

**Photodissociation of acryloyl chloride at 193 nm:
interpretation of the product energy distributions, and new
elimination pathways**

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--List of minima--

The structures are optimized at the B3LYP/6-311+G(2d,2p) level of theory. ZPE is given in kcal/mol and is calculated at this level.

The energy (in a.u.) is a CCSD(T)/6-311+G(3df,2p) single point calculation at the B3LYP/6-311+G(2d,2p) optimized geometry.

MIN1 (AC)

E= -650.7373049500 ZPE= 33.0702000000

C 1.319980 0.437682 0.000000
C 1.938009 -0.738991 0.000000
C -0.136787 0.651983 0.000000
H 1.389897 -1.669097 0.000001
H 3.017623 -0.790371 0.000000
O -0.670651 1.710857 0.000000
Cl -1.155374 -0.864706 0.000000
H 1.871843 1.368569 -0.000001

MIN2

E= -650.7369877500 ZPE= 33.0434800000

C -1.057610 -0.686338 -0.000459
C -2.344877 -0.349211 0.000337
C -0.015460 0.359227 -0.000229
H -3.117575 -1.104706 0.000308
H -2.649819 0.688097 0.001126
O -0.160103 1.534895 -0.000150
Cl 1.663672 -0.358328 0.000170
H -0.726523 -1.713035 -0.001023

MIN3

E= -650.7223013700 ZPE= 32.8982100000

C 0.534225 0.476981 0.000000
C -1.883271 0.323971 0.000000
C -0.550810 -0.293666 0.000000
H -0.497355 -1.373321 -0.000001
H -1.895319 1.431099 -0.000002
O -2.915528 -0.307427 0.000001
Cl 2.154684 -0.129315 0.000000
H 0.486399 1.556269 0.000001

MIN4

E= -650.7215610200 ZPE= 32.7601100000

C 0.592619 1.768284 -0.000158
C 0.109902 0.528121 0.000083
C -1.354048 0.284138 0.000321
H -1.944830 1.219568 0.001003
H 1.650270 1.981116 -0.000459
O -1.880793 -0.796979 -0.000322
Cl 1.137966 -0.877121 0.000049
H -0.095359 2.602937 -0.000294

MIN5

E= -650.7204656300 ZPE= 32.6485600000

C -0.002153 0.303686 0.000045
C -0.225522 1.611724 0.000103
C -1.096251 -0.712856 0.000393
H 0.573377 2.336480 -0.000080
H -1.250287 1.955640 0.000598
O -2.264834 -0.419419 -0.000416
Cl 1.617493 -0.375838 -0.000108

H -0.758245 -1.762845 0.001399
 MIN6 (CH₂ClCHCO)
 E= -650.7202205100 ZPE= 33.0592600000
 C -0.527899 0.709010 0.473072
 C 0.654611 0.674668 -0.419118
 C 1.742782 -0.000208 -0.117832
 H 0.634976 1.158927 -1.384941
 H -0.300508 0.391089 1.483488
 O 2.709141 -0.576696 0.157158
 Cl -1.896556 -0.407612 -0.086272
 H -0.983108 1.692143 0.494096
 MIN7
 E= -650.7198832200 ZPE= 32.8527800000
 C -0.522334 0.697316 -0.000159
 C 0.361613 -0.297442 0.000142
 C -1.973121 0.412355 0.000164
 H -2.619604 1.309106 0.000750
 H 0.063395 -1.334682 0.000504
 O -2.462357 -0.695283 -0.000177
 Cl 2.074451 -0.059843 -0.000015
 H -0.207547 1.731801 -0.000461
 MIN8
 E= -650.7200710100 ZPE= 32.9865500000
 C -0.634919 0.844499 0.000010
 C 0.694964 0.919603 0.000000
 C -1.433938 -0.389314 0.000021
 H -1.195829 1.770541 0.000006
 H 1.224972 1.859245 -0.000009
 O -2.645601 -0.380193 -0.000021
 Cl 1.779618 -0.441086 -0.000005
 H -0.874483 -1.338507 0.000071
 MIN9
 E= -650.7171836500 ZPE= 32.7272700000
 C -0.680548 1.092814 0.003326
 C 0.819193 1.031156 -0.004018
 C -1.480627 0.053071 0.000159
 H 1.235563 1.497920 -0.893228
 H 1.243217 1.507049 0.876652
 O -2.218808 -0.841968 -0.001684
 Cl 1.440220 -0.670269 0.001294
 H -1.160157 2.063102 0.011255
 MIN10
 E= -650.7153961200 ZPE= 32.9386000000
 C 0.590377 1.008053 -0.000007
 C -1.728472 0.002915 0.000011
 C -0.741822 1.098906 -0.000004
 H -2.779690 0.348826 0.000045
 H -1.152302 2.101559 -0.000006
 O -1.475032 -1.179948 -0.000012
 Cl 1.517608 -0.444727 0.000004
 H 1.212407 1.890323 -0.000013
 MIN11
 E= -650.7123210000 ZPE= 32.8445200000
 C -0.006273 0.350847 -0.000087
 C 0.291118 1.817895 0.000022
 C -1.208484 -0.174283 -0.000007

H 0.863561 2.098142 0.885488
H 0.865374 2.097784 -0.884380
O -2.279270 -0.630374 0.000020
Cl 1.334288 -0.794746 0.000011
H -0.635833 2.391003 -0.001029
MIN12
E= -650.6841216600 ZPE= 32.4889300000
C -0.802257 1.263819 -0.260954
C 0.132909 0.330643 0.568440
C -1.171495 -0.126418 0.057840
H 0.230419 0.564523 1.619359
H -0.533009 1.461935 -1.291884
O -1.934240 -1.030103 -0.089440
Cl 1.650712 -0.276234 -0.121795
H -1.240530 2.102084 0.266609
MIN13
E= -650.6804362600 ZPE= 32.9309900000
C -0.537567 0.459350 0.039717
C 0.677349 0.702716 -0.332352
C -1.761690 0.233057 0.440698
H -2.142758 0.629683 1.372283
H 0.990814 1.547667 -0.926959
O -2.711156 -0.494270 -0.215295
Cl 2.053597 -0.337978 0.083509
H -2.338505 -0.848309 -1.030992
MIN14
E= -650.6798528800 ZPE= 32.9670300000
C -0.687336 -0.752544 0.309087
C 0.518976 -0.480877 -0.070504
C 1.738414 -0.206253 -0.454224
H 2.093806 -0.452745 -1.445023
H 2.333692 0.757887 1.101340
O 2.683685 0.482349 0.243337
Cl -2.016966 0.358862 -0.068165
H -1.028868 -1.626544 0.849641
MIN15
E= -650.6782857300 ZPE= 32.2263200000
C -2.439822 -0.444838 0.002451
C -1.207694 -0.028571 0.022638
C 0.026396 0.376684 0.007102
H 1.228999 1.797650 0.435951
H -2.980324 -0.665459 0.916425
O 0.411830 1.677302 -0.061243
Cl 1.362365 -0.787411 -0.007405
H -2.976790 -0.584272 -0.929699
MIN16
E= -650.6786497400 ZPE= 32.6315000000
C 1.263925 -0.184059 0.127014
C 2.330435 -0.669464 -0.122636
C -0.009537 0.449123 0.427417
H 0.084300 1.652078 -1.076175
H 3.272158 -1.107831 -0.342043
O -0.175798 1.692283 -0.148429
Cl -1.370131 -0.718782 -0.086997
H -0.166786 0.563188 1.493846
MIN17

E= -650.6798454500 ZPE= 33.4726000000
C 0.013641 0.048553 0.558213
C 1.022733 1.028971 0.032962
C 1.749034 -0.028979 -0.325351
H 2.712408 -0.266117 -0.747449
H 1.106584 2.098022 0.017366
O 0.872604 -1.039056 0.067069
Cl -1.611792 0.013303 -0.178419
H -0.111804 -0.036879 1.631709

MIN18

E= -650.6769409700 ZPE= 32.7309400000
C 0.521619 0.436575 0.057430
C -0.697926 0.732848 -0.251979
C 1.746363 0.174534 0.428457
H 3.485511 -0.549261 0.089393
H -1.014269 1.649848 -0.725609
O 2.650273 -0.461752 -0.377403
Cl -2.070116 -0.348984 0.049326
H 2.098208 0.462415 1.413457

MIN19

E= -650.6765638100 ZPE= 32.5460000000
C 0.000118 0.448931 0.399438
C 2.367090 -0.614939 -0.112640
C 1.291327 -0.133456 0.096267
H -0.984349 2.054823 0.011561
H 3.318476 -1.042828 -0.308939
O -0.157609 1.647528 -0.269959
Cl -1.345642 -0.760993 -0.077315
H -0.148557 0.541443 1.473010

MIN20

E= -650.6756208000 ZPE= 33.7465900000
C 0.062298 0.048536 0.000114
C -1.024655 -0.994040 0.000016
C -0.881481 0.988878 0.000038
H -1.140803 -1.590982 0.901352
H -1.140701 -1.591088 -0.901267
O -1.983517 0.133739 -0.000077
Cl 1.776538 -0.012265 -0.000027
H -0.988485 2.060425 -0.000023

MIN21

E= -650.6735161400 ZPE= 32.7371300000
C -1.106047 -0.002494 0.093056
C -2.173984 -0.751610 -0.058156
C 0.193993 0.356647 0.557750
H -3.000163 -0.424168 -0.670819
H -2.225444 -1.712650 0.427892
O -0.602995 1.208114 -0.310166
Cl 1.657841 -0.347052 -0.139695
H 0.382506 0.756521 1.543173

MIN22

E= -650.6687069100 ZPE= 33.1444600000
C 0.415258 0.787701 -0.000025
C -0.787785 0.258440 -0.000002
C -2.221758 0.290186 0.000017
H -2.760675 0.457300 0.923656
H 0.573099 1.851534 0.000018

O -1.394694 -0.947074 -0.000014
C1 1.863031 -0.188680 0.000007
H -2.760684 0.457348 -0.923616
MIN23
E= -650.6679592100 ZPE= 32.8771800000
C 0.587665 0.442926 0.000205
C -0.775261 0.908670 0.014380
C 1.719667 0.048386 -0.004464
H -1.004255 1.479446 0.908979
H -1.007179 1.506121 -0.862005
O 2.955710 -0.367072 -0.104006
C1 -2.008287 -0.462515 -0.002382
H 3.314203 -0.586134 0.764840
MIN24
E= -650.6674710800 ZPE= 33.0760200000
C 0.000000 0.782629 0.000000
C 0.821918 -0.242318 0.000000
C -1.261916 1.455942 0.000000
H 1.893737 -0.140930 0.000000
H -1.814589 1.570073 0.923510
O 0.062714 2.137855 0.000000
C1 0.227865 -1.887034 0.000000
H -1.814589 1.570073 -0.923510
MIN25
E= -650.6653877400 ZPE= 33.0533400000
C -0.690379 0.127136 -0.000001
C 0.495779 0.301083 -0.000001
C 1.931924 0.548673 0.000000
H 2.192204 1.139916 0.884335
H 3.576312 -0.509066 0.000006
O 2.633277 -0.696864 -0.000001
C1 -2.320640 -0.121012 0.000000
H 2.192206 1.139918 -0.884332
MIN26
E= -650.6610903200 ZPE= 32.0290500000
C -1.328510 -0.638737 0.665832
C -1.348460 -0.620484 -0.639344
C -0.332671 0.191297 -0.002712
H 0.232847 1.942438 0.577696
H -1.786043 -0.949753 -1.564627
O -0.376621 1.575472 -0.071771
C1 1.433040 -0.364058 -0.010227
H -1.737673 -0.999936 1.592308
MIN27
E= -650.6613287600 ZPE= 32.8139800000
C -0.720437 1.298281 -0.249806
C -1.133606 0.099098 0.027137
C 0.157521 0.443803 0.582663
H 0.380460 0.610582 1.628940
H -1.783621 -1.639439 0.348852
O -2.055512 -0.844338 -0.123980
C1 1.696360 -0.324207 -0.141561
H -0.811725 2.247985 -0.739374
MIN28
E= -650.6604370300 ZPE= 32.8580800000
C 0.174279 0.434504 0.579806

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C -0.710199 1.276638 -0.263890
C -1.119939 0.081837 0.049534
H -2.715839 -0.696253 -0.592456
H -0.802568 2.214437 -0.776425
O -1.990051 -0.918954 0.003657
Cl 1.704447 -0.326369 -0.145564
H 0.398364 0.623843 1.621506
MIN29
E= -650.6573883700 ZPE= 31.8155700000
C -1.300549 -0.670824 -0.654323
C -1.300626 -0.670671 0.654321
C -0.301045 0.166845 -0.000031
H -1.223970 1.859260 0.001008
H -1.720773 -1.036135 1.575537
O -0.305826 1.568014 -0.000216
Cl 1.442662 -0.310755 0.000052
H -1.720583 -1.036495 -1.575506
MIN30
E= -650.6557739800 ZPE= 32.6785400000
C 0.183664 0.324381 0.081016
C -0.637139 1.288880 -0.196608
C -1.206208 0.061640 0.479762
H -0.840149 2.255010 -0.621995
H -1.750395 -0.916485 -1.112489
O -2.037178 -0.847833 -0.195609
Cl 1.786338 -0.275962 -0.023665
H -1.521684 0.086088 1.516647
MIN31
E= -650.6546405900 ZPE= 32.4565700000
C 0.199355 0.326389 0.088034
C -0.621114 1.295663 -0.159687
C -1.198622 0.062038 0.463855
H -1.521182 0.056932 1.502984
H -0.840010 2.262989 -0.572240
O -2.006331 -0.754246 -0.359506
Cl 1.790112 -0.286618 -0.032614
H -2.297779 -1.517996 0.146515
MIN32
E= -650.6530018300 ZPE= 32.6124100000
C 0.557568 0.841794 0.383434
C -2.455225 -0.711336 0.130307
C -1.557993 0.043180 -0.106989
H -3.245457 -1.388227 0.331184
H 1.108353 1.747856 0.170931
O -0.616863 0.902171 -0.399781
Cl 1.616935 -0.549826 -0.069382
H 0.318015 0.728223 1.435115
MIN33
E= -650.6501646500 ZPE= 32.3112200000
C 2.957800 0.115639 -0.000191
C -0.361783 0.569718 0.000040
C 1.799141 -0.187358 0.000114
H 3.987682 0.365203 0.000321
H -0.220456 1.158791 -0.900675
O 0.544309 -0.545371 0.000029
Cl -2.016008 -0.076927 -0.000027

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H -0.220516 1.158729 0.900804
 MIN34
 E= -650.6496604000 ZPE= 32.5351800000
 C 2.432301 -0.706200 0.146073
 C -0.534991 0.887862 0.409747
 C 1.546306 0.050878 -0.122913
 H -0.262411 0.856281 1.454137
 H -1.118367 1.750306 0.127303
 O 0.580898 0.867228 -0.440042
 Cl -1.596790 -0.562470 -0.061236
 H 3.217325 -1.377657 0.382463
 MIN35
 E= -650.6497081700 ZPE= 33.1521700000
 C -1.083433 -0.049319 -0.000333
 C -0.758943 1.412457 0.000204
 C 0.175101 0.219166 -0.000594
 H -0.893392 1.990719 0.914149
 H -0.893752 1.991666 -0.913063
 O -2.139825 -0.864629 0.000117
 Cl 1.808802 -0.281011 0.000102
 H -1.840235 -1.781989 0.000589
 MIN36
 E= -650.6462679400 ZPE= 32.8425500000
 C -0.552572 -0.224134 -0.000001
 C 0.563937 0.511690 -0.000001
 C -1.795494 0.526766 0.000000
 H -3.624692 0.150955 -0.000004
 H -0.520940 -1.310749 -0.000005
 O -2.798270 -0.345286 0.000002
 Cl 2.158962 -0.150250 0.000000
 H 0.534215 1.590405 0.000001
 MIN37
 E= -650.6454331000 ZPE= 32.3246500000
 C 0.186802 0.595006 0.000000
 C 1.019990 1.633253 0.000002
 C -1.260052 0.783246 0.000000
 H 0.589324 2.623715 0.000003
 H 2.093786 1.522753 0.000003
 O -1.946665 -0.315328 0.000002
 Cl 0.857976 -1.092306 -0.000002
 H -1.375808 -1.123678 0.000002
 MIN38
 E= -650.6456615800 ZPE= 32.7652500000
 C 0.000000 0.583459 0.000000
 C -0.380749 1.864372 0.000000
 C 1.426121 0.288971 0.000000
 H 0.386886 2.623714 0.000000
 H -1.418838 2.161569 0.000000
 O 1.637223 -1.006714 0.000000
 Cl -1.231089 -0.705636 0.000000
 H 2.590458 -1.156583 0.000000
 MIN39
 E= -650.6413605800 ZPE= 31.9026700000
 C 1.717983 0.406979 -0.000006
 C 2.745786 -0.417807 0.000022
 C -0.549108 0.741563 -0.000026

