

## Supporting Information

### **Mechanism of EnT-Mediated Amino-Sulfonylation of Alkenes with N-Sulfonyl Ketimine: A DFT Investigation**

Peng Chen,<sup>1</sup> Xin-Yuan Jiang,<sup>1,\*</sup> and Kai Chen<sup>2,\*</sup>

<sup>1</sup>College of Chemistry and Chemical Engineering, Central South University of Forestry and Technology, Changsha 410004, China;

<sup>2</sup>College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, China;

\* Correspondence: X. J., [jxyesfu@126.com](mailto:jxyesfu@126.com); K. C., [kaichen@csu.edu.cn](mailto:kaichen@csu.edu.cn)

## Table of contents

|                                                                      |           |
|----------------------------------------------------------------------|-----------|
| <b>1 Tables of energies and other thermodynamic parameters .....</b> | <b>S1</b> |
| 2 Optimized structures of selected stationary points .....           | S2        |
| 3 Comparison of different methods .....                              | S2        |
| 4 Coordinates of all stationary points .....                         | S3        |

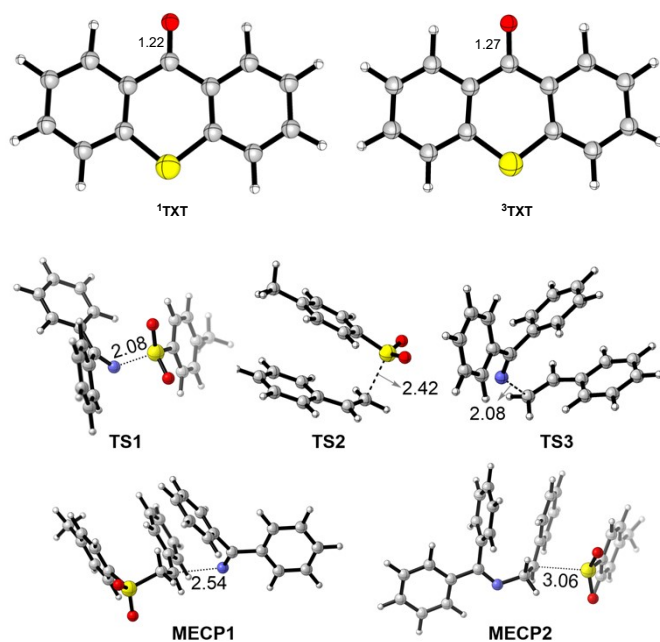
# 1 Tables of energies and other thermodynamic parameters

**Table S1. Energies and other thermodynamic parameters.**

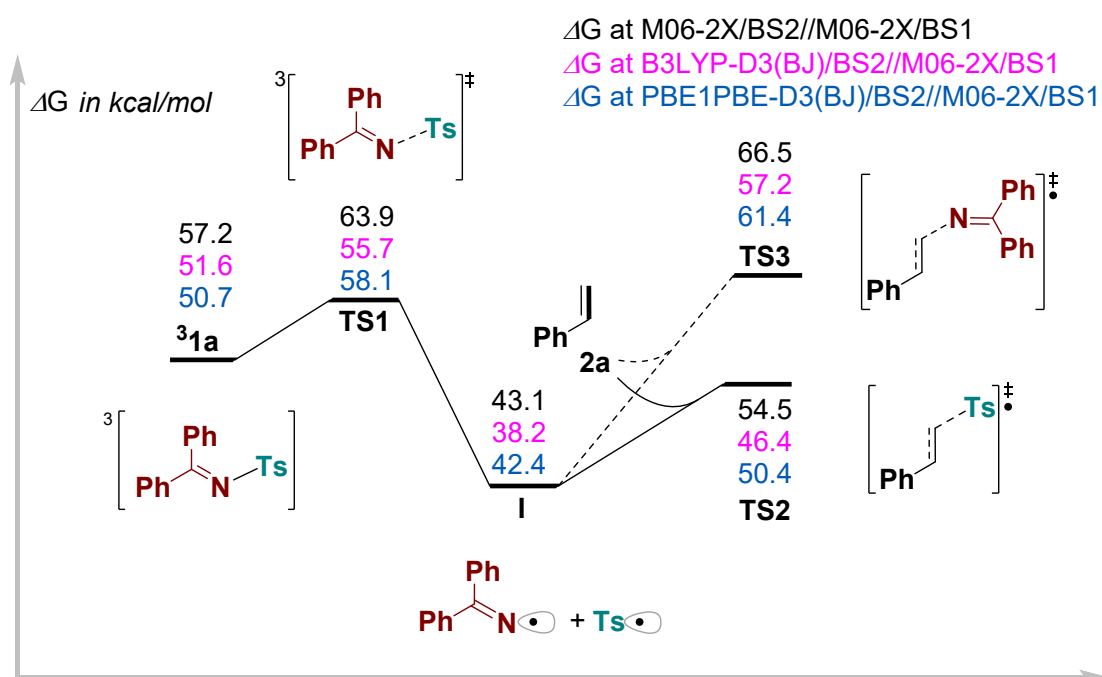
| Structures             | E <sub>ele</sub> | E <sub>ele</sub> (SP) | E <sub>0</sub> | E           | H           | G           |
|------------------------|------------------|-----------------------|----------------|-------------|-------------|-------------|
| <b>TXT</b>             | -972.86035       | -973.62948            | -972.68681     | -972.67605  | -972.67510  | -972.72411  |
| <b><sup>3</sup>TXT</b> | -972.74676       | -973.51927            | -972.57744     | -972.56626  | -972.56531  | -972.61618  |
| <b>1a</b>              | -1374.44123      | -1375.72163           | -1374.11686    | -1374.09619 | -1374.09524 | -1374.16982 |
| <b><sup>3</sup>1a</b>  | -1374.34862      | -1375.62751           | -1374.02677    | -1374.00593 | -1374.00499 | -1374.08012 |
| <b>2a</b>              | -309.28698       | -309.63118            | -309.15251     | -309.14583  | -309.14489  | -309.18364  |
| <b>TS1</b>             | -1374.33886      | -1375.61360           | -1374.01873    | -1373.99769 | -1373.99674 | -1374.07360 |
| <b>Imine-radical</b>   | -555.46771       | -556.08151            | -555.27543     | -555.26460  | -555.26366  | -555.31402  |
| <b>Ts-radical</b>      | -818.88119       | -819.54390            | -818.75428     | -818.74487  | -818.74393  | -818.79095  |
| <b>TS2</b>             | -1128.17478      | -1129.17952           | -1127.91242    | -1127.89582 | -1127.89488 | -1127.95875 |
| <b>II</b>              | -1128.19523      | -1129.20429           | -1127.93093    | -1127.91460 | -1127.91365 | -1127.97673 |
| <b>3</b>               | -1683.76382      | -1685.37864           | -1683.30012    | -1683.27260 | -1683.27166 | -1683.36096 |
| <b>TS3</b>             | -864.74417       | -865.69801            | -864.41623     | -864.39824  | -864.39729  | -864.46458  |
| <b>III</b>             | -864.79264       | -865.74309            | -864.46199     | -864.44409  | -864.44314  | -864.51061  |
| <b>3'</b>              | -1683.77217      | -1685.38341           | -1683.30877    | -1683.28096 | -1683.28002 | -1683.37117 |
| <b>MECP1</b>           |                  | -1685.28184           |                |             |             |             |
| <b>MECP2</b>           |                  | -1685.29485           |                |             |             |             |

