Supplementary Material (ESI) for Organic & Biomolecular Chemistry


**Supplementary Material (ESI) for Organic & Biomolecular Chemistry**

# Is Nucleophilic Cleavage Chemistry Practical for 4-Membered Heterocycles?

Harold D. Banks

U.S. Army Edgewood Chemical Biological Center, APG, Maryland 21010-5424

*harold.banks@us.army.mil*

## Table of Contents

Energies, Thermal Corrections, Imaginary Frequencies (if any) and Cartesian Coordinates for:



Energies (E) and thermal corrections (TC) are in hartrees, unique imaginary frequencies are in $cm^{-1}$.

**Cleavage Reactions in GAS PHASE**

**Transition State for Azetidine**: E= -229.1519685; TC=0.144781.
Imaginary Frequency = -536.6827.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | -0.390018 | -0.950654 | -0.946508 |
| 2 | 6 | -0.579804 | -0.503151 | 0.023810 |
| 3 | 1 | -0.623015 | -1.239633 | 0.816323 |
| 4 | 7 | -2.208717 | -0.065154 | -0.086337 |
| 5 | 6 | 0.124332 | 0.820904 | 0.292059 |
| 6 | 6 | 1.520729 | 0.531125 | -0.265090 |
| 7 | 1 | -2.803297 | -0.887620 | -0.212261 |
| 8 | 1 | -2.357113 | 0.567002 | -0.876697 |
| 9 | 1 | -2.502300 | 0.422584 | 0.764080 |
| 10 | 1 | -0.412104 | 1.680572 | -0.163904 |
| 11 | 1 | 0.173291 | 0.990201 | 1.374949 |
| 12 | 7 | 1.716704 | -0.882901 | -0.019070 |
| 13 | 1 | 1.493377 | 0.726379 | -1.353523 |
| 14 | 1 | 2.267486 | 1.230328 | 0.153892 |
| 15 | 1 | 2.206241 | -0.996036 | 0.876822 |

**Ground State for Azetidine** : E = -229.2678013; TC = 0.0.147117.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 1.721052 | 1.455889 | -0.873229 |
| 2 | 6 | 0.983927 | 1.046448 | -0.173730 |
| 3 | 1 | 0.417810 | 1.876589 | 0.263527 |
| 4 | 6 | 1.577654 | -0.000174 | 0.789394 |
| 5 | 7 | 0.153709 | 0.000173 | -0.843890 |
| 6 | 6 | 0.983667 | -1.046449 | -0.173947 |
| 7 | 1 | 2.660922 | -0.000324 | 0.949993 |
| 8 | 1 | 1.070356 | -0.000213 | 1.759316 |
| 9 | 1 | -0.785789 | 0.000230 | -0.436913 |
| 10 | 1 | 1.720691 | -1.455927 | -0.873531 |
| 11 | 1 | 0.417336 | -1.876538 | 0.263128 |
| 12 | 7 | -2.844376 | -0.000005 | 0.216037 |
| 13 | 1 | -3.255214 | -0.006415 | -0.715781 |
| 14 | 1 | -3.202098 | 0.822370 | 0.698469 |
| 15 | 1 | -3.201883 | -0.815789 | 0.709691 |

**Transition State for 2-Fluoroazetidine**: E = -328.2870825; TC=0.137738.
Imaginary Frequency = -699.4644.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 1.096895 | -1.545346 | -0.348610 |
| 2 | 6 | 0.771315 | -0.515822 | -0.329271 |
| 3 | 1 | 0.562874 | -0.043460 | -1.278329 |
| 4 | 7 | 2.484128 | 0.207084 | -0.142409 |
| 5 | 6 | 0.115539 | 0.079524 | 0.904883 |
| 6 | 6 | -1.308559 | -0.068833 | 0.432675 |
| 7 | 1 | 3.123040 | -0.140558 | -0.859772 |

| | | | | |
|---|---|---|---|---|
| 8 | 1 | 2.880155 | -0.008054 | 0.774345 |
| 9 | 1 | 2.420869 | 1.222794 | -0.232017 |
| 10 | 1 | 0.321505 | -0.530171 | 1.791122 |
| 11 | 1 | 0.401830 | 1.118699 | 1.089949 |
| 12 | 7 | -1.234860 | -1.213420 | -0.278456 |
| 13 | 9 | -1.420328 | 1.253692 | -0.483313 |
| 14 | 1 | -2.148441 | 0.168594 | 1.097122 |
| 15 | 1 | -2.090426 | -1.450582 | -0.787664 |

**Transition State for 2-Fluoroazetidine** @ $C_2$: E = -328.2513786;
TC=0.137017. Imaginary Frequency = -482.4612.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.202709 | 0.285110 | -1.271719 |
| 2 | 6 | 0 | 0.465314 | 0.145266 | -0.228593 |
| 3 | 7 | 0 | 1.980306 | -0.582250 | -0.294737 |
| 4 | 6 | 0 | -0.376732 | -0.790897 | 0.594424 |
| 5 | 6 | 0 | -1.725071 | -0.653191 | -0.101495 |
| 6 | 1 | 0 | 2.629370 | 0.029800 | -0.797642 |
| 7 | 1 | 0 | 1.938411 | -1.493295 | -0.759223 |
| 8 | 1 | 0 | 2.332918 | -0.708397 | 0.658793 |
| 9 | 1 | 0 | 0.041847 | -1.809347 | 0.666273 |
| 10 | 1 | 0 | -0.467144 | -0.362398 | 1.598065 |
| 11 | 7 | 0 | -1.762596 | 0.779422 | -0.189476 |
| 12 | 1 | 0 | -2.442280 | 1.086912 | -0.895876 |
| 13 | 9 | 0 | 0.914340 | 1.307400 | 0.355774 |
| 14 | 1 | 0 | -2.521472 | -1.168519 | 0.472314 |
| 15 | 1 | 0 | -1.648450 | -1.213735 | -1.069481 |

**Ground State for 2-Fluoroazetidine** : E = -328.3839197; TC = 0.139848.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 0.726971 | 1.934680 | -0.397878 |
| 2 | 6 | -0.174585 | 1.325291 | -0.294969 |
| 3 | 1 | -1.054822 | 1.906694 | -0.589912 |
| 4 | 7 | -0.077614 | -0.003526 | -0.960476 |
| 5 | 6 | -0.369205 | 0.564458 | 1.036561 |
| 6 | 6 | -0.722070 | -0.634999 | 0.161528 |
| 7 | 1 | -0.525347 | -0.134753 | -1.868592 |
| 8 | 1 | 0.569869 | 0.421931 | 1.573999 |
| 9 | 1 | -1.163749 | 0.898328 | 1.705084 |
| 10 | 9 | -2.137945 | -0.708207 | -0.009216 |
| 11 | 1 | -0.412770 | -1.654057 | 0.403455 |
| 12 | 1 | 2.106546 | -0.399858 | -0.496312 |
| 13 | 7 | 2.891739 | -0.419770 | 0.157514 |
| 14 | 1 | 3.616354 | 0.198432 | -0.201511 |
| 15 | 1 | 3.274737 | -1.362956 | 0.156619 |

**Transition State for 3-Fluoroazetidine**: E = -328.2661547; TC=0.137655.
Imaginary Frequency = -503.5557.

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

| | | | | |
|---|---|---|---|---|
| 1 | 1 | 0.283721 | -1.718551 | 0.644625 |
| 2 | 6 | 0.363729 | -0.892433 | -0.051036 |
| 3 | 1 | 0.167776 | -1.158430 | -1.086311 |
| 4 | 7 | 2.027294 | -0.624144 | -0.065164 |
| 5 | 6 | -0.195915 | 0.453087 | 0.374987 |
| 6 | 6 | -1.558822 | 0.473819 | -0.240653 |
| 7 | 1 | 2.527434 | -1.444173 | -0.415661 |
| 8 | 1 | 2.367089 | -0.410926 | 0.876915 |
| 9 | 1 | 2.228151 | 0.190946 | -0.651973 |
| 10 | 1 | -0.236119 | 0.541062 | 1.463250 |
| 11 | 9 | 0.707119 | 1.509438 | -0.055058 |
| 12 | 7 | -1.908686 | -0.869195 | 0.184725 |
| 13 | 1 | -1.415756 | 0.628944 | -1.331716 |
| 14 | 1 | -2.182354 | 1.310471 | 0.125046 |
| 15 | 1 | -2.588216 | -1.277751 | -0.465366 |

**Ground State for 3-Fluoroazetidine**: E = -328.3693544; TC = 0.139682.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 0.283721 | -1.718551 | 0.644625 |
| 2 | 6 | 0.363729 | -0.892433 | -0.051036 |
| 3 | 1 | 0.167776 | -1.158430 | -1.086311 |
| 4 | 7 | 2.027294 | -0.624144 | -0.065164 |
| 5 | 6 | -0.195915 | 0.453087 | 0.374987 |
| 6 | 6 | -1.558822 | 0.473819 | -0.240653 |
| 7 | 1 | 2.527434 | -1.444173 | -0.415661 |
| 8 | 1 | 2.367089 | -0.410925 | 0.876915 |
| 9 | 1 | 2.228151 | 0.190946 | -0.651973 |
| 10 | 1 | -0.236119 | 0.541062 | 1.463250 |
| 11 | 9 | 0.707119 | 1.509438 | -0.055058 |
| 12 | 7 | -1.908686 | -0.869195 | 0.184725 |
| 13 | 1 | -1.415756 | 0.628943 | -1.331716 |
| 14 | 1 | -2.182354 | 1.310471 | 0.125046 |
| 15 | 1 | -2.588216 | -1.277752 | -0.465366 |

**Transition State for 2,2-Difluoroazetidine**: E = -427.4103785;
TC=0.129939.
Imaginary Frequency = -658.5232.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.167198 | 0.736173 | 1.100548 |
| 2 | 6 | 0 | -1.196844 | 0.565325 | 0.032630 |
| 3 | 1 | 0 | -1.484009 | 1.397671 | -0.591439 |
| 4 | 7 | 0 | -2.875829 | -0.269696 | 0.019348 |
| 5 | 6 | 0 | -0.333032 | -0.539611 | -0.525982 |
| 6 | 6 | 0 | 0.980299 | 0.051209 | -0.074391 |
| 7 | 1 | 0 | -3.616101 | 0.369079 | 0.316108 |
| 8 | 1 | 0 | -2.871690 | -1.072678 | 0.651037 |
| 9 | 1 | 0 | -3.098831 | -0.605697 | -0.919459 |
| 10 | 1 | 0 | -0.524341 | -1.523733 | -0.090260 |
| 11 | 1 | 0 | -0.385834 | -0.588289 | -1.616159 |
| 12 | 7 | 0 | 0.797042 | 1.378436 | -0.191729 |
| 13 | 1 | 0 | 1.487736 | 1.912652 | 0.343456 |
| 14 | 9 | 0 | 2.107736 | -0.550293 | -0.697258 |
| 15 | 9 | 0 | 1.171067 | -0.432807 | 1.299402 |

**Transition State for 2,2-Difluoroazetidine @ $C_2$:** E = -427.3449513; TC = 0.129503. Imaginary Frequency = -236.2005.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.544211 | -0.070278 | 0.013177 |
| 2 | 7 | 0 | 2.027562 | 0.500714 | -0.219062 |
| 3 | 6 | 0 | -0.436560 | 0.962866 | -0.458214 |
| 4 | 6 | 0 | -1.820098 | 0.650043 | 0.118236 |
| 5 | 1 | 0 | 2.523643 | -0.118694 | -0.870896 |
| 6 | 1 | 0 | 2.529218 | 0.513823 | 0.677291 |
| 7 | 1 | 0 | 2.002994 | 1.449698 | -0.606523 |
| 8 | 1 | 0 | -0.067442 | 1.955728 | -0.156778 |
| 9 | 1 | 0 | -0.475711 | 0.886993 | -1.550590 |
| 10 | 7 | 0 | -2.012933 | -0.720467 | -0.198410 |
| 11 | 1 | 0 | -2.910078 | -1.039293 | 0.183645 |
| 12 | 9 | 0 | 0.640465 | -1.234309 | -0.641079 |
| 13 | 1 | 0 | -2.501188 | 1.417021 | -0.335301 |
| 14 | 1 | 0 | -1.768658 | 0.934260 | 1.201683 |
| 15 | 9 | 0 | 0.563924 | -0.289808 | 1.345589 |

**Ground State for 2,2-Difluoroazetidine** : E = -427.4955905; TC = 0.131611.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.011699 | 1.038427 | 1.022553 |
| 2 | 6 | 0 | -0.609208 | 0.968207 | 0.008424 |
| 3 | 1 | 0 | -1.220560 | 1.552190 | -0.679829 |
| 4 | 7 | 0 | -3.731914 | -0.326491 | 0.028892 |
| 5 | 6 | 0 | -0.289544 | -0.486867 | -0.394932 |
| 6 | 6 | 0 | 1.141748 | -0.119678 | -0.043777 |
| 7 | 1 | 0 | -4.358139 | 0.475988 | 0.023656 |
| 8 | 1 | 0 | -4.014887 | -0.924988 | 0.802154 |
| 9 | 1 | 0 | -3.899018 | -0.844955 | -0.831036 |
| 10 | 1 | 0 | -0.733171 | -1.281793 | 0.201718 |
| 11 | 1 | 0 | -0.411165 | -0.678736 | -1.461788 |
| 12 | 7 | 0 | 0.849720 | 1.265116 | -0.096681 |
| 13 | 1 | 0 | 1.301703 | 1.861249 | 0.595472 |
| 14 | 9 | 0 | 2.166351 | -0.538028 | -0.854288 |
| 15 | 9 | 0 | 1.507462 | -0.566164 | 1.230214 |

**Transition State for 3,3-Difluoroazetidine**: E = -427.3783463; TC = 0.129904.
Imaginary Frequency = -466.8560.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.223079 | 1.600178 | -0.883993 |
| 2 | 6 | 0 | 0.414784 | 1.010051 | 0.005000 |
| 3 | 1 | 0 | 0.329467 | 1.564359 | 0.931711 |
| 4 | 7 | 0 | 2.053820 | 0.695466 | -0.039334 |
| 5 | 6 | 0 | -0.186440 | -0.383806 | -0.011677 |
| 6 | 6 | 0 | -1.576377 | -0.248256 | -0.531757 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 1 | 0 | 2.589004 | 1.566771 | -0.008456 |
| 8 | 1 | 0 | 2.294261 | 0.167092 | -0.883434 |
| 9 | 1 | 0 | 2.314973 | 0.116844 | 0.765528 |
| 10 | 7 | 0 | -1.882782 | 1.090240 | -0.056124 |
| 11 | 1 | 0 | -2.310803 | 1.001418 | 0.872425 |
| 12 | 1 | 0 | -1.542059 | -0.290970 | -1.631500 |
| 13 | 1 | 0 | -2.198457 | -1.088351 | -0.185983 |
| 14 | 9 | 0 | -0.118563 | -0.882313 | 1.282385 |
| 15 | 9 | 0 | 0.695392 | -1.273822 | -0.735439 |

**Ground State for 3,3-Difluoroazetidine**: E = -427.4795382; TC = 0.131789.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.224551 | 1.735745 | 0.480372 |
| 2 | 6 | 0 | 0.377844 | 1.126615 | -0.192190 |
| 3 | 1 | 0 | 0.176125 | 1.399427 | -1.234626 |
| 4 | 7 | 0 | -2.785180 | 0.586305 | -0.020683 |
| 5 | 6 | 0 | 0.284206 | -0.381159 | -0.010899 |
| 6 | 6 | 0 | 1.804343 | -0.456021 | -0.069722 |
| 7 | 1 | 0 | -3.723576 | 0.981083 | -0.035345 |
| 8 | 1 | 0 | -2.660640 | 0.125851 | 0.878874 |
| 9 | 1 | 0 | -2.747833 | -0.140303 | -0.732648 |
| 10 | 7 | 0 | 1.821664 | 1.013556 | 0.172167 |
| 11 | 1 | 0 | 2.454453 | 1.533550 | -0.434382 |
| 12 | 1 | 0 | 2.295671 | -1.051228 | 0.703389 |
| 13 | 1 | 0 | 2.133094 | -0.770520 | -1.068056 |
| 14 | 9 | 0 | -0.396729 | -1.090189 | -0.974523 |
| 15 | 9 | 0 | -0.242881 | -0.770838 | 1.198846 |

**Transition State for *cis*-2,3-Difluoroazetidine**: E = -427.3898067; TC=0.130531.
Imaginary Frequency = -705.5336.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 0.850461 | 1.899505 | -0.276309 |
| 2 | 6 | 0.596547 | 0.941032 | 0.152006 |
| 3 | 1 | 0.351978 | 0.907797 | 1.204044 |
| 4 | 7 | 2.330456 | 0.349954 | 0.347345 |
| 5 | 6 | 0.055199 | -0.194040 | -0.716384 |
| 6 | 1 | 0.219248 | -0.010292 | -1.780720 |
| 7 | 1 | 2.861001 | 0.985508 | 0.945355 |
| 8 | 1 | 2.817894 | 0.256549 | -0.545782 |
| 9 | 1 | 2.292771 | -0.576322 | 0.776881 |
| 10 | 6 | -1.395098 | -0.082690 | -0.329097 |
| 11 | 9 | 0.689709 | -1.427717 | -0.427232 |
| 12 | 7 | -1.420703 | 1.276833 | -0.279977 |
| 13 | 1 | -2.147746 | -0.666527 | -0.873068 |
| 14 | 9 | -1.450859 | -0.779919 | 1.029999 |
| 15 | 1 | -2.303415 | 1.699178 | 0.013972 |

**Ground State for *cis*-2,3-Difluoroazetidine** : E = -427.4770485; TC = 0.132643.

| Center | Atomic | Coordinates (Angstroms) |
|---|---|---|

| Number | Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 9 | -0.349787 | 1.545837 | -0.646767 |
| 2 | 6 | 0.763779 | 0.966077 | -0.052532 |
| 3 | 6 | 1.165035 | -0.417120 | -0.585754 |
| 4 | 6 | 0.549423 | 0.269307 | 1.298644 |
| 5 | 1 | 1.579058 | 1.692211 | -0.066362 |
| 6 | 7 | 1.452599 | -0.786977 | 0.761719 |
| 7 | 9 | 0.011185 | -1.061424 | -1.119549 |
| 8 | 1 | 0.928315 | 0.768747 | 2.193640 |
| 9 | 1 | -0.494440 | -0.037029 | 1.418241 |
| 10 | 1 | 1.946249 | -0.563247 | -1.333707 |
| 11 | 7 | -2.672337 | -0.397704 | 0.433267 |
| 12 | 1 | 1.315154 | -1.759781 | 1.032359 |
| 13 | 1 | -2.114065 | -0.735117 | -0.349098 |
| 14 | 1 | -3.547517 | -0.917935 | 0.438702 |
| 15 | 1 | -2.896598 | 0.575623 | 0.236016 |

**Transition State for *trans*-2,3-Difluoroazetidine**: E = -427.388335; TC = 0.130457. Imaginary Frequency = -643.6997 $cm^{-1}$.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 1.035442 | 1.674534 | -0.662801 |
| 2 | 6 | 0.912895 | 0.874932 | 0.051754 |
| 3 | 1 | 0.967065 | 1.146302 | 1.099989 |
| 4 | 7 | 2.574275 | 0.146798 | -0.096757 |
| 5 | 6 | 0.055207 | -0.318403 | -0.296077 |
| 6 | 1 | -0.038312 | -0.482841 | -1.371420 |
| 7 | 1 | 3.299046 | 0.800356 | 0.205748 |
| 8 | 1 | 2.765099 | -0.125235 | -1.063740 |
| 9 | 1 | 2.606062 | -0.698192 | 0.477922 |
| 10 | 6 | -1.242094 | 0.131765 | 0.307017 |
| 11 | 9 | 0.604940 | -1.507584 | 0.263094 |
| 12 | 7 | -1.196093 | 1.464706 | -0.066217 |
| 13 | 9 | -2.337504 | -0.675507 | -0.248093 |
| 14 | 1 | -1.293321 | -0.126891 | 1.379255 |
| 15 | 1 | -1.751333 | 2.049486 | 0.564691 |

**Ground State for *trans*-2,3-Difluoroazetidine**: E = -427.4786664; TC = 0.132593.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 1.722366 | 0.725488 | 1.247017 |
| 2 | 6 | 1.452445 | 0.125644 | 0.376777 |
| 3 | 6 | 0.259016 | 0.616445 | -0.445484 |
| 4 | 6 | 0.647801 | -1.169572 | 0.571917 |
| 5 | 9 | 2.600318 | -0.064246 | -0.399272 |
| 6 | 7 | -0.234580 | -0.713377 | -0.525642 |
| 7 | 9 | -0.534252 | 1.467342 | 0.410361 |
| 8 | 1 | 1.193442 | -2.092223 | 0.358588 |
| 9 | 1 | 0.171774 | -1.229204 | 1.559324 |
| 10 | 1 | 0.388490 | 1.183279 | -1.369509 |
| 11 | 1 | -1.250824 | -0.848312 | -0.479989 |

| | | | | |
|---|---|---|---|---|
| 12 | 7 | -3.242119 | -0.340214 | -0.103055 |
| 13 | 1 | -2.989896 | 0.573167 | 0.273642 |
| 14 | 1 | -3.845734 | -0.183157 | -0.908302 |
| 15 | 1 | -3.802887 | -0.816863 | 0.601041 |

**Transition State for *trans*-2,4-Difluoroazetidine**: E = -427.3795835. TC = 0.130033. Imaginary frequency = -670.678.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.964786 | 0.601766 | -1.284422 |
| 2 | 6 | 0 | 0.871886 | 0.242618 | -0.273815 |
| 3 | 7 | 0 | 2.430929 | -0.763539 | -0.253091 |
| 4 | 6 | 0 | -0.133160 | -0.770069 | 0.166695 |
| 5 | 6 | 0 | -1.354501 | 0.130150 | 0.253302 |
| 6 | 1 | 0 | 3.220693 | -0.169399 | -0.514534 |
| 7 | 1 | 0 | 2.384429 | -1.557650 | -0.895169 |
| 8 | 1 | 0 | 2.593880 | -1.113754 | 0.693035 |
| 9 | 1 | 0 | -0.283291 | -1.526430 | -0.609038 |
| 10 | 1 | 0 | 0.153648 | -1.251168 | 1.107751 |
| 11 | 7 | 0 | -1.131255 | 1.036330 | -0.756885 |
| 12 | 1 | 0 | -1.669567 | 1.895749 | -0.610083 |
| 13 | 9 | 0 | 1.304929 | 1.109561 | 0.682951 |
| 14 | 9 | 0 | -2.553318 | -0.766284 | 0.098396 |
| 15 | 1 | 0 | -1.532143 | 0.505652 | 1.273078 |

**Ground State for *trans*-2,4-Difluoroazetidine**: E = -427.4798924. TC = 0.132670.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | -1.681254 | 1.547350 | -0.967954 |
| 2 | 6 | -1.491786 | 0.898977 | -0.111731 |
| 3 | 6 | -0.119784 | 1.049059 | 0.546351 |
| 4 | 6 | -1.040423 | -0.543218 | -0.379126 |
| 5 | 1 | -2.322679 | 0.924873 | 0.595847 |
| 6 | 7 | 0.008514 | -0.370703 | 0.592164 |
| 7 | 9 | 0.790279 | 1.649316 | -0.395892 |
| 8 | 9 | -1.970204 | -1.530821 | -0.022164 |
| 9 | 1 | -0.730033 | -0.787319 | -1.400390 |
| 10 | 1 | 0.043248 | 1.607464 | 1.469632 |
| 11 | 7 | 2.918568 | -0.960856 | -0.051997 |
| 12 | 1 | 0.936040 | -0.796660 | 0.472024 |
| 13 | 1 | 2.988928 | -0.023200 | -0.446367 |
| 14 | 1 | 3.601605 | -1.028607 | 0.700535 |
| 15 | 1 | 3.205857 | -1.618350 | -0.774946 |

**Transition State for *cis*-2,4-Difluoroazetidine**: E = -427.3787283. TC = 0.130146. Imaginary frequency = -698.946.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.013513 | -0.495729 | 1.408199 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 0.762083 | -0.216716 | 0.397553 |
| 3 | 7 | 0 | 2.430333 | 0.393854 | -0.064832 |
| 4 | 6 | 0 | -0.048377 | 1.008902 | 0.048351 |
| 5 | 6 | 0 | -1.447917 | 0.479848 | 0.281364 |
| 6 | 1 | 0 | 3.112822 | -0.348096 | 0.105568 |
| 7 | 1 | 0 | 2.716882 | 1.234211 | 0.441793 |
| 8 | 1 | 0 | 2.425474 | 0.595981 | -1.066905 |
| 9 | 1 | 0 | 0.215315 | 1.823163 | 0.734575 |
| 10 | 1 | 0 | 0.125704 | 1.320405 | -0.985549 |
| 11 | 7 | 0 | -1.212961 | -0.506601 | 1.185771 |
| 12 | 1 | 0 | -2.041036 | -1.054964 | 1.432340 |
| 13 | 9 | 0 | -1.846155 | -0.006338 | -1.135690 |
| 14 | 1 | 0 | -2.255903 | 1.213157 | 0.424495 |
| 15 | 9 | 0 | 0.798476 | -1.230451 | -0.498165 |

**Ground State for *cis*-2,4-Difluoroazetidine**: E = -427.4951370. TC = 0.132722.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.615537 | -1.027663 | 0.350421 |
| 2 | 1 | 0 | -0.292796 | -1.605807 | 1.222441 |
| 3 | 6 | 0 | -1.682672 | 0.045937 | 0.583051 |
| 4 | 6 | 0 | -0.543035 | 1.041793 | 0.349091 |
| 5 | 7 | 0 | 0.286543 | -0.023476 | -0.122288 |
| 6 | 1 | 0 | 1.297889 | -0.056011 | 0.044372 |
| 7 | 1 | 0 | -2.177304 | 0.063904 | 1.555826 |
| 8 | 1 | 0 | -2.415113 | 0.071081 | -0.225417 |
| 9 | 9 | 0 | -0.943733 | -1.995552 | -0.621579 |
| 10 | 9 | 0 | -0.802495 | 2.029461 | -0.624259 |
| 11 | 1 | 0 | -0.180501 | 1.597077 | 1.220317 |
| 12 | 7 | 0 | 3.341696 | -0.057905 | 0.080516 |
| 13 | 1 | 0 | 3.596956 | 0.746816 | -0.489996 |
| 14 | 1 | 0 | 3.620045 | -0.889185 | -0.438671 |
| 15 | 1 | 0 | 3.916668 | -0.023779 | 0.920692 |

**Transition State for 2-Chloroazetidine**: E = -688.2956329; TC = 0.136938.
Imaginary Frequency = -672.6771 $cm^{-1}$.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.547097 | 0.516377 | -0.013915 |
| 2 | 7 | 0 | -3.092032 | -0.585705 | -0.043486 |
| 3 | 6 | 0 | -0.464554 | -0.532265 | 0.028029 |
| 4 | 6 | 0 | 0.656810 | 0.403457 | 0.404891 |
| 5 | 1 | 0 | -3.949984 | -0.041471 | -0.151250 |
| 6 | 1 | 0 | -3.168690 | -1.141144 | 0.810322 |
| 7 | 1 | 0 | -3.021376 | -1.230875 | -0.832699 |
| 8 | 1 | 0 | -0.641442 | -1.333362 | 0.753768 |
| 9 | 1 | 0 | -0.292381 | -0.964776 | -0.960229 |
| 10 | 7 | 0 | 0.344854 | 1.547612 | -0.267579 |
| 11 | 1 | 0 | 0.789796 | 2.368989 | 0.156620 |
| 12 | 1 | 0 | 0.854919 | 0.439933 | 1.483935 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 1 | 0 | -1.804252 | 1.034021 | 0.902760 |
| 14 | 1 | 0 | -1.779323 | 1.025680 | -0.935980 |
| 15 | 17 | 0 | 2.374825 | -0.542103 | -0.091990 |

**Ground State for 2-Chloroazetidine**: E = -688.3929838; TC = 0.138961.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.369074 | 1.439029 | -0.286392 |
| 2 | 6 | 0 | -0.360415 | -0.466668 | 0.166011 |
| 3 | 6 | 0 | 0.133330 | 0.691303 | 1.042408 |
| 4 | 1 | 0 | 1.313313 | 1.976992 | -0.404552 |
| 5 | 1 | 0 | -0.469106 | 2.089043 | -0.563664 |
| 6 | 7 | 0 | 0.344632 | 0.113236 | -0.959329 |
| 7 | 1 | 0 | -0.102240 | 0.043697 | -1.874799 |
| 8 | 1 | 0 | -0.580935 | 1.112100 | 1.750417 |
| 9 | 1 | 0 | 1.072954 | 0.433017 | 1.535317 |
| 10 | 17 | 0 | -2.171059 | -0.454130 | -0.007020 |
| 11 | 1 | 0 | -0.107618 | -1.498966 | 0.411117 |
| 12 | 1 | 0 | 2.448886 | -0.547433 | -0.504348 |
| 13 | 7 | 0 | 3.224237 | -0.687618 | 0.146838 |
| 14 | 1 | 0 | 4.028900 | -0.174078 | -0.206904 |
| 15 | 1 | 0 | 3.469833 | -1.675473 | 0.132028 |

**Transition State for 3-Chloroazetidine**: E = -688.2831065; TC = 0.136491.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.675334 | 1.913244 | -0.883980 |
| 2 | 6 | 0 | -0.510708 | 1.194171 | -0.090012 |
| 3 | 1 | 0 | -0.797497 | 1.506436 | 0.908393 |
| 4 | 7 | 0 | 1.326633 | 1.748282 | 0.149883 |
| 5 | 6 | 0 | -0.477278 | -0.233209 | -0.381524 |
| 6 | 6 | 0 | -1.510936 | -0.917103 | 0.408508 |
| 7 | 1 | 0 | 1.404433 | 2.699347 | 0.515046 |
| 8 | 1 | 0 | 1.838355 | 1.679038 | -0.731006 |
| 9 | 1 | 0 | 1.756096 | 1.067298 | 0.781573 |
| 10 | 1 | 0 | -0.493007 | -0.478723 | -1.437531 |
| 11 | 7 | 0 | -2.379531 | 0.098852 | -0.224444 |
| 12 | 1 | 0 | -1.376281 | -0.846675 | 1.492893 |
| 13 | 1 | 0 | -1.727844 | -1.941702 | 0.106401 |
| 14 | 1 | 0 | -2.702888 | 0.750811 | 0.504466 |
| 15 | 17 | 0 | 1.478693 | -1.149539 | -0.020950 |

**Ground State for 3-Chloroazetidine:** E = -688.3820778; TC = 0.138873.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.154039 | -1.806558 | -1.499678 |
| 2 | 6 | 0 | 0.512908 | -1.040721 | -1.047881 |
| 3 | 1 | 0 | 0.002672 | -0.486849 | -1.842162 |
| 4 | 6 | 0 | 1.265025 | -0.203694 | 0.000478 |
| 5 | 7 | 0 | -0.370384 | -1.622156 | -0.000225 |
| 6 | 6 | 0 | 0.511573 | -1.040182 | 1.048230 |
| 7 | 1 | 0 | 2.356676 | -0.230072 | 0.001119 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 1 | 0 | -1.273539 | -1.137691 | -0.000885 |
| 9 | 1 | 0 | 1.152081 | -1.805814 | 1.501257 |
| 10 | 1 | 0 | 0.000351 | -0.485861 | 1.841556 |
| 11 | 7 | 0 | -2.755521 | 0.410713 | -0.000188 |
| 12 | 1 | 0 | -3.357001 | 0.481861 | -0.818920 |
| 13 | 1 | 0 | -2.140163 | 1.222914 | -0.000468 |
| 14 | 1 | 0 | -3.357260 | 0.482421 | 0.818303 |
| 15 | 17 | 0 | 0.800379 | 1.526667 | -0.000129 |