H 2.612576 -1.489204 0.000055
H 3.747182 -0.017449 0.000012
O 0.418505 -0.124921 0.000008
Cl -2.055275 -0.197896 -0.000001
H 1.743922 1.485844 -0.000040
MIN40
E= -650.6426474000 ZPE= 32.8348800000
C 0.462725 0.778494 0.000200
C -0.310039 -0.378851 0.000298
C 1.821308 0.504531 -0.000128
H 2.589205 1.269469 -0.000447
H 0.120525 1.807360 0.000221
O 2.288779 -0.713411 -0.000059
Cl -2.019259 -0.088980 -0.000099
H 1.463470 -1.281916 0.000146
MIN41
E= -650.6419534500 ZPE= 32.9789700000
C -2.686618 0.531542 0.000000
C 0.641886 -0.136317 0.000003
C -0.537205 -0.344555 0.000001
H -2.513075 1.128347 -0.893904
H -3.694522 0.130239 -0.000021
O -1.808566 -0.620052 -0.000001
Cl 2.275344 0.133499 -0.000001
H -2.513103 1.128324 0.893925
MIN42
E= -650.6406544200 ZPE= 32.8606000000
C -0.618613 0.773004 0.000002
C 0.716351 0.879253 0.000000
C -1.310780 -0.506399 0.000005
H 1.214685 1.837145 -0.000002
H -3.083960 -1.085299 0.000000
O -2.612989 -0.244107 -0.000003
Cl 1.837254 -0.434097 -0.000001
H -1.181877 1.705515 0.000001
MIN43
E= -650.6387512400 ZPE= 32.2284600000
C -0.565621 -0.189067 0.000000
C 0.564403 0.525364 -0.000001
C -1.809453 0.561918 -0.000002
H 0.550113 1.604258 -0.000004
H -0.536702 -1.282848 0.000003
O -2.868731 -0.216459 0.000000
Cl 2.145351 -0.164712 0.000001
H -2.670497 -1.178929 0.000002
MIN44
E= -650.6394484400 ZPE= 32.8741000000
C -0.518805 0.751491 -0.092697
C 0.335063 -0.267843 0.046170
C -1.943181 0.614058 0.196591
H -3.283187 -0.678719 0.140257
H -0.152104 1.758056 -0.239541
O -2.360092 -0.601462 -0.127799
Cl 2.062099 -0.092766 -0.002394
H 0.021891 -1.276857 0.261993
MIN45

E= -650.6373139300 ZPE= 31.7913000000
C 1.774320 0.517331 0.045506
C 2.490435 -0.578502 -0.099109
C -0.327085 -0.412881 0.376304
H 3.562834 -0.520465 0.006940
H 2.038661 -1.534547 -0.313458
O 0.370105 0.570883 -0.101641
Cl -2.020270 -0.069051 -0.062125
H 2.156226 1.506118 0.239571
MIN46
E= -650.6377683900 ZPE= 32.5352700000
C 0.199312 1.583014 0.030658
C -0.012834 0.266011 0.042178
C 1.011985 -0.738599 0.352249
H 2.823926 -1.013982 0.047558
H 1.213641 1.952350 0.080637
O 2.142986 -0.386098 -0.224988
Cl -1.633163 -0.400681 -0.052702
H -0.608469 2.299428 0.017129
MIN47
E= -650.6354125800 ZPE= 31.9141400000
C 1.067201 -1.040090 0.708576
C 0.824505 1.501588 -0.001195
C 0.312371 0.103606 0.115676
H 1.906348 1.510314 0.123443
H 0.377911 2.119744 0.776039
O 1.054718 -0.934313 -0.587509
Cl -1.442435 -0.086883 -0.009760
H 0.574927 1.930831 -0.971831
MIN48
E= -650.6349337100 ZPE= 31.6868700000
C 1.234586 -0.386021 0.000018
C 2.551855 -0.358062 -0.000013
C -0.707312 1.108330 0.000003
H 0.596099 -1.251769 0.000055
H 3.103652 -1.285196 -0.000002
O 0.550325 0.850251 0.000007
Cl -1.745644 -0.413159 -0.000006
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E= -650.6329700700 ZPE= 32.2249600000
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Cl 1.848150 -0.406222 -0.000060
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E= -650.6335343700 ZPE= 32.7068600000
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E= -650.6329714800 ZPE= 32.3998100000
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MIN54
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C 2.149775 -0.731363 0.253883
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H -0.497504 2.333609 0.183876
O 1.015689 -0.630538 -0.393012
Cl -1.522518 -0.393974 0.075285
H 1.290450 1.993448 -0.191005
MIN98
E= -650.6031670500 ZPE= 31.6040300000
C 0.641381 0.911559 0.000000
C -0.676510 0.798637 0.000000
C -2.605689 -0.581873 0.000000
H -3.039243 0.452684 0.000000
H -1.344091 1.650968 0.000000
O -1.306607 -0.445474 0.000000
Cl 1.739569 -0.423078 0.000000
H 1.108429 1.882523 -0.000001
MIN99
E= -650.6021415300 ZPE= 31.4686600000
C -1.358439 0.452666 -0.063106
C -2.181030 -0.677353 0.066460
C 0.014274 0.479527 -0.029889
H 1.631671 1.479125 0.074009
H -1.552037 -1.579190 0.000959
O 0.677699 1.624184 0.034638
Cl 1.025937 -0.933767 -0.006151
H -1.790996 1.451599 -0.088296
MIN100
E= -650.6021964200 ZPE= 31.5068300000
C 1.133393 -0.699732 0.000019
C 2.431672 -0.170829 -0.000022
C 0.077916 0.186505 0.000008
H -0.685545 1.910552 -0.000040
H 3.139055 -1.014635 -0.000016
O 0.184463 1.491559 0.000011
Cl -1.566252 -0.410306 -0.000006
H 0.839180 -1.748859 0.000043
MIN101

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E= -650.6016303000 ZPE= 31.4478000000
C -1.108984 -0.781790 0.000370
C -2.474469 -0.443377 -0.000428
C -0.098989 0.147221 0.000239
H -2.569412 0.653326 -0.000037
H -0.781915 -1.816102 0.000530
O -0.270751 1.453525 0.000064
Cl 1.590171 -0.347632 -0.000121
H 0.579086 1.911995 -0.000046
MIN102
E= -650.6006348500 ZPE= 30.9708300000
C 0.261067 1.386746 0.119841
C -1.211746 1.179602 -0.328824
C 0.845224 0.032068 0.015974
H -1.839712 1.306257 0.565110
H 0.426780 1.701162 1.159385
O 1.879374 -0.489318 -0.079518
Cl -0.811693 -0.985538 0.035395
H 0.809464 2.070769 -0.532008
MIN103
E= -650.6006025400 ZPE= 31.5968300000
C 0.543753 0.970818 0.181460
C -0.766760 1.028487 0.019440
C -1.737823 -1.139383 0.266441
H -1.190809 -1.004246 1.229395
H -1.325264 1.942839 0.146786
O -1.557801 -0.041136 -0.425437
Cl 1.508319 -0.447679 -0.074116
H 1.102040 1.841508 0.483238
MIN104
E= -650.5996086400 ZPE= 31.7437000000
C 0.289466 1.737960 0.000000
C 0.015209 0.412339 -0.000001
C 0.983014 -0.569625 0.000000
H 0.703298 -1.618305 0.000002
H 2.786409 -1.114965 0.000003
O 2.269250 -0.300437 0.000000
Cl -1.693132 -0.396176 0.000000
H -0.586593 2.387712 0.000003
MIN105
E= -650.5975331000 ZPE= 31.3370500000
C 1.616443 0.067806 -0.006789
C 3.006960 -0.353088 -0.001959
C 0.466370 0.446157 -0.002062
H 3.596291 0.245574 0.694564
H 3.463483 -0.301280 -0.990334
O -0.711712 0.916787 0.001821
Cl -2.057172 -0.403263 0.000137
H 3.067213 -1.388367 0.343726
MIN106
E= -650.5961443000 ZPE= 31.2501700000
C 0.729057 1.382182 -0.338626
C -0.125746 0.436316 0.403292
C -1.308092 -0.111199 -0.362834
H -1.117650 -0.310491 -1.430447
H -0.288544 0.465450 1.479742

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O -2.384496 -0.248194 0.153844
Cl 1.372518 -0.604843 0.006380
H 1.378044 1.869129 0.400497
MIN107
E= -650.5964555500 ZPE= 31.4981800000
C -0.165715 1.717200 0.092523
C 0.034072 0.369911 -0.038811
C -0.941634 -0.590391 0.101761
H -0.700625 -1.592183 0.447032
H -2.765527 -1.103889 0.106930
O -2.227317 -0.335952 -0.114392
Cl 1.702715 -0.326906 -0.029225
H -1.221806 1.960761 -0.074836
MIN108
E= -650.5971828500 ZPE= 32.0304900000
C -0.027878 -0.124355 0.481302
C 0.917327 0.982320 0.185943
C 1.052943 -0.994833 -0.183048
H 0.822025 1.976465 -0.222737
H 1.538552 -1.850474 0.280026
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H -0.064732 -0.377886 1.541159
MIN109
E= -650.5960744700 ZPE= 31.3491700000
C -0.654045 1.455032 0.062956
C 0.131864 0.308390 -0.466411
C 1.290755 -0.215024 0.334785
H 1.057849 -0.484907 1.381397
H 0.246165 0.224520 -1.541172
O 2.409680 -0.227482 -0.109036
Cl -1.454912 -0.511814 0.017329
H -0.459388 1.490697 1.149490
MIN110
E= -650.5921314500 ZPE= 29.5907200000
C 0.291798 1.935523 -0.257769
C 0.058019 0.628443 0.223580
C -1.414485 0.162295 0.133939
H -2.113710 0.970995 0.402767
H 1.330991 2.060746 -0.583239
O -1.757646 -0.924400 -0.210186
Cl 1.239328 -0.763157 -0.001311
H 0.163317 0.979564 1.285753
MIN111
E= -650.5947129800 ZPE= 31.9718500000
C 1.101305 -0.095309 -0.009960
C -0.157195 -0.668116 0.578641
C 1.798434 -1.105010 -0.486152
H -0.235583 -1.740910 0.425648
H -0.216821 -0.438360 1.639310
O 1.372188 1.227870 0.088667
Cl -1.618960 0.108719 -0.193592
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MIN112
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C -1.076856 0.145120 0.008502

C 0.217149 0.563849 0.632707
C -1.665920 1.209518 -0.495552
H 0.335330 1.644403 0.608479
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O -1.408746 -1.167415 0.105546
Cl 1.651116 -0.158603 -0.212915
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MIN113
E= -650.5901036100 ZPE= 29.7147400000
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C 0.018389 0.405808 0.195003
C 1.105283 -0.625225 -0.208524
H 0.731888 -1.449957 -0.836672
H 0.167220 0.585749 1.279871
O 2.245785 -0.512936 0.127923
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MIN114
E= -650.5911045700 ZPE= 31.1444900000
C 0.027024 0.635713 0.515332
C 1.453627 0.249881 0.234537
C -0.771956 1.374760 -0.514275
H -0.300945 1.128731 -1.480508
H 2.167591 1.022438 0.587145
O 1.828347 -0.730965 -0.348911
Cl -1.210753 -0.633956 0.042446
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E= -650.5907906600 ZPE= 31.1182600000
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MIN116
E= -650.5916475600 ZPE= 31.6865600000
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C -0.778218 -0.170936 0.495903
H -0.592720 -0.241720 1.562937
H -2.875564 -1.044978 -0.386739
O 0.295147 -0.722689 -0.261692
Cl 1.765952 0.177843 -0.017581
H -1.752487 1.910016 -0.343772
MIN117
E= -650.5885121000 ZPE= 29.8170700000
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C -0.015679 0.607980 0.265760
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Cl -1.373560 -0.550920 -0.008228

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H -0.119696 1.003429 1.299934
MIN118
E= -650.5919938700 ZPE= 32.1603500000
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C -1.776543 0.733273 -0.055942
H -2.231858 1.301895 0.747676
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O -1.953077 -0.651469 -0.032103
Cl 1.905647 0.073155 0.070269
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MIN119
E= -650.5903622400 ZPE= 31.3437700000
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H -2.937361 -1.318595 -0.207009
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O -0.560160 0.981123 -0.008221
Cl 1.537309 -0.566097 -0.021085
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MIN120
E= -650.5910653100 ZPE= 32.2829900000
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C 0.852350 0.693306 -0.230557
H 1.445097 1.514927 -0.617178
H 2.617069 -0.043498 0.884275
O 1.288630 -0.613126 -0.676934
Cl -1.588967 -0.269105 0.018424
H 1.023152 -0.809094 1.413811
MIN121
E= -650.5898228800 ZPE= 31.6758900000
C 1.549494 -0.465506 0.651579
C 1.549393 -0.465682 -0.651532
C 0.942634 0.699981 -0.000087
H 1.377717 1.697028 -0.000252
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MIN122
E= -650.5860601400 ZPE= 29.3537200000
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C 0.290917 1.810810 -0.089150
C 1.139782 -0.603237 0.268961
H -0.611135 2.331498 -0.426420
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E= -650.5876249400 ZPE= 31.0078100000
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H 1.988806 -1.513466 -0.361583
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E= -650.5872811900 ZPE= 31.8425500000
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Cl 1.568149 -0.547087 -0.032623
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MIN125
E= -650.5848330800 ZPE= 30.9317100000
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C -0.398067 0.298762 0.317818
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O 0.492425 -0.421662 -0.186567
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E= -650.5845874200 ZPE= 31.2979100000
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E= -650.5824513600 ZPE= 32.2696200000
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MIN129

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E= -650.5755178600 ZPE= 29.9704900000
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E= -650.5775393400 ZPE= 31.6926200000
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Cl 1.761201 0.215523 -0.097930
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MIN133
E= -650.5625188700 ZPE= 31.4220400000
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C -0.424908 0.187080 -0.000395
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Cl 2.123556 0.144536 0.000105
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E= -650.5615268000 ZPE= 31.4971100000
C -0.422452 1.189294 0.024939
C -0.943299 -0.160856 -0.475603
C 0.064859 -0.114318 0.599083
H -0.754239 -0.586783 -1.451930
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O -2.269471 -0.170069 -0.004822
C1 1.713085 -0.125165 -0.092575
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MIN135
E= -650.5598546100 ZPE= 30.7758200000
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MIN137
E= -650.5432231200 ZPE= 29.8784200000
C 2.615341 -0.409971 0.204492
C 1.591828 0.304246 -0.608381
C -0.675333 0.858220 0.333454
H 3.463093 0.271955 0.316876
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E= -650.5437356000 ZPE= 30.7306500000
C -0.292979 -0.315273 0.308828
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H 1.437110 -1.164469 0.406266
MIN139
E= -650.5407542600 ZPE= 30.7215300000
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C 0.670359 0.790014 -0.154810
C -1.808556 0.549238 -0.147814
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MIN141
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C -1.268777 -0.536812 0.062158
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MIN142
E= -650.5397988000 ZPE= 30.8107700000
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E= -650.5357639700 ZPE= 30.9329800000
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E= -650.5337207900 ZPE= 30.1959400000
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H 2.291145 -1.275007 0.194322
H 0.555414 0.753315 1.395300
O 2.651878 -0.439602 -0.187134
Cl -2.028776 -0.253245 -0.070560

H 0.426241 -0.900666 0.716830
MIN146
E= -650.5338638200 ZPE= 30.4440300000
C 0.556121 0.759596 0.309898
C -0.722652 0.891129 -0.449258
C 1.275365 -0.590712 0.174150
H 2.784933 0.510855 -0.322535
H 1.205184 1.613617 0.056101
O 2.509913 -0.424722 -0.183130
Cl -1.826234 -0.346302 0.008197
H 0.323557 0.800355 1.383384
MIN147
E= -650.5318523300 ZPE= 30.2520200000
C 0.884920 1.091940 0.110952
C -0.612566 1.089489 0.043605
C -1.339329 -0.032685 -0.647782
H -1.885531 -0.606226 1.120446
H -0.840753 1.180510 1.131342
O -1.960720 -0.832198 0.165444
Cl 1.513060 -0.520985 -0.012995
H -0.908120 2.047577 -0.395076
MIN148
E= -650.5283075300 ZPE= 30.5869800000
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C 0.918696 1.508706 -0.434547
C 1.167386 0.237521 -0.041743
H 2.047170 -1.379323 0.983712
H 2.726171 -1.044473 -0.635179
O 0.080970 0.649758 0.604677
Cl -1.763234 -0.297619 -0.097348
H 1.118858 -1.793184 -0.457967
MIN149
E= -650.5227497500 ZPE= 30.6039300000
C 2.165639 -0.866237 -0.207943
C -0.730305 1.040926 -0.018796
C 0.746265 1.195778 0.018604
H -1.152841 1.577766 0.828418
H 2.441710 -1.294138 0.772880
O 1.395867 0.117565 0.062812
Cl -1.438765 -0.645304 0.004352
H -1.086388 1.523215 -0.928973
MIN150
E= -650.5177551000 ZPE= 30.3006000000
C 0.576437 -0.634830 0.069712
C -0.405143 0.503552 0.061394
C 2.950007 0.141734 -0.267897
H -0.315479 1.097656 0.971200
H -0.221725 1.148999 -0.800683
O 1.756689 -0.164976 0.075733
Cl -2.102104 -0.076617 -0.037432
H 3.491661 0.312907 0.680705
MIN151
E= -650.5184444500 ZPE= 31.1300400000
C 0.461700 1.378448 -0.032977
C -0.144635 0.117502 0.484757
C -1.161218 -0.428047 -0.423013