Notes: E<sub>ele</sub>, ZPE, H and G(T) were the electronic energies, zero-point energies, sum of electronic and thermal enthalpies and sum of electronic and thermal free energies, respectively, which were given at the M062X/def2-SVP-SMD(DCM) level. E<sub>ele</sub>(SP) were electronic energies with solvent correction at the M06/def2TZVPP-SMD(DCM) level.

## 2 Optimized structures of selected stationary points



## 3 Comparison of different methods



**Figure S1.** Comparison of different methods.

Single point energy calculations were conducted at M06-2X/def2TZVPP-SMD(DCM), B3LYP-D3(BJ)/def2TZVPP-SMD(DCM) and PBE1PBE-D3(BJ)/def2TZVPP-SMD(DCM) theoretical levels. And the Gibbs free energies were obtained by adding the single point energies with the corresponding thermal corrections at the M06-2X/def2SVP-SMD(DCM) theoretical level. It was found that the results from all three density functionals are consistent, suggesting that our results are reliable.

#### 4 Coordinates of all stationary points

|                       |         |         |         |                       |         |         |         |
|-----------------------|---------|---------|---------|-----------------------|---------|---------|---------|
| TXT                   |         |         |         | S                     | 1.8535  | -0.0004 | -0.0000 |
| 0 imaginary frequency |         |         |         | C                     | -1.3820 | -0.0009 | 0.0000  |
| C                     | -1.3864 | -0.0000 | 2.4714  | O                     | -2.5992 | 0.0002  | 0.0000  |
| C                     | -0.6301 | -0.0003 | 1.2847  |                       |         |         |         |
| C                     | 0.7711  | -0.0002 | 1.3771  |                       |         |         |         |
| C                     | 1.3914  | 0.0002  | 2.6392  | <sup>3</sup> TXT      |         |         |         |
| C                     | 0.6240  | 0.0005  | 3.7930  | 0 imaginary frequency |         |         |         |
| C                     | -0.7758 | 0.0004  | 3.7134  | C                     | -1.3821 | -0.0000 | 2.4742  |
| H                     | -2.4726 | -0.0002 | 2.3751  | C                     | -0.6588 | -0.0001 | 1.2630  |
| H                     | 2.4814  | 0.0003  | 2.7055  | C                     | 0.7664  | -0.0000 | 1.3858  |
| H                     | 1.1188  | 0.0008  | 4.7655  | C                     | 1.4143  | 0.0000  | 2.6311  |
| H                     | -1.3780 | 0.0006  | 4.6226  | C                     | 0.6655  | 0.0001  | 3.8001  |
| C                     | -1.3864 | -0.0000 | -2.4714 | C                     | -0.7368 | 0.0000  | 3.7044  |
| C                     | -0.7758 | 0.0004  | -3.7134 | H                     | -2.4694 | -0.0001 | 2.4076  |
| C                     | 0.6240  | 0.0005  | -3.7930 | H                     | 2.5063  | 0.0001  | 2.6703  |
| C                     | 1.3914  | 0.0002  | -2.6392 | H                     | 1.1597  | 0.0001  | 4.7711  |
| C                     | 0.7711  | -0.0002 | -1.3771 | H                     | -1.3361 | 0.0001  | 4.6172  |
| C                     | -0.6301 | -0.0003 | -1.2847 | C                     | -1.3821 | -0.0000 | -2.4742 |
| H                     | -2.4726 | -0.0002 | -2.3751 | C                     | -0.7368 | 0.0000  | -3.7044 |
| H                     | -1.3780 | 0.0006  | -4.6226 | C                     | 0.6655  | 0.0001  | -3.8001 |
| H                     | 1.1188  | 0.0008  | -4.7655 | C                     | 1.4143  | 0.0000  | -2.6311 |
| H                     | 2.4814  | 0.0003  | -2.7055 | C                     | 0.7664  | -0.0000 | -1.3858 |
|                       |         |         |         | C                     | -0.6588 | -0.0001 | -1.2630 |

|   |         |         |         |
|---|---------|---------|---------|
| H | -2.4694 | -0.0001 | -2.4076 |
| H | -1.3361 | 0.0001  | -4.6172 |
| H | 1.1597  | 0.0001  | -4.7711 |
| H | 2.5063  | 0.0001  | -2.6703 |
| S | 1.8065  | -0.0000 | -0.0000 |
| C | -1.3750 | -0.0002 | 0.0000  |
| O | -2.6497 | 0.0001  | 0.0000  |

