**Supporting Information for**

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# Precursors for the Synthesis of Macroheterocyclic Compounds. Modeling of the Mechanism for Formation of 2-Amino-5-methyl-1,3,4-thiadiazole by Quantum Chemistry Methods

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**Compound, total charge (a.u.), multiplicity, Cartesian coordinates (Å) and total energy values (a.u.) of the structures optimized at the DFT/B3LYP/6-311+G(2d2p)**

**1a.**

0 1

| | | | |
|---|---|---|---|
| N | -1.725694497 | 0.363690704 | -7.336750791 |
| N | -0.902838711 | -0.737819593 | -7.636901670 |
| C | -1.326274505 | -1.802327245 | -8.374591512 |
| S | -2.797946089 | -1.853940829 | -9.162624972 |
| N | -0.447201211 | -2.850789935 | -8.386831231 |
| H | -0.664690667 | -3.578904557 | -9.045514370 |
| H | 0.534822622 | -2.666822225 | -8.247456999 |
| H | -1.714050979 | 0.988008794 | -8.136968656 |
| H | -0.197440295 | -0.901044625 | -6.935377739 |
| H | -2.682134118 | 0.020887265 | -7.265329881 |

TOTAL ENERGY = -603.470745 a.u.

**1b.**

0 1

| | | | |
|---|---|---|---|
| N | -1.734887037 | 0.259374259 | -7.336084732 |
| N | -0.802438859 | -0.691371869 | -7.786202427 |
| C | -1.136420324 | -1.868394689 | -8.435930361 |
| S | -2.807838790 | -1.846054379 | -9.099073340 |
| N | -0.389299625 | -2.878236130 | -8.622704308 |
| H | -2.667163940 | -3.065323993 | -9.639097660 |
| H | 0.530043607 | -2.766605192 | -8.197902681 |
| H | -2.047848705 | 0.832516241 | -8.108862226 |
| H | 0.022112221 | -0.737201413 | -7.208076055 |
| H | -2.533422919 | -0.179644865 | -6.891085464 |

TOTAL ENERGY = -603.442577 a.u.

**TS1.**

0 1

| | | | |
|---|---|---|---|
| N | -1.781489164 | 0.271283351 | -7.373565190 |
| N | -0.872813436 | -0.775847222 | -7.596413356 |
| C | -1.111392308 | -1.857180035 | -8.360047653 |
| S | -2.596658176 | -2.171759169 | -9.225984860 |
| N | -0.303828907 | -2.861906013 | -8.601490440 |
| H | -1.415844971 | -3.285816026 | -9.363717571 |
| H | 0.627869892 | -2.891372463 | -8.195132552 |
| H | -2.030850148 | 0.691220053 | -8.262539653 |
| H | 0.013830420 | -0.674948844 | -7.131400448 |
| H | -2.626039717 | -0.103485278 | -6.955139610 |

TOTAL ENERGY = -603.405526 a.u.

**2a.**

1 1

| | | | |
|---|---|---|---|
| C | -1.782690060 | -0.273191328 | -5.638741993 |
| N | -1.821413929 | 0.017498573 | -7.199227966 |
| N | -0.788908167 | -0.604315847 | -7.974705202 |
| C | -1.097730711 | -1.874473865 | -8.553763020 |
| S | -2.709345476 | -1.843534807 | -9.357149858 |
| C | -2.917770440 | 0.506709459 | -5.006473652 |
| H | -2.801751702 | 1.573840800 | -5.189418689 |
| H | -2.881764959 | 0.352613547 | -3.928390945 |
| H | -3.891034402 | 0.179471819 | -5.375678187 |
| N | -0.329362052 | -2.857948707 | -8.632893291 |
| H | -2.943412707 | -3.150532493 | -9.159352713 |
| H | 0.540745489 | -2.780574347 | -8.109405048 |
| O | -0.522246119 | 0.191572265 | -5.319147765 |
| H | -1.765493831 | 1.028395335 | -7.344886904 |
| H | 0.077500006 | -0.580550664 | -7.445831880 |
| O | -1.833260244 | -1.633670778 | -5.482338847 |
| H | -2.711978389 | -0.329331587 | -7.595499761 |
| H | -2.694380472 | -1.931491202 | -5.165133317 |
| H | -0.154957324 | -0.337059019 | -4.598702932 |

TOTAL ENERGY = -832.826174 a.u.