H -3.026256 -0.374715 -0.515454
H -0.190489 -0.029662 1.559629
O -2.335258 -0.111847 0.104828
Cl 1.572548 -0.383546 -0.055488
H 0.230416 1.412017 -1.112108
MIN152
E= -650.5136394000 ZPE= 29.4901800000
C 2.602048 -0.605995 0.000346
C -0.618837 0.994875 0.000139
C 0.840668 0.904738 -0.000258
H -0.888025 1.598625 0.871489
H -0.888567 1.599182 -0.870643
O 1.265825 -0.374262 -0.000343
Cl -1.667181 -0.492780 0.000018
H 3.048807 0.411847 0.000222
MIN153
E= -650.5132818600 ZPE= 29.3563400000
C -0.653157 1.002323 0.000009
C 2.633492 -0.378068 0.000159
C 0.808025 0.989527 -0.000017
H -0.955068 1.589322 -0.871592
H 2.746631 -1.484202 -0.000147
O 1.282319 -0.274272 -0.000142
Cl -1.636779 -0.540173 0.000019
H -0.955031 1.589299 0.871638
MIN154
E= -650.5118510700 ZPE= 29.2357800000
C -0.656051 -0.402352 0.000010
C 0.460367 0.571132 -0.000004
C -2.983048 -0.262146 -0.000007
H -2.716667 -1.341040 0.000011
H 0.383274 1.215388 -0.880422
O -1.787505 0.366330 0.000000
Cl 2.077797 -0.203542 0.000000
H 0.383275 1.215413 0.880428
MIN155
E= -650.5102978600 ZPE= 29.0628600000
C -0.626623 -0.466749 -0.000374
C 0.456507 0.547598 -0.000172
C -2.918561 -0.430840 0.000064
H 0.360229 1.188113 -0.881477
H 0.360031 1.188472 0.880831
O -1.774168 0.284854 0.000122
Cl 2.098530 -0.173261 0.000120
H -3.669857 0.389969 0.000531
MIN156
E= -650.5110545700 ZPE= 29.8073900000
C -0.624109 0.947933 -0.113303
C 0.795042 1.026469 0.210553
C -2.336270 -0.736262 0.239298
H -2.648898 0.100388 0.923020
H -1.205305 1.459178 0.665671
O -1.265109 -0.372011 -0.371363
Cl 1.629434 -0.443572 0.023586
H -0.733279 1.528411 -1.038044
MIN157

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E= -650.5103279600 ZPE= 29.8560500000
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C 0.320798 -0.470164 -0.208949
C -2.453670 -0.718476 0.068775
H -1.682549 -1.362125 0.570861
H -0.526911 0.843478 1.241409
O -1.933005 0.411731 -0.212719
Cl 1.981147 -0.081694 0.004714
H -0.209752 1.621410 -0.323629
MIN158
E= -650.5107196200 ZPE= 31.4067600000
C 1.328222 0.370717 0.000018
C 2.652232 0.134731 -0.000011
C 0.443169 -0.756648 0.000010
H 3.372220 0.942187 -0.000013
H 3.027928 -0.879334 -0.000039
O -1.778990 0.972645 -0.000008
Cl -1.156213 -0.454327 -0.000001
H 0.945655 1.386742 0.000038
MIN159
E= -650.5040449400 ZPE= 30.0214500000
C 0.861973 1.153888 -0.050045
C -0.525782 1.326656 0.021901
C 1.806690 0.143587 0.075867
H 1.626447 -1.878504 0.363660
H 1.352227 2.127376 -0.029592
O 1.128887 -1.191693 -0.094989
Cl -1.468890 -0.309426 0.007577
H 0.104075 -1.199871 0.010701
MIN160
E= -650.5011538000 ZPE= 28.9782100000
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C -0.007032 0.306379 0.202355
C 0.999563 -0.823990 -0.265683
H 1.315218 1.870628 -0.055175
H 0.182517 0.311529 1.288289
O 2.216378 -0.531109 0.022033
Cl -1.704198 -0.298801 -0.011204
H 2.358259 0.356604 0.435803
MIN161
E= -650.4982838800 ZPE= 29.7370800000
C 1.395705 1.090134 0.028871
C -0.599664 -1.203465 -0.022580
C -1.620183 -0.176922 0.075846
H -2.613636 -0.596310 0.306771
H 0.621530 1.828168 -0.050809
O -1.474727 1.035593 -0.076732
Cl 0.959537 -0.529906 -0.026908
H 2.422640 1.233315 0.322507
MIN162
E= -650.4969381300 ZPE= 29.7315200000
C -0.426837 0.499409 0.000011
C 2.587672 0.285405 -0.000006
C -1.611510 -0.287420 0.000003
H -1.465225 -1.385256 0.000007
H -0.360477 1.574571 0.000008

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O -2.734640 0.197693 -0.000008
C1 1.055252 -0.360916 0.000000
H 2.467575 1.380349 -0.000004
MIN163
E= -650.4952436000 ZPE= 29.5165800000
C 0.491279 -0.680642 0.000164
C -2.071639 0.993845 0.000118
C 1.428038 0.380539 -0.000124
H 1.004761 1.403181 -0.000584
H 0.708721 -1.736908 0.000418
O 2.641650 0.211982 0.000047
C1 -1.210883 -0.432112 -0.000100
H -1.347734 1.821326 0.000539
MIN164
E= -650.4915522800 ZPE= 29.6606000000
C 1.681636 1.164497 0.264473
C -0.454980 -0.696901 0.159182
C -1.378731 0.343340 -0.126512
H -0.933758 1.261946 -0.552887
H -0.668388 -1.702204 0.477461
O -2.586241 0.233671 0.035876
C1 1.207574 -0.436979 -0.104222
H 2.675765 1.133923 -0.222666
MIN165
E= -650.4911318700 ZPE= 29.7051200000
C 2.147280 1.127535 -0.004978
C -0.439900 -0.241831 -0.001105
C -1.607118 0.016488 -0.006133
H -3.245778 0.531936 0.755842
H 2.777958 0.894651 0.864025
O -2.879419 0.278784 -0.101246
C1 1.185880 -0.586955 0.009740
H 2.741636 0.908229 -0.902177
MIN166
E= -650.4921246400 ZPE= 31.0287800000
C -1.604277 0.537652 -0.103029
C -2.210855 -0.636960 0.142048
C -0.266197 0.916772 0.289406
H -3.267588 -0.761454 -0.046113
H -1.693395 -1.459521 0.615844
O 2.245095 -0.043484 0.248758
C1 0.805006 -0.217907 -0.238547
H -2.196902 1.368484 -0.475051
MIN167
E= -650.4889374000 ZPE= 29.5134700000
C -0.381326 1.013377 0.052953
C 2.269434 -0.025341 0.342298
C -1.702330 0.406001 -0.068747
H 2.357936 0.763592 1.071396
H 3.039272 -0.257817 -0.375527
O -2.063022 -0.709124 0.278890
C1 0.730319 -0.254748 -0.258606
H -2.423120 1.133708 -0.489717
MIN168
E= -650.4868314500 ZPE= 29.1668200000
C -0.510155 -0.916137 0.038905


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C 1.739908 1.055959 0.009498
C -1.436001 0.180308 0.304583
H 1.058687 1.885651 -0.056663
H 2.727157 1.065318 -0.424176
O -2.479198 0.352695 -0.291288
Cl 1.085589 -0.500250 -0.028830
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MIN169
E= -650.4824275400 ZPE= 27.9484300000
C -1.469688 1.169133 -0.194532
C 0.260420 -0.818925 -0.049543
C -0.924633 -0.103976 -0.015618
H 0.428036 -1.841291 0.230632
H 2.038423 0.598355 1.156911
O -2.128836 -0.539950 0.061490
Cl 1.708289 0.143000 -0.063876
H -1.673282 1.654138 0.764595
MIN170
E= -650.4814114400 ZPE= 29.0735000000
C 0.335933 1.052509 0.208425
C -1.845201 0.021932 0.482212
C -1.325973 -0.954796 -0.135297
H -0.874408 -1.899982 -0.344810
H -2.421723 0.632962 1.141342
O -0.924461 0.440396 -0.613682
Cl 1.590336 -0.277994 0.079351
H 0.667555 1.751878 -0.568084
MIN171
E= -650.4739985700 ZPE= 29.1706700000
C 0.839361 -0.063273 0.594446
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C 1.728316 1.058572 -0.027991
H -1.993503 1.210743 -0.732763
H 2.534014 -0.962165 -0.844621
O -2.217047 0.589091 -0.024300
Cl -0.660942 -0.581394 -0.061918
H 0.839613 -0.201707 1.665371
MIN172
E= -650.4726878300 ZPE= 29.1056300000
C 0.854663 0.004199 0.595094
C 2.042689 -0.192389 -0.358142
C 1.781558 1.039348 -0.101658
H -2.558912 0.620372 0.659103
H 2.506730 -1.064024 -0.775100
O -2.218259 0.600524 -0.246913
Cl -0.654096 -0.554770 -0.023231
H 0.844429 -0.036400 1.674462
MIN173
E= -650.4705274900 ZPE= 28.5709000000
C -0.657179 -0.819420 0.334999
C -1.807094 0.021440 0.232381
C -2.272252 1.094543 -0.341787
H 1.825133 1.641675 0.099974
H -2.704145 -0.227301 0.837138
O 2.131706 0.778118 0.409583
Cl 0.756573 -0.461163 -0.392177

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H -0.617234 -1.578928 1.099677
MIN174
E= -650.4448271700 ZPE= 29.5286200000
C 0.434924 0.839584 -0.108687
C 1.741446 0.530134 0.127883
C 2.222817 -0.780439 0.057536
H 1.558512 -1.506905 0.552868
H 2.442438 1.361822 0.082090
O -2.136986 0.221897 0.314833
Cl -0.783703 -0.409336 -0.188370
H 0.022777 1.792945 -0.411729

--List of TSs--

The structures are optimized at the B3LYP/6-311+G(2d,2p) level of theory. ZPE is given in kcal/mol and is calculated at this level.

The energy (in a.u.) is a CCSD(T)/6-311+G(3df,2p) single point calculation at the B3LYP/6-311+G(2d,2p) optimized geometry.

TS1

E= -650.7171678000 ZPE= 32.7060900000

C -0.681004 1.091534 -0.026318

C 0.817609 1.030603 0.031760

C -1.481980 0.052734 -0.001278

H 1.266842 1.537988 -0.818093

H 1.206271 1.465675 0.949247

O -2.220334 -0.842005 0.013295

Cl 1.442417 -0.669254 -0.010209

H -1.159278 2.060465 -0.088955

TS2

E= -650.7140729800 ZPE= 32.6675300000

C 0.605862 -0.430885 -0.000001

C -0.464687 0.637117 0.000000

C 1.887020 -0.154885 -0.000001

H -0.431241 1.264865 0.885728

H -0.431242 1.264865 -0.885729

O 3.022702 0.092824 0.000001

Cl -2.107183 -0.123811 0.000000

H 0.333794 -1.475624 0.000000

TS3

E= -650.7097021000 ZPE= 32.2378600000

C 0.526172 -0.504249 0.004910

C -0.457677 0.334275 0.276850

C 1.956215 -0.187642 0.333873

H 2.297704 -0.477905 1.346191

H -0.318367 1.295035 0.748400

O 2.717071 0.326436 -0.443490

Cl -2.129609 0.010431 -0.104147

H 0.339194 -1.460242 -0.469968

TS4

E= -650.7087083000 ZPE= 32.6465600000

C -0.003709 0.356762 -0.000001

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C -1.202590 -0.176387 0.000000

H -0.113078 2.330261 0.886051

H 1.363780 1.976274 -0.000010

O -2.272324 -0.635081 0.000000

Cl 1.327392 -0.803108 0.000000

H -0.113095 2.330265 -0.886041

TS5

E= -650.6704726000 ZPE= 28.4476500000

C -2.270553 0.082744 0.000002

C -3.445484 0.672942 -0.000002

C -1.167270 -0.543490 0.000005

H 1.719687 -0.254822 0.000036

H -3.544219 1.755006 0.000015

O -0.134482 -1.111098 -0.000003

Cl 2.857288 0.353402 -0.000002

H -4.373671 0.107601 -0.000025
TS6
E= -650.6692718300 ZPE= 27.9811000000
C -1.565000 -0.722472 -0.000003
C -0.994929 -1.912187 0.000000
C -1.602695 0.561130 -0.000012
H -1.586109 -2.822727 0.000078
H 1.156680 0.681314 -0.000034
O -1.792315 1.717372 0.000008
Cl 2.332887 0.169672 0.000004
H 0.084621 -2.040809 -0.000077
TS7
E= -650.6736943100 ZPE= 31.9932800000
C 2.384034 -0.578746 -0.141036
C 1.296293 -0.135483 0.092550
C -0.002815 0.424476 0.424913
H -0.125817 0.505411 1.502604
H -1.002986 1.639828 -0.715080
O -0.205809 1.670904 -0.178193
Cl -1.331535 -0.753121 -0.074268
H 3.346289 -0.970893 -0.357987
TS8
E= -650.6731162900 ZPE= 32.5130300000
C -1.594068 1.096770 0.140226
C -0.457189 0.520086 -0.166054
C 0.963037 0.700183 -0.365083
H 1.314964 1.024871 -1.360379
H -2.526355 0.565981 0.209125
O 1.803955 0.362261 0.411403
Cl -0.299748 -1.208416 -0.013488
H -1.595215 2.151900 0.434791
TS9
E= -650.6720417500 ZPE= 32.1105800000
C -0.526657 0.438929 0.082487
C 0.687511 0.726493 -0.264492
C -1.745468 0.181761 0.469955
H -3.157110 0.030270 -0.850911
H 0.977988 1.632822 -0.773310
O -2.647096 -0.553960 -0.281345
Cl 2.056554 -0.341066 0.040921
H -2.097839 0.483609 1.451637
TS10
E= -650.6642706200 ZPE= 28.9483700000
C 2.569411 0.670499 0.273594
C 2.568918 -0.671817 0.271665
C 1.420827 0.000482 -0.227608
H 3.140979 -1.552937 0.520359
H 3.142111 1.550485 0.524826
O 0.316794 0.001619 -0.716986
Cl -2.744503 -0.000371 0.177616
H -1.515826 0.000825 -0.234682
TS11
E= -650.6667525300 ZPE= 32.6475800000
C 0.579900 0.429273 0.000005
C -0.783061 0.914394 0.000002
C 1.713582 0.042873 0.000003

H -1.011502 1.499052 0.886254
H -1.011496 1.499053 -0.886252
O 2.919815 -0.469848 0.000006
Cl -1.999195 -0.457867 -0.000002
H 3.588276 0.225193 -0.000068
TS12
E= -650.6627892500 ZPE= 31.7110500000
C 0.850442 -1.120954 0.212977
C -0.352712 -1.611867 -0.237255
C 1.186264 0.190002 -0.033337
H -0.798049 -1.294488 -1.158613
H -0.752559 -2.508991 0.218647
O 1.770448 1.168760 -0.117834
Cl -1.422863 0.666754 0.075642
H 1.471720 -1.624515 0.942420
TS13
E= -650.6534356600 ZPE= 29.9774200000
C 0.799028 -0.593703 -0.245307
C 1.677929 -1.551271 0.102469
C 1.006452 0.744760 -0.022260
H 2.589455 -1.349639 0.647263
H 1.463653 -2.580384 -0.148811
O 1.152524 1.867856 0.026163
Cl -1.990882 -0.111746 0.046986
H -0.328758 -0.711853 -0.515931
TS14
E= -650.6439958100 ZPE= 30.9884100000
C -0.081577 1.414154 0.042753
C -0.599494 0.218109 -0.344514
C -1.854855 -0.195464 -0.050900
H 0.124108 -0.511997 -0.759662
H -0.641083 2.126431 0.634976
O -2.889951 -0.626426 0.161429
Cl 2.230380 -0.402854 0.070905
H 0.935677 1.624700 -0.256171
TS15
E= -650.6447235100 ZPE= 31.6318000000
C 0.206546 -0.677491 -0.000152
C -2.093980 -0.698212 0.000112
C -0.969235 0.169527 -0.000085
H -1.984613 -1.771593 -0.000103
H -3.094162 -0.285622 0.000494
O -0.956003 1.403789 -0.000059
Cl 1.746987 -0.010616 0.000068
H 0.168028 -1.755569 -0.000324
TS16
E= -650.6455999400 ZPE= 32.2323100000
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C -2.258317 -0.782209 0.000000
C -1.445233 0.096362 0.000000
H -2.966377 -1.570216 0.000000
H 1.152039 1.453574 -0.898847
O -0.646811 1.121712 0.000000
Cl 1.374113 -0.708039 0.000000
H 1.152039 1.453574 0.898847
TS17

