72130 | -3.89090 | -1.21030 |
| C | -3.66040 | -0.90030 | -0.52330 |
| C | -4.02000 | -0.23660 | 0.79410 |
| H | -3.26020 | -3.07710 | 0.74050 |
| H | -1.52540 | -3.20960 | 0.46540 |
| H | -2.76540 | -4.93290 | -0.87580 |
| H | -1.90990 | -3.79330 | -1.93750 |
| H | -3.66590 | -3.65480 | -1.71060 |
| H | -3.53210 | -0.15850 | -1.31270 |
| H | -4.42550 | -1.61600 | -0.84030 |
| H | -4.98990 | 0.26440 | 0.70260 |
| H | -4.08070 | -0.96580 | 1.60750 |
| H | -3.26660 | 0.51030 | 1.05820 |
| C | 0.48890 | -1.59340 | -1.73160 |
| C | 1.66260 | 0.43950 | -1.11800 |
| H | 1.51220 | -1.88610 | -1.95550 |
| Mg | -0.62080 | -0.52660 | -0.09530 |
| H | 0.06700 | -2.46160 | -1.19020 |
| N | 0.99110 | 1.32500 | -0.36110 |
| S | -0.27650 | 2.09960 | -1.15510 |
| C | -0.56520 | 3.49830 | 0.05510 |
| O | -1.47840 | 1.11860 | -0.89910 |
| H | 1.65520 | 0.50490 | -2.20730 |
| C | -0.75000 | 2.93070 | 1.46100 |
| H | 0.15740 | 2.44350 | 1.82020 |
| H | -1.00150 | 3.75410 | 2.13820 |
| H | -1.56480 | 2.20290 | 1.48940 |
| C | 0.65650 | 4.41560 | -0.04630 |
| H | 0.80600 | 4.78660 | -1.06640 |
| H | 0.49830 | 5.28250 | 0.60390 |

| | | | |
|---|---|---|---|
| H | 1.56580 | 3.90360 | 0.27990 |
| C | -1.84170 | 4.18840 | -0.44220 |
| H | -2.06070 | 5.03810 | 0.21240 |
| H | -1.73030 | 4.57080 | -1.46280 |
| H | -2.69580 | 3.50570 | -0.41330 |
| C | 2.85930 | -0.18760 | -0.52310 |
| C | 3.84520 | -0.72280 | -1.36820 |
| C | 3.05180 | -0.22400 | 0.86790 |
| C | 5.00130 | -1.28990 | -0.83430 |
| H | 3.70210 | -0.68840 | -2.44500 |
| C | 4.20420 | -0.80020 | 1.39760 |
| H | 2.28430 | 0.17750 | 1.51910 |
| C | 5.18220 | -1.33260 | 0.55090 |
| H | 5.75940 | -1.69650 | -1.49720 |
| H | 4.34150 | -0.83380 | 2.47460 |
| H | 6.08050 | -1.77790 | 0.96890 |
| Br | -0.34830 | -1.00630 | 2.28270 |
| C | -0.30510 | -1.31430 | -3.00670 |
| H | -0.25900 | -2.14140 | -3.73250 |
| H | -1.36570 | -1.13360 | -2.79980 |
| H | 0.07360 | -0.42340 | -3.52670 |

Gibbs free energy = -4043.013563
Temperature = 225.15 K
Only one imaginary frequency = -257.19
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -2.47750 | -2.98122 | -0.01967 |
| O | -2.38940 | -1.59532 | -0.43409 |
| C | -2.72128 | -3.89086 | -1.21034 |
| C | -3.66038 | -0.90034 | -0.52328 |
| C | -4.01999 | -0.23663 | 0.79414 |
| H | -3.26017 | -3.07706 | 0.74047 |
| H | -1.52536 | -3.20964 | 0.46537 |
| H | -2.76543 | -4.93293 | -0.87575 |
| H | -1.90988 | -3.79331 | -1.93754 |
| H | -3.66595 | -3.65485 | -1.71058 |
| H | -3.53207 | -0.15855 | -1.31271 |
| H | -4.42547 | -1.61595 | -0.84026 |
| H | -4.98994 | 0.26436 | 0.70265 |
| H | -4.08068 | -0.96575 | 1.60751 |
| H | -3.26663 | 0.51027 | 1.05815 |
| C | 0.48891 | -1.59339 | -1.73163 |
| C | 1.66257 | 0.43949 | -1.11803 |
| H | 1.51216 | -1.88613 | -1.95552 |
| Mg | -0.62083 | -0.52656 | -0.09531 |
| H | 0.06702 | -2.46161 | -1.19018 |
| N | 0.99111 | 1.32498 | -0.36112 |
| S | -0.27648 | 2.09957 | -1.15513 |
| C | -0.56524 | 3.49828 | 0.05508 |
| O | -1.47840 | 1.11863 | -0.89906 |
| H | 1.65517 | 0.50486 | -2.20727 |
| C | -0.74997 | 2.93072 | 1.46097 |
| H | 0.15741 | 2.44353 | 1.82024 |
| H | -1.00153 | 3.75406 | 2.13822 |
| H | -1.56480 | 2.20293 | 1.48944 |
| C | 0.65647 | 4.41559 | -0.04630 |
| H | 0.80604 | 4.78659 | -1.06644 |