**2b.**

1 1

| | | | |
|---|---|---|---|
| C | -1.905507736 | -0.105957688 | -6.228775912 |
| N | -1.251459286 | 0.324211374 | -7.289247250 |
| N | -0.284078858 | -0.407444680 | -7.972964980 |
| C | -0.700109617 | -1.380490510 | -8.934230968 |
| S | -2.359617790 | -1.104018603 | -9.536054961 |
| C | -2.924518160 | 0.760936082 | -5.578411765 |
| H | -2.632689582 | 0.958014845 | -4.546088228 |
| H | -3.880716030 | 0.236551423 | -5.559575956 |
| H | -3.045473914 | 1.705364825 | -6.102487589 |
| N | 0.030569407 | -2.298067959 | -9.378786308 |
| H | -2.266243627 | -2.091698509 | -10.439285290 |
| H | 0.965767314 | -2.344987689 | -8.979971315 |
| O | -1.605744060 | -1.275791360 | -5.794476104 |
| H | -1.437227266 | 1.253823860 | -7.641595899 |

H 0.455885002 -0.724283403 -7.359718359
O -2.977139765 -2.156650996 -3.812336787
H -3.544095605 -2.921205170 -3.970068500
H -2.553110237 -2.302487520 -2.958299291
H -2.150040913 -1.598829344 -4.998930708
TOTAL ENERGY = -832.863960 a.u.

**TS2.**
1 1
C -1.945353156 -0.370008471 -5.712180860
N -2.076669650 -0.161241438 -7.199459949
N -0.992441558 -0.464770830 -8.047315906
C -0.922112438 -1.770261642 -8.612002250
S -2.530984779 -2.369697546 -9.128757747
C -2.536491252 0.729888416 -4.868882703
H -1.884008891 1.601587306 -4.907048197
H -2.616563815 0.406374779 -3.830171350
H -3.528134547 1.016754730 -5.218604113
N 0.131900452 -2.408881321 -8.847030512
H -2.105545308 -3.635793080 -9.258023996
H 0.984090973 -1.985459482 -8.484630100
O -0.698078597 -0.774434920 -5.428856519
H -2.455063822 0.754573233 -7.424896625
H -0.106170628 -0.130548109 -7.687510736
O -2.886993654 -1.589258058 -5.772005329
H -2.928014975 -1.210828840 -6.930713152
H -3.687181755 -1.523392051 -5.228137315
H -0.524151864 -0.796769924 -4.478886797
TOTAL ENERGY = -832.770271 a.u.

**2b-H2O.**
1 1
C -1.925463267 -0.099470067 -6.178754899
N -1.322675609 0.225928270 -7.291881811
N -0.325071284 -0.519438192 -7.913802937
C -0.684856539 -1.400299602 -8.993419551
S -2.319477952 -1.088312747 -9.636525048
C -2.933726660 0.787457518 -5.548211352
H -2.579238111 1.108802028 -4.566164502
H -3.864604259 0.232773196 -5.411346727
H -3.133720137 1.666718586 -6.155322042
N 0.083205466 -2.262760394 -9.476369393
H -2.150439200 -1.926638851 -10.670861068
H 1.006665247 -2.326715455 -9.053909779
O -1.565124404 -1.235144306 -5.645575972
H -1.544017415 1.112724607 -7.728739282
H 0.310713770 -0.929333727 -7.241290236
H -2.043374760 -1.438958200 -4.828426990
TOTAL ENERGY = -756.405935 a.u.