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E= -650.6395992500 ZPE= 31.3015800000
C -0.096592 0.451091 0.415487
C -0.707619 1.580298 -0.209058
C -1.189227 -0.355240 0.134871
H -0.657628 2.550621 0.261076
H 0.061986 0.533888 1.485741
O -2.019944 -1.103412 -0.119532
Cl 1.747712 -0.344063 -0.093531
H -0.995285 1.534968 -1.248339
TS18
E= -650.6278399300 ZPE= 26.6006800000
C 3.062460 -0.339689 0.000044
C 2.604225 0.836070 -0.000010
C -0.807766 -0.977432 0.000003
H 1.482723 0.907942 -0.000056
H 3.158397 1.770619 -0.000018
O 0.261842 -0.500603 -0.000067
Cl -2.306709 0.328565 0.000017
H 3.324682 -1.373045 0.000091
TS19
E= -650.6291285200 ZPE= 27.9592800000
C -1.987654 0.794274 0.000013
C -0.714017 1.248267 -0.000011
C -1.521913 -0.494093 -0.000005
H 0.944750 0.433895 -0.000009
H -0.483324 2.314069 -0.000024
O -1.208290 -1.599238 -0.000003
Cl 2.208943 -0.024500 0.000003
H -3.005634 1.171742 0.000028
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E= -650.6320852000 ZPE= 30.4223600000
C 0.003476 0.514620 0.446933
C 0.348203 1.673559 -0.225457
C 1.105066 -0.549586 0.180396
H 0.458028 1.697816 -1.297590
H 0.629674 2.540397 0.351664
O 2.154219 -0.850581 -0.167279
Cl -1.587840 -0.461527 -0.097290
H -0.068646 0.580834 1.526844
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E= -650.6324257200 ZPE= 31.1067600000
C -1.298179 -0.358092 0.000004
C -2.588801 -0.679985 -0.000002
C -0.761959 0.955392 0.000000
H -2.887993 -1.718109 0.000001
H -3.367025 0.069469 -0.000011
O 0.238692 1.501633 0.000000
Cl 1.920241 -0.520515 -0.000001
H -0.404972 -1.019552 0.000011
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E= -650.6284730500 ZPE= 29.1889100000
C -0.364193 0.396773 0.500843
C -0.875631 1.656809 -0.086373
C 1.836835 0.075149 -0.392287
H -0.095097 2.416709 -0.085038
H -1.370501 1.592406 -1.057051

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O 2.742461 -0.319278 0.155064
Cl -1.319339 -0.953416 -0.051855
H -1.627395 1.980797 0.650013
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E= -650.6333709300 ZPE= 32.7121200000
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C 0.753798 1.142934 0.000000
C 1.863479 0.175883 0.000002
H 2.153657 -1.657208 0.000001
H 1.089430 2.173558 -0.000001
O 1.395379 -1.061547 -0.000001
Cl -1.494190 -0.461022 0.000000
H -1.229175 1.869207 -0.000001
TS24
E= -650.6263861000 ZPE= 29.3933500000
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C 3.078491 -0.579839 -0.000109
C 0.671999 -0.023583 0.000192
H 0.442120 -1.088531 0.000466
H 3.328912 -1.621732 -0.000072
O -0.147064 0.832133 0.000009
Cl -2.400542 -0.231175 -0.000044
H 2.376647 1.432587 -0.000110
TS25
E= -650.6302490300 ZPE= 32.1167500000
C 0.028260 0.017585 0.081397
C -0.767761 1.208926 0.071948
C -0.974379 -0.908495 0.076739
H -0.561624 2.037903 -0.603405
H -1.392097 1.450987 0.921301
O -2.069394 -0.244633 -0.181749
Cl 1.752052 -0.086703 -0.033038
H -0.992732 -1.965966 0.317233
TS26
E= -650.6284783900 ZPE= 32.2508500000
C 0.537548 1.045596 0.000000
C -0.793440 1.122190 0.000000
C -1.891408 0.104678 0.000001
H -0.519825 -1.276881 -0.000001
H -1.172243 2.138138 0.000000
O -1.489337 -1.140500 0.000000
Cl 1.488833 -0.428533 0.000000
H 1.180394 1.913017 0.000000
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E= -650.6274836500 ZPE= 31.6497400000
C -0.006221 0.227850 0.000000
C 0.248965 1.533821 0.000000
C 0.983116 -0.898694 0.000000
H 1.267955 1.908846 0.000000
H -0.527255 2.283817 0.000000
O 2.223397 -0.503838 0.000000
Cl -1.662082 -0.341648 0.000000
H 2.372357 0.468189 0.000000
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E= -650.6236982100 ZPE= 29.5831900000
C 1.099016 -0.127939 -0.591604

C 2.038109 -0.665713 0.262029
C -0.036838 0.576957 -0.084704
H 1.924852 -0.725566 1.345828
H 2.907469 -1.167713 -0.152735
O -0.207942 1.728736 0.150488
Cl -1.412429 -0.653951 0.022811
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E= -650.6269394400 ZPE= 32.0393700000
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C 0.524759 0.752441 -0.000002
C 2.009468 0.644376 0.000003
H 0.149824 1.766430 -0.000005
H -0.060366 -1.308534 0.000007
O 2.491092 -0.573561 -0.000001
Cl -2.060942 -0.080565 0.000000
H 1.840361 -1.307341 -0.000008
TS30
E= -650.6224825800 ZPE= 29.5567700000
C 1.163556 0.005364 -0.589904
C 2.098851 -0.538253 0.265970
C -0.040985 0.595572 -0.091602
H 3.014345 -0.951864 -0.146556
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O -0.260497 1.742214 0.123306
Cl -1.386966 -0.680625 0.037634
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TS31
E= -650.6246044600 ZPE= 30.9212800000
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C -1.709088 -0.171745 0.141881
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O -1.087468 -1.243189 -0.171328
Cl 1.609186 -0.309384 0.060408
H -0.062784 -1.037495 -0.260341
TS32
E= -650.6251619200 ZPE= 31.7320400000
C -0.157157 0.584872 0.537558
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C 1.639966 -0.175169 -0.333074
H 2.508465 -0.424696 -0.941560
H 1.336244 2.047355 -0.256320
O 1.041031 -1.088629 0.352607
Cl -1.566066 -0.148534 -0.196963
H -0.461130 0.993363 1.497334
TS33
E= -650.6247833300 ZPE= 31.5885100000
C 1.635639 -0.178873 0.000008
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C -0.685233 -1.185473 -0.000007
H 2.506365 1.671365 0.000005
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Cl -1.504760 0.461544 0.000004


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H 2.562624 -0.728266 0.000029
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E= -650.6113209800 ZPE= 26.0663500000
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C 1.396656 -1.382677 0.000000
C 0.968147 0.819037 0.000000
H -0.643681 -1.006206 0.000000
H 2.440603 -1.173419 0.000001
O 1.276859 1.904990 0.000000
Cl -1.629825 0.276683 0.000000
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TS35
E= -650.6085476500 ZPE= 24.6584800000
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C 1.192230 1.667924 0.010154
H 2.498626 -2.531691 -0.073832
H 3.262594 -0.824245 -0.167068
O 0.255882 2.288932 -0.010362
Cl -2.093916 -0.557964 -0.015918
H -0.792795 -0.664728 0.079405
TS36
E= -650.6184032200 ZPE= 31.1081800000
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C -0.490682 0.690226 -0.101775
C 1.729381 -0.400244 -0.216089
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H 0.831171 0.522157 1.461358
O 2.718443 0.271669 -0.195395
Cl -2.040504 -0.071968 -0.125839
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TS37
E= -650.6177611000 ZPE= 31.0260100000
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Cl -1.517646 -0.472406 -0.003692
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TS38
E= -650.6171978200 ZPE= 30.6853300000
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H -2.526471 1.257883 -0.384087
H -0.118811 1.451879 -0.549970
O -2.438047 -0.726235 -0.085242
Cl 2.026066 -0.086449 -0.120687
H -0.469073 1.178009 1.146125
TS39
E= -650.6166503900 ZPE= 30.7044000000
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C 1.588661 -0.063552 0.280591

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H 1.185252 1.812747 -0.646056
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Cl -1.497166 -0.429973 0.117497
H 2.373250 0.113280 1.043043
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E= -650.6154151800 ZPE= 30.6529200000
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C -1.036894 1.355208 -0.082779
C -0.950488 -0.347334 0.083774
H -1.226220 1.406498 -1.153441
H -0.221777 2.013339 0.194453
O -1.896413 -1.020373 -0.181849
Cl 1.711463 -0.126241 -0.142858
H -1.912196 1.578668 0.517961
TS41
E= -650.6127199600 ZPE= 28.9802000000
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H 2.992064 0.758252 0.000049
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O -0.375057 -1.775387 -0.000019
Cl -1.345058 0.793727 0.000010
H -1.065429 -0.878668 -0.000140
TS42
E= -650.6139196800 ZPE= 30.0980600000
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H 1.009771 2.147406 -0.426934
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O -2.081368 -0.959539 -0.237196
Cl 1.553728 -0.624110 -0.069789
H 0.010936 0.276274 1.481208
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H 0.492077 1.877730 -0.246475
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O 2.717283 -0.362358 -0.310251
Cl -1.972828 -0.139413 -0.225120
H -0.524701 -0.332884 1.607464
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E= -650.6137363900 ZPE= 30.5576100000
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H 0.447585 -1.386745 -0.779748
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Cl -2.118948 -0.003512 -0.024768
H -0.255071 1.458078 -0.176395
TS45

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C -1.736300 1.359783 0.000190
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H 0.314824 1.918576 0.000112
H -1.016030 3.231840 -0.000567
O -2.046157 -1.832615 -0.000147
Cl 2.251552 -0.280359 -0.000035
H 1.003403 -0.602926 0.000821
TS46
E= -650.6144762100 ZPE= 32.0599900000
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C 0.409371 0.364689 0.531792
C -1.470200 0.146044 0.350115
H 0.450678 0.465346 1.597452
H -2.978890 -0.974064 0.436874
O -2.463861 -0.524086 -0.240559
Cl 1.910479 -0.290822 -0.125933
H -0.460678 1.295902 -1.319099
TS47
E= -650.6116459100 ZPE= 30.3231400000
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C -1.344730 -0.185739 0.079547
C -0.585979 0.939701 0.425392
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O 0.171517 1.608999 -0.364658
Cl 1.546245 -0.697760 0.042527
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E= -650.6057604700 ZPE= 26.7195800000
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H -1.162029 2.066642 -0.008810
TS49
E= -650.6052853900 ZPE= 26.8234900000
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C 0.157917 1.694747 0.000006
C -1.123807 -0.599626 -0.000009
H 1.153536 2.064190 0.000019
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O -2.157792 -1.096252 0.000009
Cl 1.762062 -0.513366 0.000000
H -2.039850 1.649407 -0.000014
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E= -650.6034821900 ZPE= 25.9346300000
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H -2.887740 -1.011448 -0.000002
H 0.700130 -0.659645 -0.000009

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O -2.408325 -1.013648 -0.042428
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H 0.976654 0.127421 0.412530
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Cl -1.871046 -0.361337 -0.000199
H -1.110958 1.883190 0.000037
TS53
E= -650.6083377700 ZPE= 29.8265700000
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C -0.009878 0.583727 0.096118
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H -1.518313 -0.820568 -1.437186
O 0.130249 1.707860 -0.236647
Cl 1.381785 -0.604180 0.000377
H -2.028729 0.670850 0.801407
TS54
E= -650.6089046600 ZPE= 30.9635900000
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Cl 1.626212 -0.307832 0.033125
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TS55
E= -650.6073024000 ZPE= 30.0491400000
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H 2.024579 -0.505282 1.113362
H 1.471636 -1.420608 -0.292248
O -0.904800 1.653611 0.025625
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E= -650.6071121700 ZPE= 30.0302800000
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E= -650.6057306300 ZPE= 29.2836500000
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E= -650.6054118700 ZPE= 29.1620700000
C 1.524264 0.079723 -0.067381
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H 3.434786 -0.580269 -0.634920
H 2.648968 -1.468799 0.788061
O -0.409853 1.611764 0.036657
Cl -1.690185 -0.724404 -0.023240
H -1.293627 1.049995 0.235434
TS60
E= -650.6069139000 ZPE= 30.1068900000
C 0.992782 -0.865832 -0.074361
C 2.328899 -0.315273 -0.008763
C -0.034167 0.289018 -0.019357
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E= -650.6055118200 ZPE= 29.2580100000
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C 0.719290 1.054492 0.148442
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O 2.172281 -0.719946 -0.408368
Cl -1.662653 -0.509505 0.041950

H 0.076739 0.940015 -1.153921
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 E= -650.5997120800 ZPE= 25.6447600000
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 C 1.525823 0.599800 0.000004
 C 1.552818 -0.842951 0.000003
 H 2.572255 -1.257295 0.000007
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 Cl -2.049450 0.199489 0.000005
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 TS63
 E= -650.6060285600 ZPE= 29.7424200000
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 C -1.885938 -1.003435 0.127407
 C 0.138797 0.617683 0.002129
 H -2.954080 -0.948481 -0.145926
 H -1.838094 0.847672 0.761988
 O 0.594711 1.708812 0.057973
 Cl 1.200659 -0.831830 -0.017355
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 E= -650.6084158900 ZPE= 31.4385800000
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 C 0.653843 -0.077486 0.000248
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 O -0.245280 -0.795560 0.000056
 Cl -2.469848 0.264674 -0.000050
 H 2.335455 -1.378297 -0.000359
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 E= -650.6047582000 ZPE= 29.2446600000
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 C -1.924128 -0.880144 -0.356185
 C 0.107688 0.603797 0.024123
 H -1.319448 -0.807057 0.889122
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 E= -650.5985908800 ZPE= 25.4893500000
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 C -0.971823 0.183985 -0.000275
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 TS67
 E= -650.6047728900 ZPE= 29.6904100000
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 C -1.591734 -0.052681 0.411872

H 1.229097 1.819340 0.214299
H 0.573471 1.176351 -1.273567
O -2.248590 -0.680471 -0.400769
Cl 1.647740 -0.543838 0.035146
H -1.669736 -0.220106 1.514424
TS68
E= -650.6072970000 ZPE= 31.4710100000
C 1.754709 0.149984 0.000001
C 3.028905 -0.116643 0.000001
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O -0.462620 -0.572733 -0.000002
Cl -2.071550 0.039467 0.000001
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E= -650.6035944800 ZPE= 29.2876200000
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C 1.604045 -0.001813 0.393927
H 1.770369 0.001775 1.490399
H -1.229647 1.716225 -0.678667
O 2.198450 -0.756886 -0.350527
Cl -1.653487 -0.531647 0.039691
H -0.270319 1.503992 0.820003
TS70
E= -650.6031261400 ZPE= 29.1224600000
C -1.272055 0.277963 0.115423
C -2.404449 0.747916 -0.152050
C -0.026291 -0.449828 0.432189
H -0.226003 -1.632048 -1.077617
H -1.398429 1.512117 -0.218088
O 0.022066 -1.693852 -0.146721
Cl 1.385158 0.635018 -0.082487
H 0.116996 -0.580869 1.498384
TS71
E= -650.6004830300 ZPE= 27.5308200000
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C 1.344876 0.937485 -0.000111
C 1.836676 -0.493411 0.000133
H 1.057779 -1.264775 0.000520
H 2.105155 1.715103 -0.000564
O 3.007032 -0.752899 -0.000089
Cl -2.656260 -0.311029 -0.000054
H -1.723794 0.612443 0.000208
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E= -650.5970582500 ZPE= 25.5128200000
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C 2.392303 -0.157367 0.000000
C 0.944736 -0.169538 0.000002
H -1.581265 0.454741 0.000001
H 3.154953 -1.210722 0.000001
O 0.298349 0.854947 0.000001
Cl -2.726224 -0.157477 -0.000001
H 0.471398 -1.162074 0.000004
TS73