**Transition State for 2,2-Dichloroazetidine**: E = -1147.4322893; TC = 0.128052.
Imaginary Frequency = -620.6866 $cm^{-1}$.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.163864 | -0.567608 | 1.107418 |
| 2 | 6 | 0 | 0.564737 | -1.251804 | 0.521418 |
| 3 | 1 | 0 | 0.589811 | -2.315275 | 0.712729 |
| 4 | 7 | 0 | 2.462291 | -1.381984 | -0.570188 |
| 5 | 6 | 0 | -0.131725 | -0.671888 | -0.703120 |
| 6 | 6 | 0 | -1.336086 | -0.332402 | 0.091697 |
| 7 | 1 | 0 | 3.215342 | -1.841492 | -0.057234 |
| 8 | 1 | 0 | 2.610765 | -0.359102 | -0.499192 |
| 9 | 1 | 0 | 2.547978 | -1.658976 | -1.548494 |
| 10 | 1 | 0 | 0.398666 | 0.228462 | -1.039474 |
| 11 | 1 | 0 | -0.309943 | -1.379066 | -1.517224 |
| 12 | 7 | 0 | -1.068052 | -0.808023 | 1.255528 |
| 13 | 1 | 0 | -1.646823 | -0.662695 | 2.088363 |
| 14 | 17 | 0 | -2.706745 | 0.537740 | -0.398868 |
| 15 | 17 | 0 | 1.947281 | 1.663575 | 0.192736 |

**Ground State for 2,2-Dichloroazetidine**: E = -1147.5084421; TC = 0.130068. ]

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.549177 | -0.006670 | -0.052254 |
| 2 | 6 | 0 | -0.593352 | 2.013970 | -0.450614 |
| 3 | 6 | 0 | -1.682259 | 1.020324 | 0.014765 |
| 4 | 1 | 0 | -0.856998 | 2.711742 | -1.249267 |
| 5 | 7 | 0 | 0.183807 | 0.842755 | -0.911913 |
| 6 | 1 | 0 | 1.211562 | 0.802780 | -0.872353 |
| 7 | 1 | 0 | -2.426778 | 0.831906 | -0.761106 |
| 8 | 17 | 0 | 0.197858 | -0.225912 | 1.613981 |
| 9 | 17 | 0 | -0.873520 | -1.637733 | -0.687136 |
| 10 | 1 | 0 | -2.155501 | 1.170294 | 0.985009 |
| 11 | 1 | 0 | -0.132238 | 2.552168 | 0.386993 |
| 12 | 1 | 0 | 3.434431 | 0.306807 | 0.378772 |
| 13 | 7 | 0 | 3.063011 | 0.018803 | -0.525095 |
| 14 | 1 | 0 | 3.825295 | 0.073985 | -1.198872 |
| 15 | 1 | 0 | 2.807487 | -0.964379 | -0.437864 |

**Transition State for 2-Bromoazetidine:** E = -2801.4939786; TC = 0.136626. Imaginary frequency = -672.4135.

| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.224279 | 0.495920 | -0.045243 |
| 2 | 7 | 0 | -3.688546 | -0.783792 | -0.055255 |
| 3 | 6 | 0 | -1.059519 | -0.453407 | 0.077592 |
| 4 | 6 | 0 | -0.054624 | 0.606222 | 0.441014 |
| 5 | 1 | 0 | -4.595532 | -0.340710 | -0.212054 |
| 6 | 1 | 0 | -3.734375 | -1.301785 | 0.823643 |
| 7 | 1 | 0 | -3.530324 | -1.457688 | -0.806574 |
| 8 | 1 | 0 | -1.182781 | -1.227160 | 0.842357 |
| 9 | 1 | 0 | -0.817255 | -0.918018 | -0.880130 |
| 10 | 7 | 0 | -0.456246 | 1.681571 | -0.279886 |
| 11 | 1 | 0 | -0.110094 | 2.562274 | 0.117268 |
| 12 | 1 | 0 | 0.176713 | 0.695807 | 1.507182 |
| 13 | 1 | 0 | -2.574592 | 1.015369 | 0.838538 |
| 14 | 1 | 0 | -2.499473 | 0.917414 | -0.999162 |
| 15 | 35 | 0 | 1.940337 | -0.289210 | -0.049293 |

**Ground State for 2-Bromoazetidine:** E = -2801.5847999 ; TC = 0.138530.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.830700 | 1.830827 | -0.195717 |
| 2 | 6 | 0 | 0.357019 | -0.179825 | 0.096073 |
| 3 | 6 | 0 | 0.746243 | 0.940120 | 1.063770 |
| 4 | 1 | 0 | 1.694723 | 2.492116 | -0.301042 |
| 5 | 1 | 0 | -0.094934 | 2.391501 | -0.373556 |
| 6 | 7 | 0 | 0.927142 | 0.578695 | -0.989934 |
| 7 | 1 | 0 | 0.465015 | 0.536538 | -1.898728 |
| 8 | 1 | 0 | 0.026189 | 1.209130 | 1.836119 |
| 9 | 1 | 0 | 1.726529 | 0.737897 | 1.502324 |
| 10 | 1 | 0 | 0.722397 | -1.195262 | 0.237297 |
| 11 | 1 | 0 | 2.955603 | -0.615339 | -0.569503 |
| 12 | 7 | 0 | 3.373757 | -1.257422 | 0.105491 |
| 13 | 1 | 0 | 4.309773 | -0.919932 | 0.320969 |
| 14 | 1 | 0 | 3.478577 | -2.162541 | -0.348853 |
| 15 | 35 | 0 | -1.628398 | -0.379136 | 0.000038 |

**Transition State for 2,2-Dibromoazetidine**: E= -5373.8253295;
TC=0.127778. Imaginary Frequency = -633.208.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.448046 | 1.022555 | 1.009641 |
| 2 | 6 | 0 | -0.843733 | 1.782890 | 0.534214 |
| 3 | 1 | 0 | -0.905782 | 2.819158 | 0.838553 |
| 4 | 7 | 0 | -2.643476 | 1.931880 | -0.667530 |
| 5 | 6 | 0 | -0.011139 | 1.338412 | -0.661638 |
| 6 | 6 | 0 | 1.034025 | 0.773247 | 0.228929 |
| 7 | 1 | 0 | -3.450066 | 2.336202 | -0.190648 |
| 8 | 1 | 0 | -2.766282 | 0.906856 | -0.681364 |
| 9 | 1 | 0 | -2.653372 | 2.274126 | -1.628774 |
| 10 | 1 | 0 | -0.506698 | 0.563564 | -1.248990 |
| 11 | 1 | 0 | 0.351986 | 2.160674 | -1.286285 |
| 12 | 7 | 0 | 0.723490 | 1.224232 | 1.391499 |
| 13 | 1 | 0 | 1.182243 | 0.923270 | 2.256808 |
| 14 | 35 | 0 | -1.787928 | -1.321169 | 0.095496 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 35 | 0 | 2.432528 | -0.349301 | -0.231089 |

**Ground State for 2,2-Dibromoazetidine**: E= -5373.8253295. TC = 0.129265.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.113822 | 0.601791 | 0.215740 |
| 2 | 6 | 0 | -0.949348 | 1.865754 | 1.422955 |
| 3 | 6 | 0 | -0.070558 | 2.116749 | 0.171755 |
| 4 | 1 | 0 | -0.820963 | 2.539402 | 2.273858 |
| 5 | 7 | 0 | -0.240612 | 0.574917 | 1.569889 |
| 6 | 1 | 0 | -0.655618 | -0.288587 | 1.947403 |
| 7 | 1 | 0 | 0.859065 | 2.631685 | 0.425221 |
| 8 | 1 | 0 | -0.527013 | 2.537375 | -0.723422 |
| 9 | 1 | 0 | -2.011427 | 1.757612 | 1.170805 |
| 10 | 1 | 0 | -1.716782 | -2.567688 | 1.267671 |
| 11 | 7 | 0 | -0.858143 | -2.323410 | 1.758646 |
| 12 | 1 | 0 | -0.748400 | -2.981925 | 2.528925 |
| 13 | 1 | 0 | -0.091504 | -2.490568 | 1.106710 |
| 14 | 35 | 0 | 1.806509 | -0.232676 | -0.240138 |
| 15 | 35 | 0 | -1.268211 | -0.235999 | -1.021565 |

**Transition State for Oxetane:** E = -249.0338309; TC = 0.132922.
Imaginary frequency = -604.6319.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.499435 | -0.484628 | 0.019842 |
| 2 | 7 | 2.198411 | -0.039091 | 0.063866 |
| 3 | 6 | -0.171878 | 0.853942 | -0.232671 |
| 4 | 1 | 0.408279 | -0.901220 | 1.017265 |
| 5 | 1 | 0.554369 | -1.214492 | -0.776232 |
| 6 | 6 | -1.571176 | 0.447048 | 0.225286 |
| 7 | 1 | 2.795935 | -0.861985 | 0.168179 |
| 8 | 1 | 0.307887 | 1.691815 | 0.303258 |
| 9 | 1 | 2.452069 | 0.436785 | -0.804951 |
| 10 | 1 | 2.388443 | 0.599352 | 0.838995 |
| 11 | 1 | -0.162601 | 1.069483 | -1.307246 |
| 12 | 1 | -2.370180 | 1.064267 | -0.229631 |
| 13 | 1 | -1.635065 | 0.615073 | 1.327987 |
| 14 | 8 | -1.583287 | -0.890452 | -0.132429 |

**Ground State for Oxetane**: E = -249.1170317; TC = 0.133750.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.032922 | -0.150866 | 0.023740 |
| 2 | 6 | -0.007354 | -0.172031 | 1.552909 |
| 3 | 1 | 1.045013 | -0.147569 | -0.394214 |
| 4 | 1 | -0.584453 | 0.582979 | -0.497982 |
| 5 | 8 | -0.556755 | -1.488239 | -0.039399 |
| 6 | 6 | -0.283844 | -1.670052 | 1.379178 |
| 7 | 1 | 0.904753 | 0.119885 | 2.075550 |
| 8 | 1 | -0.858913 | 0.374921 | 1.963598 |
| 9 | 1 | -1.143205 | -2.103121 | 1.899163 |

| | | | | |
|---|---|---|---|---|
| 10 | 1 | 0.597212 | -2.307111 | 1.528419 |
| 11 | 7 | 1.270062 | 2.896724 | 0.371762 |
| 12 | 1 | 1.111042 | 3.224035 | -0.578737 |
| 13 | 1 | 0.676273 | 3.448491 | 0.987165 |
| 14 | 1 | 2.236211 | 3.111527 | 0.608982 |

**Transition State for 2-Fluorooxetane**: E = -348.1659892. TC = 0.125910.
Imaginary Frequency = -666.9846.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.598610 | 0.190363 | -1.277911 |
| 2 | 6 | 0 | 0.789833 | 0.504557 | -0.261467 |
| 3 | 1 | 0 | 1.133687 | 1.519977 | -0.122018 |
| 4 | 7 | 0 | 2.477639 | -0.256496 | -0.160538 |
| 5 | 6 | 0 | 0.103166 | -0.251757 | 0.864540 |
| 6 | 6 | 0 | -1.297130 | 0.084865 | 0.391933 |
| 7 | 1 | 0 | 3.122090 | 0.182305 | -0.820721 |
| 8 | 1 | 0 | 2.419357 | -1.251675 | -0.383636 |
| 9 | 1 | 0 | 2.868740 | -0.165696 | 0.778833 |
| 10 | 1 | 0 | 0.348150 | -1.319227 | 0.913029 |
| 11 | 1 | 0 | 0.319261 | 0.221274 | 1.828599 |
| 12 | 8 | 0 | -1.117298 | 1.224880 | -0.252874 |
| 13 | 1 | 0 | -2.130046 | 0.029450 | 1.107608 |
| 14 | 9 | 0 | -1.628905 | -1.048480 | -0.538563 |

**Ground State for 2-Fluorooxetane**: E = -348.2343011. TC = 0.127032.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.699817 | 0.385624 | 0.540001 |
| 2 | 6 | 0.184820 | 0.385034 | 0.393504 |
| 3 | 6 | 1.637579 | -0.873768 | -0.334315 |
| 4 | 1 | 2.033750 | 0.197966 | 1.562350 |
| 5 | 1 | 2.202533 | 1.261935 | 0.129203 |
| 6 | 9 | -0.233813 | 1.352338 | -0.538842 |
| 7 | 1 | 1.930579 | -0.736868 | -1.378389 |
| 8 | 8 | 0.176749 | -0.897644 | -0.200854 |
| 9 | 1 | 2.075452 | -1.788110 | 0.070224 |
| 10 | 1 | -0.499697 | 0.463334 | 1.236126 |
| 11 | 7 | -2.780208 | -0.346405 | 0.224192 |
| 12 | 1 | -3.719933 | -0.730549 | 0.297696 |
| 13 | 1 | -2.817907 | 0.440589 | -0.420552 |
| 14 | 1 | -2.186288 | -1.054690 | -0.204730 |

**Transition State for 3-Fluorooxetane**: E = -348.1447585. TC = 0.125909.
Imaginary Frequency = -567.5879.

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

| | | | | | |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.148234 | -1.166409 | -1.065487 |
| 2 | 6 | 0 | -0.291595 | -0.884547 | -0.028005 |
| 3 | 1 | 0 | -0.299493 | -1.703159 | 0.681662 |
| 4 | 7 | 0 | -2.024801 | -0.586779 | -0.071484 |
| 5 | 6 | 0 | 0.244905 | 0.474317 | 0.378495 |
| 6 | 6 | 0 | 1.598266 | 0.402192 | -0.251193 |
| 7 | 1 | 0 | -2.531166 | -1.407319 | -0.410127 |
| 8 | 1 | 0 | -2.202046 | 0.214272 | -0.681869 |
| 9 | 1 | 0 | -2.377249 | -0.343369 | 0.856897 |
| 10 | 1 | 0 | 0.301294 | 0.576885 | 1.463968 |
| 11 | 8 | 0 | 1.780012 | -0.944440 | 0.085968 |
| 12 | 9 | 0 | -0.665352 | 1.538355 | -0.051338 |
| 13 | 1 | 0 | 2.341817 | 1.093090 | 0.174943 |
| 14 | 1 | 0 | 1.527299 | 0.602014 | -1.341085 |

**Ground State for 3-Fluorooxetane**: E = -348.2183467. TC = 0.126831.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.585824 | -1.087887 | -1.871031 |
| 2 | 6 | 0 | 0.334888 | -0.435496 | -1.031950 |
| 3 | 1 | 0 | -0.201538 | 0.461077 | -1.363000 |
| 4 | 6 | 0 | 1.402791 | -0.104328 | 0.000484 |
| 5 | 6 | 0 | 0.333769 | -0.432821 | 1.032618 |
| 6 | 1 | 0 | 2.266446 | -0.772240 | 0.001816 |
| 7 | 1 | 0 | 0.583812 | -1.083057 | 1.873637 |
| 8 | 1 | 0 | -0.203054 | 0.464574 | 1.360774 |
| 9 | 7 | 0 | -2.831075 | 0.701263 | -0.000660 |
| 10 | 1 | 0 | -2.338586 | -0.193181 | -0.000282 |
| 11 | 1 | 0 | -3.433241 | 0.728084 | -0.820683 |
| 12 | 1 | 0 | -3.434504 | 0.728077 | 0.818432 |
| 13 | 8 | 0 | -0.418583 | -1.148572 | 0.000843 |
| 14 | 9 | 0 | 1.879149 | 1.207796 | -0.000966 |

**Transition State for 2,2-Difluorooxetane**: E = -447.2925542. TC = 0.118002. Imaginary Frequency = -661.3743.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.207107 | 0.597074 | 1.206649 |
| 2 | 6 | 0 | -1.158997 | 0.545421 | 0.128047 |
| 3 | 1 | 0 | -1.438944 | 1.430412 | -0.423671 |
| 4 | 7 | 0 | -2.893543 | -0.252052 | -0.038268 |
| 5 | 6 | 0 | -0.326956 | -0.540331 | -0.516901 |
| 6 | 6 | 0 | 0.979825 | 0.053145 | -0.023873 |
| 7 | 1 | 0 | -3.626138 | 0.374880 | 0.299069 |
| 8 | 1 | 0 | -2.942529 | -1.116492 | 0.503363 |
| 9 | 1 | 0 | -3.095960 | -0.481269 | -1.012793 |
| 10 | 1 | 0 | -0.537882 | -1.553393 | -0.163764 |
| 11 | 1 | 0 | -0.386840 | -0.498665 | -1.607316 |
| 12 | 9 | 0 | 2.050158 | -0.172203 | -0.901055 |
| 13 | 9 | 0 | 1.379420 | -0.686913 | 1.142236 |
| 14 | 8 | 0 | 0.707595 | 1.299307 | 0.221509 |

**Ground State for 2,2-Difluorooxetane**: E = -447.3536347. TC = 0.119193.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.060275 | 1.604364 | -0.121331 |
| 2 | 6 | 0 | -0.710009 | -0.273543 | 0.023492 |
| 3 | 6 | 0 | -0.399546 | 0.767629 | 1.078923 |
| 4 | 1 | 0 | 1.110952 | 1.888031 | -0.129128 |
| 5 | 1 | 0 | -0.595311 | 2.428057 | -0.408135 |
| 6 | 1 | 0 | -1.266194 | 1.121495 | 1.637304 |
| 7 | 1 | 0 | 0.412920 | 0.465067 | 1.738598 |
| 8 | 1 | 0 | 2.171838 | -0.405596 | -0.825392 |
| 9 | 7 | 0 | 2.701690 | -0.296428 | 0.038498 |
| 10 | 1 | 0 | 3.675616 | -0.139315 | -0.215580 |
| 11 | 1 | 0 | 2.658456 | -1.192873 | 0.519875 |
| 12 | 9 | 0 | -0.126770 | -1.504787 | 0.148361 |
| 13 | 9 | 0 | -2.041825 | -0.527625 | -0.181509 |
| 14 | 8 | 0 | -0.158384 | 0.451392 | -1.021899 |

**Transition State for *trans*-2,3-Difluorooxetane**: E = -447.2640765. TC = 0.118508.Imaginary frequency = -686.2859.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.603364 | 0.911722 | -1.440977 |
| 2 | 6 | 0 | 0.838724 | 0.716022 | -0.403875 |
| 3 | 1 | 0 | 1.022388 | 1.555946 | 0.247304 |
| 4 | 7 | 0 | 2.631885 | 0.284284 | -0.614782 |
| 5 | 6 | 0 | 0.406347 | -0.597863 | 0.211807 |
| 6 | 6 | 0 | -1.101912 | -0.598756 | 0.185417 |
| 7 | 1 | 0 | 3.162342 | 1.114658 | -0.884996 |
| 8 | 1 | 0 | 2.792250 | -0.442587 | -1.315715 |
| 9 | 1 | 0 | 2.982414 | -0.047272 | 0.287988 |
| 10 | 1 | 0 | 0.828535 | -1.476006 | -0.293997 |
| 11 | 9 | 0 | -1.402360 | -1.285112 | -1.056975 |
| 12 | 16 | 0 | -1.548512 | 1.104187 | 0.159132 |
| 13 | 9 | 0 | 0.920142 | -0.623257 | 1.527239 |
| 14 | 1 | 0 | -1.557289 | -1.214531 | 0.965290 |

**Ground State for *trans*-2,3-Difluorooxetane**: E = -447.3263376. TC = 0.119514.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.839896 | 0.695741 | -0.391674 |
| 2 | 1 | 0 | -1.168173 | 0.738294 | -1.433576 |
| 3 | 6 | 0 | -1.155262 | -0.564994 | 0.397990 |
| 4 | 6 | 0 | 0.346848 | -0.828005 | 0.356424 |
| 5 | 1 | 0 | -1.601512 | -0.383924 | 1.377124 |
| 6 | 1 | 0 | 0.884292 | -0.923269 | 1.299512 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 1 | 0 | 0.631075 | -1.624562 | -0.333394 |
| 8 | 8 | 0 | 0.556712 | 0.498283 | -0.243010 |
| 9 | 9 | 0 | -1.938211 | -1.493639 | -0.285898 |
| 10 | 9 | 0 | -1.246957 | 1.869793 | 0.221164 |
| 11 | 1 | 0 | 2.794518 | 0.488082 | -0.329188 |
| 12 | 7 | 0 | 3.486984 | -0.188503 | -0.010122 |
| 13 | 1 | 0 | 4.096672 | 0.285702 | 0.652926 |
| 14 | 1 | 0 | 4.056926 | -0.448901 | -0.812307 |

**Transition State for *cis*-2,3-Difluorooxetane**: E = -447.2703909. TC = 0.118943.
Imaginary frequency = -632.1895.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.881658 | -1.844561 | -0.399628 |
| 2 | 6 | 0 | -0.585491 | -0.927320 | 0.092575 |
| 3 | 7 | 0 | -2.325205 | -0.322847 | 0.360133 |
| 4 | 6 | 0 | -0.041329 | 0.257348 | -0.693381 |
| 5 | 6 | 0 | 1.395118 | 0.039385 | -0.311260 |
| 6 | 1 | 0 | -2.858740 | -0.983485 | 0.927740 |
| 7 | 1 | 0 | -2.825292 | -0.168494 | -0.517204 |
| 8 | 1 | 0 | -2.269293 | 0.575891 | 0.842611 |
| 9 | 8 | 0 | 1.339681 | -1.295561 | -0.275589 |
| 10 | 1 | 0 | -0.188388 | 0.125608 | -1.768273 |
| 11 | 1 | 0 | -0.346346 | -0.982540 | 1.145097 |
| 12 | 1 | 0 | 2.190627 | 0.493204 | -0.913933 |
| 13 | 9 | 0 | 1.572372 | 0.641745 | 1.006148 |
| 14 | 9 | 0 | -0.669229 | 1.490734 | -0.357285 |

**Ground State for *cis*-2,3-Difluorooxetane**: E = -447.3265368. TC = 0.119814.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.623189 | 0.138958 | 1.010344 |
| 2 | 6 | 0 | -0.242003 | 1.059427 | -0.798524 |
| 3 | 6 | 0 | -1.364104 | 0.141616 | -0.325267 |
| 4 | 1 | 0 | -1.133335 | 0.261601 | 1.966920 |
| 5 | 1 | 0 | 2.569883 | 0.325560 | 0.236912 |
| 6 | 7 | 0 | 2.707814 | -0.270544 | -0.577523 |
| 7 | 1 | 0 | 2.426055 | -1.209266 | -0.301582 |
| 8 | 1 | 0 | 3.705375 | -0.294937 | -0.779761 |
| 9 | 8 | 0 | 0.113548 | 1.272346 | 0.622498 |
| 10 | 1 | 0 | -0.513441 | 2.002317 | -1.275882 |
| 11 | 1 | 0 | 0.568891 | 0.545881 | -1.318955 |
| 12 | 1 | 0 | -2.346038 | 0.617487 | -0.270199 |
| 13 | 9 | 0 | -1.501756 | -1.077867 | -0.966207 |
| 14 | 9 | 0 | 0.194568 | -0.985868 | 1.131309 |

**Transition State for 2-Chlorooxetane**: E = -708.1763544. TC = 0.125109.
Imaginary Frequency = -686.9536.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.757271 | -0.189573 | -1.224614 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 1.145216 | 0.410515 | -0.413713 |
| 3 | 1 | 0 | 1.773078 | 1.252019 | -0.672355 |
| 4 | 7 | 0 | 2.613928 | -0.759458 | -0.107339 |
| 5 | 6 | 0 | 0.477546 | 0.299344 | 0.948162 |
| 6 | 6 | 0 | -0.851182 | 0.792460 | 0.429284 |
| 7 | 1 | 0 | 3.252553 | -0.772435 | -0.904375 |
| 8 | 1 | 0 | 2.251852 | -1.705551 | 0.025365 |
| 9 | 1 | 0 | 3.147527 | -0.504435 | 0.725270 |
| 10 | 1 | 0 | 0.508833 | -0.693566 | 1.404981 |
| 11 | 1 | 0 | 0.907824 | 1.036643 | 1.636635 |
| 12 | 8 | 0 | -0.491893 | 1.538686 | -0.586692 |
| 13 | 1 | 0 | -1.625088 | 1.162107 | 1.108914 |
| 14 | 17 | 0 | -1.762688 | -0.917201 | -0.143371 |

**Ground State for 2-Chlorooxetane**: E = -708.2391329. TC = 0.125799.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.121481 | -1.449750 | -0.071713 |
| 2 | 6 | 0 | 0.785109 | -0.697530 | -0.165801 |
| 3 | 6 | 0 | -0.051119 | -1.214517 | 0.998681 |
| 4 | 1 | 0 | -2.099848 | -1.000931 | 0.099802 |
| 5 | 1 | 0 | -1.208990 | -2.483865 | -0.417834 |
| 6 | 1 | 0 | 0.343174 | -2.080162 | 1.534926 |
| 7 | 1 | 0 | -0.331127 | -0.422005 | 1.693635 |
| 8 | 1 | 0 | -1.493650 | 1.319313 | -0.629371 |
| 9 | 7 | 0 | -1.988104 | 1.678378 | 0.187246 |
| 10 | 1 | 0 | -2.855798 | 2.103796 | -0.134606 |
| 11 | 1 | 0 | -1.413839 | 2.422685 | 0.578216 |
| 12 | 8 | 0 | -0.347423 | -0.657375 | -1.039525 |
| 13 | 1 | 0 | 1.560890 | -1.368635 | -0.544252 |
| 14 | 17 | 0 | 1.560015 | 0.893584 | 0.015174 |

**Transition State for 3-Chlorooxetane**: E = -708.1581466. TC = 0.124998.
Imaginary Frequency = -634.933.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.675334 | 1.913244 | -0.883980 |
| 2 | 6 | 0 | -0.510708 | 1.194171 | -0.090012 |
| 3 | 1 | 0 | -0.797497 | 1.506436 | 0.908393 |
| 4 | 7 | 0 | 1.326633 | 1.748282 | 0.149883 |
| 5 | 6 | 0 | -0.477278 | -0.233209 | -0.381524 |
| 6 | 6 | 0 | -1.510936 | -0.917103 | 0.408508 |
| 7 | 1 | 0 | 1.404433 | 2.699347 | 0.515046 |
| 8 | 1 | 0 | 1.838355 | 1.679038 | -0.731006 |
| 9 | 1 | 0 | 1.756096 | 1.067298 | 0.781573 |
| 10 | 1 | 0 | -0.493007 | -0.478723 | -1.437531 |
| 11 | 7 | 0 | -2.379531 | 0.098852 | -0.224444 |
| 12 | 1 | 0 | -1.376281 | -0.846675 | 1.492893 |
| 13 | 1 | 0 | -1.727844 | -1.941702 | 0.106401 |
| 14 | 1 | 0 | -2.702888 | 0.750811 | 0.504466 |
| 15 | 17 | 0 | 1.478693 | -1.149539 | -0.020950 |

**Ground State for 3-Chlorooxetane**: E = -708.2327824. TC = 0.125835.

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

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.154038 | -1.806559 | -1.499678 |
| 2 | 6 | 0 | 0.512907 | -1.040722 | -1.047881 |
| 3 | 1 | 0 | 0.002672 | -0.486849 | -1.842162 |
| 4 | 6 | 0 | 1.265025 | -0.203695 | 0.000478 |
| 5 | 7 | 0 | -0.370385 | -1.622156 | -0.000225 |
| 6 | 6 | 0 | 0.511572 | -1.040182 | 1.048230 |
| 7 | 1 | 0 | 2.356676 | -0.230074 | 0.001119 |
| 8 | 1 | 0 | -1.273540 | -1.137690 | -0.000885 |
| 9 | 1 | 0 | 1.152079 | -1.805815 | 1.501257 |
| 10 | 1 | 0 | 0.000350 | -0.485861 | 1.841556 |
| 11 | 7 | 0 | -2.755521 | 0.410715 | -0.000188 |
| 12 | 1 | 0 | -3.357001 | 0.481863 | -0.818920 |
| 13 | 1 | 0 | -2.140162 | 1.222916 | -0.000468 |
| 14 | 1 | 0 | -3.357260 | 0.482424 | 0.818303 |
| 15 | 17 | 0 | 0.800380 | 1.526666 | -0.000129 |

**Transition State for 2,2-Dichlorooxetane**: E = -1167.2955590. TC = 0.116015. Imaginary Frequency = -673.1374.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.714058 | 0.743974 | 0.934130 |
| 2 | 6 | 0 | 1.625977 | -0.267787 | 0.563362 |
| 3 | 1 | 0 | 1.992523 | -1.067001 | 1.191218 |
| 4 | 7 | 0 | 3.298303 | -0.144812 | -0.423097 |
| 5 | 6 | 0 | 0.698533 | -0.544396 | -0.601555 |
| 6 | 6 | 0 | -0.524605 | -0.169607 | 0.208279 |
| 7 | 1 | 0 | 4.095142 | -0.036661 | 0.206743 |
| 8 | 1 | 0 | 3.272765 | 0.667737 | -1.041472 |
| 9 | 1 | 0 | 3.460680 | -0.972541 | -0.998919 |
| 10 | 1 | 0 | 0.886216 | 0.034728 | -1.508765 |
| 11 | 1 | 0 | 0.678841 | -1.613685 | -0.831428 |
| 12 | 8 | 0 | -0.153243 | -0.419748 | 1.429931 |
| 13 | 17 | 0 | -0.810412 | 1.705561 | -0.102948 |
| 14 | 17 | 0 | -2.057932 | -0.969922 | -0.335276 |

**Ground State for 2,2-Dichlorooxetane**: E = -1167.3509392. TC = 0.116715.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.541801 | -1.791691 | 0.002126 |
| 2 | 6 | 0 | 0.429442 | 0.001004 | 0.063179 |
| 3 | 6 | 0 | -0.108954 | -0.901739 | 1.169413 |
| 4 | 1 | 0 | -1.590270 | -2.083595 | -0.033076 |
| 5 | 1 | 0 | 0.128967 | -2.624314 | -0.223773 |
| 6 | 1 | 0 | 0.617604 | -1.285233 | 1.885693 |
| 7 | 1 | 0 | -0.968122 | -0.450335 | 1.667137 |
| 8 | 1 | 0 | -2.539045 | 0.149132 | -0.892443 |
| 9 | 7 | 0 | -3.186583 | 0.090032 | -0.107047 |
| 10 | 1 | 0 | -4.092898 | -0.196354 | -0.473906 |
| 11 | 1 | 0 | -3.296659 | 1.034366 | 0.257973 |
| 12 | 8 | 0 | -0.292029 | -0.679290 | -0.935434 |
| 13 | 17 | 0 | 0.022692 | 1.722396 | 0.105613 |
| 14 | 17 | 0 | 2.195579 | -0.168573 | -0.185797 |

**Transition State for *trans*-2,3-Dichlorooxetane @ $C_4$:** E = -1167.2897109; TC = 0.116652. Imaginary frequency = -701.1549.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.203622 | 0.727316 | 1.558214 |
| 2 | 6 | 0 | -0.519917 | 0.894908 | 0.738812 |
| 3 | 7 | 0 | -1.779234 | 1.937393 | -0.234976 |
| 4 | 6 | 0 | -0.300545 | -0.173074 | -0.322942 |
| 5 | 6 | 0 | 0.927612 | -0.734111 | 0.360140 |
| 6 | 1 | 0 | -2.160766 | 2.685018 | 0.347118 |
| 7 | 1 | 0 | -2.551636 | 1.340867 | -0.540663 |
| 8 | 1 | 0 | -1.356010 | 2.364122 | -1.061360 |
| 9 | 8 | 0 | 0.756093 | -0.339238 | 1.598201 |
| 10 | 1 | 0 | 0.205236 | 1.693549 | 0.818014 |
| 11 | 17 | 0 | -1.680595 | -1.316130 | -0.343308 |
| 12 | 17 | 0 | 2.372960 | 0.256200 | -0.582560 |
| 13 | 1 | 0 | 1.246528 | -1.762441 | 0.164064 |
| 14 | 1 | 0 | -0.186935 | 0.196194 | -1.342470 |