**1a**

0 imaginary frequency

|   |         |         |         |
|---|---------|---------|---------|
| N | -0.0217 | 0.2041  | -0.4834 |
| C | -1.2709 | 0.2752  | -0.1825 |
| C | -1.8559 | 1.6443  | -0.1147 |
| C | -1.0142 | 2.7426  | 0.1207  |
| C | -3.2279 | 1.8578  | -0.3124 |
| C | -1.5385 | 4.0297  | 0.1680  |
| H | 0.0516  | 2.5685  | 0.2742  |
| C | -3.7470 | 3.1511  | -0.2771 |
| H | -3.8901 | 1.0145  | -0.5130 |
| C | -2.9059 | 4.2363  | -0.0328 |
| H | -0.8799 | 4.8773  | 0.3638  |
| H | -4.8136 | 3.3102  | -0.4430 |
| H | -3.3157 | 5.2474  | 0.0017  |
| C | -2.1729 | -0.8826 | 0.0784  |
| C | -2.2388 | -1.9461 | -0.8310 |
| C | -2.9731 | -0.8988 | 1.2286  |
| C | -3.0987 | -3.0146 | -0.5890 |
| H | -1.6162 | -1.9350 | -1.7271 |
| C | -3.8121 | -1.9824 | 1.4780  |
| H | -2.9273 | -0.0666 | 1.9339  |

|   |         |         |         |
|---|---------|---------|---------|
| C | -3.8797 | -3.0378 | 0.5672  |
| H | -3.1552 | -3.8354 | -1.3055 |
| H | -4.4196 | -1.9997 | 2.3841  |
| H | -4.5462 | -3.8807 | 0.7583  |
| S | 0.8590  | -1.2287 | -0.4714 |
| O | 0.4875  | -2.1017 | 0.6353  |
| O | 0.8545  | -1.7518 | -1.8337 |
| C | 2.4702  | -0.5729 | -0.1340 |
| C | 3.1992  | 0.0007  | -1.1768 |
| C | 2.9796  | -0.6529 | 1.1573  |
| C | 4.4629  | 0.5100  | -0.9053 |
| H | 2.7797  | 0.0391  | -2.1836 |
| C | 4.2509  | -0.1375 | 1.4092  |
| H | 2.3907  | -1.1176 | 1.9492  |
| C | 5.0070  | 0.4497  | 0.3886  |
| H | 5.0461  | 0.9612  | -1.7112 |
| H | 4.6636  | -0.1958 | 2.4183  |
| C | 6.3803  | 1.0008  | 0.6546  |
| H | 7.1364  | 0.4527  | 0.0725  |
| H | 6.4411  | 2.0569  | 0.3532  |
| H | 6.6421  | 0.9260  | 1.7176  |

**<sup>3</sup>1a**

0 imaginary frequency

|   |         |         |         |
|---|---------|---------|---------|
| N | -0.1568 | -0.3601 | -0.5882 |
| C | -1.4261 | 0.1654  | -0.3671 |
| C | -1.5344 | 1.6093  | -0.2893 |
| C | -0.3893 | 2.3928  | -0.0109 |
| C | -2.7482 | 2.2832  | -0.5598 |
| C | -0.4666 | 3.7791  | 0.0318  |

|   |         |         |         |
|---|---------|---------|---------|
| H | 0.5685  | 1.9087  | 0.1850  |
| C | -2.8144 | 3.6705  | -0.5118 |
| H | -3.6352 | 1.7157  | -0.8404 |
| C | -1.6799 | 4.4284  | -0.2091 |
| H | 0.4300  | 4.3591  | 0.2569  |
| H | -3.7619 | 4.1678  | -0.7271 |
| H | -1.7386 | 5.5172  | -0.1732 |
| C | -2.5142 | -0.8048 | -0.3100 |
| C | -2.3693 | -2.0648 | -0.9326 |
| C | -3.7004 | -0.5455 | 0.4100  |
| C | -3.3853 | -3.0102 | -0.8637 |
| H | -1.4519 | -2.2908 | -1.4783 |
| C | -4.7107 | -1.4992 | 0.4728  |
| H | -3.8129 | 0.3944  | 0.9509  |
| C | -4.5642 | -2.7319 | -0.1676 |
| H | -3.2573 | -3.9736 | -1.3602 |
| H | -5.6171 | -1.2822 | 1.0407  |
| H | -5.3602 | -3.4763 | -0.1146 |
| S | 0.6887  | -0.9215 | 0.8185  |
| O | 0.3575  | -0.0992 | 1.9703  |
| O | 0.4039  | -2.3486 | 0.8286  |
| C | 2.3591  | -0.6377 | 0.3437  |
| C | 2.9386  | -1.4762 | -0.6121 |
| C | 3.0627  | 0.4108  | 0.9303  |
| C | 4.2538  | -1.2406 | -0.9878 |
| H | 2.3679  | -2.2984 | -1.0473 |
| C | 4.3832  | 0.6259  | 0.5405  |
| H | 2.5857  | 1.0401  | 1.6835  |
| C | 4.9940  | -0.1891 | -0.4199 |
| H | 4.7240  | -1.8849 | -1.7337 |

|   |        |         |         |
|---|--------|---------|---------|
| H | 4.9504 | 1.4411  | 0.9936  |
| C | 6.4173 | 0.0405  | -0.8423 |
| H | 7.0325 | -0.8444 | -0.6206 |
| H | 6.4754 | 0.2131  | -1.9272 |
| H | 6.8535 | 0.9054  | -0.3272 |

## 2a

0 imaginary frequency

|   |         |         |         |
|---|---------|---------|---------|
| C | -2.2591 | 0.2683  | 0.0005  |
| C | -1.7826 | -1.0420 | 0.0007  |
| C | -0.4094 | -1.2849 | 0.0001  |
| C | 0.5121  | -0.2269 | -0.0006 |
| C | 0.0180  | 1.0883  | -0.0009 |
| C | -1.3524 | 1.3318  | -0.0003 |
| H | -2.4819 | -1.8801 | 0.0012  |
| H | -0.0377 | -2.3122 | 0.0001  |
| H | 0.7119  | 1.9308  | -0.0017 |
| H | -1.7178 | 2.3604  | -0.0006 |
| C | 1.9560  | -0.5385 | -0.0011 |
| H | 2.1934  | -1.6075 | -0.0035 |
| C | 2.9623  | 0.3413  | 0.0014  |
| H | 3.9991  | -0.0010 | 0.0008  |
| H | 2.7969  | 1.4218  | 0.0041  |
| H | -3.3332 | 0.4628  | 0.0009  |