E= -650.6063758200 ZPE= 31.5355100000
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C -0.051090 0.349235 -0.040294
C 1.042345 -0.433255 0.390984
H 0.968049 -1.062008 1.273321
H 2.241887 0.048505 -0.953972
O 2.205382 -0.582362 -0.215578
Cl -1.740616 -0.328344 -0.072417
H -0.020746 2.480438 0.286685
TS74
E= -650.5980999100 ZPE= 26.3968400000
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C 1.607603 1.292929 0.000004
C -1.030276 0.753036 0.000004
H 0.273184 1.248769 0.000015
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O -2.163543 0.868359 -0.000006
Cl -0.141254 -1.321254 0.000002
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E= -650.5958722700 ZPE= 25.3876800000
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C 1.562304 -0.974310 0.000006
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H 3.195412 0.853994 0.000016
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Cl -2.467062 0.302997 0.000002
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TS76
E= -650.5978775400 ZPE= 26.6727900000
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C 1.508296 0.970247 0.011946
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Cl -2.404495 -0.216091 -0.070007
H -2.738996 -0.715493 1.061306
TS77
E= -650.6033878800 ZPE= 30.2725200000
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C -2.018031 0.420752 -0.529833
C -0.915316 0.232190 0.080262
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H -2.938358 0.578125 -1.039021
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TS78
E= -650.6033829200 ZPE= 30.5192400000
C 0.952874 0.168942 0.140222
C -0.357052 0.695625 0.583766
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H -0.453981 1.749873 0.349732
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O 1.445825 -1.024563 0.296838
Cl -1.706948 -0.179903 -0.254050
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E= -650.6044211300 ZPE= 31.2116200000
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C 0.580891 0.496025 0.790122
C -1.692183 0.352399 -0.262812
H -2.499097 0.861491 -0.766335
H -0.420797 1.999930 -0.317109
O -2.042441 -0.917945 0.074637
Cl 1.789469 -0.294000 -0.183180
H -1.334990 -1.360012 0.555243
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E= -650.6029268700 ZPE= 30.7079600000
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C 1.081770 -0.221543 -0.492685
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H 1.272780 -0.286422 -1.554670
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E= -650.6030214400 ZPE= 30.7905200000
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C 1.291538 -0.417582 0.249812
H 0.797860 -1.170287 0.876165
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Cl -1.774201 -0.271291 0.043628
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C -0.322408 0.804510 -0.523911
C 0.729228 0.583187 0.404678
C -2.436538 -0.511658 0.000577
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Cl -1.999443 -0.308610 -0.119215
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E= -650.6025389300 ZPE= 31.5488000000
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H -1.152209 2.329567 -0.445535
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Cl -1.458815 -0.638427 -0.016392
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H -1.194695 1.740821 0.154323
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C 1.930105 -0.459612 0.000056
H 3.026974 -0.568914 0.000230
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Cl -2.074135 -0.205918 0.000018

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E= -650.5896490400 ZPE= 27.0123700000
C 0.105403 -1.618193 -0.007123
C -0.488734 -0.513201 -0.004422
C -1.412143 0.624624 -0.028395
H -0.982754 1.629665 -0.081940
H -0.116393 -2.669982 -0.017400
O -2.589028 0.370254 0.026652
Cl 1.844381 0.480048 0.006293

H 1.229735 -1.041908 0.018793
 TS118
 E= -650.5922793800 ZPE= 28.7819000000
 C -0.053340 1.576959 -0.000003
 C -1.320370 1.004821 0.000009
 C -1.437948 -0.220675 -0.000007
 H -0.021483 -1.295085 0.000022
 H 0.381282 1.947835 -0.918620
 O -1.127248 -1.431560 0.000000
 Cl 1.479227 -0.312636 0.000001
 H 0.381279 1.947916 0.918582
 TS119
 E= -650.5889949600 ZPE= 27.0808600000
 C -1.678136 -1.246935 0.070557
 C -0.486967 -0.995307 -0.212004
 C -1.603457 0.492835 0.339816
 H -1.051132 0.833585 1.216809
 H -2.657354 -1.670116 0.152306
 O -2.392418 1.105421 -0.287912
 Cl 2.591782 0.167199 -0.005337
 H 1.398895 -0.352766 -0.165312
 TS120
 E= -650.5919409100 ZPE= 29.0648800000
 C 0.462503 0.868138 -0.327742
 C -0.714023 0.998932 0.480463
 C -2.357692 0.038911 -0.302420
 H -0.627521 0.568506 1.479907
 H 0.297118 0.840292 -1.399398
 O -1.834786 -0.921484 0.051275
 Cl 1.747262 -0.429248 0.029568
 H 0.960503 1.824414 -0.095166
 TS121
 E= -650.5890842500 ZPE= 27.5074900000
 C -1.863775 0.389270 -0.008016
 C -2.122912 1.572106 0.019235
 C -1.813769 -1.022857 -0.058453
 H 2.380777 0.428372 -1.205426
 H -2.350242 2.609033 0.044667
 O -0.616149 -1.551152 0.026213
 Cl 2.328653 0.273214 0.065939
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 TS122
 E= -650.5914090400 ZPE= 29.0184200000
 C -0.183482 0.555958 0.000000
 C -0.850830 1.710403 0.000000
 C 1.274092 0.548414 0.000000
 H -0.285438 2.630887 0.000000
 H -1.929178 1.756713 0.000000
 O 1.915962 -0.582995 0.000000
 Cl -1.004389 -1.002909 0.000000
 H 2.522849 0.437163 0.000001
 TS123
 E= -650.5914339800 ZPE= 29.0372000000
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 C -0.793709 0.975370 -0.036582
 C 1.619395 0.058429 -0.289375

H 0.074092 1.050545 1.157848
H -1.370847 1.717753 -0.567290
O 2.158317 -0.908645 0.082082
Cl -1.525009 -0.602332 0.002897
H 1.039697 2.083763 -0.009132
TS124
E= -650.5913934200 ZPE= 29.1901400000
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C 1.135614 0.532105 -0.258691
C 2.227025 -0.106124 -0.005519
H -0.862796 0.951504 -0.760428
H -0.602879 0.334145 0.932125
O 3.276354 -0.619548 0.060257
Cl -2.571754 -0.375108 -0.008440
H -0.230026 1.956066 0.471746
TS125
E= -650.5866472500 ZPE= 26.7651400000
C -0.216220 1.186575 -0.090672
C 0.565686 0.248449 0.159829
C 1.975896 -0.127580 0.409858
H 2.241391 -0.162302 1.478830
H -0.470110 -0.525809 0.193484
O 2.749876 -0.408555 -0.461961
Cl -2.172827 -0.350086 -0.031885
H -0.784403 2.063338 -0.308666
TS126
E= -650.5870927700 ZPE= 27.0561900000
C -2.367938 -0.928070 -0.531610
C -1.478233 -0.992679 0.354342
C -1.643660 0.695385 0.149816
H 1.257066 0.482205 -0.225059
H -0.665788 -1.314521 0.974735
O -0.619494 1.265312 -0.073663
Cl 2.344940 -0.183533 -0.028238
H -2.560312 1.182065 0.484378
TS127
E= -650.5879621700 ZPE= 27.7246300000
C 0.442053 1.677206 0.000005
C 1.300595 0.819960 -0.000047
C 2.462931 0.021797 0.000058
H -1.312278 0.028961 -0.000478
H 1.349455 -1.561833 -0.000106
O 2.283909 -1.275036 0.000002
Cl -2.546078 -0.344554 0.000023
H -0.258594 2.476791 0.000073
TS128
E= -650.5896156700 ZPE= 28.7690100000
C -0.602811 0.921644 -0.613082
C 0.521694 0.867620 0.297368
C -1.790481 -0.774559 -0.463526
H 1.034944 1.816697 0.074639
H 0.325547 0.858875 1.368502
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Cl 1.729065 -0.463669 -0.014376
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TS129

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C -2.254072 0.234410 0.364837
H -2.609556 0.787145 1.231336
H 1.586632 0.382785 -0.327827
O -3.117421 -0.577514 -0.214507
Cl 2.849868 -0.214382 0.086715
H -3.972185 -0.560703 0.235736
TS130
E= -650.5862725000 ZPE= 27.0843500000
C -2.773042 0.423286 0.282956
C -3.024051 -0.683869 -0.257873
C -1.214265 -0.253889 0.157187
H -0.954506 -1.106222 0.786288
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Cl 2.805944 -0.062399 0.054424
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C 0.068434 0.184914 0.033319
H 0.181052 1.944726 -0.734593
H 3.086953 -1.100788 -0.107185
O 0.192740 1.497319 0.119569
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TS132
E= -650.5926799600 ZPE= 31.5571700000
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C -1.492999 -0.024857 -0.460576
H 1.295349 1.798050 0.449503
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O -1.811741 -0.485364 0.609174
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H -2.175645 -0.098871 -1.322933
TS133
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C -1.675148 0.014645 0.000000
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H 0.308292 2.912180 0.000000
O -1.750921 -1.178391 0.000000
Cl 1.539012 -0.672314 0.000000
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E= -650.5900487900 ZPE= 29.9987700000
C -0.248772 1.814526 -0.337362
C 0.012358 0.632990 0.375731
C -1.401335 -0.109350 0.283451
H -2.163194 0.394922 0.891639
H 0.412031 1.959105 -1.198712

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O -1.577820 -1.091193 -0.356018
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TS135
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C -1.304809 -0.139710 -0.349535
H -1.056214 -0.465672 -1.371707
H -0.437985 0.794590 1.425638
O -2.397725 -0.262195 0.139412
Cl 1.383721 -0.603276 0.048287
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TS136
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H 0.332993 -1.460573 0.000000
H 0.706927 1.813749 0.000000
O 2.939106 -0.179396 0.000000
Cl -2.143434 -0.100827 0.000000
H 1.513007 1.850426 -0.000001
TS137
E= -650.5862418400 ZPE= 28.0772500000
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C 2.533572 -0.434750 0.000000
C -1.360415 -0.614416 -0.000001
H 2.971014 0.551536 -0.000001
H 3.210017 -1.286417 0.000000
O -2.498916 -0.490935 0.000000
Cl -0.024869 0.991438 0.000000
H -0.415001 -1.287930 -0.000001
TS138
E= -650.5887816400 ZPE= 29.6996200000
C -0.361809 -0.555585 0.023040
C 0.375745 0.730976 -0.106409
C -2.300501 -0.318462 -0.611497
H 0.330313 1.188510 -1.089018
H 0.345013 1.467777 0.692079
O -2.519347 0.183226 0.401556
Cl 1.978649 -0.143260 0.015986
H -0.438200 -0.828258 1.081929
TS139
E= -650.5867991900 ZPE= 28.6404200000
C -0.346414 1.892876 -0.290427
C -0.053690 0.588128 0.069509
C 1.368866 0.047454 0.221817
H 2.058966 0.772291 0.691742
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O 1.733392 -1.002378 -0.217319
Cl -1.288947 -0.691870 0.014433
H -0.405284 1.359053 0.973771
TS140
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O -2.670683 -0.294553 0.000005
Cl 1.813997 -0.451045 0.000001
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E= -650.5869652600 ZPE= 29.0395900000
C -0.504122 0.772580 -0.052210
C 0.345425 -0.252275 0.036017
C -1.937175 0.533726 0.087053
H -3.141133 0.185163 0.213072
H -0.164353 1.794124 -0.137457
O -2.406156 -0.684274 -0.078097
Cl 2.065907 -0.091682 -0.002247
H 0.009550 -1.270683 0.162193
TS142
E= -650.5865362400 ZPE= 28.8503500000
C 0.050823 0.503902 0.211944
C 0.244936 1.829617 -0.089408
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Cl -1.530195 -0.498438 -0.105219
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E= -650.5856216700 ZPE= 28.5760200000
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O -2.312584 -0.578241 0.086928
Cl 1.426447 -0.677040 0.005483
H 0.076275 0.964658 1.143539
TS144
E= -650.5865088700 ZPE= 29.1636100000
C 1.111456 -0.710416 0.263443
C 2.311660 -0.426217 -0.142784
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H 2.683488 0.506247 -0.537595
H 3.001412 -1.264873 -0.052490
O -1.682259 -1.139264 -0.419035
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TS145
E= -650.5854204800 ZPE= 28.6896100000
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H -0.550675 2.318283 -0.010358
O 2.261750 -0.343761 0.096084
Cl -1.659382 -0.380847 0.021471

H 2.063400 -1.470786 -0.175333
 TS146
 E= -650.5837848600 ZPE= 27.7445700000
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 O -0.314819 1.373331 0.000000
 Cl 1.657212 -0.280301 0.000000
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 TS147
 E= -650.5852676600 ZPE= 28.6852600000
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 C 0.438437 -0.165608 0.649062
 C -1.793343 0.221628 -0.100083
 H -0.794494 0.868118 -1.075713
 H 0.123048 -1.176627 0.854978
 O -2.664895 -0.541806 -0.166774
 Cl 1.991487 -0.131229 -0.191788
 H -0.500669 1.854890 0.353390
 TS148
 E= -650.5834805400 ZPE= 27.5710400000
 C 1.136543 -0.714034 -0.030760
 C 2.331738 -0.945738 -0.050363
 C 0.293869 0.865286 0.401769
 H 0.038128 -1.053289 -0.161267
 H 3.383571 -1.112273 -0.069325
 O 0.448123 1.784830 -0.287327
 Cl -1.741466 -0.471637 -0.048655
 H 0.025345 0.671665 1.432461
 TS149
 E= -650.5861158100 ZPE= 29.3156300000
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 C 1.667234 -0.226277 0.000023
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 Cl -0.988592 -1.195547 -0.000013
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 E= -650.5852275500 ZPE= 29.3103500000
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H 0.282917 1.874858 -0.340870
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TS152
E= -650.5798880100 ZPE= 25.9787500000
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C -1.905344 -0.134348 -0.149950
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H -1.463232 1.066795 -0.149434
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Cl 1.965703 -0.514410 0.013361
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TS153
E= -650.5841079100 ZPE= 28.6962600000
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C 1.443172 1.139995 0.227934
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Cl -1.667320 -0.402648 0.130297
H -1.042075 1.757005 0.254409
TS154
E= -650.5877962800 ZPE= 31.0235900000
C -0.300205 0.230006 0.596438
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H 0.386570 2.183745 -0.358784
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C -0.919490 -0.572138 -0.381411
H -1.238228 -1.307046 -1.114294
H -2.394086 -0.028148 1.488971
O 0.413813 -0.978875 0.007989
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H -1.315579 1.780318 -0.862897
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TS157