**3a+H2O.**
1 1
C 1.069577543 -0.124382497 -0.560533532

| | | | |
|---|---|---|---|
| N | 0.759771124 | 0.203164492 | -1.786665354 |
| N | -0.428143302 | 0.877681521 | -1.984567511 |
| C | -1.243669567 | 0.873773688 | -0.836203615 |
| S | -0.201164637 | 0.239822835 | 0.541737075 |
| C | 2.389886322 | -0.686221941 | -0.191281808 |
| H | 3.012340648 | 0.106507548 | 0.231467133 |
| H | 2.895428171 | -1.101736650 | -1.062047164 |
| H | 2.268602288 | -1.446228317 | 0.579337655 |
| N | -2.430735428 | 1.244010161 | -0.860792927 |
| H | -2.944687747 | 1.228200287 | 0.011400644 |
| H | 1.754951648 | -1.364252944 | 3.453993983 |
| O | 1.272883353 | -1.648006069 | 2.669851455 |
| H | 0.790411503 | -2.433922725 | 2.947654536 |
| H | -0.886952908 | 0.698998516 | -2.870977309 |
| H | 1.414772796 | 0.168615386 | -2.558835011 |

TOTAL ENERGY = -756.421202 a.u.

**TS3.**

1 1

| | | | |
|---|---|---|---|
| C | 1.218785618 | -0.347701497 | -0.034896655 |
| N | 0.744690838 | -0.534466632 | -1.332647374 |
| N | -0.566242061 | -0.064456367 | -1.505390121 |
| C | -1.118603072 | 0.744629937 | -0.523186558 |
| S | 0.243791999 | 1.132724916 | 0.728436619 |
| C | 2.713661843 | -0.325256928 | 0.115413676 |
| H | 3.142197114 | 0.493522824 | -0.459877224 |
| H | 3.129874103 | -1.265176419 | -0.252758072 |
| H | 3.000124365 | -0.193207181 | 1.156810634 |
| N | -2.304616001 | 1.107605352 | -0.491714482 |
| H | -2.622259076 | 1.682418732 | 0.276923986 |
| H | 0.043804397 | -0.292259991 | 1.463676202 |
| O | 0.548416237 | -1.321580678 | 0.891505172 |
| H | 1.151892836 | -1.960971465 | 1.306501339 |
| H | -1.204959897 | -0.719151783 | -1.937705868 |
| H | 1.362768460 | -0.130427991 | -2.028214941 |

TOTAL ENERGY = -756.334927 a.u.

**3a.**

1 1

| | | | |
|---|---|---|---|
| C | 1.085289044 | -0.086664431 | -0.558290400 |
| N | 0.748096454 | 0.176921904 | -1.791018542 |
| N | -0.443832818 | 0.838712027 | -1.996177343 |
| C | -1.243796269 | 0.888785188 | -0.838160798 |
| S | -0.149739981 | 0.357874489 | 0.553939244 |
| C | 2.397723238 | -0.669397621 | -0.186479668 |
| H | 2.957499088 | 0.036387024 | 0.429680923 |
| H | 2.986350285 | -0.910892641 | -1.070145873 |
| H | 2.249929966 | -1.576410340 | 0.400633279 |
| N | -2.432616779 | 1.241867378 | -0.857569425 |
| H | -2.940605167 | 1.273788546 | 0.017475770 |
| H | -0.914378101 | 0.631354006 | -2.870395524 |
| H | 1.375106344 | 0.079879500 | -2.581453369 |

TOTAL ENERGY = -679.982565 a.u.

**3b.**

1 1

| | | | |
|---|---|---|---|
| C | 0.009989425 | 0.254289255 | 0.672375173 |
| N | 0.493614652 | 0.044370482 | -0.527666441 |
| N | -0.221947010 | 0.397229735 | -1.624359186 |
| C | -1.355571566 | 0.924910778 | -1.240073615 |
| S | -1.544896099 | 0.987865799 | 0.526640890 |
| C | 0.697726253 | -0.087204208 | 1.942699733 |
| H | 0.854346955 | 0.807758197 | 2.545989875 |
| H | 1.665104853 | -0.544207419 | 1.740535983 |
| H | 0.097871711 | -0.785462688 | 2.527455295 |
| N | -2.287660076 | 1.375765966 | -2.081273914 |
| H | -3.152174094 | 1.777420633 | -1.764802237 |
| H | -2.122543717 | 1.312335732 | -3.073878777 |
| H | 1.398634238 | -0.378785975 | -0.700330257 |

TOTAL ENERGY = -680.020622 a.u.