## Imine-radical

0 imaginary frequency

|   |         |        |        |
|---|---------|--------|--------|
| N | 0.0001  | 2.3898 | 0.0001 |
| C | -0.0000 | 1.1308 | 0.0001 |
| C | -1.3043 | 0.3921 | 0.0324 |

|   |         |         |         |
|---|---------|---------|---------|
| C | -2.4243 | 0.9466  | -0.6013 |
| C | -1.4282 | -0.8153 | 0.7310  |
| C | -3.6539 | 0.2952  | -0.5417 |
| H | -2.3199 | 1.8857  | -1.1476 |
| C | -2.6626 | -1.4606 | 0.7916  |
| H | -0.5611 | -1.2460 | 1.2352  |
| C | -3.7748 | -0.9088 | 0.1546  |
| H | -4.5210 | 0.7276  | -1.0436 |
| H | -2.7553 | -2.3990 | 1.3407  |
| H | -4.7383 | -1.4194 | 0.1996  |
| C | 1.3043  | 0.3921  | -0.0323 |
| C | 1.4280  | -0.8155 | -0.7307 |
| C | 2.4244  | 0.9467  | 0.6010  |
| C | 2.6624  | -1.4608 | -0.7914 |
| H | 0.5609  | -1.2463 | -1.2347 |
| C | 3.6540  | 0.2952  | 0.5413  |
| H | 2.3202  | 1.8858  | 1.1472  |
| C | 3.7748  | -0.9089 | -0.1547 |
| H | 2.7550  | -2.3993 | -1.3404 |
| H | 4.5212  | 0.7277  | 1.0429  |
| H | 4.7383  | -1.4195 | -0.1999 |

### **Ts-radical**

0 imaginary frequency

|   |         |         |         |
|---|---------|---------|---------|
| S | -2.1474 | -0.0018 | -0.2376 |
| O | -2.6491 | 1.2814  | 0.2876  |
| O | -2.6446 | -1.2852 | 0.2906  |
| C | -0.3631 | 0.0014  | -0.0997 |
| C | 0.3101  | -1.2194 | -0.0827 |
| C | 0.3054  | 1.2220  | -0.0811 |

|   |         |         |         |
|---|---------|---------|---------|
| C | 1.6988  | -1.2038 | -0.0179 |
| H | -0.2453 | -2.1580 | -0.1066 |
| C | 1.6967  | 1.2109  | -0.0158 |
| H | -0.2520 | 2.1594  | -0.1040 |
| C | 2.4109  | 0.0057  | 0.0169  |
| H | 2.2448  | -2.1493 | 0.0066  |
| H | 2.2388  | 2.1581  | 0.0103  |
| C | 3.9109  | -0.0025 | 0.1064  |
| H | 4.2308  | -0.2840 | 1.1218  |
| H | 4.3422  | -0.7381 | -0.5870 |
| H | 4.3299  | 0.9861  | -0.1199 |

### **II**

0 imaginary frequency

|   |         |         |         |
|---|---------|---------|---------|
| C | -3.3552 | -1.4099 | -0.3483 |
| C | -2.8650 | -2.2762 | 0.6363  |
| C | -1.5085 | -2.5557 | 0.7109  |
| C | -0.5873 | -1.9697 | -0.1975 |
| C | -1.1083 | -1.1100 | -1.2006 |
| C | -2.4676 | -0.8367 | -1.2666 |
| H | -3.5515 | -2.7318 | 1.3524  |
| H | -1.1271 | -3.2230 | 1.4870  |
| H | -0.4377 | -0.6469 | -1.9260 |
| H | -2.8438 | -0.1655 | -2.0414 |
| C | 0.8049  | -2.2288 | -0.0395 |
| H | 1.1096  | -2.8969 | 0.7679  |
| C | 1.8777  | -1.5484 | -0.7930 |
| H | 2.7951  | -2.1522 | -0.8685 |
| H | 1.5966  | -1.1955 | -1.7945 |
| H | -4.4220 | -1.1874 | -0.4030 |



|   |         |         |         |
|---|---------|---------|---------|
| S | 2.4927  | -0.0634 | 0.0806  |
| O | 2.8734  | -0.4783 | 1.4315  |
| O | 3.4819  | 0.5732  | -0.7904 |
| C | 1.0664  | 0.9874  | 0.1975  |
| C | 0.7685  | 1.8423  | -0.8601 |
| C | 0.2228  | 0.8657  | 1.3016  |
| C | -0.4183 | 2.5713  | -0.8183 |
| H | 1.4551  | 1.9302  | -1.7042 |
| C | -0.9592 | 1.5974  | 1.3239  |
| H | 0.4901  | 0.1965  | 2.1212  |
| C | -1.3023 | 2.4493  | 0.2621  |
| H | -0.6656 | 3.2455  | -1.6409 |
| H | -1.6347 | 1.5049  | 2.1773  |
| C | -2.6072 | 3.1953  | 0.2859  |
| H | -2.6560 | 3.9449  | -0.5144 |
| H | -3.4463 | 2.4946  | 0.1516  |
| H | -2.7555 | 3.6995  | 1.2515  |