**Transition State for *trans*-2,3-Dichlorooxetane @ $C_2$:** E = -1167.2623990; TC = 0.116316. Imaginary frequency = -542.4177. [

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.716604 | 0.188797 | 1.454563 |
| 2 | 6 | 0 | -0.582270 | -0.091742 | 0.416631 |
| 3 | 7 | 0 | -0.173517 | -1.772493 | 0.684000 |
| 4 | 6 | 0 | 0.605097 | 0.497212 | -0.325399 |
| 5 | 6 | 0 | 0.648062 | 1.853829 | 0.303546 |
| 6 | 1 | 0 | -0.951385 | -2.210013 | 1.184561 |
| 7 | 1 | 0 | 0.691209 | -1.845547 | 1.226925 |
| 8 | 1 | 0 | -0.031614 | -2.270569 | -0.199131 |
| 9 | 1 | 0 | 0.375944 | 0.576963 | -1.387471 |
| 10 | 8 | 0 | -0.742404 | 1.954978 | 0.256477 |
| 11 | 1 | 0 | 1.191661 | 2.601536 | -0.290238 |
| 12 | 1 | 0 | 1.084160 | 1.828120 | 1.321769 |
| 13 | 17 | 0 | 2.189130 | -0.532545 | -0.298208 |
| 14 | 17 | 0 | -2.101768 | -0.388481 | -0.438231 |

**Ground State for *trans*-2,3-Dichlorooxetane:** E = -1167.3491135; TC = 117425.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.055828 | -0.672419 | 0.630937 |
| 2 | 6 | 0 | -0.410135 | 1.296022 | 0.966856 |
| 3 | 6 | 0 | -0.725508 | 0.347149 | -0.186714 |
| 4 | 1 | 0 | -0.558535 | -1.341125 | 1.241256 |
| 5 | 1 | 0 | 2.339991 | 1.333223 | -0.039810 |
| 6 | 7 | 0 | 2.182982 | 1.704335 | -0.976902 |
| 7 | 1 | 0 | 2.639405 | 1.067251 | -1.627506 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 1 | 0 | 2.670044 | 2.596930 | -1.041965 |
| 9 | 8 | 0 | 0.646568 | 0.378415 | 1.411424 |
| 10 | 1 | 0 | -1.205222 | 1.365658 | 1.715546 |
| 11 | 1 | 0 | -0.003337 | 2.274467 | 0.709396 |
| 12 | 17 | 0 | -2.412194 | -0.018453 | -0.557194 |
| 13 | 1 | 0 | -0.201409 | 0.635286 | -1.097255 |
| 14 | 17 | 0 | 1.255990 | -1.670598 | -0.194524 |

**Transition State for *cis*-2,3-Dichlorooxetane @ $C_4$**: E = -1167.2900390; TC = 0.116868. Imaginary frequency = -647.8649.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.040319 | 2.200480 | -0.293714 |
| 2 | 6 | 0 | 0.661982 | 1.278061 | 0.126898 |
| 3 | 7 | 0 | 2.331867 | 0.794152 | 0.822039 |
| 4 | 6 | 0 | 0.330432 | 0.089401 | -0.775281 |
| 5 | 6 | 0 | -1.163884 | 0.309806 | -0.741793 |
| 6 | 1 | 0 | 2.684917 | 1.565244 | 1.392252 |
| 7 | 1 | 0 | 3.021202 | 0.581739 | 0.098270 |
| 8 | 1 | 0 | 2.239156 | -0.038293 | 1.406891 |
| 9 | 8 | 0 | -1.111998 | 1.641265 | -0.663245 |
| 10 | 1 | 0 | 0.677040 | 0.297647 | -1.789819 |
| 11 | 1 | 0 | 0.188566 | 1.324019 | 1.098165 |
| 12 | 17 | 0 | -1.886986 | -0.512729 | 0.802284 |
| 13 | 1 | 0 | -1.768096 | -0.130149 | -1.542148 |
| 14 | 17 | 0 | 1.035141 | -1.519828 | -0.359763 |

**Transition State for *cis*-2,3-Dichlorooxetane @ $C_2$**: E = -1167.2612435; TC = 0.116275. Imaginary frequency = -612.4285.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.190879 | -0.266238 | 1.521445 |
| 2 | 6 | 0 | -0.605106 | -0.276583 | 0.612158 |
| 3 | 7 | 0 | 0.168086 | -1.830243 | 0.902175 |
| 4 | 6 | 0 | 0.588248 | 0.664289 | 0.454813 |
| 5 | 6 | 0 | -0.085525 | 1.874047 | -0.122639 |
| 6 | 1 | 0 | -0.562736 | -2.523024 | 1.083654 |
| 7 | 1 | 0 | 0.800569 | -1.782761 | 1.706661 |
| 8 | 1 | 0 | 0.713683 | -2.117164 | 0.084202 |
| 9 | 8 | 0 | -1.237389 | 1.712750 | 0.642090 |
| 10 | 1 | 0 | -0.230908 | 1.764472 | -1.213603 |
| 11 | 1 | 0 | 0.470959 | 2.808137 | 0.056371 |
| 12 | 17 | 0 | -1.521039 | -0.711973 | -0.816079 |
| 13 | 1 | 0 | 0.972636 | 0.882465 | 1.454729 |
| 14 | 17 | 0 | 2.013008 | -0.066068 | -0.466944 |

**Ground State for *cis*-2,3-Dichlorooxetane:** E = -1167.3459604; TC = 0.117475.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.123575 | 0.448025 | 1.082977 |
| 2 | 6 | 0 | -0.191331 | -1.443600 | 0.314217 |
| 3 | 6 | 0 | 1.078119 | -0.630212 | 0.544411 |
| 4 | 1 | 0 | 0.364136 | 0.953099 | 2.018760 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 1 | 0 | -2.858846 | -0.405127 | -0.047461 |
| 6 | 7 | 0 | -3.047933 | -0.673995 | -1.012352 |
| 7 | 1 | 0 | -3.018786 | 0.176223 | -1.571546 |
| 8 | 1 | 0 | -3.998790 | -1.035214 | -1.055772 |
| 9 | 8 | 0 | -0.891633 | -0.535144 | 1.239276 |
| 10 | 1 | 0 | -0.215397 | -2.471702 | 0.679684 |
| 11 | 1 | 0 | -0.618704 | -1.364522 | -0.687820 |
| 12 | 17 | 0 | -0.326297 | 1.717481 | -0.084727 |
| 13 | 1 | 0 | 1.676068 | -1.027333 | 1.366744 |
| 14 | 17 | 0 | 2.154340 | -0.309927 | -0.808212 |

**Transition State for 2-Bromooxetane**: E = -2821.3727433. TC = 0.124741.
Imaginary Frequency = -684.5784.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.511043 | 0.927200 | -0.773925 |
| 2 | 6 | 0 | -1.683272 | 0.314953 | -0.442956 |
| 3 | 1 | 0 | -1.127246 | -0.233526 | -1.190052 |
| 4 | 7 | 0 | -2.822613 | -1.222971 | -0.089514 |
| 5 | 6 | 0 | -1.081542 | 0.445450 | 0.949264 |
| 6 | 6 | 0 | 0.095692 | 1.221089 | 0.427239 |
| 7 | 1 | 0 | -3.408757 | -1.453582 | -0.893385 |
| 8 | 1 | 0 | -3.430465 | -1.099506 | 0.721485 |
| 9 | 1 | 0 | -2.208786 | -2.019281 | 0.092543 |
| 10 | 1 | 0 | -1.711508 | 1.096062 | 1.569583 |
| 11 | 1 | 0 | -0.887328 | -0.492598 | 1.472003 |
| 12 | 8 | 0 | -0.383826 | 1.774269 | -0.648886 |
| 13 | 1 | 0 | 0.785263 | 1.778957 | 1.064814 |
| 14 | 35 | 0 | 1.524100 | -0.457887 | -0.052762 |

**Ground State for 2-Bromooxetane**: E = -2821.4298769. TC = 0.125363.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.104489 | -0.887271 | -0.027979 |
| 2 | 6 | 0 | -0.071880 | -1.048061 | -0.230930 |
| 3 | 6 | 0 | -0.988977 | -1.231421 | 0.967899 |
| 4 | 1 | 0 | -2.749890 | -0.047659 | 0.228845 |
| 5 | 1 | 0 | -2.676323 | -1.742959 | -0.397613 |
| 6 | 1 | 0 | -0.994699 | -2.223525 | 1.424356 |
| 7 | 1 | 0 | -0.859704 | -0.458494 | 1.725866 |
| 8 | 1 | 0 | -1.345382 | 1.799676 | -0.635363 |
| 9 | 7 | 0 | -1.644930 | 2.301884 | 0.200291 |
| 10 | 1 | 0 | -2.248703 | 3.067599 | -0.094336 |
| 11 | 1 | 0 | -0.809397 | 2.715965 | 0.609199 |
| 12 | 8 | 0 | -1.103791 | -0.482724 | -1.032593 |
| 13 | 35 | 0 | 1.447595 | 0.159634 | 0.012069 |
| 14 | 1 | 0 | 0.355190 | -1.948662 | -0.678595 |

**Transition State for 2,2-Dibromooxetane**: E = -5393.6825262. TC = 0.115244. Imaginary Frequency = -667.6424.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 2.351487 | 0.227389 | 0.912702 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 2.066916 | -0.759900 | 0.575481 |
| 3 | 1 | 0 | 2.352941 | -1.607465 | 1.181708 |
| 4 | 7 | 0 | 3.715978 | -0.912580 | -0.527195 |
| 5 | 6 | 0 | 1.063515 | -0.893607 | -0.553602 |
| 6 | 6 | 0 | -0.035922 | -0.341909 | 0.319465 |
| 7 | 1 | 0 | 4.558519 | -0.939609 | 0.049394 |
| 8 | 1 | 0 | 3.783288 | -0.099500 | -1.141609 |
| 9 | 1 | 0 | 3.710132 | -1.748295 | -1.113868 |
| 10 | 1 | 0 | 1.287359 | -0.341437 | -1.467475 |
| 11 | 1 | 0 | 0.871843 | -1.948037 | -0.777338 |
| 12 | 8 | 0 | 0.353368 | -0.626603 | 1.521363 |
| 13 | 35 | 0 | -1.871464 | -0.893497 | -0.178603 |
| 14 | 35 | 0 | -0.023434 | 1.745792 | -0.054886 |

**Ground State for 2,2-Dibromooxetane**: E = -5393.7320608. TC = 0.115861.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.586908 | 2.197622 | 0.077964 |
| 2 | 6 | 0 | -0.055487 | 0.273823 | 0.079744 |
| 3 | 6 | 0 | 0.365016 | 1.192569 | 1.214287 |
| 4 | 1 | 0 | 1.565037 | 2.672874 | 0.023699 |
| 5 | 1 | 0 | -0.233484 | 2.899681 | -0.089674 |
| 6 | 1 | 0 | -0.380135 | 1.410562 | 1.978806 |
| 7 | 1 | 0 | 1.316850 | 0.877396 | 1.645165 |
| 8 | 1 | 0 | 2.880819 | 0.708941 | -0.973628 |
| 9 | 7 | 0 | 3.505708 | 0.882445 | -0.186760 |
| 10 | 1 | 0 | 4.329948 | 1.361690 | -0.546564 |
| 11 | 1 | 0 | 3.813724 | -0.027967 | 0.150285 |
| 12 | 8 | 0 | 0.503073 | 1.093986 | -0.907783 |
| 13 | 35 | 0 | 0.664158 | -1.520918 | 0.050453 |
| 14 | 35 | 0 | -2.013756 | 0.183311 | -0.103323 |

**Transition State for Thietane:** E = -571.7540722; TC = 0.132922.
Imaginary frequency = -597.4165.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.800811 | -0.483616 | 0.048811 |
| 2 | 6 | -0.338887 | 0.914188 | -0.329446 |
| 3 | 1 | -0.783739 | -1.280585 | -0.680088 |
| 4 | 1 | -0.670239 | -0.797013 | 1.078234 |
| 5 | 7 | -2.594214 | -0.256532 | 0.071594 |
| 6 | 6 | 1.049837 | 1.031883 | 0.266442 |
| 7 | 1 | -0.279009 | 0.980169 | -1.421400 |
| 8 | 1 | -1.044745 | 1.688394 | 0.024148 |
| 9 | 1 | -3.066442 | -1.148921 | 0.231068 |
| 10 | 1 | -2.874380 | 0.395175 | 0.807616 |
| 11 | 1 | -2.909887 | 0.120822 | -0.824920 |
| 12 | 16 | 1.733067 | -0.626185 | -0.049350 |
| 13 | 1 | 1.628205 | 1.845941 | -0.184193 |
| 14 | 1 | 0.969828 | 1.235976 | 1.343143 |

**Ground State for Thietane**: E = -571.8346074; TC = 0.131899.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.644158 | 0.319772 | 1.132270 |
| 2 | 6 | -1.217995 | 1.184874 | -0.000021 |
| 3 | 1 | -1.281764 | 0.157127 | 2.003839 |
| 4 | 1 | 0.346713 | 0.656697 | 1.445034 |
| 5 | 16 | -0.517510 | -1.126893 | -0.000086 |
| 6 | 6 | -0.643755 | 0.319905 | -1.132221 |
| 7 | 1 | -2.310758 | 1.138198 | -0.000249 |
| 8 | 1 | -0.902810 | 2.233522 | 0.000081 |
| 9 | 1 | -1.281088 | 0.157473 | -2.004043 |
| 10 | 1 | 0.347196 | 0.656935 | -1.444624 |
| 11 | 7 | 2.780856 | 0.302685 | 0.000099 |
| 12 | 1 | 2.169946 | -0.513966 | 0.000336 |
| 13 | 1 | 3.381022 | 0.238950 | -0.819485 |
| 14 | 1 | 3.381157 | 0.239254 | 0.819618 |

**Transition State for 2-Fluorothietane**:E = -670.8600962; TC = 0.124438.
Imaginary Frequency = -598.8709.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.224838 | -0.929011 | 1.032545 |
| 2 | 6 | 0 | 1.185912 | -0.501434 | 0.038263 |
| 3 | 1 | 0 | 1.306974 | -1.198522 | -0.776506 |
| 4 | 7 | 0 | 2.923114 | 0.143439 | 0.001955 |
| 5 | 6 | 0 | 0.408932 | 0.780680 | -0.167548 |
| 6 | 6 | 0 | -0.957550 | 0.453619 | 0.391253 |
| 7 | 1 | 0 | 3.593931 | -0.626857 | 0.035913 |
| 8 | 1 | 0 | 3.105829 | 0.767060 | 0.790675 |
| 9 | 1 | 0 | 3.078173 | 0.668481 | -0.861418 |
| 10 | 1 | 0 | 0.883267 | 1.650232 | 0.313854 |
| 11 | 16 | 0 | -1.231647 | -1.240536 | -0.069627 |
| 12 | 1 | 0 | -1.002918 | 0.611663 | 1.475406 |
| 13 | 1 | 0 | 0.296577 | 0.983726 | -1.236865 |
| 14 | 9 | 0 | -1.896209 | 1.391171 | -0.138341 |

**Ground State for 2-Fluorothietane:** E = -670.9365445; TC = 0.124642.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.872867 | -1.250542 | 0.614890 |
| 2 | 6 | 0 | 0.619169 | 0.979898 | 0.198041 |
| 3 | 6 | 0 | 0.399665 | 0.012979 | 1.358140 |
| 4 | 1 | 0 | 0.148716 | -2.066008 | 0.600850 |
| 5 | 1 | 0 | 1.846944 | -1.619743 | 0.939080 |
| 6 | 1 | 0 | 0.959575 | 0.259547 | 2.265250 |
| 7 | 1 | 0 | -0.666937 | -0.041381 | 1.584888 |
| 8 | 1 | 0 | -1.921613 | -0.736417 | -0.882776 |
| 9 | 7 | 0 | -2.560374 | -0.698958 | -0.089846 |
| 10 | 1 | 0 | -3.403436 | -1.208900 | -0.346714 |
| 11 | 1 | 0 | -2.817009 | 0.279601 | 0.025459 |
| 12 | 1 | 0 | 1.415342 | 1.719233 | 0.299168 |
| 13 | 9 | 0 | -0.536812 | 1.714231 | -0.125487 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 16 | 0 | 0.990134 | -0.348457 | -0.984583 |

**Transition State for 2-Chlorothietane**:E = -1030.8763006; TC = 0.123652.
Imaginary Frequency = -619.6849.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.909944 | 0.132592 | -1.234156 |
| 2 | 6 | 0 | 1.235058 | 0.549076 | -0.290648 |
| 3 | 1 | 0 | 1.682840 | 1.532019 | -0.328963 |
| 4 | 7 | 0 | 2.839703 | -0.384501 | -0.229666 |
| 5 | 6 | 0 | 0.593360 | 0.032307 | 0.986250 |
| 6 | 6 | 0 | -0.883930 | 0.051816 | 0.666032 |
| 7 | 1 | 0 | 3.446987 | -0.101162 | -1.001133 |
| 8 | 1 | 0 | 2.645209 | -1.384102 | -0.320947 |
| 9 | 1 | 0 | 3.340498 | -0.232561 | 0.648329 |
| 10 | 1 | 0 | 0.970599 | -0.955275 | 1.292100 |
| 11 | 1 | 0 | 0.784894 | 0.742507 | 1.797323 |
| 12 | 1 | 0 | -1.535646 | -0.026169 | 1.537408 |
| 13 | 17 | 0 | -1.244915 | -1.509182 | -0.269985 |
| 14 | 16 | 0 | -1.039163 | 1.552535 | -0.272647 |

**Ground State for 2-Chlorothietane:** E = -1030.9471234; TC = 0.123628.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.878156 | 0.115558 | 0.567606 |
| 2 | 6 | 0 | 0.051346 | -1.016105 | 0.267588 |
| 3 | 6 | 0 | -0.560600 | -0.103513 | 1.330201 |
| 4 | 1 | 0 | -2.250950 | 1.141303 | 0.562631 |
| 5 | 1 | 0 | -2.674829 | -0.572144 | 0.859608 |
| 6 | 1 | 0 | -0.641262 | -0.546316 | 2.328428 |
| 7 | 1 | 0 | -0.010182 | 0.838415 | 1.379937 |
| 8 | 1 | 0 | 0.312013 | 2.172888 | -0.841271 |
| 9 | 7 | 0 | 0.659283 | 2.732386 | -0.063331 |
| 10 | 1 | 0 | 0.539456 | 3.713500 | -0.308427 |
| 11 | 1 | 0 | 1.659605 | 2.555886 | 0.007000 |
| 12 | 1 | 0 | -0.099413 | -2.080201 | 0.455479 |
| 13 | 17 | 0 | 1.791666 | -0.816287 | -0.041881 |
| 14 | 16 | 0 | -1.098955 | -0.403050 | -1.017529 |

**Transition State for 2,2-Difluorothietane**: E = -769.9765115; TC = 0.116387. Imaginary Frequency = -602.1306.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.265254 | 0.709525 | 1.093722 |
| 2 | 6 | 0 | -1.302952 | 0.557293 | 0.023764 |
| 3 | 1 | 0 | -1.559801 | 1.413001 | -0.582343 |
| 4 | 7 | 0 | -3.035257 | -0.190250 | 0.008828 |
| 5 | 6 | 0 | -0.522178 | -0.596071 | -0.567718 |
| 6 | 6 | 0 | 0.862570 | -0.340022 | -0.026586 |
| 7 | 1 | 0 | -3.727208 | 0.502361 | 0.301521 |
| 8 | 1 | 0 | -3.080602 | -0.982787 | 0.652527 |
| 9 | 1 | 0 | -3.286395 | -0.521693 | -0.924816 |
| 10 | 1 | 0 | -0.900967 | -1.583013 | -0.270088 |
| 11 | 1 | 0 | -0.499104 | -0.524656 | -1.657905 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 9 | 0 | 1.819206 | -1.051302 | -0.741457 |
| 13 | 9 | 0 | 0.906881 | -0.930043 | 1.259006 |
| 14 | 16 | 0 | 1.050419 | 1.401495 | 0.005680 |

**Ground State for 2,2-Difluorothietane:** E = -770.0446942; TC = 0.116574.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.019506 | 0.717393 | 0.000023 |
| 2 | 6 | 0 | 0.163364 | -0.576441 | -0.000006 |
| 3 | 6 | 0 | 1.670526 | -0.784306 | -0.000016 |
| 4 | 1 | 0 | 2.553336 | 1.048688 | -0.891816 |
| 5 | 1 | 0 | 2.553277 | 1.048652 | 0.891910 |
| 6 | 1 | 0 | 1.999046 | -1.322067 | 0.892612 |
| 7 | 1 | 0 | 1.999032 | -1.322006 | -0.892686 |
| 8 | 1 | 0 | -2.832082 | -0.017138 | -0.820828 |
| 9 | 7 | 0 | -2.663139 | 0.561087 | 0.000005 |
| 10 | 1 | 0 | -2.831877 | -0.017373 | 0.820719 |
| 11 | 1 | 0 | -3.354379 | 1.308875 | 0.000191 |
| 12 | 9 | 0 | -0.472228 | -1.130378 | -1.090669 |
| 13 | 9 | 0 | -0.472201 | -1.130354 | 1.090690 |
| 14 | 16 | 0 | 0.245944 | 1.221966 | -0.000021 |

**Transition State for 2,2-Dichlorothietane**: E = -1489.9868424; TC = 0.114471. Imaginary Frequency = -611.5129.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.806451 | 0.109136 | -1.089781 |
| 2 | 6 | 0 | 1.750308 | 0.513724 | -0.088325 |
| 3 | 1 | 0 | 2.169460 | 1.497502 | 0.065440 |
| 4 | 7 | 0 | 3.253509 | -0.421350 | 0.548237 |
| 5 | 6 | 0 | 0.702182 | -0.029941 | 0.861321 |
| 6 | 6 | 0 | -0.565268 | 0.070932 | 0.039681 |
| 7 | 1 | 0 | 4.099607 | -0.109903 | 0.067132 |
| 8 | 1 | 0 | 3.130794 | -1.420672 | 0.370875 |
| 9 | 1 | 0 | 3.386843 | -0.287612 | 1.552840 |
| 10 | 1 | 0 | 0.908367 | -1.048287 | 1.218120 |
| 11 | 1 | 0 | 0.609784 | 0.636743 | 1.723405 |
| 12 | 16 | 0 | -0.359093 | 1.592794 | -0.821776 |
| 13 | 17 | 0 | -2.021920 | -0.071127 | 1.090857 |
| 14 | 17 | 0 | -0.593593 | -1.413606 | -1.059877 |

**Ground State for 2,2-Dichlorothietane:**E = -1490.0538408. TC = 0.114496.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.401332 | -1.884341 | 0.481688 |
| 2 | 6 | 0 | 0.489483 | 0.143450 | 0.069570 |
| 3 | 6 | 0 | -0.233047 | -0.552281 | 1.226470 |
| 4 | 1 | 0 | -1.378864 | -2.355956 | 0.594527 |
| 5 | 1 | 0 | 0.397680 | -2.602920 | 0.675072 |
| 6 | 1 | 0 | 0.327074 | -0.575581 | 2.165310 |
| 7 | 1 | 0 | -1.214917 | -0.095095 | 1.371119 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 1 | 0 | -2.914605 | 0.175056 | -0.595558 |
| 9 | 7 | 0 | -3.332217 | 0.370754 | 0.313516 |
| 10 | 1 | 0 | -4.294747 | 0.038555 | 0.286568 |
| 11 | 1 | 0 | -3.365545 | 1.383532 | 0.415182 |
| 12 | 17 | 0 | 0.045821 | 1.837461 | -0.216642 |
| 13 | 16 | 0 | -0.167589 | -1.053599 | -1.142273 |
| 14 | 17 | 0 | 2.267135 | 0.048053 | 0.246240 |

**Transition State for 2-Bromothietane**:E = -3144.0713972; TC = 0.123161.
Imaginary Frequency = -629.2544.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.625110 | 0.723839 | -0.476221 |
| 2 | 6 | 0 | -1.749274 | 0.107439 | -0.328026 |
| 3 | 1 | 0 | -1.193858 | -0.168557 | -1.213591 |
| 4 | 7 | 0 | -2.688184 | -1.519183 | -0.236466 |
| 5 | 6 | 0 | -1.045892 | 0.048840 | 1.019032 |
| 6 | 6 | 0 | 0.256415 | 0.756724 | 0.739240 |
| 7 | 1 | 0 | -3.295532 | -1.632748 | -1.050213 |
| 8 | 1 | 0 | -3.259915 | -1.598912 | 0.606797 |
| 9 | 1 | 0 | -2.002796 | -2.278032 | -0.235858 |
| 10 | 1 | 0 | -1.612760 | 0.643663 | 1.744451 |
| 11 | 1 | 0 | -0.935606 | -0.970498 | 1.414818 |
| 12 | 1 | 0 | 0.843302 | 1.038679 | 1.613639 |
| 13 | 35 | 0 | 1.482749 | -0.670350 | -0.111557 |
| 14 | 16 | 0 | -0.235259 | 2.053817 | -0.339096 |

**Ground State for 2-Bromothietane:** E = -3144.1395738; TC = 0.123169.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.264139 | -0.589340 | 0.539015 |
| 2 | 6 | 0 | -0.059472 | -0.941503 | 0.276838 |
| 3 | 6 | 0 | -0.973076 | -0.340823 | 1.340979 |
| 4 | 1 | 0 | -2.979463 | 0.234955 | 0.539172 |
| 5 | 1 | 0 | -2.765311 | -1.526192 | 0.792206 |
| 6 | 1 | 0 | -0.906795 | -0.815791 | 2.325191 |
| 7 | 1 | 0 | -0.809680 | 0.735066 | 1.428534 |
| 8 | 1 | 0 | -0.977822 | 2.096640 | -0.814813 |
| 9 | 7 | 0 | -0.994594 | 2.759570 | -0.040901 |
| 10 | 1 | 0 | -1.555339 | 3.559615 | -0.328320 |
| 11 | 1 | 0 | -0.040000 | 3.088451 | 0.091127 |
| 12 | 1 | 0 | 0.199852 | -1.988057 | 0.440781 |
| 13 | 16 | 0 | -1.312433 | -0.749891 | -1.031567 |
| 14 | 35 | 0 | 1.645022 | -0.042098 | -0.017814 |

**Transition State for 2,2-Dibromothietane**: E = -5716.3740782; TC = 0.113702. Imaginary frequency = -619.9768.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 2.406375 | 0.070617 | 0.725740 |
| 2 | 6 | 0 | 2.140074 | -0.859387 | 0.242390 |
| 3 | 1 | 0 | 2.539047 | -1.770295 | 0.666055 |
| 4 | 7 | 0 | 3.494339 | -0.691595 | -1.099154 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | 0.929182 | -0.897545 | -0.670008 |
| 6 | 6 | 0 | -0.130053 | -0.302731 | 0.224464 |
| 7 | 1 | 0 | 4.428635 | -0.751959 | -0.689919 |
| 8 | 1 | 0 | 3.393430 | 0.225939 | -1.538515 |
| 9 | 1 | 0 | 3.414688 | -1.406774 | -1.824810 |
| 10 | 1 | 0 | 1.053765 | -0.364191 | -1.620617 |
| 11 | 16 | 0 | 0.239007 | -0.939791 | 1.798295 |
| 12 | 1 | 0 | 0.663682 | -1.939637 | -0.876245 |
| 13 | 35 | 0 | -1.935943 | -0.632953 | -0.499612 |
| 14 | 35 | 0 | 0.112534 | 1.723584 | 0.079572 |

**Ground State for 2,2-Dibromothietane:** E = -5716.4364077; TC = 0.113718.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.476701 | 2.301449 | -0.364139 |
| 2 | 6 | 0 | 0.106078 | 0.168296 | -0.054738 |
| 3 | 6 | 0 | -0.446006 | 1.011315 | -1.200531 |
| 4 | 1 | 0 | -1.362154 | 2.924864 | -0.500589 |
| 5 | 1 | 0 | 0.436552 | 2.895511 | -0.442056 |
| 6 | 1 | 0 | 0.162527 | 1.016550 | -2.108412 |
| 7 | 1 | 0 | -1.473762 | 0.706427 | -1.416113 |
| 8 | 1 | 0 | -3.221999 | 0.439307 | 0.462264 |
| 9 | 7 | 0 | -3.671052 | 0.482607 | -0.451657 |
| 10 | 1 | 0 | -4.526255 | 1.026674 | -0.349100 |
| 11 | 1 | 0 | -3.946137 | -0.467025 | -0.696155 |
| 12 | 16 | 0 | -0.490345 | 1.327872 | 1.201415 |
| 13 | 35 | 0 | -0.571648 | -1.640890 | 0.095185 |
| 14 | 35 | 0 | 2.068045 | 0.096523 | -0.132169 |

## Cleavage Reactions in AN

**Ground State for Ammonia: E =** -56.442162. **TC =** 0.037270.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.000000 | 0.000000 | 0.114589 |
| 2 | 1 | 0 | 0.000000 | 0.947508 | -0.267375 |
| 3 | 1 | 0 | -0.820566 | -0.473754 | -0.267375 |
| 4 | 1 | 0 | 0.820566 | -0.473754 | -0.267375 |

**Transition State for Azetidine:** E = -229.1973591. TC = 0.143589.
Imaginary Frequency = -801.0123.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.446131 | -0.534979 | -0.014840 |
| 2 | 7 | 0 | 2.269213 | -0.050164 | 0.084935 |
| 3 | 6 | 0 | -0.150561 | 0.841915 | -0.248695 |
| 4 | 6 | 0 | -1.554042 | 0.547823 | 0.242283 |
| 5 | 1 | 0 | 2.852733 | -0.890163 | 0.177278 |
| 6 | 1 | 0 | 2.463458 | 0.555811 | 0.890936 |
| 7 | 1 | 0 | 2.571707 | 0.447082 | -0.761394 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 1 | 0 | -0.147431 | 1.059823 | -1.323034 |
| 9 | 7 | 0 | -1.641683 | -0.842982 | -0.224458 |
| 10 | 1 | 0 | -2.137873 | -1.410237 | 0.480450 |
| 11 | 1 | 0 | 0.629188 | -1.230006 | -0.820201 |
| 12 | 1 | 0 | 0.426379 | -0.940755 | 0.989831 |
| 13 | 1 | 0 | 0.385166 | 1.648385 | 0.268937 |
| 14 | 1 | 0 | -1.566085 | 0.637550 | 1.343636 |
| 15 | 1 | 0 | -2.319122 | 1.245979 | -0.142263 |

**Ground State for Azetidine:** E = -172.8380306. TC = 0.105193.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.044067 | -0.034325 | 0.112487 |
| 2 | 1 | 0 | -1.346311 | -0.110033 | 1.166797 |
| 3 | 6 | 0 | 0.000639 | 1.076417 | -0.094316 |
| 4 | 6 | 0 | 1.044031 | -0.035550 | 0.112471 |
| 5 | 7 | 0 | -0.000606 | -1.030454 | -0.266292 |
| 6 | 1 | 0 | -0.001150 | -1.884895 | 0.309043 |
| 7 | 1 | 0 | 0.001128 | 1.916173 | 0.604534 |
| 8 | 1 | 0 | 0.000862 | 1.448200 | -1.122574 |
| 9 | 1 | 0 | 1.346026 | -0.111539 | 1.166846 |
| 10 | 1 | 0 | -1.935864 | -0.040850 | -0.522307 |
| 11 | 1 | 0 | 1.935935 | -0.043128 | -0.522151 |