| | | | |
|---|---|---|---|
| H | 0.49830 | 5.28253 | 0.60389 |
| H | 1.56579 | 3.90363 | 0.27989 |
| C | -1.84165 | 4.18838 | -0.44218 |
| H | -2.06074 | 5.03805 | 0.21242 |
| H | -1.73028 | 4.57079 | -1.46279 |
| H | -2.69578 | 3.50568 | -0.41334 |
| C | 2.85929 | -0.18764 | -0.52315 |
| C | 3.84517 | -0.72281 | -1.36821 |
| C | 3.05178 | -0.22396 | 0.86792 |
| C | 5.00129 | -1.28986 | -0.83430 |
| H | 3.70207 | -0.68835 | -2.44502 |
| C | 4.20416 | -0.80022 | 1.39757 |
| H | 2.28432 | 0.17754 | 1.51909 |
| C | 5.18221 | -1.33262 | 0.55089 |
| H | 5.75944 | -1.69653 | -1.49721 |
| H | 4.34146 | -0.83382 | 2.47461 |
| H | 6.08054 | -1.77787 | 0.96888 |
| Br | -0.34828 | -1.00633 | 2.28271 |
| C | -0.30513 | -1.31431 | -3.00670 |
| H | -0.25904 | -2.14145 | -3.73247 |
| H | -1.36569 | -1.13362 | -2.79977 |
| H | 0.07359 | -0.42340 | -3.52665 |



## 7

Gibbs free energy = -4043.113042
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

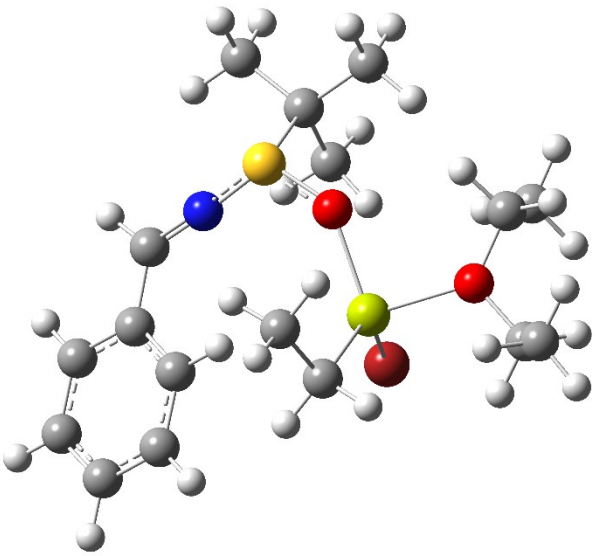
| | | | |
|---|---|---|---|
| C | -3.95096 | -1.34300 | -0.14214 |
| O | -3.12570 | -0.16980 | -0.39105 |
| C | -3.58731 | -2.46252 | -1.09759 |
| C | -3.66798 | 0.79744 | -1.33459 |
| C | -4.53276 | 1.81598 | -0.61930 |
| H | -5.00141 | -1.04952 | -0.22681 |
| H | -3.74864 | -1.62564 | 0.89250 |
| H | -4.20369 | -3.34287 | -0.88644 |
| H | -2.53636 | -2.74231 | -0.97384 |
| H | -3.75220 | -2.16957 | -2.13872 |
| H | -2.80274 | 1.27915 | -1.79306 |

| | | | |
|---|---|---|---|
| H | -4.21583 | 0.25191 | -2.10914 |
| H | -4.93690 | 2.53136 | -1.34368 |
| H | -5.37273 | 1.33808 | -0.10537 |
| H | -3.93331 | 2.36547 | 0.11257 |
| C | 0.49095 | -1.57301 | -2.12974 |
| C | 1.29879 | -0.38501 | -1.55778 |
| H | 1.17105 | -2.22897 | -2.68597 |
| Mg | -1.29219 | 0.09949 | 0.42657 |
| H | 0.11762 | -2.15729 | -1.27642 |
| N | 0.44475 | 0.34956 | -0.62448 |
| S | 0.27889 | 1.97954 | -0.70284 |
| C | 1.43571 | 2.74162 | 0.58758 |
| O | -1.11812 | 2.08809 | 0.04418 |
| H | 1.60333 | 0.25169 | -2.40295 |
| C | 1.26608 | 1.99921 | 1.90849 |
| H | 1.49564 | 0.93627 | 1.79519 |
| H | 1.94832 | 2.42098 | 2.65468 |
| H | 0.24467 | 2.09772 | 2.28884 |
| C | 2.85188 | 2.59289 | 0.02623 |
| H | 2.94921 | 3.05613 | -0.96281 |
| H | 3.56047 | 3.09245 | 0.69620 |
| H | 3.14636 | 1.54330 | -0.05037 |
| C | 1.02772 | 4.21343 | 0.69900 |
| H | 1.69603 | 4.72373 | 1.40195 |
| H | 1.10386 | 4.72989 | -0.26512 |
| H | 0.00248 | 4.31151 | 1.06596 |
| C | 2.56353 | -0.90378 | -0.87957 |
| C | 3.79317 | -0.89157 | -1.54815 |
| C | 2.50434 | -1.43794 | 0.41635 |
| C | 4.94539 | -1.39494 | -0.93684 |
| H | 3.85161 | -0.47720 | -2.55233 |
| C | 3.65247 | -1.94311 | 1.02764 |
| H | 1.55520 | -1.44264 | 0.94505 |
| C | 4.87829 | -1.92224 | 0.35445 |
| H | 5.89371 | -1.36900 | -1.46703 |
| H | 3.59065 | -2.35030 | 2.03344 |
| H | 5.77274 | -2.31008 | 0.83402 |
| Br | -1.14938 | -1.48041 | 2.25953 |
| C | -0.66797 | -1.14085 | -3.02659 |
| H | -1.22210 | -2.00726 | -3.40215 |
| H | -1.37124 | -0.50520 | -2.48208 |
| H | -0.30423 | -0.57299 | -3.89124 |