### III

0 imaginary frequency

|   |         |         |         |
|---|---------|---------|---------|
| N | -1.0132 | -1.5872 | 1.0184  |
| C | -1.3593 | -0.4682 | 0.5156  |
| C | -0.4247 | 0.6948  | 0.3345  |
| C | 0.1401  | 0.9426  | -0.9225 |
| C | -0.0984 | 1.5243  | 1.4125  |
| C | 1.0319  | 2.0000  | -1.0952 |
| H | -0.1144 | 0.2959  | -1.7658 |
| C | 0.7896  | 2.5871  | 1.2359  |
| H | -0.5442 | 1.3385  | 2.3927  |
| C | 1.3579  | 2.8239  | -0.0160 |

|   |         |         |         |
|---|---------|---------|---------|
| H | 1.4767  | 2.1797  | -2.0757 |
| H | 1.0382  | 3.2312  | 2.0813  |
| H | 2.0567  | 3.6513  | -0.1516 |
| C | -2.7732 | -0.2908 | 0.0564  |
| C | -3.2474 | 0.9560  | -0.3719 |
| C | -3.6499 | -1.3872 | 0.0597  |
| C | -4.5720 | 1.1045  | -0.7869 |
| H | -2.5815 | 1.8205  | -0.3791 |
| C | -4.9679 | -1.2383 | -0.3577 |
| H | -3.2737 | -2.3543 | 0.3946  |
| C | -5.4340 | 0.0097  | -0.7827 |
| H | -4.9288 | 2.0821  | -1.1156 |
| H | -5.6387 | -2.0994 | -0.3542 |
| H | -6.4687 | 0.1254  | -1.1105 |
| C | 4.8748  | 0.0296  | -0.6797 |
| C | 4.3447  | -0.9356 | -1.5454 |
| C | 3.1772  | -1.6072 | -1.2166 |
| C | 2.4850  | -1.3365 | -0.0038 |
| C | 3.0459  | -0.3594 | 0.8625  |
| C | 4.2168  | 0.3065  | 0.5234  |
| H | 4.8511  | -1.1608 | -2.4861 |
| H | 2.7651  | -2.3547 | -1.8984 |
| H | 2.5525  | -0.1188 | 1.8054  |
| H | 4.6228  | 1.0566  | 1.2051  |
| C | 1.2665  | -2.0174 | 0.2661  |
| H | 0.9225  | -2.7516 | -0.4674 |
| C | 0.3718  | -1.7950 | 1.4439  |
| H | 0.3799  | -2.6920 | 2.0852  |
| H | 0.7317  | -0.9577 | 2.0588  |
| H | 5.7927  | 0.5588  | -0.9400 |

**MECP-1**

|   |         |         |         |
|---|---------|---------|---------|
| C | -1.8402 | 3.5631  | 0.8129  |
| C | -1.2857 | 3.6971  | -0.4585 |
| C | -0.7733 | 2.5937  | -1.1123 |
| C | -0.8013 | 1.3165  | -0.5133 |
| C | -1.3531 | 1.2044  | 0.7802  |
| C | -1.8675 | 2.3120  | 1.4265  |
| H | -1.2580 | 4.6671  | -0.9379 |
| H | -0.3441 | 2.6924  | -2.1018 |
| H | -1.3879 | 0.2429  | 1.2731  |
| H | -2.2976 | 2.2021  | 2.4142  |
| C | -0.2917 | 0.2060  | -1.2431 |
| H | -0.0324 | 0.3666  | -2.2785 |
| C | -0.3999 | -1.2016 | -0.8030 |
| H | 0.3813  | -1.8272 | -1.2418 |
| H | -0.4024 | -1.3423 | 0.2782  |
| H | -2.2472 | 4.4266  | 1.3223  |
| S | -1.9096 | -2.0017 | -1.4043 |
| O | -1.9573 | -1.8379 | -2.8376 |
| O | -1.9280 | -3.3358 | -0.8525 |
| C | -3.2206 | -1.0683 | -0.6889 |
| C | -3.6593 | -1.3839 | 0.5888  |
| C | -3.7240 | 0.0312  | -1.3747 |
| C | -4.6062 | -0.5708 | 1.1939  |
| H | -3.2609 | -2.2494 | 1.1022  |
| C | -4.6660 | 0.8337  | -0.7555 |
| H | -3.3720 | 0.2550  | -2.3731 |
| C | -5.1083 | 0.5529  | 0.5391  |
| H | -4.9573 | -0.8078 | 2.1905  |

|   |         |         |         |
|---|---------|---------|---------|
| H | -5.0618 | 1.6965  | -1.2774 |
| C | -6.0864 | 1.4681  | 1.2147  |
| H | -6.4792 | 1.0248  | 2.1277  |
| H | -5.5968 | 2.4091  | 1.4758  |
| H | -6.9189 | 1.7077  | 0.5532  |
| N | 2.2007  | 0.6825  | -1.2082 |
| C | 2.9365  | 0.1950  | -0.3200 |
| C | 4.4288  | 0.3577  | -0.3628 |
| C | 5.0496  | 0.7982  | -1.5331 |
| C | 5.2002  | 0.1044  | 0.7685  |
| C | 6.4211  | 0.9854  | -1.5659 |
| H | 4.4481  | 0.9897  | -2.4120 |
| C | 6.5764  | 0.2958  | 0.7330  |
| H | 4.7287  | -0.2354 | 1.6811  |
| C | 7.1881  | 0.7361  | -0.4315 |
| H | 6.8959  | 1.3255  | -2.4771 |
| H | 7.1672  | 0.1004  | 1.6184  |
| H | 8.2597  | 0.8846  | -0.4585 |
| C | 2.3267  | -0.5507 | 0.8334  |
| C | 1.5761  | 0.1407  | 1.7763  |
| C | 2.4775  | -1.9312 | 0.9351  |
| C | 0.9657  | -0.5491 | 2.8167  |
| H | 1.4667  | 1.2141  | 1.6880  |
| C | 1.8534  | -2.6191 | 1.9663  |
| H | 3.0693  | -2.4633 | 0.2004  |
| C | 1.0969  | -1.9289 | 2.9079  |
| H | 0.3798  | -0.0072 | 3.5483  |
| H | 1.9556  | -3.6944 | 2.0344  |
| H | 0.6132  | -2.4668 | 3.7127  |