**Transition State for 2-Fluoroazetidine:** E = -328.3408516. TC = 0.134899
Imaginary Frequency = -736.5861.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.639122 | 1.021201 | 0.918259 |
| 2 | 6 | 0 | -1.286366 | 0.581799 | -0.004664 |
| 3 | 1 | 0 | -1.633926 | 1.016392 | -0.931851 |
| 4 | 7 | 0 | -3.032037 | -0.564876 | 0.000861 |
| 5 | 6 | 0 | -0.368036 | -0.641337 | -0.000674 |
| 6 | 6 | 0 | 0.887738 | 0.160198 | 0.004785 |
| 7 | 1 | 0 | -3.837253 | 0.051412 | -0.153746 |
| 8 | 1 | 0 | -3.185651 | -1.039640 | 0.896967 |
| 9 | 1 | 0 | -3.059553 | -1.282157 | -0.731561 |
| 10 | 1 | 0 | -0.499206 | -1.270294 | 0.886677 |
| 11 | 1 | 0 | -0.488833 | -1.266412 | -0.892278 |
| 12 | 7 | 0 | 0.426071 | 1.364835 | 0.001120 |
| 13 | 9 | 0 | 3.798918 | -0.608749 | -0.001342 |
| 14 | 1 | 0 | 1.942140 | -0.150995 | 0.007362 |
| 15 | 1 | 0 | 1.052893 | 2.195559 | 0.001706 |

**Ground State for 2-Fluoroazetidine:** E = -271.9534255. TC = 0.097599.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.497784 | -0.052846 | -0.116112 |
| 2 | 6 | 0 | 0.507584 | -0.029382 | 0.407645 |
| 3 | 6 | 0 | -0.454819 | 1.078672 | 0.002519 |
| 4 | 1 | 0 | -2.133450 | -0.073272 | -1.005133 |
| 5 | 1 | 0 | -2.117721 | -0.141484 | 0.783007 |
| 6 | 7 | 0 | -0.366699 | -1.027187 | -0.152077 |
| 7 | 1 | 0 | -0.475561 | -1.891624 | 0.398095 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 9 | 0 | 1.782350 | 0.007331 | -0.234721 |
| 9 | 1 | 0 | -0.636009 | 1.874163 | 0.727569 |
| 10 | 1 | 0 | -0.179254 | 1.500723 | -0.967078 |
| 11 | 1 | 0 | 0.737849 | -0.122836 | 1.476255 |

**Transition State for 3-Fluoroazetidine:** E = -328.3045325.
TC = 0.136146. Imaginary Frequency = -765.0728.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.370705 | -1.688977 | 0.725975 |
| 2 | 6 | 0 | 0.262324 | -0.898186 | -0.003078 |
| 3 | 1 | 0 | 0.176557 | -1.186940 | -1.044759 |
| 4 | 7 | 0 | 2.098999 | -0.594623 | -0.075020 |
| 5 | 6 | 0 | -0.218953 | 0.482036 | 0.388682 |
| 6 | 6 | 0 | -1.585691 | 0.466811 | -0.219694 |
| 7 | 1 | 0 | 2.574827 | -1.485547 | -0.264144 |
| 8 | 1 | 0 | 2.459219 | -0.226838 | 0.814280 |
| 9 | 1 | 0 | 2.350809 | 0.070572 | -0.813860 |
| 10 | 1 | 0 | -0.239354 | 0.593131 | 1.478233 |
| 11 | 9 | 0 | 0.642055 | 1.542640 | -0.082155 |
| 12 | 7 | 0 | -1.844847 | -0.931408 | 0.163434 |
| 13 | 1 | 0 | -1.488844 | 0.633108 | -1.305166 |
| 14 | 1 | 0 | -2.277245 | 1.221769 | 0.182686 |
| 15 | 1 | 0 | -2.230319 | -1.435783 | -0.648202 |

**Ground State for 3-Fluoroazetidine:** E = -271.9405895. TC = 0.097682.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.460693 | -1.050230 | -0.059829 |
| 2 | 6 | 0 | -0.460755 | 1.050270 | -0.059874 |
| 3 | 6 | 0 | 0.533115 | -0.000014 | 0.425137 |
| 4 | 1 | 0 | -0.620861 | -1.945105 | 0.547870 |
| 5 | 1 | 0 | -0.235245 | -1.328949 | -1.098570 |
| 6 | 1 | 0 | -0.620779 | 1.944976 | 0.548125 |
| 7 | 1 | 0 | -0.235252 | 1.329260 | -1.098502 |
| 8 | 1 | 0 | 0.721184 | -0.000086 | 1.502562 |
| 9 | 7 | 0 | -1.515537 | 0.000025 | 0.062267 |
| 10 | 1 | 0 | -2.196803 | -0.000372 | -0.710484 |
| 11 | 9 | 0 | 1.791834 | -0.000006 | -0.217720 |

**Transition State for 2,2-Difluoroazetidine:** E = -427.4504763.
TC = 0.127618. Imaginary Frequency = -775.9199.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.237843 | 0.935150 | 0.976634 |
| 2 | 6 | 0 | -1.147302 | 0.611754 | -0.051323 |
| 3 | 1 | 0 | -1.526634 | 1.256401 | -0.827781 |
| 4 | 7 | 0 | -2.947122 | -0.283754 | 0.057063 |
| 5 | 6 | 0 | -0.344534 | -0.632940 | -0.367610 |
| 6 | 6 | 0 | 0.974707 | 0.019938 | -0.064316 |
| 7 | 1 | 0 | -3.677156 | 0.420534 | 0.211751 |
| 8 | 1 | 0 | -3.000881 | -0.957693 | 0.828911 |
| 9 | 1 | 0 | -3.181875 | -0.783631 | -0.807892 |
| 10 | 1 | 0 | -0.573575 | -1.491867 | 0.266964 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 1 | 0 | -0.428957 | -0.913624 | -1.420770 |
| 12 | 7 | 0 | 0.728870 | 1.325750 | -0.320426 |
| 13 | 1 | 0 | 1.307879 | 1.965441 | 0.247667 |
| 14 | 9 | 0 | 2.107574 | -0.589911 | -0.726680 |
| 15 | 9 | 0 | 1.331269 | -0.267555 | 1.311964 |

**Ground State for 2,2-Difluoroazetidine**: E = -371.0683663. TC = 0.089492.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.684724 | -0.674841 | 0.860391 |
| 2 | 6 | 0 | -0.380647 | -0.043538 | -0.013732 |
| 3 | 6 | 0 | 1.671314 | 0.075294 | -0.067161 |
| 4 | 1 | 0 | 0.657356 | -0.390874 | 1.913293 |
| 5 | 1 | 0 | 0.719082 | -1.760339 | 0.746255 |
| 6 | 1 | 0 | 2.036444 | 1.009996 | 0.369814 |
| 7 | 1 | 0 | 2.499969 | -0.501745 | -0.482094 |
| 8 | 9 | 0 | -0.979928 | 1.076599 | 0.583255 |
| 9 | 7 | 0 | 0.544987 | 0.267761 | -1.029717 |
| 10 | 1 | 0 | 0.433292 | 1.171199 | -1.517390 |
| 11 | 9 | 0 | -1.466005 | -0.803716 | -0.416461 |

**Transition State for 3,3-Difluoroazetidine:** E = -427.4178991. TC = 0.128476. Imaginary Frequency = - -772.9668.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.338722 | 1.560208 | -0.950537 |
| 2 | 6 | 0 | 0.339007 | 1.013232 | -0.017441 |
| 3 | 1 | 0 | 0.409310 | 1.571382 | 0.906472 |
| 4 | 7 | 0 | 2.158676 | 0.626723 | -0.029539 |
| 5 | 6 | 0 | -0.206843 | -0.398077 | -0.026861 |
| 6 | 6 | 0 | -1.589474 | -0.200654 | -0.545965 |
| 7 | 1 | 0 | 2.668376 | 1.513962 | 0.073072 |
| 8 | 1 | 0 | 2.463844 | 0.182461 | -0.903599 |
| 9 | 1 | 0 | 2.436098 | 0.015354 | 0.749519 |
| 10 | 7 | 0 | -1.764023 | 1.170623 | -0.046002 |
| 11 | 1 | 0 | -2.025682 | 1.094493 | 0.949807 |
| 12 | 1 | 0 | -1.566756 | -0.215153 | -1.642890 |
| 13 | 1 | 0 | -2.292201 | -0.971462 | -0.199271 |
| 14 | 9 | 0 | -0.207196 | -0.878453 | 1.282783 |
| 15 | 9 | 0 | 0.601593 | -1.323734 | -0.717469 |

**Ground State for 3,3-Difluoroazetidine**: E = -371.0496966. TC = 0.089777.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.414238 | -0.023261 | 0.000043 |
| 2 | 6 | 0 | 0.661558 | -0.149466 | 1.064306 |
| 3 | 6 | 0 | 0.661514 | -0.152519 | -1.063882 |
| 4 | 1 | 0 | 0.726642 | -1.187506 | -1.421866 |
| 5 | 1 | 0 | 0.613889 | 0.546912 | -1.902519 |
| 6 | 7 | 0 | 1.654434 | 0.195807 | -0.000301 |
| 7 | 1 | 0 | 2.481065 | -0.419901 | 0.000537 |
| 8 | 9 | 0 | -1.426120 | -0.957500 | 0.001340 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 1 | 0 | 0.726640 | -1.183386 | 1.425370 |
| 10 | 1 | 0 | 0.614021 | 0.552477 | 1.900846 |
| 11 | 9 | 0 | -1.040135 | 1.209970 | -0.001680 |

**Transition State for 2-Chloroazetidine:** E = -688.3713099.
TC = 0.134867. Imaginary Frequency = -719.0856.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.760844 | 0.703402 | -1.327754 |
| 2 | 6 | 0 | -1.199944 | 0.778140 | -0.342136 |
| 3 | 1 | 0 | -1.768160 | 1.669308 | -0.112889 |
| 4 | 7 | 0 | 0.544158 | 1.861900 | 0.179492 |
| 5 | 6 | 0 | -0.918741 | -0.282960 | 0.724288 |
| 6 | 6 | 0 | -2.112238 | -1.089205 | 0.357190 |
| 7 | 1 | 0 | 0.698594 | 2.636350 | -0.473660 |
| 8 | 1 | 0 | 1.340633 | 1.220249 | 0.104008 |
| 9 | 1 | 0 | 0.542966 | 2.258540 | 1.124426 |
| 10 | 1 | 0 | 0.040634 | -0.786326 | 0.572240 |
| 11 | 1 | 0 | -0.951316 | 0.116987 | 1.743765 |
| 12 | 7 | 0 | -2.615970 | -0.393671 | -0.601559 |
| 13 | 1 | 0 | -3.481071 | -0.668258 | -1.112622 |
| 14 | 17 | 0 | 2.748406 | -0.696166 | -0.162629 |
| 15 | 1 | 0 | -2.496114 | -2.028880 | 0.765604 |

**Ground State for 2-Chlororoazetidine**: E = -631.9589100. TC = 0.096423.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.545499 | -0.108666 | -0.647653 |
| 2 | 6 | 0 | -0.014237 | 0.021072 | 0.729571 |
| 3 | 6 | 0 | 0.940523 | 1.069210 | 0.146882 |
| 4 | 1 | 0 | 2.634852 | -0.190281 | -0.690269 |
| 5 | 1 | 0 | 1.125013 | -0.197393 | -1.656881 |
| 6 | 7 | 0 | 0.906896 | -1.008929 | 0.345591 |
| 7 | 1 | 0 | 0.535096 | -1.921031 | 0.040835 |
| 8 | 1 | 0 | 0.497629 | 1.896866 | -0.408838 |
| 9 | 1 | 0 | 1.623625 | 1.448046 | 0.912422 |
| 10 | 17 | 0 | -1.603251 | 0.005424 | -0.221265 |
| 11 | 1 | 0 | -0.339937 | 0.044387 | 1.772291 |

**Transition State for 3-Chloroazetidine:** E = -688.3158740
TC = 0.135266. Imaginary Frequency = -757.7273.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.540734 | 1.938467 | 0.706313 |
| 2 | 6 | 0 | 0.320298 | 1.161051 | -0.011427 |
| 3 | 1 | 0 | 0.499877 | 1.378612 | -1.058401 |
| 4 | 7 | 0 | -1.476042 | 1.652828 | -0.069309 |
| 5 | 6 | 0 | 0.277203 | -0.295545 | 0.414637 |
| 6 | 6 | 0 | 1.552680 | -0.788956 | -0.204240 |
| 7 | 1 | 0 | -1.495930 | 2.671711 | -0.204934 |
| 8 | 1 | 0 | -1.970871 | 1.445642 | 0.807337 |
| 9 | 1 | 0 | -2.002396 | 1.221655 | -0.837315 |
| 10 | 1 | 0 | 0.315027 | -0.359442 | 1.506778 |
| 11 | 7 | 0 | 2.304467 | 0.423829 | 0.134218 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 1 | 0 | 1.402837 | -0.944271 | -1.284738 |
| 13 | 1 | 0 | 1.919314 | -1.732974 | 0.227241 |
| 14 | 1 | 0 | 2.791344 | 0.765144 | -0.708119 |
| 15 | 17 | 0 | -1.217647 | -1.257673 | -0.047197 |

**Ground State for 3-Chlororoazetidine**: E = -631.9505733. TC = 0.096661.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.074299 | 0.000019 | 0.689623 |
| 2 | 6 | 0 | 0.919019 | 1.045967 | 0.167394 |
| 3 | 6 | 0 | 0.919083 | -1.045953 | 0.167406 |
| 4 | 1 | 0 | 1.581921 | -1.375171 | 0.980330 |
| 5 | 1 | 0 | 0.516638 | -1.916892 | -0.358286 |
| 6 | 7 | 0 | 1.517350 | -0.000004 | -0.707158 |
| 7 | 1 | 0 | 2.547482 | -0.000070 | -0.721968 |
| 8 | 1 | 0 | 1.581913 | 1.375250 | 0.980266 |
| 9 | 1 | 0 | -0.320558 | 0.000076 | 1.753460 |
| 10 | 1 | 0 | 0.516673 | 1.916883 | -0.358426 |
| 11 | 17 | 0 | -1.625197 | -0.000014 | -0.204224 |

**Transition State for 2,2-Dichloroazetidine:** E = -1147.3624824.
TC = 0.126493. Imaginary Frequency = -690.1495.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.019942 | -0.007299 | -0.008791 |
| 2 | 6 | 0 | -0.007605 | 0.001426 | 1.072682 |
| 3 | 1 | 0 | 0.950714 | 0.006444 | 1.573874 |
| 4 | 7 | 0 | 0.209259 | -2.135312 | 0.900170 |
| 5 | 6 | 0 | -1.303670 | -0.158898 | 1.860294 |
| 6 | 6 | 0 | -1.487133 | 1.314100 | 1.941508 |
| 7 | 1 | 0 | 0.980556 | -2.375558 | 0.269604 |
| 8 | 1 | 0 | -0.659469 | -2.488072 | 0.485666 |
| 9 | 1 | 0 | 0.369538 | -2.638391 | 1.778528 |
| 10 | 1 | 0 | -2.081740 | -0.685364 | 1.299891 |
| 11 | 1 | 0 | -1.165091 | -0.635174 | 2.836655 |
| 12 | 7 | 0 | -0.463710 | 1.774405 | 1.321923 |
| 13 | 1 | 0 | -0.253190 | 2.786168 | 1.170175 |
| 14 | 17 | 0 | -2.757133 | 2.169371 | 2.681522 |
| 15 | 17 | 0 | -2.918200 | -2.616426 | -0.364595 |

**Ground State for 2,2-Dichlororoazetidine**: E = -1091.0616638. TC = 0.086976.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.223989 | 2.382385 | -0.669609 |
| 2 | 6 | 0 | -0.521487 | 1.994496 | 0.027136 |
| 3 | 1 | 0 | -1.033672 | 2.788707 | 0.573457 |
| 4 | 6 | 0 | -0.099012 | 0.753958 | 0.862441 |
| 5 | 6 | 0 | -1.153161 | 0.062793 | 0.064267 |
| 6 | 1 | 0 | 0.912354 | 0.383213 | 0.660137 |
| 7 | 1 | 0 | -0.299241 | 0.804915 | 1.936916 |
| 8 | 7 | 0 | -1.491411 | 1.091081 | -0.650825 |
| 9 | 1 | 0 | -2.188691 | 1.209437 | -1.425493 |
| 10 | 17 | 0 | -1.748608 | -1.492533 | 0.013688 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 17 | 0 | 3.129025 | -0.394156 | -0.145612 |

**Transition State for 2-Bromoazetidine:** E = -2801.5726209.
TC = 0.134905. Imaginary Frequency = -720.6686.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.520249 | 0.712238 | -1.335655 |
| 2 | 6 | 0 | -1.980709 | 0.739107 | -0.357283 |
| 3 | 1 | 0 | -2.698433 | 1.524573 | -0.162786 |
| 4 | 7 | 0 | -0.451833 | 2.113236 | 0.148242 |
| 5 | 6 | 0 | -1.543989 | -0.232138 | 0.741621 |
| 6 | 6 | 0 | -2.572556 | -1.240923 | 0.380090 |
| 7 | 1 | 0 | -0.406804 | 2.875197 | -0.535904 |
| 8 | 1 | 0 | 0.435978 | 1.602715 | 0.110583 |
| 9 | 1 | 0 | -0.532351 | 2.543042 | 1.075307 |
| 10 | 1 | 0 | -0.509824 | -0.565637 | 0.615713 |
| 11 | 1 | 0 | -1.663924 | 0.182239 | 1.748880 |
| 12 | 7 | 0 | -3.172579 | -0.670155 | -0.605479 |
| 13 | 1 | 0 | -3.965940 | -1.107742 | -1.119159 |
| 14 | 1 | 0 | -2.793707 | -2.222481 | 0.810090 |
| 15 | 35 | 0 | 2.160276 | -0.321200 | -0.074085 |

**Ground State for 2-Bromoazetidine**: E = -2745.1507274. TC = 0.096029.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.483183 | -0.042710 | -0.190249 |
| 2 | 6 | 0 | -0.546136 | -0.038304 | 0.513722 |
| 3 | 6 | 0 | -1.440283 | 1.080238 | -0.009352 |
| 4 | 1 | 0 | -3.063488 | -0.056432 | -1.116739 |
| 5 | 1 | 0 | -3.153149 | -0.129549 | 0.673506 |
| 6 | 7 | 0 | -1.358510 | -1.027649 | -0.164285 |
| 7 | 1 | 0 | -1.514577 | -1.899115 | 0.366281 |
| 8 | 1 | 0 | -1.664224 | 1.895640 | 0.681660 |
| 9 | 1 | 0 | -1.093791 | 1.473447 | -0.967535 |
| 10 | 1 | 0 | -0.490197 | -0.122365 | 1.606095 |
| 11 | 35 | 0 | 1.351618 | 0.001045 | -0.056514 |

**Transition State for 2,2Dibromoazetidine:** E = --5373.8763711.
TC = 0.125985. Imaginary Frequency = -694.5696.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.575855 | 1.961205 | 1.233174 |
| 2 | 6 | 0 | 0.004287 | 2.039967 | 0.323374 |
| 3 | 1 | 0 | 0.298264 | 3.025370 | -0.012646 |
| 4 | 7 | 0 | -1.889404 | 2.382248 | -0.628873 |
| 5 | 6 | 0 | 0.266109 | 0.807673 | -0.537620 |
| 6 | 6 | 0 | 1.557147 | 0.548920 | 0.152551 |
| 7 | 1 | 0 | -2.405307 | 3.129323 | -0.152952 |
| 8 | 1 | 0 | -2.423904 | 1.514696 | -0.522045 |
| 9 | 1 | 0 | -1.865464 | 2.619622 | -1.625872 |
| 10 | 1 | 0 | -0.485821 | 0.025252 | -0.398941 |
| 11 | 1 | 0 | 0.376876 | 1.033974 | -1.603555 |
| 12 | 7 | 0 | 1.629365 | 1.493880 | 1.015216 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 1 | 0 | 2.409581 | 1.638508 | 1.694861 |
| 14 | 35 | 0 | -2.918600 | -0.972324 | 0.127392 |
| 15 | 35 | 0 | 2.790790 | -0.812253 | -0.154428 |

**Ground State for 2,2-Dibromoazetidine**:E = -5317.4539551. TC = 0.086616.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.017836 | 0.510027 | -0.011490 |
| 2 | 6 | 0 | 1.135869 | 2.231482 | -0.083014 |
| 3 | 6 | 0 | 0.397886 | 1.513954 | 1.072285 |
| 4 | 1 | 0 | 1.013757 | 3.314389 | -0.162975 |
| 5 | 7 | 0 | 0.272069 | 1.461603 | -1.019321 |
| 6 | 1 | 0 | 0.619566 | 1.150277 | -1.941615 |
| 7 | 1 | 0 | -0.474643 | 2.077996 | 1.412951 |
| 8 | 1 | 0 | 0.977858 | 1.140417 | 1.916531 |
| 9 | 1 | 0 | 2.195007 | 1.955040 | -0.142853 |
| 10 | 35 | 0 | -1.767034 | -0.276550 | -0.001664 |
| 11 | 35 | 0 | 1.322875 | -1.020653 | 0.006993 |

**Transition State for Oxetane:** E = -249.0767135.
TC = 0.131967. Imaginary Frequency = -767.2942.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.376157 | -0.531018 | 0.004634 |
| 2 | 7 | 0 | 2.270652 | -0.014571 | 0.060460 |
| 3 | 6 | 0 | -0.193853 | 0.860176 | -0.201745 |
| 4 | 1 | 0 | 0.440490 | -0.934823 | 1.006738 |
| 5 | 1 | 0 | 0.592025 | -1.200067 | -0.815067 |
| 6 | 6 | 0 | -1.609944 | 0.480913 | 0.191232 |
| 7 | 1 | 0 | 2.864535 | -0.849275 | 0.120993 |
| 8 | 1 | 0 | 0.295557 | 1.633065 | 0.402900 |
| 9 | 1 | 0 | 2.547677 | 0.498945 | -0.783713 |
| 10 | 1 | 0 | 2.488885 | 0.578356 | 0.868814 |
| 11 | 1 | 0 | -0.119772 | 1.138251 | -1.258382 |
| 12 | 1 | 0 | -2.405574 | 1.002529 | -0.362881 |
| 13 | 1 | 0 | -1.777896 | 0.663484 | 1.268279 |
| 14 | 8 | 0 | -1.531832 | -0.911112 | -0.104453 |

**Ground State for Oxetane**: E = -192.6855647. TC = 0.092707.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.828953 | -0.136684 | -0.661022 |
| 2 | 6 | 0 | -1.033056 | -0.052264 | 0.083675 |
| 3 | 1 | 0 | -1.451495 | -0.129955 | 1.093909 |
| 4 | 6 | 0 | 0.000117 | 1.066011 | -0.080367 |
| 5 | 6 | 0 | 1.033048 | -0.052461 | 0.083676 |
| 6 | 1 | 0 | 0.000154 | 1.500426 | -1.082673 |
| 7 | 1 | 0 | 1.828884 | -0.137139 | -0.661063 |
| 8 | 1 | 0 | 1.451494 | -0.130275 | 1.093888 |
| 9 | 8 | 0 | -0.000123 | -1.074123 | -0.121956 |
| 10 | 1 | 0 | 0.000249 | 1.858892 | 0.670705 |

**Transition State for 2-Fluorooxetane:** E = -348.2080445.
TC = 0.124279. Imaginary Frequency = -740.5666.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.749541 | 0.455089 | -1.277751 |
| 2 | 6 | 0 | 0.758155 | 0.571602 | -0.203084 |
| 3 | 1 | 0 | 1.201352 | 1.470229 | 0.200581 |
| 4 | 7 | 0 | 2.605668 | -0.272507 | -0.171188 |
| 5 | 6 | 0 | 0.110146 | -0.473446 | 0.689466 |
| 6 | 6 | 0 | -1.283716 | 0.040798 | 0.434299 |
| 7 | 1 | 0 | 3.266441 | 0.322560 | -0.682592 |
| 8 | 1 | 0 | 2.623009 | -1.197207 | -0.614477 |
| 9 | 1 | 0 | 2.970327 | -0.382083 | 0.781246 |
| 10 | 1 | 0 | 0.296046 | -1.508236 | 0.390086 |
| 11 | 1 | 0 | 0.412498 | -0.337468 | 1.732870 |
| 12 | 8 | 0 | -1.005359 | 1.244026 | -0.106752 |
| 13 | 1 | 0 | -2.037198 | 0.026843 | 1.232215 |
| 14 | 9 | 0 | -1.909593 | -0.858679 | -0.581549 |

**Ground State for 2-Fluorooxetane**: E = -291.7853099. TC = 0.085126.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.762671 | -1.845159 | 0.640245 |
| 2 | 6 | 0 | -0.475044 | -1.038163 | -0.037742 |
| 3 | 1 | 0 | -0.223592 | -1.426300 | -1.031664 |
| 4 | 6 | 0 | 0.525090 | -0.000033 | 0.447929 |
| 5 | 6 | 0 | -0.474924 | 1.038165 | -0.037729 |
| 6 | 1 | 0 | 0.738654 | -0.000017 | 1.520516 |
| 7 | 1 | 0 | -0.762492 | 1.845200 | 0.640227 |
| 8 | 1 | 0 | -0.223494 | 1.426255 | -1.031669 |
| 9 | 8 | 0 | -1.508699 | 0.000055 | -0.114727 |
| 10 | 9 | 0 | 1.761384 | -0.000026 | -0.228288 |

**Transition State for 2,2-Difluorooxetane:** E = -447.3333294.
TC = 0.116312. Imaginary Frequency = -702.3454.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.382304 | 1.101504 | -0.924890 |
| 2 | 6 | 0 | 1.095832 | 0.622647 | -0.000045 |
| 3 | 1 | 0 | 1.378205 | 1.095457 | 0.929230 |
| 4 | 7 | 0 | 3.003758 | -0.262177 | 0.000559 |
| 5 | 6 | 0 | 0.353738 | -0.696989 | -0.005384 |
| 6 | 6 | 0 | -0.982488 | 0.003879 | -0.000702 |
| 7 | 1 | 0 | 3.720060 | 0.471583 | 0.008522 |
| 8 | 1 | 0 | 3.175727 | -0.840565 | -0.828474 |
| 9 | 1 | 0 | 3.169840 | -0.852725 | 0.822193 |
| 10 | 1 | 0 | 0.532190 | -1.292061 | -0.903797 |
| 11 | 1 | 0 | 0.534778 | -1.302390 | 0.885538 |
| 12 | 9 | 0 | -1.803981 | -0.352461 | 1.099776 |
| 13 | 9 | 0 | -1.813678 | -0.353566 | -1.092825 |
| 14 | 8 | 0 | -0.645371 | 1.278932 | -0.002252 |

**Ground State for 2,2-Difluorooxetane**: E = -390.9082960. TC = 0.076389.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.722145 | 0.000361 | -0.124154 |
| 2 | 6 | 0 | 0.382951 | -0.000147 | 0.021432 |
| 3 | 6 | 0 | -0.726174 | -0.001954 | 1.074492 |
| 4 | 1 | 0 | -2.309476 | 0.908520 | -0.270837 |
| 5 | 1 | 0 | -2.311369 | -0.906194 | -0.272972 |
| 6 | 1 | 0 | -0.739431 | -0.902532 | 1.695796 |
| 7 | 1 | 0 | -0.739130 | 0.895678 | 1.700009 |
| 8 | 9 | 0 | 1.251961 | 1.121223 | 0.007266 |
| 9 | 9 | 0 | 1.253962 | -1.119856 | 0.005057 |
| 10 | 8 | 0 | -0.507712 | 0.000333 | -1.099191 |

**Transition State for 2-Chlorooxetane:** E = -708.2124939.
TC = 0.123214. Imaginary Frequency = -732.6641.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.957807 | -0.075564 | -1.313015 |
| 2 | 6 | 0 | 1.156293 | 0.467110 | -0.398606 |
| 3 | 1 | 0 | 1.823582 | 1.315405 | -0.452275 |
| 4 | 7 | 0 | 2.825082 | -0.708023 | -0.137967 |
| 5 | 6 | 0 | 0.490189 | 0.040231 | 0.899134 |
| 6 | 6 | 0 | -0.816028 | 0.680010 | 0.508284 |
| 7 | 1 | 0 | 3.498541 | -0.520137 | -0.888396 |
| 8 | 1 | 0 | 2.610472 | -1.710475 | -0.167217 |
| 9 | 1 | 0 | 3.303496 | -0.523608 | 0.750367 |
| 10 | 1 | 0 | 0.495715 | -1.033532 | 1.094228 |
| 11 | 1 | 0 | 0.936016 | 0.567529 | 1.750509 |
| 12 | 8 | 0 | -0.404253 | 1.488991 | -0.466923 |
| 13 | 1 | 0 | -1.508438 | 1.090307 | 1.250135 |
| 14 | 17 | 0 | -1.978910 | -0.775871 | -0.198591 |

**Ground State for 2-Chlorooxetane**: E = -651.8048500. TC = 0.084170.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.282068 | 0.000208 | 1.727947 |
| 2 | 6 | 0 | 0.030972 | 0.027268 | 0.664671 |
| 3 | 6 | 0 | -0.945477 | 1.060509 | 0.112879 |
| 4 | 6 | 0 | -1.617753 | -0.142316 | -0.556118 |
| 5 | 1 | 0 | -1.552016 | 1.504340 | 0.906719 |
| 6 | 1 | 0 | -2.680362 | -0.304355 | -0.366710 |
| 7 | 1 | 0 | -1.385786 | -0.274904 | -1.616768 |
| 8 | 8 | 0 | -0.799164 | -1.055136 | 0.265686 |
| 9 | 1 | 0 | -0.535573 | 1.838895 | -0.532254 |
| 10 | 17 | 0 | 1.615208 | 0.000243 | -0.210177 |

**Transition State for 2-Bromoooxetane:** E = -2821.4124581.
TC = 0.122295. Imaginary Frequency = -494.5211.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.801088 | 0.934229 | -0.683373 |
| 2 | 6 | 0 | -1.885835 | 0.387778 | -0.494762 |
| 3 | 1 | 0 | -1.516792 | -0.256930 | -1.282566 |
| 4 | 7 | 0 | -3.304381 | -1.335690 | -0.086304 |
| 5 | 6 | 0 | -1.294051 | 0.287910 | 0.905929 |
| 6 | 6 | 0 | -0.326113 | 1.336776 | 0.526659 |
| 7 | 1 | 0 | -3.931208 | -1.455723 | -0.887894 |
| 8 | 1 | 0 | -3.902379 | -1.200721 | 0.734703 |
| 9 | 1 | 0 | -2.821922 | -2.230205 | 0.044147 |
| 10 | 1 | 0 | -1.982397 | 0.631280 | 1.688600 |
| 11 | 1 | 0 | -0.877938 | -0.681678 | 1.177987 |
| 12 | 8 | 0 | -0.718007 | 1.687112 | -0.627461 |
| 13 | 1 | 0 | 0.445143 | 1.885569 | 1.071128 |
| 14 | 35 | 0 | 1.922837 | -0.395648 | -0.053311 |

**Ground State for 2-Bromooxetane**: E = -2764.9964819. TC = 0.083643.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.367337 | -0.018720 | 1.814951 |
| 2 | 6 | 0 | -0.563321 | 0.017296 | 0.740531 |
| 3 | 6 | 0 | -1.473245 | 1.060877 | 0.111758 |
| 4 | 6 | 0 | -2.067745 | -0.135709 | -0.641726 |
| 5 | 1 | 0 | -2.162334 | 1.480463 | 0.850644 |
| 6 | 1 | 0 | -3.145123 | -0.299438 | -0.582051 |
| 7 | 1 | 0 | -1.705977 | -0.263491 | -1.666079 |
| 8 | 8 | 0 | -1.351868 | -1.054174 | 0.268979 |
| 9 | 1 | 0 | -1.010305 | 1.856008 | -0.473446 |
| 10 | 35 | 0 | 1.252340 | 0.000680 | -0.095978 |