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C 0.070690 0.440866 0.045505
C 0.172794 1.798574 -0.039446
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E= -650.5839647600 ZPE= 28.8770900000
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H 0.206191 2.616578 -0.087844
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Cl -1.570719 -0.572248 0.018998
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H -0.035860 -1.202611 0.374365
TS162
E= -650.5870641800 ZPE= 31.3381400000
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Cl -1.736644 -0.421441 -0.059911
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E= -650.5822635700 ZPE= 28.3972300000
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Cl 1.477537 -0.618295 0.035906
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TS164
E= -650.5835271700 ZPE= 29.2268100000
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C -0.983017 -0.866669 0.369411
H -1.361294 1.703694 0.711219
H 0.046303 2.216307 -0.298763
O -2.022679 -0.581957 -0.252082
Cl 1.671292 -0.226356 -0.068280
H -1.631754 0.640718 -0.675575
TS165
E= -650.5778285100 ZPE= 25.6767200000
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C -2.373704 -0.869515 0.000001
C 0.316898 1.764745 -0.000001
H -2.649413 -1.923218 -0.000001
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Cl 1.809542 -0.559561 0.000000
H 0.116936 -0.755951 0.000001
TS166
E= -650.5860856800 ZPE= 30.8728100000
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C -1.445852 -0.211494 -0.359558
H -1.261801 -0.437381 -1.424409
H -0.244461 -0.075249 1.484230
O -2.547055 -0.203999 0.126349
Cl 1.641723 -0.415540 -0.028635
H 0.474341 1.446704 -1.074373
TS167
E= -650.5852216000 ZPE= 30.3846500000
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C -0.044783 0.332026 0.061327
C 0.938849 -0.597068 -0.186240
H 0.708421 -1.517098 -0.718931
H 2.536576 -0.734476 0.890635
O 2.259987 -0.377249 0.038025
Cl -1.718538 -0.297117 0.048158
H 1.241715 1.928076 0.147765
TS168
E= -650.5854916300 ZPE= 30.7220200000
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C -1.508161 -1.118113 0.054011
C -0.672853 0.087978 0.107199
H -2.521233 -0.827583 0.342311
H -1.132872 -1.872653 0.738393
O -0.759155 1.225694 -0.543403
Cl 1.434898 -0.361083 -0.087073
H -1.538717 -1.512570 -0.960097
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E= -650.5792998900 ZPE= 26.8555900000
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C 0.329570 -1.747217 -0.000426
C 1.321090 0.752972 -0.091571
H -0.946343 -1.492999 0.104150
H 0.861603 -2.681262 0.022222
O 2.502068 0.613009 0.109324
Cl -2.008314 0.392513 0.024272
H 0.794226 1.700560 -0.235821
TS170
E= -650.5809058300 ZPE= 28.0875500000
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C 1.874815 -1.639856 0.000000
C 1.272911 0.814979 0.000000
H 2.252176 1.282876 0.000000
H -0.619977 1.049903 0.000000
O 0.286566 1.609011 0.000000
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E= -650.5834776900 ZPE= 29.7731200000
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C 0.728542 0.794847 -0.172546
C -1.693759 0.026481 0.501651
H 1.076813 1.776039 -0.443566
H -3.423998 -0.638364 0.205895
O -2.645095 -0.451599 -0.326749
Cl 1.997386 -0.394450 0.023616
H -1.418276 1.332675 0.483275
TS172
E= -650.5855035100 ZPE= 31.1089600000
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C -1.615947 0.889787 0.164635
C -1.121925 -0.078525 -0.667573
H -0.683713 0.094252 -1.638419
H -2.170225 0.635395 1.052590
O -0.743083 -1.207263 0.024460
Cl 1.592203 0.200150 -0.061191
H -1.611242 1.924645 -0.152006
TS173
E= -650.5843263300 ZPE= 30.5220700000
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C 0.223955 -0.604209 -0.106235
C -0.937122 0.113131 0.013030
H -2.376610 -0.907576 0.851901
H 0.188265 -1.658167 -0.346888
O -2.104262 -0.682286 -0.042639
Cl 1.808637 0.001901 0.036178

H -1.920997 1.869295 -0.273463
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C 1.562414 -0.878426 0.000005
C 2.878605 -0.575450 -0.000006
H 1.000324 -1.796222 0.000014
H 2.429470 0.924180 -0.000011
O 0.406931 1.308453 0.000003
Cl -2.345380 -0.256980 -0.000002
H -1.299017 0.517567 0.000010
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E= -650.5776162100 ZPE= 26.8425400000
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C -2.432568 -1.220375 0.000006
C -1.221386 0.252852 0.000005
H -0.893134 -0.904711 0.000025
H 1.431471 0.439053 0.000028
O -0.343508 1.087717 0.000008
Cl 2.546398 -0.229199 -0.000004
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E= -650.5821901900 ZPE= 29.7942100000
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C -1.923349 -1.012990 -0.122277
C -0.103368 0.885112 0.496923
H -2.072852 -1.215221 -1.176519
H -2.535682 -1.543112 0.601738
O -0.412173 1.625502 -0.451152
Cl 1.514931 -0.544819 -0.082310
H 0.374924 1.154560 1.433936
TS177
E= -650.5827059900 ZPE= 30.1537800000
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C 0.030451 0.416485 0.364525
C 1.202334 -0.284792 -0.364972
H 0.986741 -0.556985 -1.408796
H 0.175657 0.350592 1.440734
O 2.242310 -0.503012 0.182961
Cl -1.481548 -0.547727 -0.002875
H -0.083235 2.506560 0.439166
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E= -650.5790295200 ZPE= 27.9932600000
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C -2.298549 -0.427838 0.000000
C 0.256035 0.166358 0.000000
H -1.076030 1.125892 0.000000
H -2.618020 -1.444081 0.000000
O -0.292806 -0.900664 0.000000
Cl 2.047905 0.148419 0.000000
H -2.999548 1.603533 0.000000
TS179
E= -650.5795856000 ZPE= 28.5789700000
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C 1.753548 0.472777 0.397279

H 0.904556 0.258946 1.059400
H 0.834441 -2.155091 0.119582
O 2.597525 0.419326 -0.382770
Cl -1.669698 0.614853 -0.018715
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TS180
E= -650.5797418000 ZPE= 28.7355300000
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H 1.637786 -0.918919 0.799888
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E= -650.5787044000 ZPE= 28.6804500000
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C -2.193568 -0.966399 -0.079535
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H -1.745633 -1.858894 0.314071
H -3.182835 -0.975094 -0.513516
O -1.181358 1.293379 -0.144359
Cl 1.915687 -0.164086 -0.245694
H 0.750637 0.770970 1.437936
TS182
E= -650.5785927900 ZPE= 28.6182400000
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C 2.264720 -0.693531 -0.022718
C 0.030660 0.760182 0.175811
H 2.579544 -1.333454 -0.841580
H 2.906117 -0.626706 0.849041
O -0.293233 1.882254 -0.153864
Cl -1.410989 -0.803084 -0.013294
H 0.136732 0.472401 1.288595
TS183
E= -650.5774667800 ZPE= 28.0282700000
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Cl 3.231414 -0.125184 -0.001250
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H 2.180867 1.032125 1.075672
H 3.155482 -0.017313 -0.031767
O -2.834782 0.031663 0.115070
Cl 0.852346 -0.600503 -0.019846
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 H 1.657489 -2.225033 -0.000010
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 Cl -1.184950 -0.806871 0.000001
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 E= -650.5755971300 ZPE= 27.8167100000
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 E= -650.5769508800 ZPE= 28.7731800000
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 O 2.358823 -0.778302 -0.419802
 Cl -2.004597 -0.455367 0.064573
 H 2.168753 -0.126986 1.512790
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 E= -650.5779703000 ZPE= 29.7396700000
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 H 1.891554 -2.018042 -0.064931
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 E= -650.5753678500 ZPE= 28.5454200000
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 C -0.382205 1.101613 -0.167268
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 H 2.024000 -0.206702 1.511756
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E= -650.5719323700 ZPE= 26.6636200000
C -0.167995 1.465814 -0.000443
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Cl 1.598142 -0.135827 0.000127
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Cl 1.963478 -0.215069 0.000000
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C 0.940423 -0.480543 0.398787
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E= -650.5670439100 ZPE= 26.1094000000
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H -1.539314 1.883867 0.121939
H 0.210762 2.337602 -0.332916
O -1.100764 -0.585731 0.669726
Cl 1.460436 -0.274134 -0.035717
H -2.449181 -0.885775 -0.767861
TS215
E= -650.5690192500 ZPE= 29.4644200000
C 0.494689 0.058764 0.004284
C -2.223452 1.090221 -0.042229
C -2.002142 -0.131350 0.012483
H -2.679476 2.029219 0.148613
H 0.023037 0.116957 0.962417
O -1.504689 -1.238086 0.000554
Cl 2.180216 0.089604 -0.000769
H 0.015713 0.129427 -0.949617
TS216
E= -650.5682165200 ZPE= 29.3318500000
C 0.385136 0.843274 0.496314
C 1.058709 1.682173 -0.238584
C 0.801168 -0.742128 0.421731
H 1.009396 2.006540 -1.266661
H 0.007152 1.066803 1.482462
O 1.485008 -1.241300 -0.399571
Cl -1.575027 -0.154716 -0.142457
H 0.408773 -1.212687 1.325760
TS217
E= -650.5631777000 ZPE= 26.2927900000
C -0.038002 0.594597 0.000000
C -0.036333 1.925325 -0.000003
C 1.144879 -0.189041 0.000002
H -1.014081 2.401415 -0.000007
H 1.815891 1.758376 0.000009
O 1.772348 -1.143145 -0.000003
Cl -1.401223 -0.601718 0.000001
H 2.416939 1.229279 0.000015
TS218
E= -650.5693357500 ZPE= 30.2373000000
C -0.036471 0.324676 0.520028
C 0.877184 1.201744 -0.110338
C 1.887380 -0.272275 -0.277139
H 1.360838 1.930470 0.529225
H 0.638502 1.550322 -1.105414

O 1.051439 -1.157710 0.044363
Cl -1.577153 -0.109901 -0.126608
H 0.032202 0.124324 1.578312
TS219
E= -650.5659900400 ZPE= 28.1807900000
C -0.476809 1.970121 -0.059295
C -0.329425 0.693843 0.112167
C -1.158038 -0.503973 -0.377578
H -0.814170 -0.901769 -1.340427
H 0.174679 2.812337 -0.231137
O -2.062815 -0.944362 0.257918
Cl 1.696726 -0.462826 0.018688
H 0.083309 0.552427 1.138766
TS220
E= -650.5694798000 ZPE= 30.3718400000
C -0.820969 1.276881 0.222414
C 0.313941 0.634604 -0.406899
C 1.268740 -0.276225 0.278249
H 0.909575 -0.805903 1.173746
H 0.672575 0.992890 -1.371834
O 2.432379 -0.263559 -0.056453
Cl -1.457982 -0.546678 -0.071585
H -0.825755 1.403454 1.304070
TS221
E= -650.5629037100 ZPE= 26.2723600000
C -0.015904 0.367041 -0.095626
C -0.199165 1.720590 -0.280051
C -1.169805 -0.310627 -0.010977
H 0.586972 2.330609 -0.708003
H 0.226850 2.482961 1.293142
O -2.162587 -0.885932 0.039124
Cl 1.487829 -0.637679 0.032152
H -0.496966 2.452404 0.875200
TS222
E= -650.5669165700 ZPE= 28.7935300000
C 0.960915 -1.166141 0.422229
C -1.417353 0.611376 0.901267
C 1.678994 -0.163389 0.055407
H -1.869025 0.080580 1.721176
H -0.970123 1.585431 1.003918
O 2.151167 0.870641 -0.267602
Cl -1.345972 -0.124949 -0.557097
H 1.176009 -2.198071 0.612945
TS223
E= -650.5601828000 ZPE= 24.6145000000
C 3.628957 -0.469912 -0.000003
C 2.352545 -0.184516 0.000000
C 1.200457 0.438540 0.000001
H 1.232425 -0.982165 0.000010
H -1.779533 0.400163 -0.000002
O 0.232125 1.104197 0.000000
Cl -2.844165 -0.320565 0.000000
H 3.949159 -1.506644 0.000003
TS224
E= -650.5605708200 ZPE= 25.0985800000
C -2.137450 -0.218127 -0.000101

C -1.424006 -1.209500 0.000120
C 0.879232 1.489642 0.000052
H -1.107355 0.670461 0.000683
H -0.739650 -2.025396 0.000284
O -0.303248 1.623394 -0.000006
Cl 1.379456 -0.722579 -0.000049
H -3.084420 0.279527 -0.000505
TS225
E= -650.5691914500 ZPE= 30.6086900000
C 0.727757 1.316081 0.053774
C 1.966080 -0.405900 -0.468447
C 0.043038 0.142835 0.171890
H 0.301304 2.214014 -0.365029
H 2.801707 -0.526168 0.260500
O 0.843240 -0.904663 0.254500
Cl -1.640963 -0.128992 -0.066296
H 1.626187 1.424221 0.652264
TS226
E= -650.5630128300 ZPE= 26.8783500000
C 1.104377 0.053961 -0.345895
C 2.137472 -0.394218 0.255539
C -0.144423 0.604607 -0.056933
H 2.937648 -1.174660 -0.579860
H 3.265202 -0.392507 -0.560847
O -0.490656 1.736694 0.069247
Cl -1.378638 -0.782539 0.015088
H 2.574681 -0.609321 1.213959
TS227
E= -650.5685726200 ZPE= 30.4721100000
C -1.584034 0.998528 0.280836
C 0.035107 -0.269096 -0.189817
C -1.308460 -0.117166 -0.567991
H -1.799745 -0.509193 -1.452389
H -1.556057 0.858996 1.346191
O -0.687071 -1.207381 0.410465
Cl 1.638081 0.216504 -0.010071
H -1.850683 1.955082 -0.144473
TS228
E= -650.5694251100 ZPE= 31.0146100000
C -0.367676 0.700678 -0.124407
C 0.525955 1.692788 -0.001523
C -1.556991 0.273185 0.056740
H 0.298490 2.545004 0.633004
H 1.447302 1.692105 -0.558185
O -2.239576 -0.816100 -0.048761
Cl 1.630221 -0.766097 0.028385
H -3.150671 -0.684571 0.247869
TS229
E= -650.5604387400 ZPE= 25.4976700000
C 1.247300 -0.329827 -0.000001
C 2.142132 -1.174442 0.000001
C 1.072978 1.269505 -0.000002
H 2.895094 -1.926565 0.000003
H 0.067618 -0.659106 -0.000004
O -0.091222 1.672477 0.000001
Cl -1.654559 -0.605552 0.000000

H -0.879884 0.908816 0.000006
 TS230
 E= -650.5682828900 ZPE= 30.5286400000
 C -1.817949 -0.569209 -0.602494
 C -0.885223 0.810780 0.024869
 C 0.452218 0.924137 -0.147306
 H -1.530358 1.671076 -0.020867
 H -1.533638 -1.610110 -0.862302
 O -1.432587 -0.341261 0.662070
 Cl 1.596638 -0.364534 0.020738
 H 0.887579 1.871953 -0.416341
 TS231
 E= -650.5677163900 ZPE= 30.2178200000
 C -0.353817 -0.280139 -0.000270
 C 2.361747 -0.694410 0.000145
 C 0.366389 0.789437 0.000160
 H 3.433670 -0.875398 -0.000148
 H 1.592126 -1.476922 0.000596
 O 1.985977 0.474043 -0.000183
 Cl -2.091948 -0.128905 0.000020
 H 0.403590 1.862028 0.000472
 TS232
 E= -650.5652906000 ZPE= 28.7089800000
 C 1.230154 -0.018714 -0.020896
 C 2.387706 -0.683181 0.161994
 C -0.029057 0.387349 0.003547
 H 2.115807 0.765421 0.150549
 H 2.945462 -0.826885 -0.773260
 O -0.390960 1.697882 -0.102836
 Cl -1.324144 -0.798454 -0.003772
 H -0.955956 1.939395 0.641656
 TS233
 E= -650.5651810400 ZPE= 28.6681700000
 C -0.880431 -0.025739 1.020395
 C 1.979583 1.124023 -0.121242
 C 1.788035 -0.119339 -0.120773
 H 2.593047 1.924197 0.221574
 H 0.182150 0.089059 1.014281
 O 1.365018 -1.244686 -0.137674
 Cl -1.738213 0.126338 -0.395855
 H -1.468833 -0.077198 1.924784
 TS234
 E= -650.5629252000 ZPE= 27.4644800000
 C -2.697445 -0.029507 -0.000241
 C -1.680179 -0.878389 0.000058
 C -1.671195 1.091832 0.000022
 H 1.389644 0.180110 0.000108
 H -1.437938 -1.935232 0.000166
 O -0.645543 0.140657 0.000308
 Cl 2.663202 -0.022651 -0.000074
 H -3.768888 -0.088680 -0.000516
 TS235
 E= -650.5645143700 ZPE= 28.6491300000
 C -2.514661 -0.475593 0.165182
 C -1.204849 -0.218112 -0.020685
 C -0.000950 0.332646 -0.004838

H 0.580559 2.016471 0.705348
H -1.356147 -1.391808 0.124560
O 0.174415 1.678593 -0.103009
Cl 1.455455 -0.658016 -0.004175
H -3.039715 -0.700784 -0.772818
TS236
E= -650.5615895000 ZPE= 26.8669900000
C 1.003180 0.617471 -0.001024
C -0.166324 1.154356 -0.107969
C 2.213272 0.214884 0.152080
H -0.410361 2.178366 0.146477
H -1.289285 0.370304 -0.233904
O 2.916876 -0.837731 -0.089525
Cl -2.574959 -0.415627 0.021700
H 3.838169 -0.701426 0.176215
TS237
E= -650.5615905300 ZPE= 27.0600500000
C -0.600748 0.743693 -0.525596
C 0.308354 1.130785 0.636631
C -1.650814 -0.041377 -0.184310
H 0.433334 -0.089957 -0.710813
H -0.708300 1.403278 -1.378368
O -2.481905 -0.723744 0.215787
Cl 1.868075 -0.414883 -0.041894
H 0.032170 0.531041 1.514730
TS238
E= -650.5583984300 ZPE= 25.1343000000
C 0.565821 -0.515627 0.000002
C -0.529210 0.136964 0.000001
C 1.847393 0.082788 0.000000
H 1.510550 1.311543 0.000001
H -0.153306 1.466686 0.000003
O 2.997610 -0.200695 -0.000001
Cl -2.192166 -0.082443 -0.000001
H 0.624671 2.004117 -0.000002
TS239
E= -650.5647316200 ZPE= 29.1554100000
C 0.256385 -0.666481 0.000000
C -0.513164 0.393046 0.000000
C 2.543654 -0.471451 0.000000
H -0.255412 1.438083 -0.000001
H 2.690154 -1.033194 -0.934064
O 2.343409 0.730816 0.000000
Cl -2.211378 -0.044053 0.000000
H 2.690155 -1.033195 0.934062
TS240
E= -650.5605733500 ZPE= 26.7800800000
C -1.515418 -0.275088 -0.604126
C -1.368229 -1.303227 0.276391
C 1.277656 -0.500831 -0.139151
H -1.030805 -1.253736 1.310310
H -1.859967 -2.225810 -0.018912
O 2.389850 -0.348387 -0.004744
Cl -0.398755 1.168632 0.104502
H 0.186764 -1.125222 -0.228659
TS241