**MECP-2**

|   |         |         |         |
|---|---------|---------|---------|
| N | -2.1493 | -1.4439 | 0.4524  |
| C | -3.0255 | -0.5555 | 0.2096  |
| C | -2.8153 | 0.9125  | 0.4198  |
| C | -2.6201 | 1.7422  | -0.6810 |
| C | -2.8020 | 1.4558  | 1.7016  |
| C | -2.3951 | 3.1004  | -0.5006 |
| H | -2.6368 | 1.3207  | -1.6792 |
| C | -2.5798 | 2.8151  | 1.8807  |
| H | -2.9630 | 0.8119  | 2.5578  |
| C | -2.3720 | 3.6382  | 0.7803  |
| H | -2.2350 | 3.7369  | -1.3611 |
| H | -2.5711 | 3.2298  | 2.8803  |
| H | -2.1964 | 4.6967  | 0.9212  |
| C | -4.3478 | -0.9892 | -0.3343 |
| C | -5.4223 | -0.1031 | -0.3951 |
| C | -4.5317 | -2.3045 | -0.7697 |
| C | -6.6578 | -0.5224 | -0.8744 |
| H | -5.3006 | 0.9187  | -0.0604 |
| C | -5.7611 | -2.7198 | -1.2510 |
| H | -3.6998 | -2.9936 | -0.7248 |
| C | -6.8304 | -1.8299 | -1.3039 |
| H | -7.4835 | 0.1759  | -0.9099 |
| H | -5.8886 | -3.7409 | -1.5867 |
| H | -7.7914 | -2.1573 | -1.6791 |
| C | 2.1578  | 2.5630  | -1.4521 |
| C | 2.2204  | 1.3855  | -2.1987 |
| C | 1.5313  | 0.2654  | -1.7847 |
| C | 0.7445  | 0.2827  | -0.6050 |
| C | 0.6865  | 1.4923  | 0.1298  |

|   |         |         |         |
|---|---------|---------|---------|
| C | 1.3853  | 2.6062  | -0.2921 |
| H | 2.8163  | 1.3483  | -3.1018 |
| H | 1.5837  | -0.6513 | -2.3598 |
| H | 0.0869  | 1.5515  | 1.0292  |
| H | 1.3277  | 3.5203  | 0.2845  |
| C | 0.1089  | -0.9085 | -0.1910 |
| H | 0.2313  | -1.7818 | -0.8237 |
| C | -0.8268 | -1.0700 | 0.9614  |
| H | -0.4879 | -1.9072 | 1.5768  |
| H | -0.8429 | -0.1805 | 1.5884  |
| H | 2.7066  | 3.4391  | -1.7715 |
| S | 2.2967  | -1.0759 | 1.9373  |
| O | 2.4569  | -0.0360 | 2.9482  |
| O | 2.2792  | -2.4737 | 2.3575  |
| C | 3.5958  | -0.8763 | 0.7370  |
| C | 3.8418  | -1.9196 | -0.1461 |
| C | 4.2576  | 0.3379  | 0.6341  |
| C | 4.7989  | -1.7462 | -1.1306 |
| H | 3.3020  | -2.8532 | -0.0540 |
| C | 5.2159  | 0.4892  | -0.3581 |
| H | 4.0389  | 1.1413  | 1.3244  |
| C | 5.4972  | -0.5426 | -1.2530 |
| H | 5.0126  | -2.5583 | -1.8150 |
| H | 5.7538  | 1.4260  | -0.4386 |
| C | 6.5069  | -0.3590 | -2.3481 |
| H | 7.0217  | -1.2942 | -2.5662 |
| H | 6.0133  | -0.0336 | -3.2670 |
| H | 7.2450  | 0.3962  | -2.0823 |

**TS1**

1 imaginary frequency, -374.9553 cm<sup>-1</sup>

|   |         |         |         |
|---|---------|---------|---------|
| N | -0.3678 | -0.4052 | -1.0406 |
| C | -1.4541 | 0.2126  | -0.6434 |
| C | -1.4083 | 1.6642  | -0.4090 |
| C | -0.1719 | 2.2894  | -0.1600 |
| C | -2.5688 | 2.4553  | -0.4837 |
| C | -0.1035 | 3.6650  | 0.0311  |
| H | 0.7387  | 1.6895  | -0.1115 |
| C | -2.4918 | 3.8321  | -0.2933 |
| H | -3.5301 | 1.9921  | -0.7100 |
| C | -1.2632 | 4.4413  | -0.0303 |
| H | 0.8610  | 4.1348  | 0.2308  |
| H | -3.3990 | 4.4353  | -0.3564 |
| H | -1.2085 | 5.5205  | 0.1213  |
| C | -2.6395 | -0.6354 | -0.3881 |
| C | -2.8192 | -1.8171 | -1.1291 |
| C | -3.5408 | -0.3299 | 0.6459  |
| C | -3.8922 | -2.6597 | -0.8568 |
| H | -2.1140 | -2.0626 | -1.9250 |
| C | -4.6118 | -1.1790 | 0.9124  |
| H | -3.3863 | 0.5601  | 1.2575  |
| C | -4.7940 | -2.3412 | 0.1607  |
| H | -4.0274 | -3.5697 | -1.4434 |
| H | -5.3033 | -0.9356 | 1.7207  |
| H | -5.6356 | -3.0028 | 0.3728  |
| S | 0.6467  | -1.2291 | 0.5837  |
| O | 0.1535  | -0.5439 | 1.7799  |
| O | 0.4289  | -2.6636 | 0.3954  |
| C | 2.3467  | -0.8408 | 0.3178  |
| C | 3.0591  | -1.5824 | -0.6279 |

|   |        |         |         |
|---|--------|---------|---------|
| C | 2.9179 | 0.2351  | 0.9955  |
| C | 4.3789 | -1.2340 | -0.8850 |
| H | 2.5857 | -2.4213 | -1.1406 |
| C | 4.2444 | 0.5623  | 0.7238  |
| H | 2.3356 | 0.7929  | 1.7310  |
| C | 4.9905 | -0.1603 | -0.2164 |
| H | 4.9525 | -1.8061 | -1.6174 |
| H | 4.7108 | 1.3944  | 1.2547  |
| C | 6.4218 | 0.1917  | -0.5092 |
| H | 7.0864 | -0.6442 | -0.2436 |
| H | 6.5616 | 0.3895  | -1.5822 |
| H | 6.7390 | 1.0786  | 0.0537  |