Gibbs free energy = -4043.093263
Temperature = 225.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -3.95097 | -1.34298 | -0.14209 |
| O | -3.12572 | -0.16977 | -0.39097 |
| C | -3.58739 | -2.46243 | -1.09765 |
| C | -3.66801 | 0.79748 | -1.33448 |
| C | -4.53274 | 1.81603 | -0.61916 |
| H | -5.00142 | -1.04948 | -0.22667 |
| H | -3.74858 | -1.62569 | 0.89251 |
| H | -4.20375 | -3.34279 | -0.88651 |
| H | -2.53643 | -2.74224 | -0.97399 |
| H | -3.75235 | -2.16941 | -2.13875 |

| | | | |
|---|---|---|---|
| H | -2.80277 | 1.27918 | -1.79298 |
| H | -4.21589 | 0.25196 | -2.10902 |
| H | -4.93690 | 2.53142 | -1.34353 |
| H | -5.37271 | 1.33815 | -0.10521 |
| H | -3.93327 | 2.36551 | 0.11269 |
| C | 0.49092 | -1.57291 | -2.12979 |
| C | 1.29876 | -0.38493 | -1.55779 |
| H | 1.17100 | -2.22884 | -2.68607 |
| Mg | -1.29218 | 0.09950 | 0.42662 |
| H | 0.11760 | -2.15724 | -1.27649 |
| N | 0.44472 | 0.34961 | -0.62447 |
| S | 0.27885 | 1.97959 | -0.70277 |
| C | 1.43569 | 2.74164 | 0.58765 |
| O | -1.11815 | 2.08811 | 0.04428 |
| H | 1.60329 | 0.25179 | -2.40294 |
| C | 1.26608 | 1.99919 | 1.90854 |
| H | 1.49564 | 0.93625 | 1.79521 |
| H | 1.94834 | 2.42095 | 2.65473 |
| H | 0.24468 | 2.09768 | 2.28891 |
| C | 2.85186 | 2.59291 | 0.02627 |
| H | 2.94916 | 3.05618 | -0.96277 |
| H | 3.56046 | 3.09246 | 0.69623 |
| H | 3.14634 | 1.54333 | -0.05037 |
| C | 1.02771 | 4.21344 | 0.69911 |
| H | 1.69603 | 4.72373 | 1.40205 |
| H | 1.10383 | 4.72992 | -0.26501 |
| H | 0.00247 | 4.31152 | 1.06608 |
| C | 2.56350 | -0.90373 | -0.87961 |
| C | 3.79313 | -0.89153 | -1.54821 |
| C | 2.50432 | -1.43790 | 0.41630 |
| C | 4.94535 | -1.39493 | -0.93693 |
| H | 3.85155 | -0.47716 | -2.55240 |
| C | 3.65246 | -1.94309 | 1.02757 |
| H | 1.55519 | -1.44260 | 0.94503 |
| C | 4.87827 | -1.92223 | 0.35436 |
| H | 5.89366 | -1.36900 | -1.46714 |
| H | 3.59066 | -2.35029 | 2.03338 |
| H | 5.77272 | -2.31009 | 0.83391 |
| Br | -1.14925 | -1.48061 | 2.25941 |
| C | -0.66803 | -1.14072 | -3.02659 |
| H | -1.22215 | -2.00712 | -3.40219 |
| H | -1.37130 | -0.50511 | -2.48203 |
| H | -0.30432 | -0.57281 | -3.89122 |