**Transition State for 2-Aminooxetane**: E = -304.3355358. TC = 0.149142.
Imaginary Frequency = -688.8103.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.199883 | 1.081115 | 0.880088 |
| 2 | 6 | 0 | -0.987111 | 0.553019 | -0.042282 |
| 3 | 1 | 0 | -1.220901 | 1.057746 | -0.969921 |
| 4 | 7 | 0 | -2.773519 | -0.308125 | -0.031143 |
| 5 | 6 | 0 | -0.114677 | -0.704664 | -0.004100 |
| 6 | 6 | 0 | 1.209989 | -0.004262 | 0.395693 |
| 7 | 1 | 0 | -3.481981 | 0.433094 | -0.061936 |
| 8 | 1 | 0 | -2.881303 | -0.862776 | 0.824298 |
| 9 | 1 | 0 | -2.860738 | -0.911973 | -0.855357 |
| 10 | 1 | 0 | -0.480425 | -1.482707 | 0.682992 |
| 11 | 1 | 0 | -0.034380 | -1.139217 | -1.012454 |
| 12 | 1 | 0 | 1.330208 | -0.043836 | 1.500479 |
| 13 | 7 | 0 | 2.473207 | -0.520332 | -0.167639 |
| 14 | 1 | 0 | 2.735643 | -1.436582 | 0.210968 |
| 15 | 1 | 0 | 2.426075 | -0.553474 | -1.191092 |
| 16 | 8 | 0 | 0.890083 | 1.324156 | -0.089057 |

**Ground State for 2-Aminooxetane**: E = -247.9457171. TC = 0.110401.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.355405 | -0.099112 | -0.401548 |
| 2 | 6 | 0 | 0.514648 | -0.006164 | 0.497355 |
| 3 | 6 | 0 | -0.526161 | 1.061666 | 0.154405 |
| 4 | 1 | 0 | -1.358625 | -0.179603 | -1.493082 |
| 5 | 1 | 0 | -2.368506 | -0.226662 | -0.010959 |
| 6 | 1 | 0 | 0.813369 | -0.096725 | 1.551028 |
| 7 | 1 | 0 | -0.202033 | 1.822135 | -0.560567 |
| 8 | 1 | 0 | -0.967612 | 1.535515 | 1.034214 |
| 9 | 8 | 0 | -0.437233 | -1.076981 | 0.192191 |
| 10 | 7 | 0 | 1.624456 | -0.024154 | -0.427976 |
| 11 | 1 | 0 | 2.081058 | 0.895487 | -0.440385 |
| 12 | 1 | 0 | 2.330532 | -0.703556 | -0.123212 |

**Transition State for Thietane:** E = -571.7926361.
TC = 0.130379. Imaginary Frequency = -742.7596.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.688699 | -0.814006 | 1.072040 |
| 2 | 6 | 0 | 0.650846 | -0.504517 | 0.036003 |
| 3 | 1 | 0 | 0.817716 | -1.260574 | -0.715265 |
| 4 | 7 | 0 | 2.672577 | -0.226352 | 0.069982 |
| 5 | 6 | 0 | 0.297926 | 0.933786 | -0.302028 |
| 6 | 6 | 0 | -1.115303 | 1.062607 | 0.239046 |
| 7 | 1 | 0 | 3.138779 | -1.129752 | 0.206971 |
| 8 | 1 | 0 | 2.971655 | 0.396161 | 0.828428 |
| 9 | 1 | 0 | 3.016319 | 0.168197 | -0.812375 |
| 10 | 1 | 0 | 1.007392 | 1.652519 | 0.126985 |
| 11 | 1 | 0 | 0.303932 | 1.051608 | -1.391157 |
| 12 | 16 | 0 | -1.676737 | -0.658521 | -0.042894 |
| 13 | 1 | 0 | -1.724697 | 1.816545 | -0.268033 |
| 14 | 1 | 0 | -1.100852 | 1.288852 | 1.310707 |

**Ground State for Thietane**: E = -515.3973209. TC = 0.090413

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.344897 | 1.134793 | 0.153050 |
| 2 | 6 | 0 | -1.323328 | -0.000001 | -0.187738 |
| 3 | 6 | 0 | -0.344880 | -1.134799 | 0.153061 |
| 4 | 1 | 0 | -0.343648 | 2.005130 | -0.506974 |
| 5 | 1 | 0 | -0.419410 | 1.458961 | 1.194921 |
| 6 | 1 | 0 | -1.546510 | 0.000018 | -1.258986 |
| 7 | 1 | 0 | -2.264397 | -0.000022 | 0.372887 |
| 8 | 1 | 0 | -0.343575 | -2.005017 | -0.507131 |
| 9 | 1 | 0 | -0.419444 | -1.459147 | 1.194862 |
| 10 | 16 | 0 | 1.088475 | 0.000007 | -0.074989 |

**Transition State for 2-Fluorothietane:** E = -670.9002695.
TC = 0.122622. Imaginary Frequency = -718.7473. [2FthietTS-acn]

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

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.264885 | 1.002981 | 0.950707 |
| 2 | 6 | 0 | -1.060532 | 0.548940 | -0.008879 |
| 3 | 1 | 0 | -1.332274 | 1.100342 | -0.894778 |
| 4 | 7 | 0 | -2.989643 | -0.196685 | -0.013132 |
| 5 | 6 | 0 | -0.384414 | -0.806537 | -0.074768 |
| 6 | 6 | 0 | 1.005905 | -0.477042 | 0.415916 |
| 7 | 1 | 0 | -3.650720 | 0.585211 | -0.074497 |
| 8 | 1 | 0 | -3.212511 | -0.724646 | 0.837651 |
| 9 | 1 | 0 | -3.163849 | -0.810774 | -0.816290 |
| 10 | 1 | 0 | -0.894567 | -1.571948 | 0.520083 |
| 11 | 16 | 0 | 1.152684 | 1.245555 | -0.057232 |
| 12 | 1 | 0 | 1.150231 | -0.640344 | 1.488735 |
| 13 | 1 | 0 | -0.328235 | -1.141559 | -1.115796 |
| 14 | 9 | 0 | 1.979511 | -1.327057 | -0.209089 |

**Ground State for 2-Fluorothietane**: E = -614.5007763. TC = 0.082793.

| | | | | | |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.207232 | -0.307997 | 1.455084 |
| 2 | 6 | 0 | 0.744779 | -0.056260 | 0.497294 |
| 3 | 6 | 0 | 0.077473 | 1.301471 | 0.311327 |
| 4 | 6 | 0 | -1.157184 | 0.772178 | -0.440826 |
| 5 | 1 | 0 | -0.194098 | 1.727890 | 1.282041 |
| 6 | 1 | 0 | -2.122681 | 1.126748 | -0.075557 |
| . 7 | 1 | 0 | -1.101048 | 0.890857 | -1.524773 |
| 8 | 1 | 0 | 0.699340 | 2.018635 | -0.233754 |
| 9 | 9 | 0 | 1.757475 | -0.255998 | -0.483908 |
| 10 | 16 | 0 | -0.768527 | -0.953531 | 0.077835 |

**Transition State for 2,2-Difluorothietane:** E = -770.0141041.
TC = 0.114514. Imaginary Frequency = -703.0132.

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.415572 | 0.832797 | 1.072588 |
| 2 | 6 | 0 | -1.244169 | 0.585323 | 0.034700 |
| 3 | 1 | 0 | -1.608701 | 1.264136 | -0.720515 |
| 4 | 7 | 0 | -3.137312 | -0.283506 | 0.005423 |
| 5 | 6 | 0 | -0.530799 | -0.700351 | -0.334755 |
| 6 | 6 | 0 | 0.899974 | -0.343070 | -0.020532 |
| 7 | 1 | 0 | -3.831826 | 0.450703 | 0.181055 |
| 8 | 1 | 0 | -3.260268 | -1.002350 | 0.726959 |
| 9 | 1 | 0 | -3.363527 | -0.708870 | -0.900532 |
| 10 | 1 | 0 | -0.876532 | -1.568406 | 0.235200 |
| 11 | 1 | 0 | -0.638157 | -0.902266 | -1.404873 |
| 12 | 9 | 0 | 1.811821 | -0.924543 | -0.906313 |
| 13 | 9 | 0 | 1.277522 | -0.895828 | 1.217904 |
| 14 | 16 | 0 | 0.900103 | 1.421921 | -0.006790 |

**Ground State for 2,2-Difluorothietane**: E = -713.6180599. TC = 0.075111.

| Center Number | Atomic Number | Atomic Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.598437 | 0.658007 | 0.010628 |
| 2 | 6 | 0 | -0.581268 | 0.066928 | -0.003980 |
| 3 | 6 | 0 | 0.223044 | 1.352761 | -0.064229 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 1 | 0 | 2.147068 | 0.852999 | 0.932809 |
| 5 | 1 | 0 | 2.238336 | 0.828546 | -0.855853 |
| 6 | 1 | 0 | 0.051592 | 1.882937 | -1.005154 |
| 7 | 1 | 0 | 0.003225 | 2.015278 | 0.777701 |
| 8 | 9 | 0 | -1.383699 | -0.049901 | 1.115815 |
| 9 | 9 | 0 | -1.447173 | -0.128410 | -1.061321 |
| 10 | 16 | 0 | 0.849772 | -1.027571 | 0.000346 |

**Transition State for 2-Chlorothietane:** E = -1030.9103379.
TC = 0.121787. Imaginary Frequency = -714.4890.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.804856 | 0.830551 | 0.956522 |
| 2 | 6 | 0 | -1.517339 | 0.451089 | -0.014667 |
| 3 | 1 | 0 | -1.919590 | 0.941316 | -0.887163 |
| 4 | 7 | 0 | -3.217858 | -0.718305 | -0.011905 |
| 5 | 6 | 0 | -0.543606 | -0.706883 | -0.113131 |
| 6 | 6 | 0 | 0.708070 | -0.076658 | 0.458998 |
| 7 | 1 | 0 | -4.043819 | -0.112027 | -0.062331 |
| 8 | 1 | 0 | -3.302025 | -1.286781 | 0.837891 |
| 9 | 1 | 0 | -3.252306 | -1.352942 | -0.817213 |
| 10 | 1 | 0 | -0.871455 | -1.600581 | 0.430191 |
| 11 | 16 | 0 | 0.483082 | 1.629782 | -0.072989 |
| 12 | 1 | 0 | 0.737622 | -0.155142 | 1.550271 |
| 13 | 1 | 0 | -0.393508 | -0.964229 | -1.166770 |
| 14 | 17 | 0 | 2.221346 | -0.903166 | -0.092790 |

**Ground State for 2-Fluorothietane**: E = -974.5100941. TC = 0.081997.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.848204 | 0.556989 | -0.088904 |
| 2 | 6 | 0 | 0.286400 | 0.167586 | 0.499415 |
| 3 | 6 | 0 | -0.515981 | 1.324953 | -0.091672 |
| 4 | 1 | 0 | -2.485932 | 0.689913 | -0.964927 |
| 5 | 1 | 0 | -2.426526 | 0.708019 | 0.825440 |
| 6 | 1 | 0 | -0.485910 | 2.254974 | 0.485521 |
| 7 | 1 | 0 | -0.192851 | 1.520031 | -1.118456 |
| 8 | 1 | 0 | 0.364937 | 0.196302 | 1.590304 |
| 9 | 17 | 0 | 1.944458 | -0.044999 | -0.115555 |
| 10 | 16 | 0 | -0.960175 | -1.056339 | -0.047905 |

**Transition State for 2-Bromoothietane:** E = -3144.1044209.
TC = 0.121271. Imaginary Frequency = -724.3685.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.643796 | 0.876347 | -0.346261 |
| 2 | 6 | 0 | -1.770318 | 0.242092 | -0.332475 |
| 3 | 1 | 0 | -1.411294 | -0.140158 | -1.278628 |
| 4 | 7 | 0 | -3.052772 | -1.359496 | -0.230332 |
| 5 | 6 | 0 | -1.034009 | -0.104020 | 0.951584 |
| 6 | 6 | 0 | 0.285446 | 0.613063 | 0.767397 |
| 7 | 1 | 0 | -3.757059 | -1.270067 | -0.970896 |
| 8 | 1 | 0 | -3.552481 | -1.409128 | 0.664493 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 1 | 0 | -2.570036 | -2.254279 | -0.368637 |
| 10 | 1 | 0 | -1.560399 | 0.352496 | 1.798975 |
| 11 | 1 | 0 | -0.952353 | -1.180218 | 1.134350 |
| 12 | 1 | 0 | 0.819162 | 0.891699 | 1.679020 |
| 13 | 35 | 0 | 1.597168 | -0.635074 | -0.131529 |
| 14 | 16 | 0 | -0.236871 | 1.960661 | -0.275976 |

**Ground State for 2-Bromothietane**: E = -3087.7030034. TC = 0.081379.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.087956 | -0.100733 | 1.841028 |
| 2 | 6 | 0 | -0.301291 | 0.067453 | 0.783028 |
| 3 | 6 | 0 | -1.068941 | 1.326096 | 0.372678 |
| 4 | 6 | 0 | -1.896230 | 0.631527 | -0.719929 |
| 5 | 1 | 0 | -1.710149 | 1.633565 | 1.206403 |
| 6 | 1 | 0 | -2.956237 | 0.889197 | -0.767568 |
| 7 | 1 | 0 | -1.445736 | 0.701040 | -1.713270 |
| 8 | 1 | 0 | -0.459486 | 2.176930 | 0.054695 |
| 9 | 16 | 0 | -1.555099 | -1.009887 | 0.044610 |
| 10 | 35 | 0 | 1.461141 | -0.036922 | -0.112849 |

**Halide Displacement Reactions in AN**

**Transition State for Fluorocyclobutane:** E = -312.3154340.
TC = 0.150630. Imaginary Frequency = - -563.4248

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.271509 | -0.535176 | -0.000016 |
| 2 | 1 | 0 | -0.294233 | -1.614885 | -0.000020 |
| 3 | 7 | 0 | -2.079581 | -0.341559 | -0.000012 |
| 4 | 1 | 0 | -2.477636 | -0.787501 | -0.829790 |
| 5 | 1 | 0 | -2.358007 | 0.641764 | -0.000612 |
| 6 | 1 | 0 | -2.477505 | -0.786455 | 0.830389 |
| 7 | 6 | 0 | 0.744843 | 1.348254 | 0.000019 |
| 8 | 1 | 0 | 0.383413 | 2.382365 | 0.000039 |
| 9 | 1 | 0 | 1.832762 | 1.334436 | 0.000019 |
| 10 | 6 | 0 | 0.148097 | 0.430122 | 1.104616 |
| 11 | 1 | 0 | -0.685416 | 0.887705 | 1.656995 |
| 12 | 1 | 0 | 0.861723 | 0.003977 | 1.805976 |
| 13 | 6 | 0 | 0.148147 | 0.430139 | -1.104623 |
| 14 | 1 | 0 | 0.861815 | 0.004010 | -1.805948 |
| 15 | 1 | 0 | -0.685330 | 0.887724 | -1.657053 |
| 16 | 9 | 0 | 1.664224 | -1.178029 | 0.000012 |

**Ground State for Fluorocyclobutane:** E = -255.9329401. TC = 0.110303.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.432316 | -1.077261 | -0.106968 |
| 2 | 6 | 0 | -1.541944 | 0.000007 | -0.002426 |
| 3 | 6 | 0 | -0.432304 | 1.077257 | -0.106958 |
| 4 | 6 | 0 | 0.519325 | -0.000009 | 0.396760 |
| 5 | 1 | 0 | -0.524203 | -2.000930 | 0.470802 |
| 6 | 1 | 0 | -0.214680 | -1.309542 | -1.154827 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 1 | 0 | -2.015031 | -0.000008 | 0.983947 |
| 8 | 1 | 0 | -2.316450 | 0.000033 | -0.773060 |
| 9 | 1 | 0 | -0.524137 | 2.000946 | 0.470786 |
| 10 | 1 | 0 | -0.214743 | 1.309531 | -1.154828 |
| 11 | 1 | 0 | 0.646085 | 0.000001 | 1.485073 |
| 12 | 9 | 0 | 1.831844 | 0.000001 | -0.156705 |

**Ground State for Chlorocyclobutane:** E = -615.9327035.
TC = 0.108773.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.869804 | 1.076763 | -0.106658 |
| 2 | 6 | 0 | -1.980932 | -0.000062 | -0.046338 |
| 3 | 6 | 0 | -0.869688 | -1.076753 | -0.106640 |
| 4 | 6 | 0 | 0.065006 | 0.000051 | 0.446895 |
| 5 | 1 | 0 | -0.619019 | 1.317351 | -1.145057 |
| 6 | 1 | 0 | -0.983515 | 1.997873 | 0.472132 |
| 7 | 1 | 0 | -2.722472 | -0.000091 | -0.849716 |
| 8 | 1 | 0 | -2.493425 | -0.000110 | 0.920353 |
| 9 | 1 | 0 | -0.618812 | -1.317334 | -1.145022 |
| 10 | 1 | 0 | -0.983328 | -1.997867 | 0.472159 |
| 11 | 1 | 0 | 0.084115 | 0.000076 | 1.541671 |
| 12 | 17 | 0 | 1.780527 | 0.000006 | -0.081769 |

**Transition State for Chlorocyclobutane:** E = -672.1835728.
TC = 0.147790. Imaginary Frequency = -619.7673.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.273080 | -0.441683 | 0.000293 |
| 2 | 1 | 0 | 0.203054 | -1.517710 | 0.000660 |
| 3 | 7 | 0 | 2.409162 | -1.012322 | 0.000004 |
| 4 | 1 | 0 | 2.620607 | -1.583660 | 0.825226 |
| 5 | 1 | 0 | 3.070456 | -0.228323 | -0.000685 |
| 6 | 1 | 0 | 2.620013 | -1.584612 | -0.824711 |
| 7 | 6 | 0 | 0.221546 | 1.693810 | -0.000306 |
| 8 | 1 | 0 | 0.983427 | 2.478074 | -0.000538 |
| 9 | 1 | 0 | -0.768621 | 2.152716 | -0.000398 |
| 10 | 6 | 0 | 0.381853 | 0.602252 | -1.095970 |
| 11 | 1 | 0 | 1.368518 | 0.608350 | -1.565300 |
| 12 | 1 | 0 | -0.375479 | 0.558736 | -1.879380 |
| 13 | 17 | 0 | -2.066481 | -0.571159 | 0.000027 |
| 14 | 6 | 0 | 0.381951 | 0.602863 | 1.095961 |
| 15 | 1 | 0 | -0.375194 | 0.559771 | 1.879577 |
| 16 | 1 | 0 | 1.368673 | 0.609163 | 1.565183 |

**Transition State for 2-Fluoroazetidine:** E = -328.3698657.
TC = 0.135624. Imaginary Frequency = -210.2841

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.521692 | -0.180248 | 0.658159 |
| 2 | 1 | 0 | 0.626775 | -0.850674 | 1.507558 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 7 | 0 | 2.330087 | -1.089821 | -0.149392 |
| 4 | 1 | 0 | 3.094126 | -1.012589 | 0.529968 |
| 5 | 1 | 0 | 2.645316 | -0.635457 | -1.013004 |
| 6 | 1 | 0 | 2.205789 | -2.086415 | -0.357958 |
| 7 | 7 | 0 | 0.658818 | 1.126094 | 0.684129 |
| 8 | 6 | 0 | 0.035128 | 1.347909 | -0.635417 |
| 9 | 1 | 0 | 0.767294 | 1.615541 | -1.402716 |
| 10 | 1 | 0 | -0.787272 | 2.066237 | -0.609123 |
| 11 | 6 | 0 | -0.342589 | -0.161985 | -0.573172 |
| 12 | 1 | 0 | -0.025342 | -0.789459 | -1.407086 |
| 13 | 1 | 0 | -1.403494 | -0.331421 | -0.336170 |
| 14 | 1 | 0 | 1.150354 | 1.750101 | 1.348699 |
| 15 | 9 | 0 | -3.386807 | -0.668204 | 0.144361 |

**Ground State for 2-Fluoroazetidine:** E = -271.9534255. TC = 0.097599.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.497784 | -0.052846 | -0.116112 |
| 2 | 6 | 0 | 0.507584 | -0.029382 | 0.407645 |
| 3 | 6 | 0 | -0.454819 | 1.078672 | 0.002519 |
| 4 | 1 | 0 | -2.133450 | -0.073272 | -1.005133 |
| 5 | 1 | 0 | -2.117721 | -0.141484 | 0.783007 |
| 6 | 7 | 0 | -0.366699 | -1.027187 | -0.152077 |
| 7 | 1 | 0 | -0.475561 | -1.891624 | 0.398095 |
| 8 | 9 | 0 | 1.782350 | 0.007331 | -0.234721 |
| 9 | 1 | 0 | -0.636009 | 1.874163 | 0.727569 |
| 10 | 1 | 0 | -0.179254 | 1.500723 | -0.967078 |
| 11 | 1 | 0 | 0.737849 | -0.122836 | 1.476255 |

**Transition State for 2-Chloroazetidine:** E = -688.3991133.
TC = 0.135550. Imaginary Frequency = -222.815.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.621595 | -0.348896 | -0.209248 |
| 2 | 1 | 0 | -0.192462 | -1.304785 | -0.491194 |
| 3 | 7 | 0 | -2.515662 | -1.373757 | 0.031284 |
| 4 | 1 | 0 | -2.751408 | -1.857678 | -0.841443 |
| 5 | 1 | 0 | -3.286131 | -0.729230 | 0.238778 |
| 6 | 1 | 0 | -2.497490 | -2.078115 | 0.776871 |
| 7 | 7 | 0 | -0.778150 | 0.693396 | -0.992207 |
| 8 | 6 | 0 | -0.992051 | 1.657486 | 0.103083 |
| 9 | 1 | 0 | -2.029849 | 1.995423 | 0.173511 |
| 10 | 1 | 0 | -0.303533 | 2.504893 | 0.070377 |
| 11 | 6 | 0 | -0.609663 | 0.480284 | 1.048219 |
| 12 | 1 | 0 | -1.321388 | 0.213474 | 1.829877 |
| 13 | 1 | 0 | 0.399972 | 0.570791 | 1.454688 |
| 14 | 1 | 0 | -0.824529 | 0.774233 | -2.023435 |
| 15 | 17 | 0 | 2.894315 | -0.356455 | -0.006700 |

**Ground State for 2-Chloroazetidine:** E = -631.9589493. TC = 0.096608.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.928465 | -0.052969 | -0.145829 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 0.044035 | -0.026791 | 0.465633 |
| 3 | 6 | 0 | -0.889364 | 1.079223 | -0.021011 |
| 4 | 1 | 0 | -2.558089 | -0.075137 | -1.039156 |
| 5 | 1 | 0 | -2.552413 | -0.140579 | 0.751914 |
| 6 | 1 | 0 | 0.115417 | -0.105744 | 1.557688 |
| 7 | 1 | 0 | -0.587042 | 1.467359 | -0.996592 |
| 8 | 1 | 0 | -1.090180 | 1.898469 | 0.672190 |
| 9 | 7 | 0 | -0.795858 | -1.026945 | -0.173637 |
| 10 | 1 | 0 | -0.923793 | -1.894702 | 0.369656 |
| 11 | 17 | 0 | 1.753522 | 0.002481 | -0.111353 |

**Transition State for 3-Chloroazetidine:** E = -688.3456908.
TC = 0.135983. Imaginary Frequency = -657.535.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.436501 | 0.566985 | 1.068875 |
| 2 | 6 | 0 | -0.436263 | 0.566652 | -1.068916 |
| 3 | 1 | 0 | 0.446265 | 0.984494 | 1.557093 |
| 4 | 1 | 0 | -1.155792 | 0.253713 | 1.829946 |
| 5 | 1 | 0 | -0.573904 | 2.382722 | -0.000074 |
| 6 | 1 | 0 | 0.446581 | 0.984070 | -1.557036 |
| 7 | 1 | 0 | -1.155448 | 0.253329 | -1.830075 |
| 8 | 1 | 0 | 0.066532 | -1.520166 | 0.000281 |
| 9 | 6 | 0 | -0.100092 | -0.455786 | 0.000159 |
| 10 | 1 | 0 | -2.353387 | -1.731436 | -0.824392 |
| 11 | 1 | 0 | -2.355530 | -1.727161 | 0.826947 |
| 12 | 1 | 0 | -2.824373 | -0.370648 | -0.002858 |
| 13 | 7 | 0 | -2.161649 | -1.152034 | 0.000038 |
| 14 | 17 | 0 | 2.206222 | -0.333000 | 0.000034 |
| 15 | 7 | 0 | -1.011149 | 1.449889 | -0.000198 |

**Ground State for 3-Chloroazetidine:** E = -631.9505733. TC = 0.096661.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.074299 | 0.000019 | 0.689623 |
| 2 | 6 | 0 | 0.919019 | 1.045967 | 0.167394 |
| 3 | 6 | 0 | 0.919083 | -1.045953 | 0.167406 |
| 4 | 1 | 0 | 1.581921 | -1.375171 | 0.980330 |
| 5 | 1 | 0 | 0.516638 | -1.916892 | -0.358286 |
| 6 | 7 | 0 | 1.517350 | -0.000004 | -0.707158 |
| 7 | 1 | 0 | 2.547482 | -0.000070 | -0.721968 |
| 8 | 1 | 0 | 1.581913 | 1.375250 | 0.980266 |
| 9 | 1 | 0 | -0.320558 | 0.000076 | 1.753460 |
| 10 | 1 | 0 | 0.516673 | 1.916883 | -0.358426 |
| 11 | 17 | 0 | -1.625197 | -0.000014 | -0.204224 |

**Transition State for 2,2-Dichloroazetidine:** E = -1147.5071610.
TC = 0.125940. Imaginary Frequency = -283.5000.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.735228 | 0.023507 | 0.045427 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 7 | 0 | -2.832700 | -0.473923 | -0.200572 |
| 3 | 1 | 0 | -3.348945 | -0.060643 | 0.584687 |
| 4 | 1 | 0 | -3.024386 | -1.482557 | -0.193882 |
| 5 | 1 | 0 | -3.232102 | -0.090977 | -1.065304 |
| 6 | 7 | 0 | -0.293123 | -0.673746 | 1.063049 |
| 7 | 6 | 0 | 0.085485 | -1.832316 | 0.224937 |
| 8 | 1 | 0 | -0.614401 | -2.665381 | 0.334369 |
| 9 | 1 | 0 | 1.120201 | -2.139009 | 0.379850 |
| 10 | 6 | 0 | -0.179244 | -0.906876 | -0.995361 |
| 11 | 1 | 0 | -0.855880 | -1.253604 | -1.775597 |
| 12 | 1 | 0 | 0.755214 | -0.514284 | -1.403707 |
| 13 | 1 | 0 | -0.348377 | -0.513955 | 2.088644 |
| 14 | 17 | 0 | 3.106427 | 0.232545 | -0.078292 |
| 15 | 17 | 0 | -0.965053 | 1.711467 | 0.040856 |

**Ground State for 2,2-Dichloroazetidine:** E = -1147.5071610.
TC = 0.087497.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.009903 | -0.532327 | -0.088657 |
| 2 | 6 | 0 | -0.013643 | -0.129967 | -0.002304 |
| 3 | 6 | 0 | 0.986471 | -0.576019 | 1.066511 |
| 4 | 1 | 0 | 2.698126 | -1.375349 | -0.183493 |
| 5 | 1 | 0 | 2.557807 | 0.415891 | -0.132890 |
| 6 | 7 | 0 | 0.855865 | -0.595302 | -1.025991 |
| 7 | 1 | 0 | 0.883711 | -0.076282 | -1.919072 |
| 8 | 1 | 0 | 1.126485 | 0.088477 | 1.919846 |
| 9 | 1 | 0 | 0.780080 | -1.597077 | 1.396603 |
| 10 | 17 | 0 | -1.648594 | -0.849800 | -0.009906 |
| 11 | 17 | 0 | -0.229856 | 1.681643 | 0.024473 |

**Transition State for 2-Bromoazetidine:** E = -2801.6015183.
TC = 0.135577. Imaginary Frequency = -234.5142.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.260151 | -0.343363 | -0.139548 |
| 2 | 1 | 0 | -0.764359 | -1.288758 | -0.329768 |
| 3 | 7 | 0 | -3.105150 | -1.432158 | 0.014173 |
| 4 | 1 | 0 | -3.255978 | -1.960346 | -0.851874 |
| 5 | 1 | 0 | -3.917285 | -0.818440 | 0.141259 |
| 6 | 1 | 0 | -3.106569 | -2.105922 | 0.788006 |
| 7 | 7 | 0 | -1.399829 | 0.645735 | -0.993181 |
| 8 | 6 | 0 | -1.741919 | 1.657375 | 0.022345 |
| 9 | 1 | 0 | -2.795997 | 1.948540 | -0.005039 |
| 10 | 1 | 0 | -1.091335 | 2.534552 | -0.007423 |
| 11 | 6 | 0 | -1.383545 | 0.555634 | 1.063703 |
| 12 | 1 | 0 | -2.143412 | 0.299414 | 1.802607 |
| 13 | 1 | 0 | -0.416328 | 0.721365 | 1.542897 |
| 14 | 1 | 0 | -1.370832 | 0.665232 | -2.027433 |
| 15 | 35 | 0 | 2.191732 | -0.163101 | 0.003452 |

**Ground State for 2-Bromoazetidine:** E = -2745.1520877. TC = 0.095828.

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

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.003243 | -0.088844 | -0.726767 |
| 2 | 6 | 0 | 0.602503 | -0.005172 | 0.802886 |
| 3 | 6 | 0 | 1.473432 | 1.069644 | 0.152722 |
| 4 | 1 | 0 | 3.082957 | -0.163799 | -0.880398 |
| 5 | 1 | 0 | 1.478595 | -0.161561 | -1.687614 |
| 6 | 7 | 0 | 1.468345 | -1.005082 | 0.306840 |
| 7 | 1 | 0 | 1.122502 | -1.948087 | 0.074935 |
| 8 | 1 | 0 | 0.973144 | 1.905089 | -0.337423 |
| 9 | 1 | 0 | 2.230281 | 1.435786 | 0.853279 |
| 10 | 1 | 0 | 0.325339 | -0.013246 | 1.859274 |
| 11 | 35 | 0 | -1.256180 | 0.003646 | -0.097228 |

**Transition State for 2-Fluorooxetane:** E = -348.1976540.
TC = 0.123618. Imaginary Frequency = -383.9887.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.032642 | -0.449869 | -0.070195 |
| 2 | 1 | 0 | 0.021668 | -1.517014 | -0.227823 |
| 3 | 7 | 0 | -2.230787 | -0.717100 | 0.025956 |
| 4 | 1 | 0 | -2.519462 | -1.301053 | -0.765390 |
| 5 | 1 | 0 | -2.751996 | 0.162367 | -0.052972 |
| 6 | 1 | 0 | -2.562822 | -1.184228 | 0.876046 |
| 7 | 6 | 0 | 0.181461 | 1.549060 | -0.081764 |
| 8 | 1 | 0 | -0.700079 | 2.179067 | -0.205949 |
| 9 | 1 | 0 | 1.111000 | 2.094113 | -0.243254 |
| 10 | 6 | 0 | 0.153636 | 0.514230 | 1.058600 |
| 11 | 1 | 0 | -0.692246 | 0.567976 | 1.743208 |
| 12 | 1 | 0 | 1.094857 | 0.405461 | 1.595512 |
| 13 | 9 | 0 | 2.173251 | -1.038017 | 0.009632 |
| 14 | 8 | 0 | 0.106112 | 0.409329 | -1.053452 |