**TS4.**

1 1

| | | | |
|---|---|---|---|
| C | -0.036906496 | 0.242589292 | 0.691229979 |
| N | 0.372473216 | 0.067935986 | -0.539166302 |
| N | -0.540055361 | 0.285749790 | -1.527434172 |
| C | -1.641243226 | 0.916975782 | -1.048831999 |
| S | -1.682669182 | 0.848157156 | 0.721049916 |
| C | 0.765562511 | -0.059393142 | 1.900565135 |
| H | 0.868697395 | 0.831445339 | 2.521491505 |
| H | 1.758984248 | -0.411774722 | 1.626988397 |
| H | 0.273878869 | -0.828915651 | 2.498500653 |
| N | -2.199841063 | 1.491381840 | -2.056393192 |
| H | -3.157231843 | 1.812269004 | -2.095541208 |
| H | -0.971617168 | 0.893293310 | -2.591782105 |
| H | 1.270669385 | -0.331147743 | -0.789165875 |

TOTAL ENERGY = -679.914112 a.u.

**3c.**

0 1

| | | | |
|---|---|---|---|
| C | 1.072437132 | -0.110785389 | -0.615126737 |
| N | 0.750090212 | 0.075300981 | -1.840956291 |
| N | -0.510049345 | 0.574220169 | -1.959987135 |
| C | -1.263719364 | 0.814953723 | -0.831187085 |
| S | -0.199893504 | 0.330574975 | 0.546678533 |
| C | 2.391781250 | -0.648633230 | -0.180956843 |
| H | 2.915196671 | 0.061958977 | 0.460806033 |
| H | 3.001027907 | -0.843270065 | -1.061193875 |
| H | 2.273678201 | -1.577541739 | 0.379351873 |
| N | -2.443352179 | 1.279061310 | -0.859689890 |
| H | -2.859786364 | 1.397753716 | 0.054591106 |
| H | -0.867158110 | 0.759996215 | -2.881456400 |

TOTAL ENERGY = -679.646495 a.u.

**4.**

0 1

| | | | |
|---|---|---|---|
| C | 1.050455427 | -0.122654942 | -0.610174258 |
| N | 0.721859141 | 0.103600171 | -1.835509442 |
| N | -0.550568509 | 0.589479209 | -2.001427785 |
| C | -1.190428878 | 0.716709077 | -0.880539800 |
| S | -0.256409225 | 0.240050053 | 0.528629089 |
| C | 2.381765671 | -0.632320973 | -0.171879509 |
| H | 2.880704775 | 0.074347500 | 0.493027208 |
| H | 3.000390039 | -0.779060944 | -1.054616117 |
| H | 2.292597026 | -1.582487267 | 0.356599650 |
| N | -2.507187393 | 1.106790709 | -0.797358341 |
| H | -2.767347687 | 1.642405580 | 0.014678587 |
| H | -2.851898987 | 1.499199295 | -1.661682135 |

TOTAL ENERGY = -679.651977 a.u.

**TS5.**

0 1

| | | | |
|---|---|---|---|
| C | 0.000829930 | 0.256285819 | 0.654331167 |
| N | 0.424716918 | 0.059382497 | -0.544286413 |
| N | -0.504223624 | 0.404269498 | -1.468153279 |
| C | -1.612124666 | 1.007900679 | -1.018760434 |
| S | -1.651368691 | 0.994983261 | 0.719537515 |
| C | 0.746101141 | -0.090383094 | 1.896426809 |
| H | 0.902494901 | 0.785614833 | 2.527719350 |
| H | 1.715285195 | -0.498059269 | 1.616546376 |
| H | 0.210679899 | -0.836818091 | 2.486213845 |
| N | -2.213650440 | 1.510402179 | -2.081303221 |
| H | -3.215582458 | 1.620746311 | -2.124820521 |
| H | -1.051882608 | 0.848130790 | -2.585088197 |

TOTAL ENERGY = -679.566452 a.u.