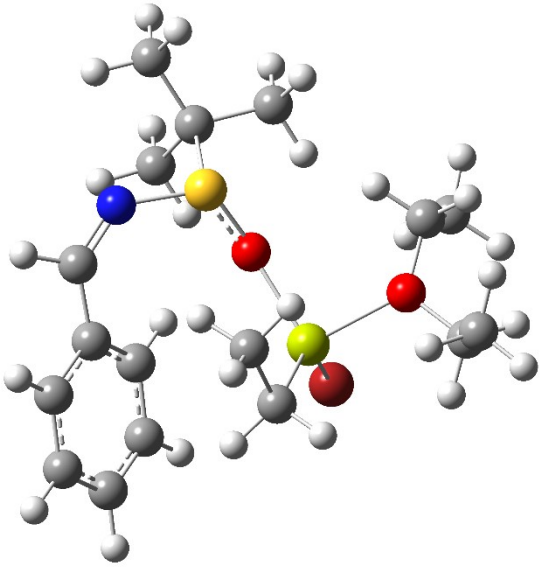


## TS 6-6′Z

Gibbs free energy = -4043.023545
Temperature = 298.15 K
Only one imaginary frequency = -193.62
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.42198 | -2.57795 | 1.55614 |
| C | -2.92491 | 1.31119 | 0.48372 |
| H | -0.48947 | -3.12492 | 1.26367 |
| Mg | 0.96186 | -0.99297 | 0.21244 |
| N | -1.71888 | 1.58620 | 0.77593 |
| S | -0.26732 | 1.93972 | 1.28162 |
| C | 0.18705 | 3.34659 | 0.07791 |
| O | 0.80076 | 0.86399 | 0.96448 |
| H | -3.63686 | 2.14113 | 0.38660 |
| C | -0.77787 | 4.49073 | 0.38304 |
| H | -1.81488 | 4.21125 | 0.17747 |
| H | -0.52369 | 5.33887 | -0.26160 |
| H | -0.70077 | 4.82562 | 1.42297 |
| C | 0.04941 | 2.82666 | -1.34927 |
| H | -0.99594 | 2.63471 | -1.60578 |
| H | 0.60886 | 1.90071 | -1.49890 |
| H | 0.43546 | 3.58594 | -2.03833 |
| C | 1.63330 | 3.71369 | 0.41593 |
| H | 1.93198 | 4.56022 | -0.21129 |
| H | 2.30838 | 2.88164 | 0.21190 |
| H | 1.74601 | 4.01543 | 1.46300 |
| C | -3.48161 | -0.02143 | 0.25056 |
| C | -4.80854 | -0.11735 | -0.20575 |
| C | -2.73928 | -1.19340 | 0.47324 |
| C | -5.37717 | -1.36486 | -0.45191 |
| H | -5.38482 | 0.78900 | -0.37213 |
| C | -3.31012 | -2.43692 | 0.22885 |
| H | -1.72356 | -1.12763 | 0.84281 |
| C | -4.62777 | -2.52501 | -0.23618 |
| H | -6.39990 | -1.43422 | -0.80963 |
| H | -2.73037 | -3.33813 | 0.40162 |
| H | -5.07024 | -3.49848 | -0.42667 |
| Br | 0.33454 | -0.95013 | -2.16803 |

| | | | |
|---|---|---|---|
| H | 1.21243 | -3.35014 | 1.55222 |
| C | 0.25168 | -2.06757 | 3.00008 |
| H | 1.16155 | -1.56111 | 3.35324 |
| H | -0.55545 | -1.32413 | 3.07121 |
| H | 0.02022 | -2.84736 | 3.74729 |
| C | 3.82469 | 0.26929 | 0.21029 |
| O | 3.03984 | -0.94655 | 0.23061 |
| C | 3.82781 | 0.90451 | -1.16846 |
| C | 3.74539 | -2.15648 | -0.13743 |
| C | 4.43694 | -2.76885 | 1.06698 |
| H | 4.83854 | 0.03878 | 0.55381 |
| H | 3.35406 | 0.92359 | 0.94640 |
| H | 4.42977 | 1.81969 | -1.15530 |
| H | 2.80852 | 1.15642 | -1.47040 |
| H | 4.24868 | 0.22765 | -1.91842 |
| H | 2.98719 | -2.83444 | -0.53956 |
| H | 4.44928 | -1.92877 | -0.94508 |
| H | 4.93012 | -3.70325 | 0.77807 |
| H | 5.19682 | -2.09621 | 1.47723 |
| H | 3.70558 | -2.98727 | 1.85082 |

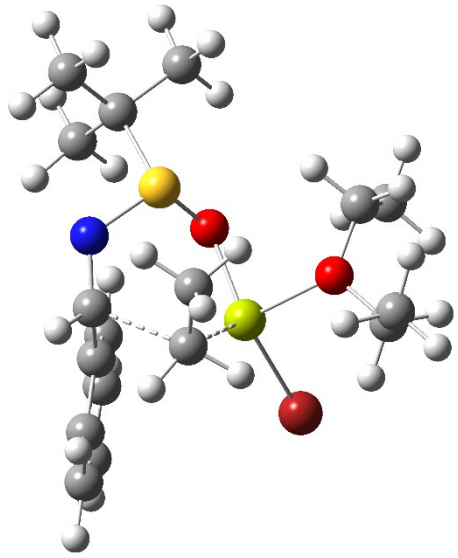


## 6′Z

Gibbs free energy = -4043.04183
Temperature = 298.15 K
No imaginary frequencies
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -3.76271 | 1.19158 | 1.15598 |
| O | -2.72706 | 0.22530 | 0.85272 |
| C | -3.93229 | 1.34887 | 2.65575 |
| C | -3.16385 | -1.14895 | 0.73896 |
| C | -3.67341 | -1.46417 | -0.65610 |
| H | -4.69283 | 0.88463 | 0.66641 |
| H | -3.44124 | 2.13159 | 0.69826 |
| H | -4.70904 | 2.09169 | 2.86739 |
| H | -2.99525 | 1.68569 | 3.10865 |