E= -650.5611664900 ZPE= 27.2323100000
C -0.405361 -0.073724 -0.045932
C 0.143375 1.121471 -0.183222
C 2.290598 0.318140 0.160515
H 1.331711 1.148089 -0.391090
H 0.074216 -1.041170 0.004780
O 2.518943 -0.798030 -0.108020
Cl -2.152610 -0.171259 0.049538
H 2.865227 0.993400 0.820151
TS242
E= -650.5674615300 ZPE= 31.2013700000
C -2.391609 -0.276641 0.282191
C 0.573657 0.939701 0.063907
C -0.708656 0.769664 -0.150863
H 1.016794 1.897502 0.267691
H -2.754983 -1.151071 0.807063
O -1.280791 -0.431098 -0.412767
Cl 1.770178 -0.384298 0.050156
H -2.948859 0.639080 0.203306
TS243
E= -650.5638820600 ZPE= 29.7057300000
C -0.461852 -0.947444 -0.088069
C 0.743456 -0.284481 0.097283
C 2.172309 -0.259515 -0.116974
H 2.853378 -0.441339 0.703512
H 0.311603 -0.831440 1.129199
O 1.328271 0.949460 0.048493
Cl -1.827751 0.177872 -0.026794
H 2.557145 -0.398080 -1.118612
TS244
E= -650.5603884000 ZPE= 27.7438400000
C -1.615572 0.052581 -0.208403
C -1.728464 1.301980 0.177297
C 2.149169 0.902510 -0.332957
H -2.656697 1.834504 0.012172
H -0.929865 1.851239 0.677212
O 1.974755 0.008811 0.402384
Cl -0.384322 -1.086006 -0.030993
H 1.491199 1.163432 -1.197201
TS245
E= -650.5620127900 ZPE= 28.9633400000
C -1.246592 1.059807 -0.342519
C -0.160783 1.346317 0.382156
C -0.695581 -1.554535 0.140304
H 0.308986 2.286709 0.098532
H -0.044903 1.053058 1.410608
O -1.508094 -0.725571 0.071084
Cl 1.519091 -0.209016 -0.103702
H -1.406140 0.908541 -1.394521
TS246
E= -650.5543954800 ZPE= 24.2854800000
C 2.743380 0.495143 -0.000129
C 1.529958 0.485848 0.000255
C -1.080036 -1.412120 -0.000087
H 0.462965 0.897343 0.000460
H 0.948569 -0.722808 0.000171

O 0.091379 -1.615503 0.000044
Cl -1.477061 0.876056 -0.000038
H 3.807671 0.443311 -0.000566
TS247
E= -650.5610661300 ZPE= 28.5083900000
C 0.146941 0.352051 0.589790
C -0.720053 1.273821 -0.212848
C -1.307602 0.128501 -0.110096
H -0.713535 2.281821 -0.579488
H -0.867960 -0.897277 0.571183
O -2.008732 -0.942617 -0.092166
Cl 1.683920 -0.288658 -0.147080
H 0.308996 0.537339 1.644916
TS248
E= -650.5589043500 ZPE= 27.2806800000
C -0.538737 1.103703 -0.020113
C 0.869425 1.020399 -0.125689
C -1.384860 0.050688 0.116493
H 0.417302 -1.130340 1.084502
H -1.001945 2.063318 0.179390
O -2.258132 -0.697517 -0.093950
Cl 1.380748 -0.593489 -0.045553
H 1.502017 1.687728 0.437954
TS249
E= -650.5582871000 ZPE= 26.9478300000
C -2.818206 -0.209592 -0.000061
C -1.828753 -0.894304 -0.000112
C -0.109100 1.578840 0.000314
H -3.726866 0.342647 0.000049
H -0.886082 -1.413914 -0.000138
O 1.009129 1.654920 -0.000293
Cl 1.538123 -0.941100 0.000047
H -1.071827 0.980933 0.000793
TS250
E= -650.5645259400 ZPE= 30.8648800000
C -0.007711 1.333688 -0.034265
C -1.363720 0.951059 0.234963
C 0.739460 0.229171 -0.213432
H 2.205496 -0.232417 0.917927
H -2.098765 1.040718 -0.564946
O 1.973459 -0.216919 -0.023690
Cl -0.733100 -0.971027 -0.003395
H 0.360121 2.351002 -0.029339
TS251
E= -650.5590647400 ZPE= 27.4518500000
C 0.117207 1.620704 0.061180
C 1.231469 0.933461 -0.063850
C -1.893498 -0.176395 0.400500
H -1.027800 0.597391 0.254598
H 2.117530 1.546595 -0.216128
O -2.747314 -0.290757 -0.408532
Cl 1.529332 -0.785782 -0.030181
H -1.840925 -0.726247 1.355887
TS252
E= -650.5572809200 ZPE= 26.9384100000
C 0.995750 -0.651058 0.522445

C 1.796771 -1.298031 -0.401343
C 0.524446 0.747379 0.227616
H -0.150030 -1.101130 0.147789
H 1.897653 -0.770239 -1.356813
O 0.699667 1.812218 -0.135942
Cl -1.660402 -0.267167 -0.081243
H 0.980066 -0.874278 1.585369
TS253
E= -650.5596165000 ZPE= 28.6962200000
C -0.944888 0.563112 -0.381528
C 0.249460 1.087459 0.127672
C -1.995327 -0.124180 -0.022230
H 0.865163 1.702118 -0.514299
H 0.710812 0.722486 1.051235
O -2.994734 -0.707031 0.091843
Cl 2.301310 -0.454368 -0.010007
H -0.595847 1.797562 0.554948
TS254
E= -650.5541983600 ZPE= 25.3858700000
C 0.085790 0.317044 0.000000
C -0.420191 1.490900 0.000000
C -0.966378 -0.759400 0.000000
H -1.874633 1.397585 0.000000
H -2.633181 0.931741 0.000000
O -2.133625 -0.769454 0.000000
Cl 1.733891 -0.292786 0.000000
H -0.094662 2.512396 0.000000
TS255
E= -650.5581150300 ZPE= 28.5622200000
C -1.192310 0.077847 0.142340
C -2.218735 -0.717579 -0.059316
C 0.438800 0.679891 0.638416
H -2.451734 -1.505226 0.638290
H -2.856088 -0.570541 -0.921574
O -0.547363 1.091333 -0.386220
Cl 1.645883 -0.405000 -0.129899
H -0.459814 -0.010861 1.252688
TS256
E= -650.5616415800 ZPE= 30.8269700000
C -0.368240 0.836819 0.384957
C -1.418518 0.635406 -0.492761
C -0.841220 -0.420455 0.762341
H -1.054332 -0.906012 1.707012
H -2.246433 1.156654 -0.940889
O -1.424157 -0.839299 -0.401157
Cl 1.793298 -0.090003 -0.142923
H -0.024163 1.683181 0.945599
TS257
E= -650.5615851800 ZPE= 30.9145300000
C -1.412002 0.673580 0.783145
C 0.302899 -0.841904 0.204861
C -0.955641 -0.731743 -0.298359
H -1.647297 -1.563201 -0.286344
H 0.621397 -1.777463 0.642037
O -1.431238 0.509887 -0.633903
Cl 1.592574 0.273986 -0.035595

H -2.209500 0.004206 1.182769
TS258
E= -650.5609229000 ZPE= 30.5590000000
C -1.925544 -0.004787 -0.046436
C -3.084367 -0.643381 0.006776
C -0.888784 0.677178 0.129385
H -3.618286 -0.771772 0.939809
H -3.508666 -1.087071 -0.884970
O 0.293267 1.008521 -0.162190
Cl 2.318780 -0.470275 0.015935
H 0.753722 1.611294 0.433434
TS259
E= -650.5594743800 ZPE= 29.6638700000
C 0.475274 -0.918794 -0.104952
C -0.713839 -0.222776 0.076749
C -1.640574 0.890731 0.004059
H -1.974574 1.381599 0.908010
H -0.214889 -0.688858 1.125992
O -2.028733 -0.537525 -0.093228
Cl 1.848598 0.215947 -0.012986
H -1.732010 1.441402 -0.922550
TS260
E= -650.5544695500 ZPE= 26.7810600000
C 0.498297 0.778160 -0.146610
C 1.940354 -1.010573 0.500376
C 1.035903 -0.566694 -0.459860
H 0.957877 -0.779718 -1.530522
H 2.325252 -1.986117 0.175751
O 0.510182 1.878777 0.111471
Cl -1.654592 -0.375677 0.068693
H -0.083840 -1.083230 -0.068208
TS261
E= -650.5586109700 ZPE= 29.4752400000
C -0.798695 1.181604 0.108146
C 0.049264 0.006635 -0.048932
C -0.877071 -0.952101 -0.059316
H -0.942557 -2.014506 0.089509
H -1.961955 0.512576 0.797107
O -2.052466 -0.149931 -0.043845
Cl 1.768599 -0.030832 0.013314
H -0.982933 1.808698 -0.761593
TS262
E= -650.5617355800 ZPE= 31.5016600000
C -0.623542 -0.131930 0.808116
C -1.044562 1.054578 0.054345
C -0.640589 -0.032071 -1.027475
H -0.496744 1.983534 0.120729
H -2.126261 1.165043 0.017552
O -1.081029 -1.041070 -0.066487
Cl 1.493021 0.013757 -0.023716
H -0.257960 -0.397348 1.786862
TS263
E= -650.5561042300 ZPE= 27.9897800000
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C -1.745792 -0.500714 0.000001
C 0.432126 -0.416067 -0.000002

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H -3.790593 -0.397222 0.000000
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Cl 2.099044 0.056367 0.000000
H -2.937164 1.254193 0.000000
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E= -650.5514500400 ZPE= 25.1567600000
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C 0.628880 1.744026 0.000000
C -1.373316 0.513022 0.000000
H 2.459248 1.842704 0.000000
H 2.867657 1.201138 0.000000
O -1.997384 -0.512634 0.000000
Cl 0.947393 -1.005400 0.000000
H -1.851411 1.499429 0.000000
TS265
E= -650.5568728400 ZPE= 28.8965800000
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C -1.884115 -1.210714 0.069601
C -0.781332 0.725292 -0.452465
H -0.639949 0.611006 -1.526678
H -1.370503 -2.139775 -0.053029
O 0.001499 1.142592 0.333089
Cl 1.990185 -0.318578 0.008046
H -2.948187 0.655414 0.436930
TS266
E= -650.5553573400 ZPE= 28.0510200000
C -0.427920 1.069529 0.145120
C 0.806294 0.948962 -0.282328
C -1.477512 -0.480817 0.075825
H -0.803255 -1.295183 -0.197415
H -0.907453 0.215550 1.024967
O -2.644060 -0.372068 -0.122469
Cl 1.799655 -0.414678 0.023703
H -1.136115 1.879660 0.117542
TS267
E= -650.5524712900 ZPE= 26.2453000000
C 0.501143 -0.037094 -0.000002
C -0.644239 -0.686508 -0.000001
C 1.915572 -0.400658 0.000000
H 2.083027 -1.488112 0.000002
H 0.503800 1.292150 -0.424267
O 2.820831 0.401588 0.000001
Cl -2.134831 0.143333 0.000001
H 0.503801 1.292152 0.424263
TS268
E= -650.5510848000 ZPE= 25.4183800000
C 0.300430 -0.058752 -0.024517
C -0.491149 0.974622 0.020487
C -1.889537 0.452797 -0.022893
H -0.354522 2.043003 0.060849
H -1.126451 -1.863725 0.088467
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H 0.782658 -0.886873 1.352369
H 1.327375 1.916584 0.094394
O 1.876051 -0.970147 -0.379302
Cl -1.523379 -0.604466 -0.043509
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TS270
E= -650.5551368200 ZPE= 28.6677400000
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O 2.554437 0.398676 0.191632
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H 0.674926 -1.608834 0.440900
H 3.164312 -1.082393 0.000019
O 0.052436 1.639390 0.000003
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C 1.712451 -0.844003 -0.372954
C 0.218495 0.487269 -0.162868
H 0.473525 0.041189 -1.251995
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O 0.262023 1.705454 -0.019177
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H -1.992023 0.965382 1.507335
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H 3.442287 -0.727370 -0.366266
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E= -650.5484078700 ZPE= 25.8343600000
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H -0.584081 1.531713 -1.248606
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O -2.961137 -0.567627 -0.307733
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E= -650.5515476200 ZPE= 27.9443200000
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C -0.717027 0.995998 -0.293610
C 1.779634 -0.036737 0.056674
H 2.679882 0.516858 -0.236395
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Cl -1.575188 -0.420383 0.053391
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TS282
E= -650.5488973400 ZPE= 26.3141400000
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C -0.326563 1.071930 -0.097750
C 1.939432 -0.048227 -0.030040
H -1.383666 0.674031 1.190586
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TS283
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H 3.039285 0.391141 0.000012
H 0.594574 -1.686116 0.419334
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E= -650.5517440700 ZPE= 28.4625900000
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H -0.173543 0.199281 1.433073
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Cl 1.562963 -0.381829 -0.070803
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H 0.199933 -1.331069 0.423457
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O -2.665457 -0.430349 -0.214153
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 H -2.990978 -0.518333 -0.615670
 O -2.269346 -1.002707 -0.195654
 Cl 1.773104 -0.433593 -0.041792
 H -0.582997 2.360904 -0.770354
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 E= -650.5451942600 ZPE= 24.9408300000
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 C -0.168563 1.628334 -0.075192
 C -1.255626 -0.518299 -0.167055
 H 1.967724 2.213693 0.057683
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 Cl 1.478438 -0.603478 0.047480
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E= -650.5493459400 ZPE= 28.6075700000
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O -2.539529 -0.538097 0.000012
Cl 1.747943 -0.413261 0.000007
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E= -650.5495446400 ZPE= 30.8798100000
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O 1.575600 0.343664 -0.391197
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E= -650.5410776600 ZPE= 25.7579100000
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H 0.511545 -0.701414 -0.000030
H 1.819961 -2.141907 -0.000024
O 0.411634 1.294729 -0.000008
Cl -2.282921 -0.253948 0.000004
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TS308
E= -650.5392944100 ZPE= 24.6881100000
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 TS309
 E= -650.5459281900 ZPE= 29.1752500000
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 O 0.108673 -0.957293 -0.224354
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 E= -650.5406510100 ZPE= 25.9185300000
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 Cl -1.999836 -0.156927 0.000000
 H 0.171260 -1.124306 0.000002
 TS311
 E= -650.5425242000 ZPE= 27.8368000000
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 C 1.850472 -1.204705 0.000000
 H 0.718685 -1.028876 -0.000003
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 O 2.414856 -0.082936 0.000001
 Cl -1.880441 -0.386375 0.000000
 H 1.713761 0.711014 -0.000002
 TS312
 E= -650.5453906600 ZPE= 29.6883300000
 C 0.642887 0.665634 -0.078789
 C -0.271917 1.454949 -0.142899
 C -1.866827 0.069352 0.599298
 H -1.199156 -0.524089 1.258831
 H -0.866928 2.319554 -0.298546
 O -2.308950 -0.706275 -0.377487
 Cl 1.850523 -0.451637 0.010233
 H -1.946067 -1.607040 -0.379999
 TS313
 E= -650.5449551200 ZPE= 29.4270400000
 C 0.856402 0.990218 0.000002
 C -1.578738 1.313972 -0.000002
 C -1.832741 -0.015625 0.000000
 H 0.259462 1.016131 -0.917505
 H 1.499476 1.865110 0.000008
 O -2.227557 -1.113193 0.000001
 Cl 1.831325 -0.513130 -0.000001