**Compound, total charge (a.u.), multiplicity, Cartesian coordinates (Å) and total energy values (a.u.) of the structures optimized at the MP2/6-311+G(2d2p)**

**1a.**

0 1

| | | | |
|---|---|---|---|
| N | 2.002892450 | 0.512352512 | 0.056594168 |
| N | 1.132867514 | -0.586231360 | -0.069396167 |
| C | -0.222524744 | -0.443490354 | -0.016791324 |
| S | -0.989805280 | 1.023143655 | -0.005555594 |
| N | -0.885927203 | -1.644456132 | 0.063921094 |
| H | -1.876716537 | -1.569997799 | -0.085833142 |
| H | -0.454603042 | -2.443792018 | -0.371068536 |
| H | 2.051252358 | 0.965259565 | -0.847436983 |
| H | 1.523058935 | -1.436851013 | 0.300544762 |
| H | 1.547031332 | 1.183050712 | 0.669703621 |

TOTAL ENERGY = -601.711877 a.u.

**1b.**

0 1

| | | | |
|---|---|---|---|
| N | -1.945450587 | 0.542982774 | -0.108957781 |
| N | -1.161209829 | -0.594053613 | 0.168820932 |
| C | 0.216713914 | -0.615411652 | 0.011913171 |
| S | 0.938189675 | 1.015533040 | 0.016728391 |
| N | 0.963479502 | -1.650419299 | -0.072816288 |
| H | 2.166824293 | 0.505810931 | -0.068838415 |
| H | 0.405492039 | -2.502922137 | -0.060436366 |
| H | -1.897606613 | 1.178800370 | 0.673357458 |
| H | -1.623729932 | -1.447805141 | -0.097065098 |
| H | -1.616227312 | 1.018212725 | -0.939578960 |

TOTAL ENERGY = -601.681269 a.u.

**TS1.**

0 1

| | | | |
|---|---|---|---|
| N | -2.051331514 | -0.559278239 | 0.039028345 |
| N | -1.222502189 | 0.571359871 | -0.055440747 |
| C | 0.122121566 | 0.520872622 | -0.008685553 |
| S | 1.057354933 | -0.941795037 | -0.004908271 |
| N | 0.961556841 | 1.534961890 | 0.023114751 |
| H | 1.868292068 | 0.473346224 | 0.033037392 |
| H | 0.623973861 | 2.492945577 | 0.026598716 |
| H | -1.924741879 | -1.116069784 | -0.795766772 |
| H | -1.691485516 | 1.449620901 | 0.076910464 |
| H | -1.745891902 | -1.119596681 | 0.825222003 |

TOTAL ENERGY = -601.627146 a.u.

**2a.**

1 1

| | | | |
|---|---|---|---|
| C | -1.690262511 | 0.095579286 | -0.141458786 |
| N | -0.551326543 | 0.404024172 | 0.857752571 |

| | | | |
|---|---|---|---|
| N | 0.418637417 | -0.638792103 | 1.012192083 |
| C | 1.496177476 | -0.590691407 | 0.070787609 |
| S | 2.196876429 | 1.051421442 | -0.008332441 |
| C | -2.592669200 | 1.303003339 | -0.203829541 |
| H | -2.997508908 | 1.526648215 | 0.779099715 |
| H | -3.426111458 | 1.077345840 | -0.863845154 |
| H | -2.065634781 | 2.174934714 | -0.587290419 |
| N | 2.005685881 | -1.574031859 | -0.533829636 |
| H | 2.575001894 | 0.914816817 | -1.280574727 |
| H | 1.478226466 | -2.439175303 | -0.428313525 |
| O | -2.251245247 | -1.016976471 | 0.460104461 |
| H | -0.953743426 | 0.605129383 | 1.775352478 |
| H | -0.075556536 | -1.526804651 | 1.011929863 |
| O | -1.096977559 | -0.262524343 | -1.328158759 |
| H | -0.013701956 | 1.224814642 | 0.531498922 |
| H | -1.190266226 | 0.434663746 | -1.987301242 |
| H | -2.727989674 | -1.528219525 | -0.205583063 |

TOTAL ENERGY = -829.902829 a.u.