| | | | |
|---|---|---|---|
| H | -4.22754 | 0.40424 | 3.12358 |
| H | -2.28356 | -1.74776 | 0.97690 |
| H | -3.92308 | -1.34098 | 1.50495 |
| H | -3.94959 | -2.52257 | -0.71772 |
| H | -4.55591 | -0.86582 | -0.90360 |
| H | -2.90001 | -1.24895 | -1.39802 |
| C | -0.22149 | 2.29754 | 1.61376 |
| C | 3.22745 | -0.61345 | 0.94736 |
| H | 0.59944 | 2.94988 | 1.27753 |
| Mg | -0.91407 | 0.94400 | 0.11159 |
| H | -1.00873 | 2.99043 | 1.95911 |
| N | 2.46620 | -1.64059 | 1.09751 |
| S | 0.81477 | -1.87294 | 0.89876 |
| C | 0.90619 | -3.32327 | -0.32615 |
| O | 0.02634 | -0.83211 | 0.08261 |
| H | 4.22156 | -0.75862 | 1.38277 |
| C | 1.60535 | -2.83885 | -1.59459 |
| H | 2.64374 | -2.55496 | -1.40365 |
| H | 1.60569 | -3.65672 | -2.32311 |
| H | 1.07275 | -1.99241 | -2.03660 |
| C | 1.64095 | -4.47713 | 0.35524 |
| H | 1.16275 | -4.76281 | 1.29811 |
| H | 1.60981 | -5.34533 | -0.31177 |
| H | 2.68648 | -4.23123 | 0.55189 |
| C | -0.56251 | -3.66316 | -0.60379 |
| H | -0.59444 | -4.50302 | -1.30517 |
| H | -1.09286 | -3.96491 | 0.30583 |
| H | -1.08180 | -2.81601 | -1.05710 |
| C | 3.04203 | 0.70339 | 0.32226 |
| C | 3.80723 | 1.76365 | 0.84777 |
| C | 2.21499 | 0.94389 | -0.78858 |
| C | 3.70365 | 3.04351 | 0.31118 |
| H | 4.46808 | 1.58004 | 1.69050 |
| C | 2.12434 | 2.22442 | -1.33042 |
| H | 1.65142 | 0.13555 | -1.23290 |
| C | 2.86032 | 3.27603 | -0.78003 |
| H | 4.28305 | 3.85673 | 0.73744 |
| H | 1.45727 | 2.39086 | -2.16938 |
| H | 2.78308 | 4.27290 | -1.20392 |
| Br | -1.37792 | 1.25087 | -2.30151 |
| C | 0.26831 | 1.47444 | 2.82232 |
| H | -0.52140 | 0.81404 | 3.20966 |
| H | 1.10535 | 0.81864 | 2.54551 |
| H | 0.62145 | 2.07224 | 3.68135 |



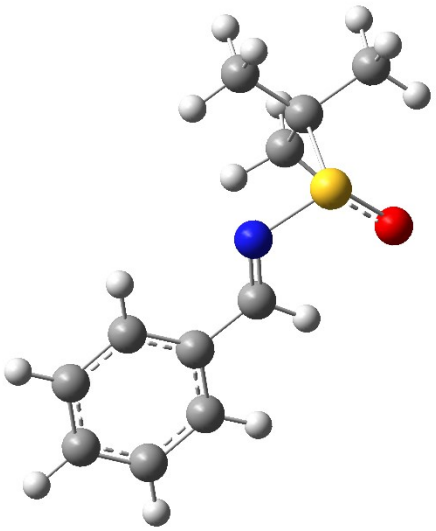
## TS 6′Z-7

Gibbs free energy = -4043.010716
Temperature = 298.15 K
Only one imaginary frequency = -321.69
Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -2.54845 | -2.81649 | 0.35495 |
| O | -1.21560 | -2.32676 | 0.04575 |
| C | -2.54015 | -3.70546 | 1.58464 |
| C | -0.41436 | -3.21711 | -0.77565 |
| C | -0.61654 | -2.93757 | -2.25346 |
| H | -2.94386 | -3.33400 | -0.52533 |
| H | -3.16343 | -1.92759 | 0.51241 |
| H | -3.55625 | -4.06483 | 1.78040 |
| H | -2.19495 | -3.14916 | 2.46010 |
| H | -1.89310 | -4.57775 | 1.44837 |
| H | 0.62058 | -3.04149 | -0.47784 |
| H | -0.67139 | -4.24882 | -0.51733 |
| H | -0.00801 | -3.62941 | -2.84602 |
| H | -1.66393 | -3.06553 | -2.54289 |
| H | -0.30936 | -1.91527 | -2.49064 |
| C | -0.72681 | -0.18488 | 2.35147 |
| C | 0.96397 | 1.28168 | 1.73384 |
| H | -0.98042 | 0.59267 | 3.07226 |
| Mg | -0.85094 | -0.27871 | 0.05271 |
| H | -1.72787 | -0.53207 | 2.01615 |
| N | 2.07511 | 0.58866 | 1.43729 |
| S | 2.05350 | -0.61141 | 0.31000 |
| C | 3.69580 | -0.38330 | -0.58508 |
| O | 0.95081 | -0.37963 | -0.79954 |
| H | 0.95936 | 1.59773 | 2.77828 |
| C | 3.76134 | 0.99308 | -1.23802 |
| H | 3.65609 | 1.78938 | -0.49647 |
| H | 4.73551 | 1.10523 | -1.72662 |
| H | 2.98797 | 1.10638 | -2.00250 |
| C | 4.78815 | -0.56885 | 0.47315 |
| H | 4.70141 | -1.53437 | 0.98311 |
| H | 5.76386 | -0.53978 | -0.02385 |
| H | 4.75731 | 0.22628 | 1.22181 |