**Ground State for 2-Fluorooxetane:** E = -291.7853099. TC = 0.085128.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.762343 | -1.846015 | 0.639078 |
| 2 | 6 | 0 | -0.475259 | -1.038172 | -0.038227 |
| 3 | 1 | 0 | -0.224729 | -1.425464 | -1.032769 |
| 4 | 6 | 0 | 0.524896 | -0.000031 | 0.447465 |
| 5 | 6 | 0 | -0.475143 | 1.038176 | -0.038212 |
| 6 | 1 | 0 | 0.737516 | -0.000019 | 1.520226 |
| 7 | 1 | 0 | -0.762182 | 1.846058 | 0.639052 |
| 8 | 1 | 0 | -0.224645 | 1.425415 | -1.032777 |
| 9 | 8 | 0 | -1.508494 | 0.000051 | -0.113720 |
| 10 | 9 | 0 | 1.761930 | -0.000024 | -0.227690 |

**Transition State for 2-Chlorooxetane:** E = -708.2223341.
TC = 0.121945. Imaginary Frequency = -212.5777.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.222676 | -0.312264 | -0.042187 |
| 2 | 1 | 0 | -0.171996 | -1.386682 | -0.165099 |
| 3 | 7 | 0 | -2.730621 | -1.088905 | 0.026644 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 1 | 0 | -2.880864 | -1.671447 | -0.801567 |
| 5 | 1 | 0 | -3.405560 | -0.321627 | -0.038414 |
| 6 | 1 | 0 | -3.017605 | -1.654501 | 0.830461 |
| 7 | 6 | 0 | -0.486886 | 1.670615 | -0.111541 |
| 8 | 1 | 0 | -1.446932 | 2.159663 | -0.276712 |
| 9 | 1 | 0 | 0.363607 | 2.329218 | -0.286883 |
| 10 | 6 | 0 | -0.375544 | 0.674477 | 1.056676 |
| 11 | 1 | 0 | -1.294490 | 0.533721 | 1.628262 |
| 12 | 1 | 0 | 0.482358 | 0.791314 | 1.717067 |
| 13 | 17 | 0 | 2.354787 | -0.546819 | 0.008907 |
| 14 | 8 | 0 | -0.379363 | 0.492705 | -1.045340 |

**Ground State for 2-Chlorooxetane:** E = -651.8048500. TC = 0.084170.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.282068 | 0.000208 | 1.727947 |
| 2 | 6 | 0 | 0.030972 | 0.027268 | 0.664671 |
| 3 | 6 | 0 | -0.945477 | 1.060509 | 0.112879 |
| 4 | 6 | 0 | -1.617753 | -0.142316 | -0.556118 |
| 5 | 1 | 0 | -1.552016 | 1.504340 | 0.906719 |
| 6 | 1 | 0 | -2.680362 | -0.304355 | -0.366710 |
| 7 | 1 | 0 | -1.385786 | -0.274904 | -1.616768 |
| 8 | 8 | 0 | -0.799164 | -1.055136 | 0.265686 |
| 9 | 1 | 0 | -0.535573 | 1.838895 | -0.532254 |
| 10 | 17 | 0 | 1.615208 | 0.000243 | -0.210177 |

**Transition State for 2-Bromooxetane:** E = -2821.4222808.
TC = 0.121770. Imaginary Frequency = -189.4920.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.820581 | -0.246121 | -0.028544 |
| 2 | 1 | 0 | -0.658694 | -1.311394 | -0.136825 |
| 3 | 7 | 0 | -3.233436 | -1.280526 | 0.028508 |
| 4 | 1 | 0 | -3.346836 | -1.758676 | -0.869447 |
| 5 | 1 | 0 | -4.006536 | -0.612534 | 0.096276 |
| 6 | 1 | 0 | -3.402428 | -1.985974 | 0.751144 |
| 7 | 6 | 0 | -1.303525 | 1.694115 | -0.124491 |
| 8 | 1 | 0 | -2.314941 | 2.063253 | -0.295026 |
| 9 | 1 | 0 | -0.536734 | 2.446616 | -0.309208 |
| 10 | 6 | 0 | -1.077632 | 0.732812 | 1.057476 |
| 11 | 1 | 0 | -1.971708 | 0.496913 | 1.637721 |
| 12 | 1 | 0 | -0.235719 | 0.956042 | 1.711354 |
| 13 | 8 | 0 | -1.058078 | 0.524613 | -1.043562 |
| 14 | 35 | 0 | 1.908077 | -0.246066 | 0.003895 |

**Ground State for 2-Bromooxetane:** E = -2764.9964819. TC = 0.083643.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.367337 | -0.018720 | 1.814951 |
| 2 | 6 | 0 | -0.563321 | 0.017296 | 0.740531 |
| 3 | 6 | 0 | -1.473245 | 1.060877 | 0.111758 |
| 4 | 6 | 0 | -2.067745 | -0.135709 | -0.641726 |
| 5 | 1 | 0 | -2.162334 | 1.480463 | 0.850644 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 1 | 0 | -3.145123 | -0.299438 | -0.582051 |
| 7 | 1 | 0 | -1.705977 | -0.263491 | -1.666079 |
| 8 | 8 | 0 | -1.351868 | -1.054174 | 0.268979 |
| 9 | 1 | 0 | -1.010305 | 1.856008 | -0.473446 |
| 10 | 35 | 0 | 1.252340 | 0.000680 | -0.095978 |

**HALIDE DISPLACEMENT REACTIONS in the GAS PHASE**

**Transition State for Fluorocyclobutane:** E = -312.3154340.
TC = 0.150630. Imaginary Frequency = -563.4139.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.271634 | -0.535101 | -0.000010 |
| 2 | 1 | 0 | 0.294397 | -1.614796 | -0.000013 |
| 3 | 7 | 0 | 2.079675 | -0.341358 | -0.000007 |
| 4 | 1 | 0 | 2.477662 | -0.786421 | 0.830279 |
| 5 | 1 | 0 | 2.358053 | 0.641982 | -0.000385 |
| 6 | 1 | 0 | 2.477746 | -0.787082 | -0.829898 |
| 7 | 6 | 0 | -0.745296 | 1.347984 | 0.000012 |
| 8 | 1 | 0 | -0.384447 | 2.382297 | 0.000017 |
| 9 | 1 | 0 | -1.833202 | 1.333513 | 0.000026 |
| 10 | 6 | 0 | -0.148123 | 0.430161 | -1.104607 |
| 11 | 1 | 0 | 0.685320 | 0.888081 | -1.656810 |
| 12 | 1 | 0 | -0.861502 | 0.003905 | -1.806165 |
| 13 | 6 | 0 | -0.148093 | 0.430150 | 1.104602 |
| 14 | 1 | 0 | -0.861445 | 0.003884 | 1.806181 |
| 15 | 1 | 0 | 0.685371 | 0.888069 | 1.656775 |
| 16 | 9 | 0 | -1.664045 | -1.178122 | 0.000006 |

**Ground State for Fluorocyclobutane**: E = -312.2639963. TC = 0.151471.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.222459 | -0.019921 | -1.076229 |
| 2 | 6 | 0 | -2.103556 | -0.687039 | 0.009607 |
| 3 | 6 | 0 | -1.223448 | 0.011882 | 1.076071 |
| 4 | 6 | 0 | -0.146438 | 0.084877 | -0.000898 |
| 5 | 1 | 0 | -0.991223 | -0.569857 | -1.992053 |
| 6 | 1 | 0 | -1.597891 | 0.977174 | -1.326275 |
| 7 | 1 | 0 | -1.973569 | -1.772789 | 0.025710 |
| 8 | 1 | 0 | -3.171661 | -0.458316 | 0.005736 |
| 9 | 1 | 0 | -0.993070 | -0.510753 | 2.007958 |
| 10 | 1 | 0 | -1.599091 | 1.015926 | 1.296202 |
| 11 | 1 | 0 | 0.550650 | -0.756130 | 0.011818 |
| 12 | 1 | 0 | 3.730256 | -0.698023 | 0.830073 |
| 13 | 7 | 0 | 3.132141 | -0.635435 | 0.009183 |
| 14 | 1 | 0 | 3.729771 | -0.721937 | -0.809886 |
| 15 | 1 | 0 | 2.721387 | 0.296666 | -0.004282 |
| 16 | 9 | 0 | 0.649429 | 1.256365 | -0.017844 |

**Transition State for Chlorocyclobutane:** E = -312.3154340.
TC= 0.149864. Imaginary Frequency = -590.9614.

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

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.407182 | -0.474881 | 0.000009 |
| 2 | 1 | 0 | 0.119259 | -1.512430 | -0.000077 |
| 3 | 7 | 0 | 2.285606 | -1.001509 | 0.000003 |
| 4 | 1 | 0 | 2.482469 | -1.566485 | 0.828648 |
| 5 | 1 | 0 | 2.922330 | -0.202971 | -0.000426 |
| 6 | 1 | 0 | 2.482313 | -1.567157 | -0.828236 |
| 7 | 6 | 0 | 0.213093 | 1.655170 | -0.000008 |
| 8 | 1 | 0 | 0.931890 | 2.480378 | -0.000021 |
| 9 | 1 | 0 | -0.801255 | 2.051154 | -0.000011 |
| 10 | 6 | 0 | 0.424587 | 0.578088 | -1.102133 |
| 11 | 1 | 0 | 1.392397 | 0.664963 | -1.611619 |
| 12 | 1 | 0 | -0.360431 | 0.480403 | -1.849112 |
| 13 | 17 | 0 | -2.059839 | -0.528330 | 0.000009 |
| 14 | 6 | 0 | 0.424619 | 0.578103 | 1.102134 |
| 15 | 1 | 0 | -0.360331 | 0.480436 | 1.849188 |
| 16 | 1 | 0 | 1.392494 | 0.664999 | 1.611490 |

**Ground State for Chlorocyclobutane**: E = -672.3696321. TC = 0.150579.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.328530 | -0.234513 | 1.076271 |
| 2 | 6 | 0 | 2.119293 | -1.016779 | -0.000272 |
| 3 | 6 | 0 | 1.333818 | -0.227228 | -1.075384 |
| 4 | 6 | 0 | 0.263742 | -0.017708 | -0.001461 |
| 5 | 1 | 0 | 1.025842 | -0.745608 | 1.994351 |
| 6 | 1 | 0 | 1.832184 | 0.704634 | 1.325811 |
| 7 | 1 | 0 | 1.855250 | -2.078132 | -0.004467 |
| 8 | 1 | 0 | 3.208000 | -0.918970 | 0.002696 |
| 9 | 1 | 0 | 1.035668 | -0.731976 | -1.998447 |
| 10 | 1 | 0 | 1.838579 | 0.713637 | -1.316047 |
| 11 | 1 | 0 | -0.486952 | -0.810611 | -0.005704 |
| 12 | 17 | 0 | -0.650254 | 1.521286 | 0.001552 |
| 13 | 1 | 0 | -3.368048 | -1.651653 | -0.820842 |
| 14 | 7 | 0 | -2.848468 | -1.341384 | -0.002363 |
| 15 | 1 | 0 | -3.362304 | -1.653492 | 0.819043 |
| 16 | 1 | 0 | -2.856929 | -0.322642 | -0.001162 |

**Transition State for 2-Fluoroazetidine:** E = -328.3017640.
TC= 0.138610. Imaginary Frequency = -493.1080.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.267250 | -0.444484 | 0.032597 |
| 2 | 1 | 0 | -0.201476 | -1.520157 | 0.074124 |
| 3 | 7 | 0 | -2.182120 | -0.402333 | 0.004845 |
| 4 | 1 | 0 | -2.492441 | -0.949791 | -0.799942 |
| 5 | 1 | 0 | -2.448979 | 0.569435 | -0.159421 |
| 6 | 1 | 0 | -2.655008 | -0.748606 | 0.842878 |
| 7 | 7 | 0 | 0.052146 | 0.346407 | -1.058224 |
| 8 | 6 | 0 | 0.738557 | 1.333121 | -0.165112 |
| 9 | 1 | 0 | 0.431167 | 2.366439 | -0.347477 |
| 10 | 1 | 0 | 1.820034 | 1.211849 | -0.198430 |
| 11 | 6 | 0 | 0.123436 | 0.598968 | 1.053667 |
| 12 | 1 | 0 | -0.706434 | 1.123957 | 1.537472 |
| 13 | 1 | 0 | 0.838083 | 0.228045 | 1.784078 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 1 | 0 | 0.633814 | -0.128771 | -1.747120 |
| 15 | 9 | 0 | 1.791400 | -1.187395 | 0.095620 |

**Transition State for 2-Chloroazetidine:** E = -688.3336221. TC= 0.138156.
Imaginary Frequency = -371.9539.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.570757 | -0.362478 | 0.012156 |
| 2 | 1 | 0 | -0.142065 | -1.353648 | 0.048701 |
| 3 | 7 | 0 | -2.451013 | -1.079217 | 0.001584 |
| 4 | 1 | 0 | -2.549547 | -1.742061 | -0.769450 |
| 5 | 1 | 0 | -3.072274 | -0.290024 | -0.182442 |
| 6 | 1 | 0 | -2.749583 | -1.541930 | 0.862722 |
| 7 | 7 | 0 | -0.473686 | 0.484595 | -1.028655 |
| 8 | 6 | 0 | -0.233070 | 1.660878 | -0.151598 |
| 9 | 1 | 0 | -0.891460 | 2.508826 | -0.354016 |
| 10 | 1 | 0 | 0.821575 | 1.940384 | -0.166298 |
| 11 | 6 | 0 | -0.569401 | 0.735539 | 1.048293 |
| 12 | 1 | 0 | -1.522818 | 0.929478 | 1.545302 |
| 13 | 1 | 0 | 0.236378 | 0.620409 | 1.772323 |
| 14 | 1 | 0 | 0.107720 | 0.252705 | -1.832052 |
| 15 | 17 | 0 | 2.263196 | -0.550907 | 0.047741 |

**Transition State for 3-Chloroazetidine**:E = -688.3083976. TC = 0.138420.
Imaginary Frequency = -628.4952.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.462418 | 0.536941 | -1.067540 |
| 2 | 6 | 0 | 0.462529 | 0.536836 | 1.067582 |
| 3 | 1 | 0 | -0.463566 | 0.943652 | -1.470698 |
| 4 | 1 | 0 | 1.139362 | 0.269869 | -1.886980 |
| 5 | 1 | 0 | 0.776426 | 2.343688 | 0.000072 |
| 6 | 1 | 0 | -0.463406 | 0.943533 | 1.470869 |
| 7 | 1 | 0 | 1.139560 | 0.269683 | 1.886915 |
| 8 | 1 | 0 | -0.180590 | -1.519723 | -0.000076 |
| 9 | 6 | 0 | 0.195078 | -0.513201 | -0.000039 |
| 10 | 1 | 0 | 2.255135 | -1.705214 | 0.828598 |
| 11 | 1 | 0 | 2.255375 | -1.704881 | -0.828868 |
| 12 | 1 | 0 | 2.627010 | -0.301593 | 0.000283 |
| 13 | 7 | 0 | 2.046324 | -1.145935 | -0.000054 |
| 14 | 17 | 0 | -2.226207 | -0.265834 | 0.000013 |
| 15 | 7 | 0 | 1.102257 | 1.376895 | 0.000004 |

**Transition State for 2,2-Dichloroazetidine:** E = -1147.4735691. TC= 0.127758. Imaginary Frequency = -329.5316.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.922675 | 0.070429 | -0.117192 |
| 2 | 7 | 0 | -0.095063 | -0.356010 | 1.703946 |
| 3 | 1 | 0 | -1.039378 | -0.497714 | 1.296164 |
| 4 | 1 | 0 | -0.173847 | 0.360238 | 2.427987 |
| 5 | 1 | 0 | 0.212828 | -1.222780 | 2.146873 |
| 6 | 7 | 0 | 0.021446 | 0.728413 | -0.821952 |
| 7 | 6 | 0 | 0.450620 | 2.023735 | -0.243032 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 1 | 0 | -0.232912 | 2.357723 | 0.542880 |
| 9 | 1 | 0 | 0.595079 | 2.802252 | -0.993886 |
| 10 | 6 | 0 | 1.716094 | 1.285516 | 0.277020 |
| 11 | 1 | 0 | 1.984390 | 1.387635 | 1.327786 |
| 12 | 1 | 0 | 2.593079 | 1.433071 | -0.358951 |
| 13 | 1 | 0 | -0.989964 | 0.390864 | -0.958929 |
| 14 | 17 | 0 | -2.656470 | -0.226392 | -0.214691 |
| 15 | 17 | 0 | 1.422924 | -1.532207 | -0.438524 |

**Transition State for 2-Bromoazetidine:** E = -2801.5372993. TC= 0.138019.
Imaginary Frequency = -363.5883.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.131501 | -0.331148 | 0.034411 |
| 2 | 1 | 0 | -0.570994 | -1.252527 | 0.108113 |
| 3 | 7 | 0 | -2.892423 | -1.314619 | -0.006047 |
| 4 | 1 | 0 | -2.867616 | -1.999773 | -0.763377 |
| 5 | 1 | 0 | -3.619222 | -0.631545 | -0.225069 |
| 6 | 1 | 0 | -3.144768 | -1.801558 | 0.856478 |
| 7 | 7 | 0 | -1.115955 | 0.497104 | -1.023574 |
| 8 | 6 | 0 | -1.073557 | 1.715576 | -0.173866 |
| 9 | 1 | 0 | -1.839001 | 2.456152 | -0.416809 |
| 10 | 1 | 0 | -0.070067 | 2.145840 | -0.169868 |
| 11 | 6 | 0 | -1.312246 | 0.778580 | 1.041517 |
| 12 | 1 | 0 | -2.294634 | 0.848117 | 1.513830 |
| 13 | 1 | 0 | -0.517650 | 0.792601 | 1.787825 |
| 14 | 1 | 0 | -0.488974 | 0.327324 | -1.808669 |
| 15 | 35 | 0 | 1.845011 | -0.232573 | 0.026072 |

**Transition State for 2-Fluorooxetane:** E = -348.1414171. TC= 0.125749.
Imaginary Frequency = -484.1120.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.254337 | -0.439900 | -0.052784 |
| 2 | 1 | 0 | -0.146641 | -1.497884 | -0.239478 |
| 3 | 7 | 0 | -2.105613 | -0.431085 | 0.041681 |
| 4 | 1 | 0 | -2.452683 | -0.786956 | -0.851818 |
| 5 | 1 | 0 | -2.434450 | 0.530493 | 0.146863 |
| 6 | 1 | 0 | -2.488671 | -1.004007 | 0.797806 |
| 7 | 6 | 0 | 0.693505 | 1.329592 | -0.073573 |
| 8 | 1 | 0 | 0.331055 | 2.359258 | -0.114302 |
| 9 | 1 | 0 | 1.754550 | 1.230044 | -0.286745 |
| 10 | 6 | 0 | 0.225955 | 0.424840 | 1.083705 |
| 11 | 1 | 0 | -0.572072 | 0.868325 | 1.689930 |
| 12 | 1 | 0 | 1.004529 | -0.025935 | 1.690778 |
| 13 | 9 | 0 | 1.799801 | -1.154024 | -0.065571 |
| 14 | 8 | 0 | -0.055658 | 0.480410 | -1.034843 |

**Transition State for 2-Chlorooxetane:** E = -708.1705615. TC= 0.125208.
Imaginary Frequency = -427.4127.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.488419 | -0.373558 | -0.048842 |
| 2 | 1 | 0 | -0.099893 | -1.368197 | -0.200958 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 7 | 0 | -2.366279 | -1.044527 | 0.034679 |
| 4 | 1 | 0 | -2.537171 | -1.557835 | -0.832213 |
| 5 | 1 | 0 | -3.017551 | -0.258465 | 0.064999 |
| 6 | 1 | 0 | -2.564972 | -1.666106 | 0.821527 |
| 7 | 6 | 0 | -0.284278 | 1.621198 | -0.096424 |
| 8 | 1 | 0 | -1.036830 | 2.404945 | -0.194391 |
| 9 | 1 | 0 | 0.730110 | 1.967898 | -0.285383 |
| 10 | 6 | 0 | -0.395031 | 0.622103 | 1.072125 |
| 11 | 1 | 0 | -1.309178 | 0.727895 | 1.662132 |
| 12 | 1 | 0 | 0.482866 | 0.514880 | 1.702970 |
| 13 | 17 | 0 | 2.202315 | -0.513971 | -0.010257 |
| 14 | 8 | 0 | -0.564552 | 0.508215 | -1.046028 |

**Data for Strain Energy Calculations at the MP2(Full)/6-31+G(d) Level**

**Azetidine: See Ref 3a.**

**2-Fluoroazetidine**: E = -271.7050876. TC = 0.098725.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.500000 | -0.056775 | -0.093444 |
| 2 | 6 | 0 | 0.519075 | -0.025843 | 0.394581 |
| 3 | 6 | 0 | -0.454366 | 1.075665 | -0.014796 |
| 4 | 1 | 0 | -2.160740 | -0.088456 | -0.963240 |
| 5 | 1 | 0 | -2.099073 | -0.127816 | 0.823083 |
| 6 | 7 | 0 | -0.370131 | -1.018776 | -0.156493 |
| 7 | 1 | 0 | -0.455690 | -1.903300 | 0.342448 |
| 8 | 9 | 0 | 1.778380 | 0.004115 | -0.220916 |
| 9 | 1 | 0 | -0.623239 | 1.890322 | 0.691012 |
| 10 | 1 | 0 | -0.188623 | 1.468869 | -0.997579 |
| 11 | 1 | 0 | 0.724601 | -0.103498 | 1.469926 |

**(2-Fluoroethyl)methylether**: E = -292.7320218. TC = 0.109923.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.225185 | 0.507823 | 0.000019 |
| 2 | 1 | 0 | 1.271798 | 1.130115 | 0.895212 |
| 3 | 1 | 0 | 1.271765 | 1.130155 | -0.895147 |
| 4 | 6 | 0 | -0.005885 | -0.368881 | 0.000017 |
| 5 | 1 | 0 | -0.012980 | -1.011113 | -0.892229 |
| 6 | 1 | 0 | -0.013016 | -1.011075 | 0.892290 |
| 7 | 6 | 0 | -2.352925 | -0.190434 | -0.000000 |
| 8 | 1 | 0 | -2.444680 | -0.819774 | 0.894575 |
| 9 | 1 | 0 | -3.140786 | 0.562433 | -0.000040 |
| 10 | 1 | 0 | -2.444666 | -0.819853 | -0.894522 |
| 11 | 8 | 0 | -1.117120 | 0.513463 | -0.000023 |
| 12 | 9 | 0 | 2.361252 | -0.328850 | -0.000019 |

**3-Fluoroazetidine**: E = -271.6905037. TC = 0.098425.

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

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.571130 | -0.000012 | 0.515194 |
| 2 | 6 | 0 | 0.484450 | 1.051717 | 0.168503 |
| 3 | 6 | 0 | 0.484481 | -1.051719 | 0.168486 |
| 4 | 1 | 0 | 0.968126 | -1.445408 | 1.073944 |
| 5 | 1 | 0 | 0.150174 | -1.878364 | -0.464164 |
| 6 | 7 | 0 | 1.256166 | 0.000021 | -0.541888 |
| 7 | 1 | 0 | 2.261163 | 0.000018 | -0.371995 |
| 8 | 1 | 0 | 0.968080 | 1.445462 | 1.073944 |
| 9 | 9 | 0 | -1.628768 | -0.000008 | -0.408681 |
| 10 | 1 | 0 | -1.018663 | -0.000041 | 1.510690 |
| 11 | 1 | 0 | 0.150070 | 1.878340 | -0.464174 |

**2-Fluoropropylethylamine**. E = -351.2499643. TC = 0.183114.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.544356 | 1.036653 | 0.123405 |
| 2 | 1 | 0 | -2.321518 | 2.051938 | -0.219440 |
| 3 | 1 | 0 | -2.593954 | 1.035935 | 1.215647 |
| 4 | 1 | 0 | -3.519681 | 0.743032 | -0.271752 |
| 5 | 6 | 0 | -1.478734 | 0.081159 | -0.354503 |
| 6 | 1 | 0 | -1.425845 | 0.037396 | -1.446594 |
| 7 | 6 | 0 | -0.106742 | 0.346986 | 0.216920 |
| 8 | 1 | 0 | -0.175262 | 0.322780 | 1.321060 |
| 9 | 1 | 0 | 0.192221 | 1.359930 | -0.074227 |
| 10 | 6 | 0 | 2.180574 | -0.508199 | 0.301720 |
| 11 | 1 | 0 | 2.122381 | -0.514198 | 1.405729 |
| 12 | 1 | 0 | 2.740998 | -1.399607 | 0.001792 |
| 13 | 6 | 0 | 2.925458 | 0.733874 | -0.164436 |
| 14 | 1 | 0 | 3.949355 | 0.730426 | 0.222799 |
| 15 | 1 | 0 | 2.963551 | 0.757744 | -1.257013 |
| 16 | 1 | 0 | 2.446102 | 1.652387 | 0.185277 |
| 17 | 7 | 0 | 0.854848 | -0.610219 | -0.313111 |
| 18 | 1 | 0 | 0.483702 | -1.546687 | -0.149296 |
| 19 | 9 | 0 | -1.855909 | -1.233599 | 0.057685 |

**2,2-Difluoroazetidine**: E = -370.7563719 TC = 0.090825.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.677526 | -0.659177 | 0.873149 |
| 2 | 6 | 0 | -0.394087 | -0.046218 | -0.012743 |
| 3 | 6 | 0 | 1.663164 | 0.074312 | -0.067893 |
| 4 | 1 | 0 | 0.648172 | -0.357103 | 1.919739 |
| 5 | 1 | 0 | 0.711890 | -1.744903 | 0.775596 |
| 6 | 1 | 0 | 2.016314 | 1.021812 | 0.351975 |
| 7 | 1 | 0 | 2.502828 | -0.501907 | -0.460684 |
| 8 | 9 | 0 | -0.949474 | 1.104308 | 0.550424 |
| 9 | 7 | 0 | 0.545427 | 0.221029 | -1.039645 |
| 10 | 1 | 0 | 0.432395 | 1.088817 | -1.562176 |
| 11 | 9 | 0 | -1.473771 | -0.800688 | -0.383980 |

**1,1-Difluoro-1-propylethylamine**: E = -450.3099247. TC = 0.175364.

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

| | | | | |
|---|---|---|---|---|
| 1 | 1 | -1.471149 | 1.558344 | -0.915412 |
| 2 | 6 | -1.577471 | 0.949853 | -0.009880 |
| 3 | 1 | -1.435703 | 1.608546 | 0.852028 |
| 4 | 6 | -0.439331 | -0.041719 | 0.007993 |
| 5 | 6 | -2.948240 | 0.284406 | 0.027508 |
| 6 | 7 | 0.834552 | 0.550597 | 0.000263 |
| 7 | 9 | -0.612531 | -0.943231 | -1.068561 |
| 8 | 9 | -0.533492 | -0.856570 | 1.123483 |
| 9 | 1 | -3.730579 | 1.048562 | 0.029449 |
| 10 | 1 | -3.062811 | -0.322129 | 0.928701 |
| 11 | 1 | -3.098207 | -0.358185 | -0.842556 |
| 12 | 1 | 0.880878 | 1.258641 | -0.731507 |
| 13 | 6 | 1.984917 | -0.362296 | -0.065237 |
| 14 | 1 | 1.891800 | -1.061788 | 0.768110 |
| 15 | 6 | 3.267996 | 0.441116 | 0.061993 |
| 16 | 1 | 1.985167 | -0.947060 | -0.994512 |
| 17 | 1 | 3.278817 | 0.996897 | 1.002880 |
| 18 | 1 | 3.369013 | 1.155822 | -0.762037 |
| 19 | 1 | 4.137899 | -0.221788 | 0.034466 |

**3,3-Difluoroazetidine**: E = -370.7371284. TC = 0.090739.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.420399 | -0.014163 | -0.000015 |
| 2 | 6 | 0 | 0.661426 | -0.134160 | 1.066200 |
| 3 | 6 | 0 | 0.661587 | -0.135894 | -1.065900 |
| 4 | 1 | 0 | 0.704930 | -1.161223 | -1.453219 |
| 5 | 1 | 0 | 0.625872 | 0.586343 | -1.884297 |
| 6 | 7 | 0 | 1.653491 | 0.182446 | -0.000133 |
| 7 | 1 | 0 | 2.481842 | -0.411197 | 0.000440 |
| 8 | 9 | 0 | -1.397212 | -0.978345 | 0.000728 |
| 9 | 1 | 0 | 0.704803 | -1.158878 | 1.455139 |
| 10 | 1 | 0 | 0.625576 | 0.589426 | 1.883408 |
| 11 | 9 | 0 | -1.062026 | 1.198757 | -0.000978 |

**trans-2,3-Difluoroazetidine:** E = -370.7364727. TC = 0.091433.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.662806 | -0.258109 | 0.383393 |
| 2 | 6 | 0 | 0.670672 | -0.187921 | -0.346784 |
| 3 | 6 | 0 | -0.754259 | 1.252768 | 0.142664 |
| 4 | 1 | 0 | -0.563600 | -0.557903 | 1.427785 |
| 5 | 1 | 0 | -1.337232 | 1.455427 | -0.764000 |
| 6 | 1 | 0 | -1.090946 | 1.892179 | 0.961305 |
| 7 | 7 | 0 | 0.718829 | 1.226898 | -0.052004 |
| 8 | 1 | 0 | 1.121091 | 1.838677 | -0.760026 |
| 9 | 9 | 0 | 1.725139 | -0.916119 | 0.200364 |
| 10 | 9 | 0 | -1.646261 | -1.037529 | -0.219559 |
| 11 | 1 | 0 | 0.607337 | -0.474265 | -1.403924 |

**(*R,S*)-(1,2-Difluoropropyl)ethylamine (*anti* conformation)**: E = -450.2926588. TC = 0.175940.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.386426 | 0.568389 | 0.532854 |
| 2 | 7 | -0.949288 | 0.181412 | 0.685041 |
| 3 | 6 | 1.238230 | -0.394750 | -0.281420 |
| 4 | 1 | 0.826749 | 0.768936 | 1.513113 |
| 5 | 9 | 0.525743 | 1.823864 | -0.193803 |
| 6 | 1 | -1.444030 | 0.819110 | 1.306182 |
| 7 | 1 | 0.864002 | -0.427029 | -1.308651 |
| 8 | 6 | 2.708323 | -0.056386 | -0.247191 |
| 9 | 6 | -1.731604 | -0.122940 | -0.516098 |
| 10 | 9 | 1.064172 | -1.689188 | 0.256137 |
| 11 | 6 | -3.182749 | -0.350478 | -0.127520 |
| 12 | 1 | -1.327089 | -1.037748 | -0.958085 |
| 13 | 1 | -1.660647 | 0.680487 | -1.262836 |
| 14 | 1 | 3.074759 | -0.074905 | 0.783187 |
| 15 | 1 | 2.875592 | 0.937602 | -0.668207 |
| 16 | 1 | 3.269768 | -0.789776 | -0.830689 |
| 17 | 1 | -3.620414 | 0.555836 | 0.304840 |
| 18 | 1 | -3.257768 | -1.157390 | 0.606340 |
| 19 | 1 | -3.776887 | -0.620117 | -1.005236 |

***cis*-2,3-Difluoroazetidine**: E = -370.7296382. TC = 0.091361.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.588910 | 0.494270 | 0.527014 |
| 2 | 6 | 0 | 0.687653 | -0.360151 | 0.421727 |
| 3 | 6 | 0 | -1.322743 | -0.722433 | -0.047191 |
| 4 | 1 | 0 | -1.851262 | -1.293220 | 0.726741 |
| 5 | 1 | 0 | -1.993312 | -0.516491 | -0.885041 |
| 6 | 7 | 0 | -0.004212 | -1.273818 | -0.449574 |
| 7 | 1 | 0 | 0.171547 | -2.270078 | -0.335029 |
| 8 | 1 | 0 | 1.037951 | -0.765639 | 1.380152 |
| 9 | 9 | 0 | -0.577472 | 1.567627 | -0.356521 |
| 10 | 9 | 0 | 1.786566 | 0.256873 | -0.161260 |
| 11 | 1 | 0 | -0.873283 | 0.871539 | 1.510921 |