**2b.**

1 1

| | | | |
|---|---|---|---|
| C | 1.077600326 | 0.749978522 | -0.275793642 |
| N | -0.063583709 | 1.308508760 | -0.619349455 |
| N | -1.125206486 | 0.608116570 | -1.186434684 |
| C | -1.755834402 | -0.369283410 | -0.354721411 |
| S | -1.621929904 | 0.015865815 | 1.374166112 |
| C | 2.116071744 | 1.544246884 | 0.425968219 |
| H | 3.059698925 | 1.468642964 | -0.107298799 |
| H | 2.255286798 | 1.128629822 | 1.422081057 |
| H | 1.827801211 | 2.586052174 | 0.512112817 |
| N | -2.420657912 | -1.357901281 | -0.778602200 |
| H | -2.389965210 | -1.023261604 | 1.707179884 |
| H | -2.424047135 | -1.444549726 | -1.793043202 |
| O | 1.223134850 | -0.491014371 | -0.574580231 |
| H | -0.220145086 | 2.285904074 | -0.420057660 |
| H | -0.877573946 | 0.246197185 | -2.099099314 |
| O | 3.421037590 | -1.497861866 | 0.270235575 |
| H | 3.372491885 | -2.163319891 | 0.963895027 |
| H | 4.076982918 | -1.822790414 | -0.354437469 |
| H | 2.097768152 | -0.882988933 | -0.251112477 |

TOTAL ENERGY = -829.939105 a.u.

**TS2.**

1 1

| | | | |
|---|---|---|---|
| C | -1.700621920 | 0.004532929 | 0.070534556 |
| N | -0.596104352 | -0.209443942 | -0.913187959 |
| N | 0.423963295 | 0.761423630 | -1.000200236 |
| C | 1.506962939 | 0.602927147 | -0.087781638 |
| S | 2.068548210 | -1.085058716 | -0.025862369 |
| C | -3.046821991 | -0.444004632 | -0.417349310 |
| H | -3.413249871 | 0.265788577 | -1.153901082 |
| H | -3.752084629 | -0.478686687 | 0.410629171 |

| | | | |
|---|---|---|---|
| H | -2.992677318 | -1.431109964 | -0.870287490 |
| N | 2.104805458 | 1.535982214 | 0.524249968 |
| H | 2.770434250 | -0.873745806 | 1.089202795 |
| H | 1.651443466 | 2.441898804 | 0.416555217 |
| O | -1.599502400 | 1.243768581 | 0.586624622 |
| H | -0.934434393 | -0.450899736 | -1.838910590 |
| H | 0.046618726 | 1.702686335 | -0.989937440 |
| O | -1.099955794 | -1.009812756 | 1.037081419 |
| H | -0.362111385 | -1.146277447 | 0.078013800 |
| H | -1.692633928 | -1.744343744 | 1.262566528 |
| H | -2.370485598 | 1.466758592 | 1.122969126 |

TOTAL ENERGY = -829.828463 a.u.

**2b-H2O.**

1 1

| | | | |
|---|---|---|---|
| C | -1.109628497 | 0.151808771 | 0.112824457 |
| N | -0.540552942 | 1.247537756 | -0.577860082 |
| N | 0.855802861 | 1.278844775 | -0.444174743 |
| C | 1.482709819 | 0.107179770 | -0.066167436 |
| S | 0.159180795 | -1.266195467 | -0.343695373 |
| C | -2.498035846 | -0.189450848 | -0.350440363 |
| H | -2.533625282 | -0.374543370 | -1.420456569 |
| H | -3.149286172 | 0.652129587 | -0.118422814 |
| H | -2.860421911 | -1.063992543 | 0.179062694 |
| N | 2.647705919 | -0.011284263 | 0.346443479 |
| H | 3.031442728 | -0.925140173 | 0.542991376 |
| H | 0.320660516 | -1.764312375 | 0.891557646 |
| O | -0.924265778 | 0.224848283 | 1.483363731 |
| H | -1.482834839 | 0.932225855 | 1.835934876 |
| H | 1.222787285 | 2.103539343 | 0.013017773 |
| H | -0.796647625 | 1.266539378 | -1.558407106 |

TOTAL ENERGY = -753.802257 a.u.