| | | | |
|---|---|---|---|
| C | 3.72128 | -1.50664 | -1.62737 |
| H | 4.66409 | -1.45246 | -2.18131 |
| H | 3.66293 | -2.49566 | -1.15984 |
| H | 2.89873 | -1.40684 | -2.34112 |
| C | 0.22809 | 2.27166 | 0.88373 |
| C | -0.77412 | 3.04670 | 1.50469 |
| C | 0.55494 | 2.55650 | -0.45081 |
| C | -1.44187 | 4.04526 | 0.80698 |
| H | -1.02446 | 2.85650 | 2.54450 |
| C | -0.12045 | 3.55863 | -1.15138 |
| H | 1.33241 | 1.99421 | -0.94237 |
| C | -1.11963 | 4.30437 | -0.53057 |
| H | -2.21222 | 4.62739 | 1.30481 |
| H | 0.14632 | 3.75628 | -2.18572 |
| H | -1.64131 | 5.08494 | -1.07670 |
| Br | -2.78239 | 0.55165 | -1.14868 |
| C | 0.03697 | -1.33195 | 3.00069 |
| H | 0.11924 | -2.18787 | 2.32300 |
| H | 1.05894 | -1.02417 | 3.25275 |
| H | -0.43162 | -1.69393 | 3.92843 |

**6. Cartesian coordinates of the subunits used to calculate the deformation and interaction energies of TS 4'-5 and TS 6-7**

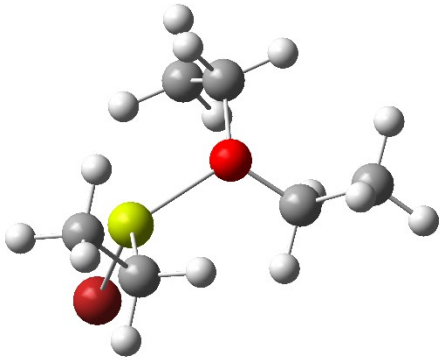


**Im 4'**

Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | 0.60708 | -0.64167 | -0.27956 |
| N | -0.29111 | 0.12291 | -0.79877 |
| S | -1.87393 | -0.50775 | -0.95293 |
| C | -2.70927 | 0.51463 | 0.40748 |
| O | -1.95869 | -1.94211 | -0.38068 |
| H | 0.36827 | -1.64352 | 0.09011 |
| C | -2.66094 | 1.97896 | -0.03160 |
| H | -1.63416 | 2.34567 | -0.10131 |
| H | -3.19024 | 2.57999 | 0.71552 |
| H | -3.15732 | 2.13182 | -0.99577 |
| C | -1.97739 | 0.26539 | 1.72425 |
| H | -0.99293 | 0.73872 | 1.73649 |
| H | -1.85738 | -0.80512 | 1.91458 |

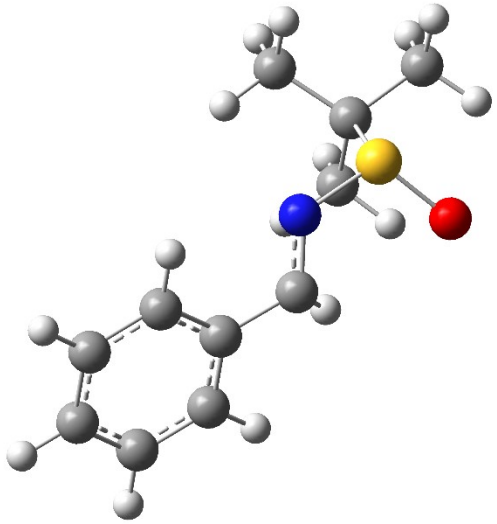
| | | | |
|---|---|---|---|
| H | -2.57115 | 0.69342 | 2.53866 |
| C | -4.14478 | -0.02110 | 0.45051 |
| H | -4.71036 | 0.56486 | 1.18209 |
| H | -4.16830 | -1.06893 | 0.75877 |
| H | -4.64820 | 0.07662 | -0.51749 |
| C | 2.00007 | -0.23660 | -0.11959 |
| C | 2.88045 | -1.15618 | 0.47844 |
| C | 2.47522 | 1.02124 | -0.53412 |
| C | 4.22086 | -0.81994 | 0.66051 |
| H | 2.49940 | -2.12443 | 0.79498 |
| C | 3.81332 | 1.34938 | -0.34965 |
| H | 1.78934 | 1.72366 | -0.99697 |
| C | 4.68700 | 0.43035 | 0.24731 |
| H | 4.89946 | -1.53078 | 1.12190 |
| H | 4.18248 | 2.31907 | -0.66977 |
| H | 5.73163 | 0.69248 | 0.38813 |



## Gr 4′

Cartesian coordinates:

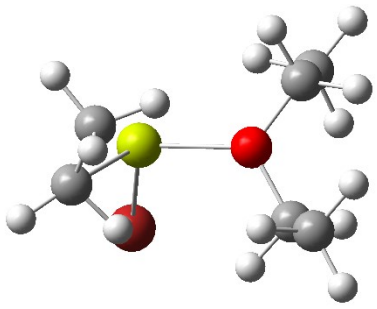
| | | | |
|---|---|---|---|
| C | 1.26818 | 2.53837 | -0.34638 |
| H | 2.10295 | 2.46225 | -1.06351 |
| Mg | 0.62348 | 0.62501 | 0.36652 |
| Br | 1.57862 | -1.56091 | -0.34747 |
| H | 0.46796 | 3.04857 | -0.91147 |
| C | 1.70131 | 3.45475 | 0.81629 |
| H | 0.88248 | 3.60836 | 1.53313 |
| H | 2.53152 | 3.01688 | 1.38873 |
| H | 2.03765 | 4.46110 | 0.51091 |
| C | -2.20184 | -0.18400 | 1.30241 |
| O | -1.41699 | 0.30747 | 0.18436 |
| C | -1.82936 | -1.60982 | 1.66718 |
| C | -1.92757 | -0.01970 | -1.13384 |
| C | -2.98514 | 0.97495 | -1.57561 |
| H | -3.26321 | -0.08894 | 1.05252 |
| H | -1.97999 | 0.49996 | 2.12382 |
| H | -2.43494 | -1.94067 | 2.51815 |
| H | -0.77323 | -1.66197 | 1.94043 |
| H | -2.00458 | -2.29760 | 0.83467 |
| H | -1.06304 | 0.01167 | -1.80367 |
| H | -2.30136 | -1.04877 | -1.12781 |
| H | -3.32654 | 0.72389 | -2.58562 |
| H | -3.85508 | 0.96197 | -0.91185 |
| H | -2.57156 | 1.98803 | -1.59033 |



**Im TS 4′-5**

Cartesian coordinates:

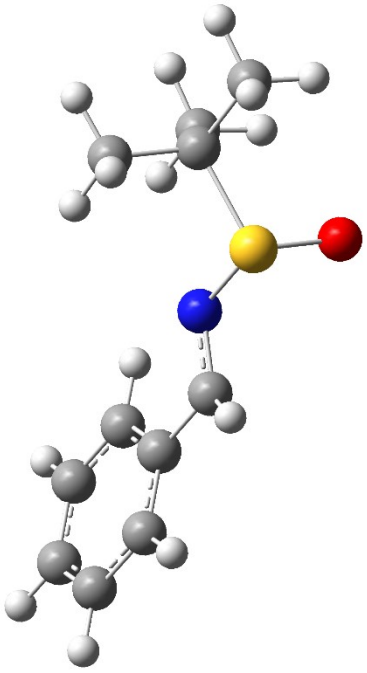
| | | | |
|---|---|---|---|
| C | 0.54497 | -0.78595 | -0.37978 |
| N | -0.27755 | 0.03274 | -1.06383 |
| S | -1.89758 | -0.33555 | -1.03297 |
| C | -2.57891 | 0.52046 | 0.52025 |
| O | -2.10857 | -1.85723 | -0.66298 |
| H | 0.18144 | -1.33330 | 0.49451 |
| C | -2.28353 | 2.01178 | 0.35560 |
| H | -1.20744 | 2.20446 | 0.33868 |
| H | -2.71809 | 2.55570 | 1.20150 |
| H | -2.72474 | 2.41572 | -0.56264 |
| C | -1.93174 | -0.06418 | 1.77198 |
| H | -0.86668 | 0.17513 | 1.83154 |
| H | -2.05960 | -1.14975 | 1.81092 |
| H | -2.41700 | 0.36605 | 2.65544 |
| C | -4.08309 | 0.22828 | 0.48694 |
| H | -4.56285 | 0.72858 | 1.33513 |
| H | -4.27879 | -0.84471 | 0.56898 |
| H | -4.55089 | 0.60217 | -0.43055 |
| C | 1.94465 | -0.34642 | -0.16452 |
| C | 2.70959 | -0.98398 | 0.82539 |
| C | 2.51554 | 0.69164 | -0.91354 |
| C | 4.02382 | -0.58620 | 1.06396 |
| H | 2.26461 | -1.79541 | 1.39712 |
| C | 3.83243 | 1.08523 | -0.67396 |
| H | 1.92003 | 1.18508 | -1.67448 |
| C | 4.59026 | 0.44938 | 0.31372 |
| H | 4.60618 | -1.08332 | 1.83460 |
| H | 4.26776 | 1.89164 | -1.25763 |
| H | 5.61481 | 0.75929 | 0.49873 |



## Gr TS 4′-5

Cartesian coordinates:

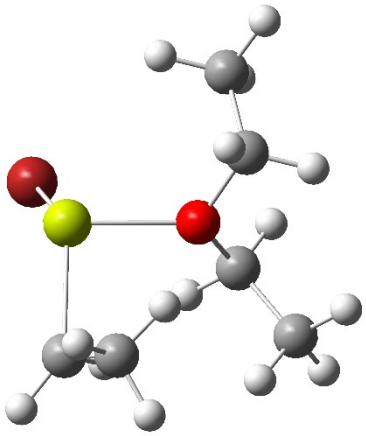
| | | | |
|---|---|---|---|
| C | 0.55040 | 2.66610 | -0.17181 |
| H | 0.24187 | 3.64162 | 0.18940 |
| Mg | -0.25971 | 0.65617 | -0.74040 |
| Br | -2.34394 | -0.01811 | 0.30582 |
| H | 0.57346 | 2.03569 | 0.74193 |
| C | 1.89667 | 2.70839 | -0.87161 |
| H | 2.34792 | 1.71470 | -0.98155 |
| H | 1.77608 | 3.12992 | -1.88056 |
| H | 2.62931 | 3.33866 | -0.34918 |
| C | 1.63241 | -1.67260 | -0.98449 |
| O | 1.18035 | -0.61091 | -0.09412 |
| C | 0.50085 | -2.63562 | -1.29438 |
| C | 1.36068 | -0.86046 | 1.32650 |
| C | 2.73222 | -0.39923 | 1.77937 |
| H | 2.48357 | -2.17262 | -0.51348 |
| H | 1.97781 | -1.16534 | -1.88648 |
| H | 0.86804 | -3.43993 | -1.94066 |
| H | -0.31023 | -2.11961 | -1.81827 |
| H | 0.09673 | -3.08148 | -0.38038 |
| H | 0.56780 | -0.30251 | 1.83251 |
| H | 1.19162 | -1.92459 | 1.51944 |
| H | 2.84584 | -0.57797 | 2.85382 |
| H | 3.52713 | -0.94042 | 1.25692 |
| H | 2.85525 | 0.67134 | 1.58931 |



## Im TS 6-7

Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -0.79314 | -1.02906 | 0.00359 |
| N | 0.26277 | -0.20702 | -0.12742 |
| S | 1.75829 | -0.96027 | 0.05495 |
| C | 2.82469 | 0.56219 | 0.27698 |
| O | 2.07209 | -1.43603 | -1.41052 |
| H | -0.71488 | -1.96845 | 0.55333 |
| C | 2.57216 | 1.53763 | -0.87084 |
| H | 1.54985 | 1.91772 | -0.85782 |
| H | 3.26444 | 2.38047 | -0.76977 |
| H | 2.74975 | 1.06299 | -1.83915 |
| C | 2.45114 | 1.15579 | 1.63801 |
| H | 2.59669 | 0.43670 | 2.45190 |
| H | 3.09880 | 2.01686 | 1.83412 |
| H | 1.41274 | 1.49776 | 1.65075 |
| C | 4.26555 | 0.03651 | 0.25813 |
| H | 4.94970 | 0.87824 | 0.40603 |
| H | 4.44802 | -0.68910 | 1.05842 |
| H | 4.50199 | -0.43138 | -0.70188 |
| C | -2.13529 | -0.41498 | -0.02538 |
| C | -3.21395 | -1.09560 | 0.56263 |
| C | -2.34822 | 0.85270 | -0.59203 |
| C | -4.48507 | -0.52362 | 0.58010 |
| H | -3.04975 | -2.07287 | 1.00892 |
| C | -3.62208 | 1.41639 | -0.58095 |
| H | -1.51781 | 1.37089 | -1.05691 |
| C | -4.69286 | 0.73326 | 0.00528 |
| H | -5.31113 | -1.05669 | 1.04170 |
| H | -3.78123 | 2.39261 | -1.03003 |
| H | -5.68354 | 1.17870 | 0.01423 |



## Gr TS 6-7

Cartesian coordinates:

| | | | |
|---|---|---|---|
| C | -1.05540 | 0.94153 | 1.31498 |
| O | -0.99400 | 0.69043 | -0.11099 |
| C | -2.46929 | 0.76414 | 1.83844 |
| C | -1.29507 | 1.83674 | -0.94865 |
| C | -0.04021 | 2.62731 | -1.27381 |
| H | -0.66247 | 1.94354 | 1.51787 |
| H | -0.36971 | 0.22565 | 1.77471 |
| H | -2.48749 | 0.94039 | 2.91938 |

| | | | |
|---|---|---|---|
| H | -2.82262 | -0.25314 | 1.64609 |
| H | -3.16392 | 1.46755 | 1.36827 |
| H | -1.74416 | 1.42610 | -1.85398 |
| H | -2.04270 | 2.45222 | -0.43858 |
| H | -0.29953 | 3.49433 | -1.89122 |
| H | 0.45658 | 2.98293 | -0.36627 |
| H | 0.66512 | 2.00360 | -1.82933 |
| C | -1.19789 | -2.46022 | -0.12176 |
| H | -1.14296 | -3.49177 | 0.21849 |
| Mg | 0.21040 | -0.86186 | -0.83532 |
| H | -1.10582 | -1.86040 | 0.80383 |
| Br | 2.29393 | -0.26990 | 0.29071 |
| C | -2.52459 | -2.17185 | -0.82241 |
| H | -3.40097 | -2.45770 | -0.21969 |
| H | -2.63980 | -1.10959 | -1.06437 |
| H | -2.60516 | -2.72407 | -1.76902 |