## TS2

1 imaginary frequency, -260.5016 cm<sup>-1</sup>

|   |         |         |         |
|---|---------|---------|---------|
| C | -3.2900 | -1.1708 | -0.2767 |
| C | -2.8204 | -1.9505 | 0.7823  |
| C | -1.4884 | -2.3537 | 0.8140  |
| C | -0.5948 | -1.9821 | -0.2090 |
| C | -1.0879 | -1.2095 | -1.2798 |
| C | -2.4182 | -0.8081 | -1.3090 |
| H | -3.4957 | -2.2431 | 1.5882  |
| H | -1.1178 | -2.9554 | 1.6472  |
| H | -0.4223 | -0.9141 | -2.0930 |
| H | -2.7815 | -0.2033 | -2.1425 |
| C | 0.8058  | -2.3710 | -0.0972 |
| H | 1.0580  | -2.9974 | 0.7635  |
| C | 1.8265  | -1.9439 | -0.9052 |
| H | 2.8197  | -2.3858 | -0.7921 |
| H | 1.6348  | -1.4231 | -1.8477 |

|   |         |         |         |
|---|---------|---------|---------|
| H | -4.3329 | -0.8500 | -0.3027 |
| S | 2.6087  | 0.1142  | 0.1085  |
| O | 3.0363  | -0.2213 | 1.4765  |
| O | 3.5214  | 0.8325  | -0.7995 |
| C | 1.0790  | 1.0213  | 0.2087  |
| C | 0.6955  | 1.8254  | -0.8645 |
| C | 0.2378  | 0.7936  | 1.2947  |
| C | -0.5648 | 2.4128  | -0.8383 |
| H | 1.3776  | 1.9837  | -1.7018 |
| C | -1.0229 | 1.3866  | 1.2987  |
| H | 0.5652  | 0.1562  | 2.1179  |
| C | -1.4449 | 2.1927  | 0.2334  |
| H | -0.8807 | 3.0465  | -1.6702 |
| H | -1.6973 | 1.2097  | 2.1393  |
| C | -2.8154 | 2.8105  | 0.2274  |
| H | -2.7529 | 3.8947  | 0.4098  |
| H | -3.3027 | 2.6721  | -0.7486 |
| H | -3.4541 | 2.3706  | 1.0044  |

### TS3

1 imaginary frequency, -592.4727 cm<sup>-1</sup>

|   |         |         |         |
|---|---------|---------|---------|
| C | -3.4659 | -0.9410 | -2.1616 |
| C | -4.0118 | -0.1296 | -1.1655 |
| C | -3.5011 | -0.1727 | 0.1296  |
| C | -2.4351 | -1.0302 | 0.4603  |
| C | -1.8954 | -1.8444 | -0.5565 |
| C | -2.4071 | -1.7993 | -1.8490 |
| H | -4.8376 | 0.5445  | -1.4008 |
| H | -3.9228 | 0.4708  | 0.9057  |
| H | -1.0537 | -2.5040 | -0.3351 |

|   |         |         |         |
|---|---------|---------|---------|
| H | -1.9726 | -2.4334 | -2.6242 |
| C | -1.8968 | -1.0114 | 1.8140  |
| H | -2.2931 | -0.2322 | 2.4704  |
| C | -0.8841 | -1.8142 | 2.2748  |
| H | -0.6213 | -1.7844 | 3.3327  |
| H | -0.6359 | -2.7410 | 1.7567  |
| H | -3.8613 | -0.9052 | -3.1782 |
| N | 0.9938  | -1.1791 | 1.6810  |
| C | 1.1777  | -0.2418 | 0.8521  |
| C | 2.5255  | -0.2003 | 0.1731  |
| C | 3.2231  | -1.3933 | -0.0612 |
| C | 3.1063  | 1.0193  | -0.1973 |
| C | 4.4799  | -1.3661 | -0.6603 |
| H | 2.7643  | -2.3408 | 0.2255  |
| C | 4.3689  | 1.0432  | -0.7897 |
| H | 2.5732  | 1.9543  | -0.0154 |
| C | 5.0566  | -0.1475 | -1.0247 |
| H | 5.0113  | -2.3008 | -0.8478 |
| H | 4.8165  | 1.9986  | -1.0692 |
| H | 6.0415  | -0.1269 | -1.4945 |
| C | 0.2133  | 0.8544  | 0.5098  |
| C | -0.0872 | 1.1309  | -0.8299 |
| C | -0.3765 | 1.6151  | 1.5231  |
| C | -0.9952 | 2.1387  | -1.1493 |
| H | 0.3817  | 0.5434  | -1.6226 |
| C | -1.2703 | 2.6368  | 1.2004  |
| H | -0.1294 | 1.4034  | 2.5653  |
| C | -1.5853 | 2.8952  | -0.1341 |
| H | -1.2430 | 2.3342  | -2.1940 |
| H | -1.7225 | 3.2328  | 1.9952  |