**3a+H2O.**

1 1

| | | | |
|---|---|---|---|
| C | -1.493808535 | -0.515999461 | -0.030803326 |
| N | -0.418650355 | -1.225877113 | 0.190406370 |
| N | 0.740792963 | -0.559030121 | 0.411851133 |
| C | 0.643265721 | 0.800945278 | 0.123240327 |
| S | -1.130983151 | 1.160314665 | -0.087540824 |
| C | -2.840948207 | -1.118677356 | -0.173694342 |
| H | -3.492431648 | -0.768848415 | 0.623706337 |
| H | -2.783664889 | -2.203081079 | -0.130667719 |
| H | -3.281174791 | -0.826237825 | -1.123375809 |
| N | 1.661544517 | 1.543945888 | 0.053737915 |
| H | 1.470851500 | 2.520588498 | -0.137046299 |
| H | 3.552508916 | -0.169632859 | -0.271057655 |
| O | 3.249313747 | -1.084276118 | -0.300139222 |
| H | 4.009096154 | -1.627778036 | -0.076811562 |
| H | 1.650586923 | -1.018778395 | 0.199600914 |
| H | -0.423691825 | -2.232514434 | 0.309097599 |

TOTAL ENERGY = -753.861030 a.u.

**TS3.**

1 1

| | | | |
|---|---|---|---|
| C | 1.212280981 | -0.329951328 | -0.051744606 |
| N | 0.764667653 | -0.529908975 | -1.356978651 |
| N | -0.546859360 | -0.052524509 | -1.527377979 |
| C | -1.092295436 | 0.718927724 | -0.509508348 |
| S | 0.290440089 | 1.183536153 | 0.664139087 |
| C | 2.698740139 | -0.342747624 | 0.128232631 |
| H | 3.154815421 | 0.450491766 | -0.457019216 |
| H | 3.090844657 | -1.300438981 | -0.210995370 |
| H | 2.963985844 | -0.193034089 | 1.170611441 |
| N | -2.305882654 | 1.019803741 | -0.433845451 |
| H | -2.590855511 | 1.592324197 | 0.350361929 |
| H | 0.060512489 | -0.205423223 | 1.422690219 |
| O | 0.498792523 | -1.274704283 | 0.858764564 |
| H | 1.091624991 | -1.921844175 | 1.278320859 |
| H | -1.189344646 | -0.724300492 | -1.926195193 |
| H | 1.381860522 | -0.083961072 | -2.026579585 |

TOTAL ENERGY = -753.749501 a.u.

**3a.**

1 1

| | | | |
|---|---|---|---|
| C | -0.042851145 | 0.270279403 | 0.689174999 |
| N | 0.402516000 | 0.044056549 | -0.517061469 |
| N | -0.465724035 | 0.257005437 | -1.554284678 |
| C | -1.607734330 | 0.979249673 | -1.152465280 |
| S | -1.625325618 | 0.928154475 | 0.673806790 |
| C | 0.742692755 | -0.054132789 | 1.903563162 |
| H | 0.847249289 | 0.832322218 | 2.523893437 |
| H | 1.730710553 | -0.421074854 | 1.639258140 |
| H | 0.226533701 | -0.814621633 | 2.485329071 |
| N | -2.389876995 | 1.492363478 | -1.986358298 |
| H | -3.202752832 | 1.964962153 | -1.608905228 |
| H | -0.041533450 | 0.531770537 | -2.433393179 |
| H | 1.282774187 | -0.418835333 | -0.714087376 |

TOTAL ENERGY = -677.787754 a.u.

**3b.**

1 1

| | | | |
|---|---|---|---|
| C | 0.000072873 | 0.268546370 | 0.690430585 |
| N | 0.487796663 | 0.043262031 | -0.517817528 |
| N | -0.216905869 | 0.389650078 | -1.608686761 |
| C | -1.350500669 | 0.943562107 | -1.211044177 |
| S | -1.527725491 | 1.022539091 | 0.534303254 |
| C | 0.691085289 | -0.090163254 | 1.954475726 |
| H | 0.860242560 | 0.794833934 | 2.562163855 |
| H | 1.651472542 | -0.549221056 | 1.735670981 |
| H | 0.093719875 | -0.792976601 | 2.529472113 |
| N | -2.247597619 | 1.460368933 | -2.064358008 |
| H | -3.188274572 | 1.647302277 | -1.766508361 |
| H | -2.105489108 | 1.285111650 | -3.046392624 |

| | | | |
|---|---|---|---|
| H | 1.386671368 | -0.397615019 | -0.679517694 |

TOTAL ENERGY = -677.824957 a.u.