**(*R,S*)-1-(1,2-Difluoropropyl)ethylamine (syn conformation)**: E = -450.2945662. TC = 0.175969.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 1 | 3.348184 | 1.218187 | 0.688024 |
| 2 | 6 | 3.362982 | 0.509944 | -0.147219 |
| 3 | 1 | 3.338338 | 1.077660 | -1.080818 |
| 4 | 6 | 2.181719 | -0.441853 | -0.072961 |
| 5 | 1 | 4.305559 | -0.043050 | -0.095706 |
| 6 | 7 | 0.926277 | 0.310529 | -0.185902 |
| 7 | 1 | 2.220223 | -1.030235 | 0.853981 |
| 8 | 1 | 2.211129 | -1.145627 | -0.911504 |
| 9 | 6 | -0.246341 | -0.472631 | -0.219675 |
| 10 | 1 | 0.868510 | 1.018457 | 0.546347 |

| | | | | |
|---|---|---|---|---|
| 11 | 6 | -1.480618 | 0.365322 | -0.494048 |
| 12 | 9 | -0.466055 | -1.170729 | 1.015823 |
| 13 | 1 | -0.150374 | -1.260125 | -0.972240 |
| 14 | 1 | -1.339717 | 0.874602 | -1.452041 |
| 15 | 6 | -1.854320 | 1.329336 | 0.606166 |
| 16 | 9 | -2.556348 | -0.534621 | -0.674625 |
| 17 | 1 | -2.799289 | 1.815121 | 0.352019 |
| 18 | 1 | -1.095387 | 2.110308 | 0.716128 |
| 19 | 1 | -1.970031 | 0.798440 | 1.552762 |

***trans*-2,3-Difluoroazetidine**: E = -370.7364727. TC = 0.091433.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.662806 | -0.258109 | 0.383393 |
| 2 | 6 | 0 | 0.670672 | -0.187921 | -0.346784 |
| 3 | 6 | 0 | -0.754259 | 1.252768 | 0.142664 |
| 4 | 1 | 0 | -0.563600 | -0.557903 | 1.427785 |
| 5 | 1 | 0 | -1.337232 | 1.455427 | -0.764000 |
| 6 | 1 | 0 | -1.090946 | 1.892179 | 0.961305 |
| 7 | 7 | 0 | 0.718829 | 1.226898 | -0.052004 |
| 8 | 1 | 0 | 1.121091 | 1.838677 | -0.760026 |
| 9 | 9 | 0 | 1.725139 | -0.916119 | 0.200364 |
| 10 | 9 | 0 | -1.646261 | -1.037529 | -0.219559 |
| 11 | 1 | 0 | 0.607337 | -0.474265 | -1.403924 |

***cis*-2,3-Difluoroazetidine**: E = -370.7364727. TC = 0.091433.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.662806 | -0.258109 | 0.383393 |
| 2 | 6 | 0 | 0.670672 | -0.187921 | -0.346784 |
| 3 | 6 | 0 | -0.754259 | 1.252768 | 0.142664 |
| 4 | 1 | 0 | -0.563600 | -0.557903 | 1.427785 |
| 5 | 1 | 0 | -1.337232 | 1.455427 | -0.764000 |
| 6 | 1 | 0 | -1.090946 | 1.892179 | 0.961305 |
| 7 | 7 | 0 | 0.718829 | 1.226898 | -0.052004 |
| 8 | 1 | 0 | 1.121091 | 1.838677 | -0.760026 |
| 9 | 9 | 0 | 1.725139 | -0.916119 | 0.200364 |
| 10 | 9 | 0 | -1.646261 | -1.037529 | -0.219559 |
| 11 | 1 | 0 | 0.607337 | -0.474265 | -1.403924 |

**(*R,S*)-1-(1,2-Difluoropropyl)ethylamine (*anti* conformation)**: E = -450.2926588. TC = 0.175940.

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.386426 | 0.568389 | 0.532854 |
| 2 | 7 | -0.949288 | 0.181412 | 0.685041 |
| 3 | 6 | 1.238230 | -0.394750 | -0.281420 |
| 4 | 1 | 0.826749 | 0.768936 | 1.513113 |
| 5 | 9 | 0.525743 | 1.823864 | -0.193803 |
| 6 | 1 | -1.444030 | 0.819110 | 1.306182 |
| 7 | 1 | 0.864002 | -0.427029 | -1.308651 |
| 8 | 6 | 2.708323 | -0.056386 | -0.247191 |

| | | | | |
|---|---|---|---|---|
| 9 | 6 | -1.731604 | -0.122940 | -0.516098 |
| 10 | 9 | 1.064172 | -1.689188 | 0.256137 |
| 11 | 6 | -3.182749 | -0.350478 | -0.127520 |
| 12 | 1 | -1.327089 | -1.037748 | -0.958085 |
| 13 | 1 | -1.660647 | 0.680487 | -1.262836 |
| 14 | 1 | 3.074759 | -0.074905 | 0.783187 |
| 15 | 1 | 2.875592 | 0.937602 | -0.668207 |
| 16 | 1 | 3.269768 | -0.789776 | -0.830689 |
| 17 | 1 | -3.620414 | 0.555836 | 0.304840 |
| 18 | 1 | -3.257768 | -1.157390 | 0.606340 |
| 19 | 1 | -3.776887 | -0.620117 | -1.005236 |

***cis*-2,4-Difluoroazetidine**: E = -370.7493441. TC = 0.091230.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.039064 | -0.014168 | 0.385284 |
| 2 | 1 | 0 | -1.583285 | -0.059798 | 1.333529 |
| 3 | 6 | 0 | -0.000025 | 1.101014 | 0.238918 |
| 4 | 6 | 0 | 1.039103 | -0.014150 | 0.385317 |
| 5 | 7 | 0 | 0.000015 | -0.988138 | 0.194826 |
| 6 | 1 | 0 | -0.000044 | -1.882258 | 0.678614 |
| 7 | 1 | 0 | -0.000047 | 1.892679 | 0.989385 |
| 8 | 1 | 0 | -0.000001 | 1.519032 | -0.768998 |
| 9 | 9 | 0 | -2.025209 | -0.051620 | -0.610375 |
| 10 | 9 | 0 | 2.025187 | -0.051612 | -0.610405 |
| 11 | 1 | 0 | 1.583394 | -0.059789 | 1.333589 |

***trans*-2,4-Difluoroazetidine**: E = -370.7503172. TC = 0.091263.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.837964 | -0.043648 | -0.413122 |
| 2 | 1 | 0 | 0.833491 | -0.166844 | -1.500167 |
| 3 | 6 | 0 | 0.000646 | 1.107306 | 0.160575 |
| 4 | 6 | 0 | -1.002474 | 0.012201 | 0.529810 |
| 5 | 7 | 0 | 0.028783 | -0.965768 | 0.347851 |
| 6 | 1 | 0 | -0.196092 | -1.897351 | 0.003512 |
| 7 | 1 | 0 | -1.544861 | -0.003037 | 1.476011 |
| 8 | 9 | 0 | -2.008918 | -0.065072 | -0.477228 |
| 9 | 1 | 0 | -0.365140 | 1.867951 | -0.529417 |
| 10 | 1 | 0 | 0.494914 | 1.557498 | 1.023255 |
| 11 | 9 | 0 | 2.182184 | -0.051927 | -0.030741 |

***bis*-(1-Fluoroethyl)amine**: E = -411.1332255. TC = 0.145134.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.393419 | -0.641828 | 0.575699 |
| 2 | 1 | 0 | 2.245210 | -1.687784 | 0.854015 |
| 3 | 1 | 0 | 2.480175 | -0.036500 | 1.483053 |
| 4 | 1 | 0 | 3.320294 | -0.544553 | 0.007691 |
| 5 | 6 | 0 | 1.229567 | -0.162041 | -0.252015 |
| 6 | 1 | 0 | 1.113661 | -0.721566 | -1.183002 |
| 7 | 7 | 0 | 0.015361 | -0.179550 | 0.459044 |
| 8 | 6 | 0 | -1.202048 | 0.058912 | -0.229840 |
| 9 | 1 | 0 | -1.016923 | 0.520892 | -1.203651 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 6 | 0 | -2.191446 | 0.841387 | 0.596185 |
| 11 | 1 | 0 | -1.815095 | 1.852378 | 0.776072 |
| 12 | 1 | 0 | -3.146903 | 0.904791 | 0.072641 |
| 13 | 1 | 0 | -2.354428 | 0.335908 | 1.552730 |
| 14 | 9 | 0 | 1.546646 | 1.181539 | -0.686230 |
| 15 | 9 | 0 | -1.810556 | -1.195637 | -0.549268 |
| 16 | 1 | 0 | 0.064720 | 0.181576 | 1.406449 |

***bis*-(1-Fluoroethyl)amine** (gauche conformation): E = -411.1342946.
TC = 0.145269

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.315498 | -1.908275 | 0.311046 |
| 2 | 6 | 0 | -2.404354 | -0.896951 | -0.092076 |
| 3 | 1 | 0 | -2.441819 | -0.947637 | -1.184292 |
| 4 | 6 | 0 | -1.225437 | -0.060161 | 0.340270 |
| 5 | 1 | 0 | -3.332019 | -0.443554 | 0.262446 |
| 6 | 7 | 0 | -0.000011 | -0.583226 | -0.145586 |
| 7 | 1 | 0 | -1.157284 | 0.038751 | 1.427276 |
| 8 | 9 | 0 | -1.465395 | 1.267328 | -0.134927 |
| 9 | 6 | 0 | 1.225339 | -0.059616 | 0.340002 |
| 10 | 1 | 0 | -0.000057 | -0.723483 | -1.155070 |
| 11 | 6 | 0 | 2.404348 | -0.897124 | -0.090712 |
| 12 | 1 | 0 | 1.156752 | 0.040845 | 1.426840 |
| 13 | 9 | 0 | 1.465538 | 1.267078 | -0.137131 |
| 14 | 1 | 0 | 2.442016 | -0.949664 | -1.182833 |
| 15 | 1 | 0 | 2.315356 | -1.907773 | 0.314063 |
| 16 | 1 | 0 | 3.331966 | -0.443173 | 0.263240 |

**2-Chloroazetidine**: E = -631.7109146. TC = -631.7109146.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.930492 | -0.059882 | -0.127503 |
| 2 | 6 | 0 | 0.056325 | -0.020938 | 0.456631 |
| 3 | 6 | 0 | -0.890910 | 1.075230 | -0.035338 |
| 4 | 1 | 0 | -2.578465 | -0.095825 | -1.006683 |
| 5 | 1 | 0 | -2.539640 | -0.131346 | 0.783575 |
| 6 | 7 | 0 | -0.795390 | -1.017986 | -0.173136 |
| 7 | 1 | 0 | -0.897498 | -1.904382 | 0.322526 |
| 8 | 1 | 0 | -1.083783 | 1.909453 | 0.641213 |
| 9 | 1 | 0 | -0.595902 | 1.439887 | -1.020729 |
| 10 | 1 | 0 | 0.111055 | -0.081111 | 1.550216 |
| 11 | 17 | 0 | 1.749555 | 0.001339 | -0.107112 |

**1-(1-Chloroethyl)methylamine**: E = -632.9204556. TC = 0.121393.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.162427 | 1.546051 | -0.017768 |
| 2 | 1 | 0 | -1.330662 | 1.553630 | -1.098716 |
| 3 | 1 | 0 | -0.758577 | 2.515369 | 0.286882 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 1 | 0 | -2.122455 | 1.381314 | 0.474740 |
| 5 | 6 | 0 | -0.174345 | 0.463873 | 0.354751 |
| 6 | 1 | 0 | -0.029904 | 0.396326 | 1.434859 |
| 7 | 6 | 0 | 2.132372 | -0.287437 | 0.089314 |
| 8 | 1 | 0 | 1.902188 | -1.318878 | -0.206604 |
| 9 | 1 | 0 | 3.061566 | 0.027652 | -0.389506 |
| 10 | 1 | 0 | 2.278785 | -0.259158 | 1.172225 |
| 11 | 17 | 0 | -0.959033 | -1.175973 | -0.065285 |
| 12 | 7 | 0 | 1.078672 | 0.658893 | -0.263919 |
| 13 | 1 | 0 | 0.978323 | 0.748110 | -1.274382 |

**3-Chloroazetidine**: E = -631.7020306. TC = 0.097572.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.920702 | 1.048171 | 0.165056 |
| 2 | 6 | 0 | 0.080981 | 0.000000 | 0.676754 |
| 3 | 6 | 0 | -0.920702 | -1.048171 | 0.165056 |
| 4 | 1 | 0 | -1.564029 | 1.394587 | 0.988122 |
| 5 | 1 | 0 | -0.520200 | 1.907773 | -0.378641 |
| 6 | 1 | 0 | -1.564029 | -1.394587 | 0.988122 |
| 7 | 1 | 0 | -0.520200 | -1.907773 | -0.378641 |
| 8 | 7 | 0 | -1.526787 | 0.000000 | -0.689008 |
| 9 | 1 | 0 | -2.545462 | -0.000000 | -0.736854 |
| 10 | 17 | 0 | 1.626388 | -0.000000 | -0.202423 |
| 11 | 1 | 0 | 0.315371 | 0.000000 | 1.740937 |

**2-Chloropropylmethylamine**: E = -671.6519250. TC = 0.150376.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.772115 | 1.542676 | 0.062038 |
| 2 | 1 | 0 | -1.433346 | 2.537457 | -0.266754 |
| 3 | 1 | 0 | -1.872827 | 1.547269 | 1.156000 |
| 4 | 1 | 0 | -2.758594 | 1.348406 | -0.376305 |
| 5 | 6 | 0 | -0.754345 | 0.494849 | -0.387773 |
| 6 | 1 | 0 | -0.664610 | 0.435475 | -1.476770 |
| 7 | 6 | 0 | 0.628884 | 0.666410 | 0.235994 |
| 8 | 1 | 0 | 0.548741 | 0.589095 | 1.340877 |
| 9 | 1 | 0 | 0.970527 | 1.688045 | -0.001097 |
| 10 | 6 | 0 | 3.011333 | -0.039169 | 0.102079 |
| 11 | 1 | 0 | 3.136440 | -0.083078 | 1.201752 |
| 12 | 1 | 0 | 3.655930 | -0.797575 | -0.357377 |
| 13 | 1 | 0 | 3.338756 | 0.949366 | -0.246220 |
| 14 | 17 | 0 | -1.425557 | -1.241127 | 0.093159 |
| 15 | 7 | 0 | 1.615223 | -0.266512 | -0.343505 |
| 16 | 1 | 0 | 1.324346 | -1.238305 | -0.227300 |

**2,2-Dichloroazetidine**: E = -1090.7582015. TC = 0.088658.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.027877 | -0.127107 | -0.000756 |
| 2 | 6 | 0 | -1.998212 | -0.550786 | -0.089110 |
| 3 | 6 | 0 | -0.972789 | -0.590570 | 1.063925 |
| 4 | 1 | 0 | -2.681942 | -1.396639 | -0.187231 |
| 5 | 7 | 0 | -0.846932 | -0.607187 | -1.022753 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 1 | 0 | -0.875187 | -0.096767 | -1.905863 |
| 7 | 1 | 0 | -0.753433 | -1.610048 | 1.386104 |
| 8 | 17 | 0 | 0.200542 | 1.681283 | 0.023862 |
| 9 | 17 | 0 | 1.656409 | -0.828220 | -0.010589 |
| 10 | 1 | 0 | -1.117667 | 0.068307 | 1.919511 |
| 11 | 1 | 0 | -2.552674 | 0.394154 | -0.123245 |

**1-(1,1-Dichloroethyl)methyl amine**: E = -1091.9602822. TC = 0.112383.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.077398 | -0.327475 | 1.662891 |
| 2 | 1 | 0 | -0.027513 | -1.394477 | 1.894701 |
| 3 | 1 | 0 | -1.032567 | 0.080336 | 1.999206 |
| 4 | 1 | 0 | 0.722974 | 0.197920 | 2.185004 |
| 5 | 6 | 0 | 0.077184 | -0.149638 | 0.167582 |
| 6 | 6 | 0 | -2.273285 | -0.661416 | -0.312768 |
| 7 | 1 | 0 | -2.845724 | -1.212450 | -1.060883 |
| 8 | 1 | 0 | -2.541078 | -1.056341 | 0.668299 |
| 9 | 1 | 0 | -2.546287 | 0.400623 | -0.365067 |
| 10 | 7 | 0 | -0.854814 | -0.903528 | -0.579364 |
| 11 | 1 | 0 | -0.647915 | -0.834483 | -1.574893 |
| 12 | 17 | 0 | 1.709016 | -0.668206 | -0.339481 |
| 13 | 17 | 0 | -0.030027 | 1.666720 | -0.177993 |

***trans*-2,3-Dichloroazetidine**: E = -1090.7546304. TC = 0.089330.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.323460 | 1.394221 | 0.605126 |
| 2 | 6 | 0 | -0.527322 | -0.113378 | -0.575161 |
| 3 | 6 | 0 | 0.558525 | -0.127327 | 0.515553 |
| 4 | 1 | 0 | 1.211188 | 2.030070 | 0.623167 |
| 5 | 1 | 0 | -0.348056 | 1.649602 | 1.435083 |
| 6 | 1 | 0 | -0.407946 | -0.720180 | -1.473164 |
| 7 | 1 | 0 | 0.353559 | -0.729701 | 1.398738 |
| 8 | 7 | 0 | -0.333016 | 1.304263 | -0.716565 |
| 9 | 1 | 0 | -1.143433 | 1.887973 | -0.918438 |
| 10 | 17 | 0 | -2.126069 | -0.606378 | 0.140818 |
| 11 | 17 | 0 | 2.157706 | -0.580016 | -0.100968 |

**(*R,S*)-1-(1,2-Dichloropropyl)methylamine (*anti* conformation)**: E = -1131.1315863. TC = 0.143268.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.942905 | 0.402152 | -0.334901 |
| 2 | 1 | 0 | -0.868551 | 0.461753 | -1.424144 |
| 3 | 6 | 0 | 0.425966 | 0.015907 | 0.218158 |
| 4 | 1 | 0 | 0.374735 | -0.061665 | 1.316317 |
| 5 | 6 | 0 | 2.089177 | -1.754720 | 0.259899 |
| 6 | 1 | 0 | 1.895360 | -1.966704 | 1.323302 |
| 7 | 1 | 0 | 2.346265 | -2.686992 | -0.246548 |
| 8 | 1 | 0 | 2.944114 | -1.080049 | 0.188728 |
| 9 | 6 | 0 | -1.523676 | 1.673913 | 0.252804 |
| 10 | 1 | 0 | -0.913282 | 2.533590 | -0.028298 |
| 11 | 1 | 0 | -2.537784 | 1.826277 | -0.122988 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 1 | 0 | -1.566107 | 1.610559 | 1.344150 |
| 13 | 17 | 0 | -2.078263 | -0.957406 | 0.016240 |
| 14 | 17 | 0 | 1.562891 | 1.385200 | -0.089693 |
| 15 | 7 | 0 | 0.943330 | -1.156504 | -0.422650 |
| 16 | 1 | 0 | 0.191900 | -1.837254 | -0.519028 |

***cis*-2,3-Dichloroazetidine**: E = -1090.7544565. TC = 0.089393.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.046990 | 1.547087 | -0.650329 |
| 2 | 6 | 0 | 0.780944 | 0.189574 | 0.719136 |
| 3 | 6 | 0 | -0.667467 | 0.638144 | 0.419646 |
| 4 | 1 | 0 | -0.444755 | 2.559972 | -0.748227 |
| 5 | 1 | 0 | -0.007261 | 1.050732 | -1.627122 |
| 6 | 1 | 0 | 1.080904 | 0.004806 | 1.751096 |
| 7 | 7 | 0 | 1.204998 | 1.445095 | 0.138220 |
| 8 | 1 | 0 | 2.094506 | 1.451648 | -0.361209 |
| 9 | 17 | 0 | 1.280631 | -1.274848 | -0.205834 |
| 10 | 17 | 0 | -1.898854 | -0.527967 | -0.039821 |
| 11 | 1 | 0 | -1.047517 | 1.216202 | 1.263333 |

**1-(1,2-Dichloropropyl)methylamine** (gauche conformation): E = -1131.1383529. TC = 0.143502.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.855054 | 0.988952 | 1.045343 |
| 2 | 1 | 0 | -1.910604 | 1.682327 | 0.205006 |
| 3 | 1 | 0 | -1.450950 | 1.520179 | 1.914091 |
| 4 | 1 | 0 | -2.864223 | 0.647120 | 1.286972 |
| 5 | 6 | 0 | -0.971151 | -0.198414 | 0.721487 |
| 6 | 1 | 0 | -0.998928 | -0.928296 | 1.535665 |
| 7 | 6 | 0 | 0.503359 | 0.142262 | 0.543100 |
| 8 | 1 | 0 | 0.848124 | 0.635682 | 1.457128 |
| 9 | 6 | 0 | 2.733490 | -0.808008 | 0.321755 |
| 10 | 1 | 0 | 3.029125 | -0.381376 | 1.284050 |
| 11 | 1 | 0 | 3.217487 | -1.780694 | 0.215796 |
| 12 | 1 | 0 | 3.078859 | -0.142109 | -0.479153 |
| 13 | 7 | 0 | 1.287113 | -1.007393 | 0.318606 |
| 14 | 1 | 0 | 0.974443 | -1.504844 | -0.514511 |
| 15 | 17 | 0 | 0.701128 | 1.449672 | -0.750695 |
| 16 | 17 | 0 | -1.606833 | -1.064083 | -0.715505 |

**2-Bromoazetidine**: E = -2742.1397124. TC = 0.097317.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.564173 | 0.018872 | 0.789113 |
| 2 | 6 | 0 | -1.997777 | -0.108718 | -0.713373 |
| 3 | 6 | 0 | -1.467181 | 1.069403 | 0.136281 |
| 4 | 1 | 0 | -3.077983 | -0.193984 | -0.854600 |
| 5 | 7 | 0 | -1.450507 | -1.005873 | 0.330170 |
| 6 | 1 | 0 | -1.069368 | -1.916247 | 0.075835 |
| 7 | 1 | 0 | -2.216662 | 1.437553 | 0.842037 |
| 8 | 1 | 0 | -0.983733 | 1.900088 | -0.376732 |
| 9 | 1 | 0 | -1.482806 | -0.187926 | -1.678603 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 35 | 0 | 1.242275 | 0.002418 | -0.098355 |
| 11 | 1 | 0 | -0.320735 | 0.039651 | 1.851173 |

**1-Bromoethylmethylamine**:E = -2743.3478932. TC =0.121035.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.368443 | 2.090944 | -0.032759 |
| 2 | 1 | 0 | 0.188822 | 2.153097 | -1.109786 |
| 3 | 1 | 0 | 1.253897 | 2.683876 | 0.217592 |
| 4 | 1 | 0 | -0.501340 | 2.502504 | 0.481938 |
| 5 | 6 | 0 | 0.609226 | 0.657758 | 0.378330 |
| 6 | 1 | 0 | 0.690174 | 0.521727 | 1.457664 |
| 7 | 6 | 0 | 2.057573 | -1.279350 | 0.081156 |
| 8 | 1 | 0 | 1.274058 | -1.991756 | -0.207308 |
| 9 | 1 | 0 | 2.995489 | -1.545548 | -0.409915 |
| 10 | 1 | 0 | 2.204340 | -1.339346 | 1.162396 |
| 11 | 7 | 0 | 1.714365 | 0.093989 | -0.268346 |
| 12 | 1 | 0 | 1.667515 | 0.230895 | -1.277111 |
| 13 | 35 | 0 | -1.142427 | -0.362557 | -0.028497 |

**2,2-Dibromoazetidine** : E = -5311.6130424. TC = 0.087847.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.012613 | 0.490929 | -0.008706 |
| 2 | 6 | 0 | 1.134295 | 2.219430 | -0.083450 |
| 3 | 6 | 0 | 0.386471 | 1.508311 | 1.068393 |
| 4 | 1 | 0 | 1.018927 | 3.302163 | -0.169689 |
| 5 | 7 | 0 | 0.272342 | 1.453560 | -1.019063 |
| 6 | 1 | 0 | 0.627925 | 1.133473 | -1.919974 |
| 7 | 1 | 0 | -0.490229 | 2.071111 | 1.395870 |
| 8 | 1 | 0 | 0.958815 | 1.139352 | 1.918462 |
| 9 | 1 | 0 | 2.192704 | 1.937905 | -0.128838 |
| 10 | 35 | 0 | -1.766656 | -0.276774 | -0.002779 |
| 11 | 35 | 0 | 1.326233 | -1.010967 | 0.007927 |

**2,2-Dibromoethylmethylamine**: E = -5312.8192635. TC = 0.111391.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.006674 | -0.302599 | 2.050451 |
| 2 | 1 | 0 | -0.899988 | -0.001435 | 2.582547 |
| 3 | 1 | 0 | 0.889480 | 0.087393 | 2.567869 |
| 4 | 1 | 0 | 0.071957 | -1.390681 | 2.021794 |
| 5 | 6 | 0 | -0.044548 | 0.258534 | 0.648186 |
| 6 | 6 | 0 | -0.134983 | 2.362235 | -0.636088 |
| 7 | 1 | 0 | -1.039621 | 2.108558 | -1.188880 |
| 8 | 1 | 0 | -0.144982 | 3.432568 | -0.422810 |
| 9 | 1 | 0 | 0.744193 | 2.115342 | -1.243834 |
| 10 | 35 | 0 | 1.608645 | -0.443144 | -0.324565 |
| 11 | 35 | 0 | -1.556132 | -0.524487 | -0.317447 |
| 12 | 7 | 0 | -0.137606 | 1.651851 | 0.640678 |
| 13 | 1 | 0 | 0.541386 | 2.043378 | 1.293718 |

**Oxetane**: See Ref 10.

**2-Fluorooxetane**: E = -291.5512313. TC = 0.085852.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.981555 | -0.059945 | 1.484204 |
| 2 | 6 | 0 | 0.531501 | 0.003565 | 0.491728 |
| 3 | 6 | 0 | -0.499274 | 1.064702 | 0.132785 |
| 4 | 6 | 0 | -1.322768 | -0.126200 | -0.377657 |
| 5 | 1 | 0 | -0.932128 | 1.562507 | 1.002763 |
| 6 | 1 | 0 | -2.315600 | -0.270123 | 0.052428 |
| 7 | 1 | 0 | -1.353567 | -0.246674 | -1.463529 |
| 8 | 8 | 0 | -0.359817 | -1.054310 | 0.224170 |
| 9 | 1 | 0 | -0.164853 | 1.799893 | -0.600138 |
| 10 | 9 | 0 | 1.600708 | -0.000398 | -0.416692 |

**1-(1-Fluoroethyl)methylether**: E = -331.9322372. TC = 0.139560.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.366064 | 0.379227 | 0.284390 |
| 2 | 1 | 0 | 1.348172 | 0.480786 | 1.378644 |
| 3 | 1 | 0 | 1.272172 | 1.374961 | -0.159837 |
| 4 | 8 | 0 | 0.248043 | -0.429510 | -0.126184 |
| 5 | 6 | 0 | -0.972660 | 0.026701 | 0.330267 |
| 6 | 1 | 0 | -0.939302 | 0.244467 | 1.406477 |
| 7 | 6 | 0 | -2.045818 | -0.946817 | -0.061416 |
| 8 | 1 | 0 | -3.022680 | -0.567559 | 0.246059 |
| 9 | 1 | 0 | -2.030548 | -1.073836 | -1.145722 |
| 10 | 1 | 0 | -1.863629 | -1.911482 | 0.417646 |
| 11 | 9 | 0 | -1.263492 | 1.281538 | -0.271872 |
| 12 | 6 | 0 | 2.621014 | -0.320082 | -0.183649 |
| 13 | 1 | 0 | 3.503530 | 0.259123 | 0.105097 |
| 14 | 1 | 0 | 2.694355 | -1.315121 | 0.261543 |
| 15 | 1 | 0 | 2.613405 | -0.423279 | -1.271129 |

**3-Fluorooxetane**: E = -291.5352287. TC = 0.085622.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.478760 | -1.032895 | -0.051312 |
| 2 | 6 | 0 | 0.528865 | -0.000109 | 0.434709 |
| 3 | 6 | 0 | -0.478605 | 1.032902 | -0.051244 |
| 4 | 1 | 0 | 0.716708 | -0.000181 | 1.509985 |
| 5 | 1 | 0 | -0.754158 | 1.858165 | 0.609091 |
| 6 | 1 | 0 | -0.237592 | 1.399007 | -1.056070 |
| 7 | 8 | 0 | -1.509353 | 0.000114 | -0.086719 |
| 8 | 1 | 0 | -0.238009 | -1.399239 | -1.056094 |
| 9 | 1 | 0 | -0.754533 | -1.857917 | 0.609223 |
| 10 | 9 | 0 | 1.768157 | -0.000015 | -0.212811 |

**1-(2-Fluoropropyl)methylether**: E = -331.9119233. TC = 0.139508.

| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.997503 | 0.043515 | -0.334970 |
| 2 | 1 | 0 | -0.928522 | 0.191015 | -1.417037 |
| 3 | 6 | 0 | 0.309592 | -0.495243 | 0.187862 |
| 4 | 1 | 0 | 0.329094 | -0.382352 | 1.282914 |
| 5 | 1 | 0 | 0.390986 | -1.567859 | -0.053798 |
| 6 | 6 | 0 | 2.629250 | -0.130664 | 0.141179 |
| 7 | 1 | 0 | 2.834806 | -1.200411 | -0.002280 |
| 8 | 1 | 0 | 3.379860 | 0.457754 | -0.386289 |
| 9 | 1 | 0 | 2.666670 | 0.102054 | 1.213533 |
| 10 | 8 | 0 | 1.369936 | 0.226770 | -0.411533 |
| 11 | 6 | 0 | -2.186078 | -0.808876 | 0.045922 |
| 12 | 1 | 0 | -3.110036 | -0.319763 | -0.270185 |
| 13 | 1 | 0 | -2.126607 | -1.788124 | -0.438641 |
| 14 | 1 | 0 | -2.221935 | -0.951920 | 1.129734 |
| 15 | 9 | 0 | -1.189486 | 1.332561 | 0.221595 |

**2,2-Difluorooxetane:** E = -390.1332569. TC = 0.076872.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.714377 | 0.000116 | -0.117647 |
| 2 | 6 | 0 | 0.392327 | -0.000059 | 0.013180 |
| 3 | 6 | 0 | -0.713572 | -0.000421 | 1.077717 |
| 4 | 1 | 0 | -2.309368 | 0.904436 | -0.255072 |
| 5 | 1 | 0 | -2.310231 | -0.903598 | -0.255293 |
| 6 | 1 | 0 | -0.719129 | -0.899131 | 1.699926 |
| 7 | 1 | 0 | -0.719030 | 0.897583 | 1.700940 |
| 8 | 9 | 0 | 1.246422 | 1.123146 | 0.002820 |
| 9 | 9 | 0 | 1.247284 | -1.122536 | 0.002653 |
| 10 | 8 | 0 | -0.521483 | -0.000324 | -1.097407 |

**(2,2-Difluoropropyl)methylether**: E = -430.9567805. TC = 0.131754.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.874425 | -0.001911 | 0.000001 |
| 2 | 6 | 0 | 0.493810 | 0.641252 | 0.000081 |
| 3 | 1 | 0 | 0.575208 | 1.278831 | -0.894003 |
| 4 | 1 | 0 | 0.575187 | 1.278586 | 0.894337 |
| 5 | 6 | 0 | 2.786742 | 0.186335 | -0.000003 |
| 6 | 1 | 0 | 2.955504 | 0.799235 | 0.895515 |
| 7 | 1 | 0 | 3.476788 | -0.656856 | -0.000197 |
| 8 | 1 | 0 | 2.955403 | 0.799565 | -0.895314 |
| 9 | 8 | 0 | 1.476266 | -0.365869 | -0.000040 |
| 10 | 6 | 0 | -2.027950 | 0.963935 | -0.000085 |
| 11 | 1 | 0 | -2.957723 | 0.391820 | -0.000158 |
| 12 | 1 | 0 | -1.992847 | 1.592316 | 0.892483 |
| 13 | 1 | 0 | -1.992695 | 1.592305 | -0.892654 |
| 14 | 9 | 0 | -0.981826 | -0.827052 | -1.106321 |
| 15 | 9 | 0 | -0.981954 | -0.827005 | 1.106359 |