|                       |         |         |         |   |         |         |         |
|-----------------------|---------|---------|---------|---|---------|---------|---------|
| H                     | -2.2897 | 3.6904  | -0.3849 | C | 4.9966  | -0.4182 | 0.6586  |
|                       |         |         |         | H | 4.9159  | 1.4190  | 1.7888  |
| <b>3</b>              |         |         |         | H | 4.8665  | -2.1031 | -0.6890 |
| 0 imaginary frequency |         |         |         | C | 6.0271  | -1.0685 | 1.5386  |
| C                     | 2.0148  | -3.0226 | 1.6902  | H | 6.4463  | -0.3555 | 2.2600  |
| C                     | 1.4615  | -3.5166 | 0.5077  | H | 5.5745  | -1.9004 | 2.1011  |
| C                     | 0.7529  | -2.6658 | -0.3390 | H | 6.8478  | -1.4891 | 0.9401  |
| C                     | 0.5848  | -1.3136 | -0.0187 | N | -1.6163 | -0.7726 | -0.8870 |
| C                     | 1.1327  | -0.8285 | 1.1723  | C | -2.4934 | -0.1451 | -0.2111 |
| C                     | 1.8472  | -1.6773 | 2.0197  | C | -3.9052 | -0.6527 | -0.2582 |
| H                     | 1.5880  | -4.5672 | 0.2400  | C | -4.2532 | -1.6605 | -1.1713 |
| H                     | 0.3287  | -3.0487 | -1.2705 | C | -4.8908 | -0.1454 | 0.5989  |
| H                     | 1.0254  | 0.2226  | 1.4449  | C | -5.5546 | -2.1476 | -1.2243 |
| H                     | 2.2809  | -1.2800 | 2.9397  | H | -3.4831 | -2.0506 | -1.8371 |
| C                     | -0.1986 | -0.4387 | -0.9952 | C | -6.1959 | -0.6381 | 0.5467  |
| H                     | 0.0781  | -0.7858 | -2.0032 | H | -4.6418 | 0.6358  | 1.3187  |
| C                     | 0.1692  | 1.0489  | -0.9813 | C | -6.5316 | -1.6378 | -0.3640 |
| H                     | -0.5633 | 1.6295  | -1.5625 | H | -5.8122 | -2.9288 | -1.9416 |
| H                     | 0.2733  | 1.5222  | 0.0029  | H | -6.9519 | -0.2362 | 1.2233  |
| H                     | 2.5771  | -3.6839 | 2.3521  | H | -7.5529 | -2.0203 | -0.4066 |
| S                     | 1.6881  | 1.4189  | -1.8808 | C | -2.2446 | 1.0542  | 0.6579  |
| O                     | 1.6314  | 0.7164  | -3.1657 | C | -1.6743 | 0.8857  | 1.9232  |
| O                     | 1.8199  | 2.8769  | -1.8589 | C | -2.5917 | 2.3373  | 0.2189  |
| C                     | 3.0216  | 0.7280  | -0.9337 | C | -1.4148 | 1.9972  | 2.7273  |
| C                     | 3.5262  | 1.4493  | 0.1444  | H | -1.4309 | -0.1184 | 2.2765  |
| C                     | 3.5017  | -0.5409 | -1.2558 | C | -2.3238 | 3.4460  | 1.0197  |
| C                     | 4.5126  | 0.8665  | 0.9376  | H | -3.0587 | 2.4667  | -0.7604 |
| H                     | 3.1495  | 2.4511  | 0.3595  | C | -1.7288 | 3.2780  | 2.2722  |
| C                     | 4.4866  | -1.1062 | -0.4538 | H | -0.9663 | 1.8602  | 3.7129  |
| H                     | 3.0983  | -1.0743 | -2.1182 | H | -2.5808 | 4.4458  | 0.6657  |

|                       |         |         |         |   |         |         |         |
|-----------------------|---------|---------|---------|---|---------|---------|---------|
| H                     | -1.5194 | 4.1472  | 2.8981  | C | -2.4389 | 1.8755  | 1.1025  |
|                       |         |         |         | C | -1.7087 | 1.5014  | -0.0315 |
| <b>3'</b>             |         |         |         | C | -2.0594 | 2.0380  | -1.2769 |
| 0 imaginary frequency |         |         |         | C | -3.1221 | 2.9347  | -1.3819 |
| N                     | 1.6255  | -0.2051 | -0.5675 | H | -4.0662 | 3.0510  | 1.8880  |
| C                     | 2.8371  | -0.0787 | -0.1979 | H | -2.1743 | 1.4518  | 2.0741  |
| C                     | 3.4926  | 1.2250  | 0.1477  | H | -1.5202 | 1.7336  | -2.1759 |
| C                     | 4.0496  | 1.4230  | 1.4177  | H | -3.3888 | 3.3444  | -2.3577 |
| C                     | 3.5488  | 2.2580  | -0.7955 | C | -0.6128 | 0.4752  | 0.0878  |
| C                     | 4.6414  | 2.6428  | 1.7425  | H | -0.4115 | 0.2399  | 1.1429  |
| H                     | 4.0165  | 0.6165  | 2.1538  | C | 0.6865  | 0.8801  | -0.6194 |
| C                     | 4.1537  | 3.4729  | -0.4735 | H | 0.4616  | 1.0879  | -1.6774 |
| H                     | 3.1221  | 2.1034  | -1.7892 | H | 1.0306  | 1.8208  | -0.1552 |
| C                     | 4.6971  | 3.6680  | 0.7967  | H | -4.6819 | 3.9990  | -0.3327 |
| H                     | 5.0649  | 2.7922  | 2.7373  | S | -1.1828 | -1.1359 | -0.6028 |
| H                     | 4.1997  | 4.2699  | -1.2175 | O | -1.1226 | -1.0256 | -2.0634 |
| H                     | 5.1674  | 4.6198  | 1.0496  | O | -0.4952 | -2.2326 | 0.0835  |
| C                     | 3.6582  | -1.3273 | -0.1011 | C | -2.8961 | -1.2311 | -0.1236 |
| C                     | 5.0577  | -1.2915 | -0.0628 | C | -3.2102 | -1.6966 | 1.1532  |
| C                     | 3.0005  | -2.5679 | -0.0687 | C | -3.8833 | -0.8097 | -1.0092 |
| C                     | 5.7907  | -2.4778 | 0.0035  | C | -4.5430 | -1.7145 | 1.5508  |
| H                     | 5.5818  | -0.3348 | -0.0965 | H | -2.4189 | -2.0417 | 1.8211  |
| C                     | 3.7352  | -3.7472 | 0.0040  | C | -5.2134 | -0.8363 | -0.5942 |
| H                     | 1.9080  | -2.5771 | -0.0978 | H | -3.6082 | -0.4649 | -2.0072 |
| C                     | 5.1323  | -3.7059 | 0.0394  | C | -5.5614 | -1.2809 | 0.6878  |
| H                     | 6.8812  | -2.4394 | 0.0254  | H | -4.8033 | -2.0747 | 2.5487  |
| H                     | 3.2169  | -4.7074 | 0.0353  | H | -5.9972 | -0.5055 | -1.2786 |
| H                     | 5.7062  | -4.6327 | 0.0956  | C | -6.9963 | -1.3139 | 1.1360  |
| C                     | -3.8478 | 3.3003  | -0.2475 | H | -7.3284 | -2.3516 | 1.2919  |
| C                     | -3.5035 | 2.7694  | 0.9963  | H | -7.1192 | -0.7859 | 2.0929  |

H -7.6578 -0.8499 0.3933