**TS4.**

1 1

| | | | |
|---|---|---|---|
| C | -0.050728433 | 0.252661034 | 0.694416170 |
| N | 0.365561809 | 0.070032689 | -0.541296763 |
| N | -0.544163963 | 0.268023451 | -1.519867946 |
| C | -1.643548476 | 0.916468946 | -1.038996029 |
| S | -1.686615703 | 0.840768577 | 0.718256646 |
| C | 0.762183434 | -0.055565983 | 1.895376852 |
| H | 0.868741810 | 0.828844845 | 2.518311312 |
| H | 1.751473903 | -0.399105488 | 1.604540928 |
| H | 0.282122344 | -0.833331604 | 2.485341051 |
| N | -2.186384824 | 1.510180503 | -2.056173797 |
| H | -3.152195477 | 1.809946307 | -2.093606760 |
| H | -0.954043846 | 0.876908351 | -2.574303697 |
| H | 1.268298708 | -0.327265387 | -0.780487234 |

TOTAL ENERGY = -677.694995 a.u.

**3c.**

0 1

| | | | |
|---|---|---|---|
| C | 1.066983526 | -0.109261968 | -0.604374571 |
| N | 0.753508976 | 0.074398848 | -1.850311231 |
| N | -0.504696428 | 0.572558625 | -1.959151731 |
| C | -1.253338384 | 0.810771082 | -0.827104001 |
| S | -0.198670882 | 0.330680174 | 0.539513235 |
| C | 2.385707800 | -0.646468285 | -0.177608595 |
| H | 2.909911637 | 0.062746493 | 0.458965218 |
| H | 2.985342105 | -0.837370398 | -1.062367513 |
| H | 2.269304784 | -1.574265674 | 0.377961653 |
| N | -2.443232432 | 1.279110998 | -0.865842882 |
| H | -2.841741344 | 1.390240526 | 0.058089337 |
| H | -0.868826850 | 0.760449222 | -2.876895631 |

TOTAL ENERGY = -677.444673 a.u.

**4.**

0 1

| | | | |
|---|---|---|---|
| C | 1.039585622 | -0.126499787 | -0.595087867 |
| N | 0.726613781 | 0.117404654 | -1.844427377 |
| N | -0.544856296 | 0.603821425 | -2.004034467 |
| C | -1.186637263 | 0.710989538 | -0.865206890 |
| S | -0.261462004 | 0.209747254 | 0.521077705 |
| C | 2.374975751 | -0.630154320 | -0.169077680 |
| H | 2.873341359 | 0.078240853 | 0.488438151 |
| H | 2.980971540 | -0.769482626 | -1.058826596 |
| H | 2.294693620 | -1.579675403 | 0.354374814 |
| N | -2.516036201 | 1.084811952 | -0.782276157 |
| H | -2.739788826 | 1.686728229 | -0.006982288 |
| H | -2.837469683 | 1.470125700 | -1.658224203 |

TOTAL ENERGY = -677.45031 a.u.

**TS5.**

0 1

| | | | |
|---|---|---|---|
| C | -0.013281451 | 0.271985464 | 0.660447142 |
| N | 0.432209462 | 0.048065296 | -0.550775323 |
| N | -0.512927389 | 0.383659220 | -1.463612482 |
| C | -1.613729124 | 1.008918685 | -1.011738814 |
| S | -1.631353173 | 1.008713650 | 0.719596536 |
| C | 0.739220665 | -0.086600968 | 1.892811433 |
| H | 0.887405812 | 0.778583686 | 2.534396818 |
| H | 1.708184206 | -0.477230210 | 1.597597843 |
| H | 0.214625812 | -0.848137386 | 2.465902891 |
| N | -2.204698168 | 1.543835750 | -2.077069990 |
| H | -3.212974007 | 1.597774498 | -2.121515042 |
| H | -1.041407146 | 0.832887728 | -2.567678014 |

TOTAL ENERGY = -677.339719 a.u.