***trans*-2,3-Difluorooxetane**: E = -390.5786256. TC = 0.078442.

| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.651452 | -0.281364 | 0.407548 |
| 2 | 6 | 0 | 0.644671 | -0.255319 | -0.390093 |
| 3 | 6 | 0 | -0.624617 | 1.237485 | 0.267886 |
| 4 | 1 | 0 | -0.556117 | -0.692253 | 1.413775 |
| 5 | 1 | 0 | 0.629586 | -0.665754 | -1.402998 |
| 6 | 1 | 0 | -1.372362 | 1.618631 | -0.431439 |
| 7 | 1 | 0 | -0.601489 | 1.830611 | 1.184319 |
| 8 | 8 | 0 | 0.700896 | 1.161005 | -0.350334 |
| 9 | 9 | 0 | 1.722868 | -0.819133 | 0.272239 |
| 10 | 9 | 0 | -1.713801 | -0.912432 | -0.235910 |

**1,2-Difluoropropylmethylether** (*anti* conformation): E = -430.958648.
TC = 0.132462.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.558864 | -0.292410 | 0.182206 |
| 2 | 1 | 0 | 2.534035 | -0.552277 | 1.246536 |
| 3 | 1 | 0 | 2.890147 | 0.741072 | 0.055396 |
| 4 | 1 | 0 | 3.229741 | -0.967008 | -0.346803 |
| 5 | 6 | 0 | 0.267502 | 0.223835 | 0.210192 |
| 6 | 6 | 0 | -1.071435 | -0.229812 | -0.333059 |
| 7 | 1 | 0 | -1.006621 | -0.287790 | -1.423489 |
| 8 | 6 | 0 | -2.232858 | 0.609808 | 0.135633 |
| 9 | 1 | 0 | -2.143745 | 1.628669 | -0.247275 |
| 10 | 1 | 0 | -3.165509 | 0.172681 | -0.228068 |
| 11 | 1 | 0 | -2.264625 | 0.642257 | 1.228280 |
| 12 | 8 | 0 | 1.264867 | -0.485599 | -0.406542 |
| 13 | 1 | 0 | 0.316653 | 0.150150 | 1.305410 |
| 14 | 9 | 0 | 0.402287 | 1.604804 | -0.083605 |
| 15 | 9 | 0 | -1.251338 | -1.550526 | 0.138329 |

**1,2-Difluoropropylmethylether (*gauche* conformation)**: E = -430.9558637.
TC = 0.132518.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.594768 | 0.053668 | -0.194148 |
| 2 | 1 | 0 | 2.742523 | -0.619921 | -1.047196 |
| 3 | 1 | 0 | 2.760126 | -0.487094 | 0.739977 |
| 4 | 1 | 0 | 3.280235 | 0.896457 | -0.265160 |
| 5 | 6 | 0 | 0.280516 | -0.324997 | -0.287306 |
| 6 | 6 | 0 | -1.060429 | 0.367301 | -0.407198 |
| 7 | 6 | 0 | -2.221149 | -0.596794 | -0.457071 |
| 8 | 1 | 0 | -2.239808 | -1.206299 | 0.448322 |
| 9 | 1 | 0 | -3.156767 | -0.038431 | -0.531150 |
| 10 | 1 | 0 | -2.138622 | -1.254148 | -1.328582 |
| 11 | 8 | 0 | 1.276905 | 0.618501 | -0.224351 |
| 12 | 1 | 0 | 0.438926 | -1.032855 | -1.116134 |
| 13 | 1 | 0 | -1.025660 | 1.016554 | -1.288729 |
| 14 | 9 | 0 | -1.220694 | 1.208064 | 0.706878 |
| 15 | 9 | 0 | 0.283091 | -1.121102 | 0.877323 |

***cis*-2,3-Difluorooxetane**: E = -390.5778789. TC = 0.078673.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.705144 | 0.329797 | 0.446055 |
| 2 | 6 | 0 | 0.612079 | -0.440629 | 0.520043 |
| 3 | 6 | 0 | 0.069860 | 1.292501 | -0.448374 |
| 4 | 1 | 0 | -1.005002 | 0.758283 | 1.405004 |
| 5 | 1 | 0 | -0.051548 | 1.083426 | -1.513898 |
| 6 | 1 | 0 | 0.021421 | 2.361799 | -0.238123 |
| 7 | 8 | 0 | 1.310422 | 0.700661 | 0.075085 |
| 8 | 9 | 0 | -1.791459 | -0.323982 | -0.107606 |
| 9 | 9 | 0 | 0.645188 | -1.459141 | -0.426858 |
| 10 | 1 | 0 | 1.007416 | -0.850708 | 1.450168 |

**2-Chlorooxetane**: E = -651.5542897. TC = 0.084732.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.280254 | -0.016087 | 1.723053 |
| 2 | 6 | 0 | 0.035896 | 0.018445 | 0.661364 |
| 3 | 6 | 0 | -0.939376 | 1.062698 | 0.120055 |
| 4 | 6 | 0 | -1.602382 | -0.139087 | -0.562618 |
| 5 | 1 | 0 | -1.553878 | 1.494899 | 0.913354 |
| 6 | 1 | 0 | -2.670145 | -0.296982 | -0.401102 |
| 7 | 1 | 0 | -1.349958 | -0.264211 | -1.619499 |
| 8 | 8 | 0 | -0.810664 | -1.050896 | 0.267827 |
| 9 | 1 | 0 | -0.524309 | 1.849382 | -0.510306 |
| 10 | 17 | 0 | 1.608148 | -0.000716 | -0.209466 |

**Chloromethylmethyl ether**: E = -652.7572662. TC = 0.108162.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.072639 | -0.307326 | 0.072507 |
| 2 | 1 | 0 | -2.237771 | -0.212388 | 1.152612 |
| 3 | 1 | 0 | -2.967389 | -0.000999 | -0.467310 |
| 4 | 1 | 0 | -1.822355 | -1.342995 | -0.173305 |
| 5 | 8 | 0 | -1.034358 | 0.578957 | -0.354471 |
| 6 | 6 | 0 | 0.158200 | 0.440135 | 0.341376 |
| 7 | 1 | 0 | -0.023900 | 0.383741 | 1.421398 |
| 8 | 6 | 0 | 1.062658 | 1.583746 | -0.036221 |
| 9 | 1 | 0 | 2.020281 | 1.503784 | 0.482233 |
| 10 | 1 | 0 | 1.236814 | 1.573482 | -1.114018 |
| 11 | 1 | 0 | 0.577993 | 2.523996 | 0.239878 |
| 12 | 17 | 0 | 0.976581 | -1.138800 | -0.057158 |

**2,2-Dichlorooxetane**: E = -1110.5986336. TC = 0.075569.

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

| | | | | | |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 2.580032 | -1.369262 | -0.319056 |
| 2 | 6 | 0 | 1.994189 | -0.466033 | -0.144256 |
| 3 | 1 | 0 | 2.607357 | 0.430402 | -0.265862 |
| 4 | 6 | 0 | 1.051208 | -0.445358 | 1.062726 |
| 5 | 6 | 0 | -0.004018 | -0.075315 | 0.020561 |
| 6 | 1 | 0 | 0.871844 | -1.436841 | 1.481215 |
| 7 | 1 | 0 | 1.232122 | 0.282803 | 1.853137 |
| 8 | 17 | 0 | -0.392108 | 1.671835 | 0.005018 |
| 9 | 17 | 0 | -1.505428 | -1.002812 | -0.002786 |
| 10 | 8 | 0 | 0.839810 | -0.420032 | -1.052695 |

**1-(1,1-Dichloroethyl)ethyl ether:** E = -1150.9795942. TC = 0.129352.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.291147 | 0.116665 | 1.662837 |
| 2 | 6 | 0 | -0.528652 | 0.019994 | 0.364111 |
| 3 | 1 | 0 | -2.362292 | 0.193504 | 1.471771 |
| 4 | 1 | 0 | -0.950081 | 1.002399 | 2.202739 |
| 5 | 1 | 0 | -1.086620 | -0.776754 | 2.256355 |
| 6 | 8 | 0 | 0.804150 | -0.059065 | 0.661438 |
| 7 | 17 | 0 | -0.893246 | 1.479715 | -0.648293 |
| 8 | 17 | 0 | -1.094604 | -1.428102 | -0.559953 |
| 9 | 6 | 0 | 1.744219 | -0.239170 | -0.423501 |
| 10 | 6 | 0 | 3.113831 | 0.044414 | 0.145134 |
| 11 | 1 | 0 | 1.491398 | 0.450852 | -1.233641 |
| 12 | 1 | 0 | 1.659285 | -1.266691 | -0.788427 |
| 13 | 1 | 0 | 3.872934 | -0.112479 | -0.627511 |
| 14 | 1 | 0 | 3.178423 | 1.077551 | 0.493890 |
| 15 | 1 | 0 | 3.327695 | -0.624700 | 0.982011 |

**3-Chlorooxetane**: E = -651.5467881. TC = 0.084693.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.070290 | 0.000000 | 0.494089 |
| 2 | 6 | 0 | -0.907472 | -1.029135 | -0.068498 |
| 3 | 6 | 0 | -0.907472 | 1.029135 | -0.068498 |
| 4 | 1 | 0 | 0.101710 | 0.000000 | 1.583992 |
| 5 | 1 | 0 | -1.202159 | -1.870811 | 0.562519 |
| 6 | 1 | 0 | -0.634035 | -1.370963 | -1.073813 |
| 7 | 1 | 0 | -1.202161 | 1.870812 | 0.562518 |
| 8 | 1 | 0 | -0.634036 | 1.370964 | -1.073813 |
| 9 | 8 | 0 | -1.938861 | -0.000001 | -0.121545 |
| 10 | 17 | 0 | 1.738206 | 0.000000 | -0.101859 |

**1-(2-Chloropropyl)methyl Ether**: E = 691.9223035. E = 0.138569.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.839393 | -0.082649 | 0.156550 |
| 2 | 1 | 0 | 2.816051 | -0.374370 | 1.214720 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 1 | 0 | 3.232146 | 0.939935 | 0.073035 |
| 4 | 1 | 0 | 3.483576 | -0.766163 | -0.396280 |
| 5 | 6 | 0 | 0.616643 | 0.674054 | 0.206062 |
| 6 | 1 | 0 | 0.885762 | 1.727599 | 0.021254 |
| 7 | 1 | 0 | 0.606013 | 0.504638 | 1.294143 |
| 8 | 6 | 0 | -0.756425 | 0.416166 | -0.372953 |
| 9 | 1 | 0 | -0.676496 | 0.406186 | -1.463148 |
| 10 | 6 | 0 | -1.769068 | 1.448750 | 0.088239 |
| 11 | 1 | 0 | -1.467206 | 2.443935 | -0.254847 |
| 12 | 1 | 0 | -2.758266 | 1.227636 | -0.318244 |
| 13 | 1 | 0 | -1.843370 | 1.460155 | 1.179694 |
| 14 | 8 | 0 | 1.546763 | -0.184326 | -0.425141 |
| 15 | 17 | 0 | -1.307975 | -1.225463 | 0.093142 |

***cis*-2,3-Dichlorooxetane:** E = -1110.5948458. TC = 0.076378.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.684406 | 0.603529 | 0.431669 |
| 2 | 6 | 0 | -0.787095 | 0.227757 | 0.674565 |
| 3 | 6 | 0 | 0.116799 | 1.557145 | -0.614817 |
| 4 | 1 | 0 | 1.068287 | 1.141504 | 1.300254 |
| 5 | 1 | 0 | -1.156968 | 0.148929 | 1.696876 |
| 6 | 1 | 0 | 0.469184 | 2.589884 | -0.622653 |
| 7 | 1 | 0 | 0.087400 | 1.135705 | -1.623953 |
| 8 | 8 | 0 | -1.187923 | 1.439142 | 0.042339 |
| 9 | 17 | 0 | 1.876420 | -0.598686 | -0.040038 |
| 10 | 17 | 0 | -1.349901 | -1.216593 | -0.197476 |

**1,2-Dichloropropylmethylether (*gauche* conformation):** E = -1150.9712794. TC = 0.130198.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.647437 | -0.851449 | 0.329311 |
| 2 | 1 | 0 | 2.925021 | -0.464425 | 1.317412 |
| 3 | 1 | 0 | 3.019099 | -0.180743 | -0.449772 |
| 4 | 1 | 0 | 3.059900 | -1.849564 | 0.191355 |
| 5 | 6 | 0 | 0.512768 | 0.145065 | 0.521674 |
| 6 | 6 | 0 | -0.949788 | -0.227933 | 0.704395 |
| 7 | 6 | 0 | -1.819400 | 0.939254 | 1.131709 |
| 8 | 1 | 0 | -1.885068 | 1.689689 | 0.341901 |
| 9 | 1 | 0 | -2.827116 | 0.585873 | 1.361011 |
| 10 | 1 | 0 | -1.402799 | 1.406923 | 2.030631 |
| 11 | 8 | 0 | 1.227323 | -1.002382 | 0.231395 |
| 12 | 17 | 0 | 0.729704 | 1.416275 | -0.747012 |
| 13 | 1 | 0 | 0.873382 | 0.613534 | 1.448702 |
| 14 | 17 | 0 | -1.610676 | -0.993129 | -0.764141 |
| 15 | 1 | 0 | -0.950571 | -1.005341 | 1.474676 |

***trans*-2,3-Dichlorooxetane:** E = -1110.5960168. TC = 0.076265.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.631924 | 0.120636 | 0.444304 |
| 2 | 6 | 0 | 0.610798 | 0.120719 | -0.439389 |
| 3 | 6 | 0 | -0.620285 | 1.630740 | 0.208094 |
| 4 | 1 | 0 | -0.399534 | -0.152184 | 1.474035 |
| 5 | 1 | 0 | 0.428851 | -0.140259 | -1.486118 |
| 6 | 1 | 0 | -1.285665 | 1.950698 | -0.599761 |
| 7 | 1 | 0 | -0.708572 | 2.287118 | 1.075842 |
| 8 | 17 | 0 | -2.027048 | -0.815957 | -0.091322 |
| 9 | 17 | 0 | 2.008948 | -0.799532 | 0.108060 |
| 10 | 8 | 0 | 0.765137 | 1.535670 | -0.253323 |

**(*R,S*)-1,2-Dichloropropylmethylether (*anti* conformation):**
E = -1150.9733875. TC = 0.130316.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.866952 | -1.881394 | 0.221937 |
| 2 | 1 | 0 | 1.546702 | -2.150382 | 1.234952 |
| 3 | 1 | 0 | 2.787861 | -1.292092 | 0.262743 |
| 4 | 1 | 0 | 2.027122 | -2.782382 | -0.367875 |
| 5 | 6 | 0 | 0.429491 | -0.011056 | 0.207277 |
| 6 | 6 | 0 | -0.915370 | 0.419958 | -0.355233 |
| 7 | 1 | 0 | -0.832409 | 0.445238 | -1.445071 |
| 8 | 6 | 0 | -1.436842 | 1.734373 | 0.194888 |
| 9 | 1 | 0 | -0.802723 | 2.562383 | -0.126215 |
| 10 | 1 | 0 | -2.451378 | 1.907041 | -0.170295 |
| 11 | 1 | 0 | -1.465677 | 1.712692 | 1.288455 |
| 12 | 8 | 0 | 0.830424 | -1.156501 | -0.447959 |
| 13 | 17 | 0 | -2.082414 | -0.885881 | 0.039987 |
| 14 | 17 | 0 | 1.641561 | 1.323098 | -0.040009 |
| 15 | 1 | 0 | 0.376229 | -0.154476 | 1.294136 |

**2-Bromooxetane:** E = -2761.9781931. TC =0.084235.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.367717 | -0.030547 | 1.809403 |
| 2 | 6 | 0 | -0.553273 | 0.010652 | 0.736609 |
| 3 | 6 | 0 | -1.464609 | 1.063180 | 0.117589 |
| 4 | 6 | 0 | -2.048287 | -0.133499 | -0.646550 |
| 5 | 1 | 0 | -2.161787 | 1.472366 | 0.853664 |
| 6 | 1 | 0 | -3.127303 | -0.293058 | -0.615243 |
| 7 | 1 | 0 | -1.665832 | -0.254788 | -1.664042 |
| 8 | 8 | 0 | -1.360108 | -1.050258 | 0.270631 |
| 9 | 1 | 0 | -0.997947 | 1.864806 | -0.454206 |
| 10 | 35 | 0 | 1.245670 | 0.000037 | -0.095443 |

**Bromomethylethyl ether**: E = -2802.3601564. TC = 0.137950.

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

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.868331 | -0.545643 | 0.291540 |
| 2 | 1 | 0 | 1.375134 | -1.449433 | -0.082372 |
| 3 | 1 | 0 | 1.818347 | -0.552306 | 1.389311 |
| 4 | 8 | 0 | 1.154946 | 0.601013 | -0.200147 |
| 5 | 6 | 0 | -0.065129 | 0.835323 | 0.401455 |
| 6 | 6 | 0 | -0.603338 | 2.144602 | -0.110368 |
| 7 | 1 | 0 | -1.578802 | 2.360494 | 0.330426 |
| 8 | 1 | 0 | 0.099610 | 2.940207 | 0.155459 |
| 9 | 1 | 0 | -0.700397 | 2.101248 | -1.196780 |
| 10 | 6 | 0 | 3.293175 | -0.438543 | -0.197561 |
| 11 | 1 | 0 | 3.866469 | -1.311022 | 0.131034 |
| 12 | 1 | 0 | 3.316736 | -0.399151 | -1.289158 |
| 13 | 1 | 0 | 3.770187 | 0.461971 | 0.196297 |
| 14 | 1 | 0 | -0.001607 | 0.774743 | 1.494033 |
| 15 | 35 | 0 | -1.376100 | -0.620266 | -0.052499 |

**2,2-Dibromooxetane**: E = -5331.4490599. TC = 0.074698.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.007839 | 0.463112 | 0.012411 |
| 2 | 6 | 0 | 0.265466 | 1.533260 | 1.065536 |
| 3 | 6 | 0 | 0.774059 | 2.338350 | -0.137838 |
| 4 | 1 | 0 | -0.666225 | 1.931021 | 1.472186 |
| 5 | 1 | 0 | 0.352860 | 3.330281 | -0.306192 |
| 6 | 1 | 0 | 1.859665 | 2.339440 | -0.263425 |
| 7 | 8 | 0 | 0.161130 | 1.359806 | -1.054115 |
| 8 | 1 | 0 | 0.966696 | 1.283678 | 1.861199 |
| 9 | 35 | 0 | 1.426253 | -0.900883 | 0.001179 |
| 10 | 35 | 0 | -1.714431 | -0.406866 | -0.000365 |

**1,1-Dibromoethylmethyl ether**: E = -5332.6572202. TC = 0.098365.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000021 | -0.196147 | 2.063978 |
| 2 | 6 | 0 | 0.000001 | 0.275164 | 0.632977 |
| 3 | 1 | 0 | 0.000039 | -1.285965 | 2.102996 |
| 4 | 1 | 0 | -0.894165 | 0.192081 | 2.558325 |
| 5 | 1 | 0 | 0.894204 | 0.192107 | 2.558309 |
| 6 | 8 | 0 | -0.000031 | 1.633283 | 0.617314 |
| 7 | 6 | 0 | -0.000102 | 2.303548 | -0.655593 |
| 8 | 1 | 0 | -0.898432 | 2.038713 | -1.216637 |
| 9 | 1 | 0 | 0.897928 | 2.038371 | -1.216957 |
| 10 | 1 | 0 | 0.000149 | 3.363942 | -0.410497 |
| 11 | 35 | 0 | 1.581863 | -0.484270 | -0.308037 |
| 12 | 35 | 0 | -1.581835 | -0.484327 | -0.308026 |

**Thietane**: See Ref. 10.

**2-Fluorothietane**: E = -614.1629452. TC = 0.083390.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.201028 | -0.336200 | 1.445620 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | 0.748129 | -0.074422 | 0.488297 |
| 3 | 6 | 0 | 0.097698 | 1.296219 | 0.321255 |
| 4 | 6 | 0 | -1.137078 | 0.787573 | -0.444028 |
| 5 | 1 | 0 | -0.178181 | 1.712916 | 1.294162 |
| 6 | 1 | 0 | -2.099873 | 1.165195 | -0.095870 |
| 7 | 1 | 0 | -1.061698 | 0.907515 | -1.526166 |
| 8 | 1 | 0 | 0.733389 | 2.010780 | -0.209672 |
| 9 | 9 | 0 | 1.749088 | -0.271220 | -0.482981 |
| 10 | 16 | 0 | -0.786809 | -0.942215 | 0.077850 |

**1-(1-Fluoroethylmethyl) sulfide**: E = -714.4040618. TC = 0.098174.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.072288 | -0.444174 | -0.000007 |
| 2 | 1 | 0 | -3.058722 | 0.023990 | 0.000073 |
| 3 | 1 | 0 | -1.968858 | -1.057342 | 0.895375 |
| 4 | 1 | 0 | -1.968954 | -1.057245 | -0.895466 |
| 5 | 6 | 0 | 0.633022 | -0.074458 | 0.000000 |
| 6 | 6 | 0 | 1.881208 | 0.760604 | -0.000024 |
| 7 | 1 | 0 | 1.910847 | 1.387119 | 0.892949 |
| 8 | 1 | 0 | 2.739276 | 0.085094 | -0.000024 |
| 9 | 1 | 0 | 1.910828 | 1.387097 | -0.893013 |
| 10 | 16 | 0 | -0.869018 | 0.905884 | 0.000004 |
| 11 | 9 | 0 | 0.649356 | -0.928578 | 1.095114 |
| 12 | 9 | 0 | 0.649335 | -0.928609 | -1.095088 |

**2,2-Difluorothietane** : E = -713.2081387. TC = 0.075616.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.580767 | 0.670092 | 0.029254 |
| 2 | 6 | 0 | -0.590225 | 0.058915 | -0.010320 |
| 3 | 6 | 0 | 0.209624 | 1.337769 | -0.197929 |
| 4 | 1 | 0 | 2.028932 | 0.906645 | 0.994784 |
| 5 | 1 | 0 | 2.305755 | 0.832918 | -0.768701 |
| 6 | 1 | 0 | 0.086583 | 1.714238 | -1.215826 |
| 7 | 1 | 0 | -0.061041 | 2.115692 | 0.520197 |
| 8 | 9 | 0 | -1.308965 | 0.034049 | 1.162303 |
| 9 | 9 | 0 | -1.502221 | -0.211155 | -0.996597 |
| 10 | 16 | 0 | 0.858715 | -1.023512 | 0.003260 |

**1-(1,1-Difluoroethyl)methyl Sulfide**: E = -714.4040618. TC = 0.098174.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.072288 | -0.444174 | -0.000007 |
| 2 | 1 | 0 | -3.058722 | 0.023990 | 0.000073 |
| 3 | 1 | 0 | -1.968858 | -1.057342 | 0.895375 |
| 4 | 1 | 0 | -1.968954 | -1.057245 | -0.895466 |
| 5 | 6 | 0 | 0.633022 | -0.074458 | 0.000000 |
| 6 | 6 | 0 | 1.881208 | 0.760604 | -0.000024 |
| 7 | 1 | 0 | 1.910847 | 1.387119 | 0.892949 |
| 8 | 1 | 0 | 2.739276 | 0.085094 | -0.000024 |
| 9 | 1 | 0 | 1.910828 | 1.387097 | -0.893013 |
| 10 | 16 | 0 | -0.869018 | 0.905884 | 0.000004 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 9 | 0 | 0.649356 | -0.928578 | 1.095114 |
| 12 | 9 | 0 | 0.649335 | -0.928609 | -1.095088 |

**2-Chlorothietane**: E = -974.1705009. TC = 0.082420.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 0.555984 | -0.143730 | 1.726866 |
| 2 | 6 | 0 | 0.292116 | 0.036779 | 0.685402 |
| 3 | 6 | 0 | -0.485382 | 1.321223 | 0.368532 |
| 4 | 6 | 0 | -1.440125 | 0.665011 | -0.639084 |
| 5 | 1 | 0 | -1.028711 | 1.644917 | 1.261510 |
| 6 | 1 | 0 | -2.489655 | 0.956431 | -0.570869 |
| 7 | 1 | 0 | -1.097667 | 0.745606 | -1.672909 |
| 8 | 1 | 0 | 0.121494 | 2.151408 | -0.003788 |
| 9 | 16 | 0 | -1.071979 | -0.995685 | 0.058423 |
| 10 | 17 | 0 | 1.817092 | -0.091868 | -0.244982 |

(**1-Chloromethyl)methylsulfide**: E = -975.3659112. TC = 0.105066.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.067301 | -0.706049 | 0.310846 |
| 2 | 1 | 0 | 2.069195 | -0.698448 | 1.403851 |
| 3 | 1 | 0 | 1.672687 | -1.655820 | -0.053780 |
| 4 | 1 | 0 | 3.095153 | -0.590058 | -0.039692 |
| 5 | 6 | 0 | -0.470790 | 0.350179 | 0.416114 |
| 6 | 1 | 0 | -0.332250 | 0.221575 | 1.492586 |
| 7 | 6 | 0 | -1.424161 | 1.496270 | 0.133308 |
| 8 | 1 | 0 | -1.577114 | 1.615150 | -0.942332 |
| 9 | 1 | 0 | -2.392016 | 1.301013 | 0.600664 |
| 10 | 1 | 0 | -1.015432 | 2.425906 | 0.539414 |
| 11 | 16 | 0 | 1.121376 | 0.681182 | -0.351303 |
| 12 | 17 | 0 | -1.205667 | -1.197684 | -0.149498 |

**2,2-Dichlorothietane**: E = -1433.2110926. TC = 0.073389.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.996561 | 0.050017 | 0.579344 |
| 2 | 6 | 0 | -0.201241 | -0.035726 | 0.103313 |
| 3 | 6 | 0 | 0.681442 | -0.112699 | 1.354125 |
| 4 | 1 | 0 | 2.822070 | -0.584467 | 0.905543 |
| 5 | 1 | 0 | 2.324084 | 1.088575 | 0.501695 |
| 6 | 1 | 0 | 0.458371 | 0.633046 | 2.122130 |
| 7 | 1 | 0 | 0.610073 | -1.116156 | 1.780752 |
| 8 | 17 | 0 | -1.600975 | -1.117004 | 0.073689 |
| 9 | 16 | 0 | 1.193044 | -0.517241 | -0.973085 |
| 10 | 17 | 0 | -0.761606 | 1.637317 | -0.189068 |

**(1,1-Dichloroethyl)methylsulfide**: E = -1434.4053269. TC = 0.096018.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.293719 | 0.000095 | 1.540298 |
| 2 | 1 | 0 | 2.342296 | 0.000249 | 1.235865 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 1 | 0 | 1.096565 | 0.892810 | 2.138874 |
| 4 | 1 | 0 | 1.096804 | -0.892736 | 2.138779 |
| 5 | 6 | 0 | 0.401821 | 0.000044 | 0.311109 |
| 6 | 6 | 0 | -2.192179 | -0.000090 | -0.712327 |
| 7 | 1 | 0 | -1.960106 | -0.895680 | -1.290700 |
| 8 | 1 | 0 | -3.256910 | -0.000523 | -0.467426 |
| 9 | 1 | 0 | -1.960704 | 0.895989 | -1.290182 |
| 10 | 16 | 0 | -1.314593 | -0.000246 | 0.862275 |
| 11 | 17 | 0 | 0.784204 | -1.449912 | -0.679370 |
| 12 | 17 | 0 | 0.783758 | 1.450120 | -0.679224 |

2-Bromothietane: E = -3084.5977579. TC = 0.081953.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.090031 | -0.109450 | 1.833843 |
| 2 | 6 | 0 | -0.295227 | 0.060571 | 0.777991 |
| 3 | 6 | 0 | -1.060102 | 1.325722 | 0.378984 |
| 4 | 6 | 0 | -1.882656 | 0.637797 | -0.721017 |
| 5 | 1 | 0 | -1.706868 | 1.628685 | 1.209007 |
| 6 | 1 | 0 | -2.938200 | 0.908456 | -0.782573 |
| 7 | 1 | 0 | -1.418446 | 0.707248 | -1.707321 |
| 8 | 1 | 0 | -0.444943 | 2.175329 | 0.070930 |
| 9 | 16 | 0 | -1.563464 | -1.005394 | 0.043274 |
| 10 | 35 | 0 | 1.458338 | -0.039100 | -0.112343 |

**(1-Bromomethyl)methylsulfide: E** = -3085.7927512. TC = 0.104581.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.973441 | -1.371386 | 0.306240 |
| 2 | 1 | 0 | 1.917821 | -1.364079 | 1.397765 |
| 3 | 1 | 0 | 1.235711 | -2.067637 | -0.095714 |
| 4 | 1 | 0 | 2.973599 | -1.694462 | 0.009018 |
| 5 | 6 | 0 | 0.199319 | 0.723417 | 0.458085 |
| 6 | 1 | 0 | 0.288285 | 0.574145 | 1.536375 |
| 7 | 6 | 0 | -0.176561 | 2.150320 | 0.108899 |
| 8 | 1 | 0 | -0.311889 | 2.253986 | -0.970384 |
| 9 | 1 | 0 | -1.107825 | 2.431074 | 0.605767 |
| 10 | 1 | 0 | 0.617783 | 2.829407 | 0.435438 |
| 11 | 16 | 0 | 1.729221 | 0.286547 | -0.362714 |
| 12 | 35 | 0 | -1.293092 | -0.473180 | -0.067262 |

**2,2-Dibromothietane**: E = -5654.0680955. TC = 0.072571.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.624686 | 1.816538 | 0.575520 |
| 2 | 6 | 0 | -0.050367 | 0.301707 | 0.117553 |
| 3 | 6 | 0 | -0.546857 | 1.046953 | 1.355829 |
| 4 | 1 | 0 | -1.763385 | 2.863050 | 0.852421 |
| 5 | 1 | 0 | -2.583854 | 1.295041 | 0.547610 |
| 6 | 1 | 0 | -0.879425 | 0.413207 | 2.182123 |
| 7 | 1 | 0 | 0.233243 | 1.731729 | 1.699632 |
| 8 | 16 | 0 | -0.696409 | 1.576318 | -0.996839 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 35 | 0 | 1.848965 | -0.037197 | 0.017913 |
| 10 | 35 | 0 | -1.007039 | -1.406098 | -0.064364 |

**(1,1-Dibromoethyl)methylsulfide**: E = -5655.2647866. TC = 0.095268.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.104009 | -0.423752 | 2.046370 |
| 2 | 1 | 0 | -0.238645 | -1.506965 | 2.052868 |
| 3 | 1 | 0 | 0.817771 | -0.171686 | 2.578104 |
| 4 | 1 | 0 | -0.957373 | 0.045719 | 2.544889 |
| 5 | 6 | 0 | -0.016356 | 0.079741 | 0.618400 |
| 6 | 6 | 0 | 0.431920 | 2.196296 | -1.123668 |
| 7 | 1 | 0 | -0.305103 | 1.655666 | -1.721088 |
| 8 | 1 | 0 | 0.278849 | 3.269847 | -1.257277 |
| 9 | 1 | 0 | 1.441317 | 1.930655 | -1.438819 |
| 10 | 16 | 0 | 0.179993 | 1.856147 | 0.629956 |
| 11 | 35 | 0 | 1.479545 | -0.826491 | -0.285067 |
| 12 | 35 | 0 | -1.644860 | -0.488803 | -0.345921 |