H 0.259455 1.016125 0.917504
TS314
E= -650.5404079000 ZPE= 27.1309100000
C 0.128969 0.657078 -0.203297
C 2.289920 -0.153717 -0.009867
C 3.447763 -0.083879 0.267146
H 4.476260 -0.011175 0.519526
H 0.620837 1.545061 0.230828
O 1.012377 -0.301438 -0.345390
Cl -2.761802 -0.111778 0.110098
H -1.445388 0.260957 -0.182789
TS315
E= -650.5435515700 ZPE= 29.2056900000
C 0.577211 0.551984 -0.237822
C -0.599811 -0.015904 0.156953
C -1.867276 0.186796 0.462017
H -2.738726 -0.707228 -1.001336
H 0.687816 1.493897 -0.758824
O -2.947908 -0.218493 -0.187847
Cl 2.167235 -0.218133 -0.006152
H 0.130443 0.332280 1.080637
TS316
E= -650.5368370600 ZPE= 25.3209400000
C -1.149521 -0.639226 -0.000001
C -2.503058 -0.337601 0.000001
C -3.530196 0.402568 0.000002
H -1.768827 0.925785 -0.000001
H -0.667159 -1.612372 -0.000001
O -0.477736 0.439280 -0.000002
Cl 2.810950 0.015123 0.000001
H 1.568372 0.360818 -0.000002
TS317
E= -650.5461803000 ZPE= 31.3035800000
C -1.002353 0.831351 0.445156
C 0.204694 -0.608007 0.611647
C -1.006496 -0.853309 -0.023509
H -1.663401 -1.673204 0.272396
H -1.642647 0.938160 1.309172
O -1.649080 0.176848 -0.663514
Cl 1.629823 0.083943 -0.155270
H -0.383379 1.673019 0.166366
TS318
E= -650.5391387000 ZPE= 26.9717300000
C -0.702335 0.766926 0.000024
C 0.543299 0.468321 -0.000169
C 1.552840 -0.533663 -0.000087
H 1.282018 -1.587736 -0.000209
H 1.451096 1.520370 -0.000038
O 2.740638 -0.186887 0.000123
Cl -2.080273 -0.223490 0.000033
H 2.343608 1.152290 0.000105
TS319
E= -650.5420971400 ZPE= 28.9269000000
C 2.345737 0.890192 0.145464
C -0.488059 -0.240835 0.743305
C -1.602961 0.110086 0.141751

H -0.376206 -0.291825 1.812081
H 1.604347 1.707029 0.204747
O -2.587216 0.405151 -0.388229
Cl 0.898903 -0.596843 -0.245861
H 2.659938 0.933259 -0.914482
TS320
E= -650.5429826800 ZPE= 29.5834700000
C -1.428013 0.461569 0.343799
C -2.567308 -0.440188 0.052470
C 0.607556 0.871712 0.129758
H -2.545260 -0.893900 -0.942012
H -3.505714 0.077941 0.246015
O -0.460315 0.250603 -0.527764
Cl 1.915754 -0.312527 0.056127
H -2.507743 -1.234462 0.807785
TS321
E= -650.5344137600 ZPE= 24.2584700000
C -0.470492 0.359339 0.000003
C -0.554797 1.633690 -0.000010
C 2.285802 0.163329 0.000034
H -1.114663 2.547392 -0.000042
H 0.764624 2.171406 0.409163
O 2.751153 -0.865005 -0.000021
Cl -1.763937 -0.759312 0.000002
H 0.764672 2.171392 -0.409144
TS322
E= -650.5418063600 ZPE= 28.9777000000
C 0.342763 0.812436 -0.037047
C -1.636172 -1.095468 -0.172773
C -0.892613 0.010834 0.072725
H -0.914494 -0.820625 1.052662
H 0.313518 1.343576 -0.985652
O -2.195134 0.417999 0.007708
Cl 1.815433 -0.221465 -0.004705
H 0.415826 1.531150 0.773868
TS323
E= -650.5392925900 ZPE= 27.4939400000
C -3.352395 -0.783809 0.000005
C -0.185194 0.558916 -0.000059
C -2.437436 -0.018062 0.000013
H 1.887265 0.526848 -0.000010
H -0.148700 -0.550638 -0.000134
O -1.466815 0.888023 0.000027
Cl 2.941364 -0.243951 0.000010
H -4.157077 -1.475492 -0.000002
TS324
E= -650.5386991000 ZPE= 27.2066600000
C 0.590739 0.925908 -0.010445
C -0.753692 0.764928 -0.345587
C -1.734005 -0.009124 -0.054145
H -0.013208 1.318895 1.024564
H 1.138299 1.752001 -0.447205
O -2.706859 -0.640094 0.106477
Cl 1.823574 -0.543425 -0.012926
H 0.910767 1.197804 1.251625
TS325

E= -650.5397718700 ZPE= 27.9431400000
C 0.514415 1.327924 0.119205
C -0.719565 1.441687 -0.068823
C -1.395477 -1.319251 0.136169
H -0.288815 -1.446150 0.287908
H -1.534806 2.130202 -0.095536
O -1.909982 -0.297635 -0.088168
Cl 1.489134 -0.523870 -0.055457
H 1.391963 1.900658 0.336432

TS326

E= -650.5328752100 ZPE= 23.6509100000
C 0.125003 -0.041568 -0.000007
C -1.109509 -0.101669 -0.000002
C 2.817887 -0.086667 -0.000013
H 0.992229 -0.775981 -0.000013
H 0.834044 0.958335 -0.000007
O 3.967464 -0.008553 0.000014
Cl -2.739827 0.018361 0.000004
H 2.010784 0.953349 -0.000015

TS327

E= -650.5373809000 ZPE= 26.4906200000
C -0.520544 0.550713 0.000021
C 0.738052 0.878218 -0.000011
C -1.541015 -0.485558 0.000015
H -1.102657 -1.497938 0.000044
H -1.356244 1.681165 -0.409116
O -2.734423 -0.295370 -0.000020
Cl 1.978326 -0.303628 -0.000003
H -1.356208 1.681168 0.409134

TS328

E= -650.5318381700 ZPE= 23.3464900000
C -0.784136 0.584435 -0.000009
C -0.638504 1.891066 0.000004
C -1.789355 -0.256291 -0.000001
H 0.326530 2.582877 0.000007
H 0.885271 -0.347217 -0.000022
O -2.529424 -1.144973 0.000003
Cl 2.200595 -0.483200 0.000001
H 0.885445 1.823271 -0.000003

TS329

E= -650.5364316800 ZPE= 26.5140100000
C -2.544120 0.445862 0.000000
C -3.243566 -0.596148 0.000000
C 0.446969 -0.182101 0.000000
H -2.157371 -1.016120 0.000000
H -4.091497 -1.248480 0.000000
O 0.142666 1.057979 0.000000
Cl 2.236451 -0.311988 0.000000
H -0.867831 1.098894 0.000000

TS330

E= -650.5364678700 ZPE= 26.6153800000
C 0.688754 0.692997 0.043643
C -0.566681 0.640398 -0.082515
C 1.885312 0.019459 0.390584
H -1.080869 1.662828 -0.864453
H -1.184171 1.878536 -0.047096

O 2.637196 -0.541933 -0.386897
Cl -1.940592 -0.435667 0.024876
H 2.113224 0.083306 1.473563
TS331
E= -650.5407707800 ZPE= 29.3445700000
C 0.308662 -0.739769 0.469926
C -1.305646 1.436992 0.091877
C -1.385194 0.220475 -0.084651
H -0.915590 2.409384 0.254206
H 0.063589 -0.546976 1.499461
O -1.619022 -1.015263 -0.267676
Cl 1.634661 0.147141 -0.151700
H 0.308009 -1.747887 0.103725
TS332
E= -650.5323918700 ZPE= 24.1339700000
C 0.180542 -1.180395 -0.000001
C -0.646252 -0.220791 -0.000002
C 2.439161 0.554095 0.000003
H -0.017403 0.975144 -0.416432
H -0.017400 0.975149 0.416415
O 3.472851 0.103372 -0.000001
Cl -2.327463 0.267232 0.000001
H -0.021849 -2.237673 0.000003
TS333
E= -650.5303413500 ZPE= 22.9606800000
C 1.419720 0.794034 -0.000037
C 0.203284 1.241939 0.000015
C 2.199435 -0.239671 -0.000001
H 0.514691 2.708638 0.000022
H -0.349115 2.274205 0.000052
O 3.024477 -1.058160 0.000012
Cl -2.689445 -0.443217 0.000001
H -1.575458 0.239310 -0.000053
TS334
E= -650.5323390900 ZPE= 24.2367800000
C 0.437348 0.243541 0.000033
C 0.241801 1.508505 -0.000001
C -2.209046 -1.088191 0.000035
H -1.150753 1.766952 -0.411195
H -1.150719 1.766978 0.411295
O -2.815592 -0.132212 -0.000037
Cl 1.965543 -0.528332 -0.000010
H 0.591355 2.522276 -0.000050
TS335
E= -650.5404873300 ZPE= 29.4408100000
C -1.015930 0.003281 -0.692716
C -1.903013 -0.672118 0.266420
C 0.750882 1.190415 0.295675
H -2.859733 -0.148253 0.093332
H -1.651004 -0.576804 1.324006
O -0.474235 1.145722 -0.047161
Cl 1.375044 -0.580288 -0.013131
H -2.062775 -1.705302 -0.033092
TS336
E= -650.5369512600 ZPE= 27.4229800000
C 1.082467 0.060383 0.221265

C 1.069259 1.412332 0.034279
C 0.388537 -1.111967 0.693901
H 0.926585 2.032799 0.908861
H 1.577465 1.843528 -0.817485
O 1.219440 -1.006248 -0.523822
Cl -1.600637 0.056238 -0.081668
H -0.290311 1.053132 -0.209119
TS337
E= -650.5412480100 ZPE= 30.7148300000
C 0.097071 0.872740 0.205959
C -1.121164 1.222271 -0.545510
C -1.289491 0.051362 0.321517
H -2.001285 0.131059 1.140136
H -0.642965 -1.778845 0.411111
O -1.144316 -1.223819 -0.199568
Cl 1.485312 -0.186979 -0.036170
H 0.429975 1.738745 0.768384
TS338
E= -650.5349512500 ZPE= 27.1234300000
C 1.865530 0.423567 0.078431
C 2.914200 -0.305876 -0.037009
C -1.716162 0.779054 -0.053262
H 2.847322 -1.383576 -0.154317
H 3.897021 0.159139 -0.027706
O -0.697304 1.518829 -0.004352
Cl -1.162141 -1.022297 0.013570
H 0.209080 1.072388 0.057191
TS339
E= -650.5299440600 ZPE= 24.0316400000
C 0.576423 0.320867 0.000063
C -0.138071 1.368359 0.000008
C -3.051845 0.265378 0.000025
H 0.200415 2.390828 -0.000162
H -0.160591 -0.800035 0.419591
O -2.697644 -0.808583 -0.000062
Cl 2.198999 -0.355861 -0.000027
H -0.160698 -0.800112 -0.419048
TS340
E= -650.5348106600 ZPE= 27.1922500000
C -2.168062 -0.728853 -0.153154
C -0.169013 0.508332 1.070923
C -1.125685 0.023793 0.150661
H -2.500331 -1.477211 0.550016
H 0.669609 0.574426 -0.688836
O -0.469696 1.096488 -0.452346
Cl 1.709736 -0.357806 -0.092252
H -2.700671 -0.606062 -1.084695
TS341
E= -650.5341397300 ZPE= 27.0316500000
C -0.062075 -0.700294 0.640363
C 0.048294 2.204533 0.010992
C -1.224170 -0.439973 0.077579
H -0.013435 -1.132859 1.623983
H 0.022060 2.309435 1.113559
O -2.273900 -0.256157 -0.369203
Cl 1.442793 -0.471868 -0.230740

H 1.082793 2.508846 -0.234938
TS342
E= -650.5345820500 ZPE= 27.5423300000
C -2.400162 0.345216 0.149856
C -3.275434 -0.569640 -0.067946
C 0.444454 -0.108028 0.092476
H -2.834981 -1.471369 -0.498980
H -4.315163 -0.607574 0.227000
O 0.211198 1.131544 -0.108970
Cl 2.214066 -0.363653 0.007874
H -0.791708 1.203399 -0.036427
TS343
E= -650.5284422200 ZPE= 23.9780300000
C 0.602451 0.456876 0.000000
C -0.573137 0.838671 0.000000
C -1.966754 0.007893 0.000000
H -2.674092 1.156211 0.000000
H -2.337104 2.130019 0.000000
O -2.200281 -1.130191 0.000000
Cl 2.082484 -0.233775 0.000000
H -1.164139 1.908835 0.000000
TS344
E= -650.5354240800 ZPE= 28.6257100000
C 2.015676 -0.089943 0.000000
C -2.101882 -0.840636 0.000001
C -0.795211 -0.622347 -0.000002
H -2.420518 -1.877103 0.000000
H -2.882782 -0.088670 0.000003
O 1.580660 -1.139145 0.000000
Cl -0.259240 1.145534 0.000000
H 2.353598 0.922404 0.000000
TS345
E= -650.5337018200 ZPE= 27.6822300000
C -0.879095 0.153475 0.070256
C -1.543027 -1.160589 -0.073129
C 0.360078 0.141376 0.588886
H -2.423536 0.050919 -0.353134
H -1.795631 -1.681403 0.844376
O -1.729743 1.091055 -0.137320
Cl 1.858744 -0.005136 -0.120827
H -1.169266 -1.816201 -0.854694
TS346
E= -650.5315614900 ZPE= 26.5547500000
C -0.685564 0.965018 0.000000
C 0.612612 0.848527 0.000000
C 1.811672 0.011510 0.000000
H 2.773120 0.567068 0.000000
H 1.199074 2.107659 0.415593
O 1.756216 -1.190690 0.000000
Cl -1.744313 -0.365129 0.000000
H 1.199074 2.107659 -0.415593
TS347
E= -650.5329573500 ZPE= 27.8153600000
C 0.368102 1.145108 -0.621953
C -0.645505 1.334648 0.296850
C -1.801439 -0.215816 -0.062193

H -1.319761 2.148983 0.055560
 H -0.583016 1.096128 1.358208
 O -1.170039 -1.248657 -0.070297
 Cl 1.399758 -0.335081 0.086504
 H -0.059731 -1.143114 0.001816
 TS348
 E= -650.5243503500 ZPE= 22.5289300000
 C 1.330879 0.750536 -0.000083
 C 1.024528 1.957515 0.000047
 C 1.315010 -0.556987 -0.000084
 H 0.007755 2.540451 0.000112
 H -1.452888 1.191503 0.000058
 O 1.391378 -1.697129 0.000080
 Cl -1.799955 -0.304420 -0.000011
 H -1.109152 2.113831 0.000102
 TS349
 E= -650.5348643300 ZPE= 29.2985400000
 C 1.615695 0.646917 -0.243615
 C 2.450031 -0.554353 -0.049556
 C -0.379556 0.396753 -0.458603
 H 2.996002 -0.298182 0.876603
 H 1.932534 -1.499794 0.120129
 O 0.396164 0.401827 0.551419
 Cl -1.965311 -0.218935 -0.003503
 H 3.195425 -0.630634 -0.837877
 TS350
 E= -650.5298559900 ZPE= 26.4143900000
 C 0.518646 0.426942 -0.002836
 C -0.724947 0.771704 -0.128902
 C 1.746149 0.037047 0.183180
 H 2.719389 -0.138890 1.028473
 H -1.080313 1.769548 -0.343618
 O 2.820522 -0.400046 -0.351180
 Cl -2.080914 -0.355430 0.017959
 H 1.933191 0.197857 1.510637
 TS351
 E= -650.5315777400 ZPE= 27.4997500000
 C 1.409171 -0.123563 0.126352
 C 2.425655 -0.698542 -0.189258
 C 0.363353 0.578173 0.735878
 H -0.985708 0.714727 -0.577718
 H -0.665570 2.200530 0.174157
 O -0.197484 1.525264 -0.338167
 Cl -1.486697 -0.732498 -0.026631
 H 3.315943 -1.201299 -0.476197
 TS352
 E= -650.5292075100 ZPE= 26.1052600000
 C -2.142191 -0.876298 -0.040467
 C -2.715778 0.278625 -0.068088
 C -1.283512 0.792854 -0.197333
 H -3.660052 0.762601 -0.212095
 H 1.365780 0.043564 0.142070
 O -0.517162 0.004863 0.457980
 Cl 2.646475 -0.017722 -0.070640
 H -1.709619 -1.714897 -0.557614
 TS353

E= -650.5343559100 ZPE= 29.5548600000
C -0.923030 0.175220 -0.094257
C -1.980770 -0.560923 0.108060
C 1.080336 1.130228 0.427500
H -1.985192 -1.621760 -0.065034
H -2.864043 -0.059326 0.482302
O -0.389576 1.284530 -0.235640
Cl 1.016633 -0.852787 -0.041182
H 1.623869 1.435074 -0.479872
TS354
E= -650.5280981800 ZPE= 25.7620500000
C 0.886961 0.630389 0.090090
C -3.306418 0.432736 0.013763
C -2.263877 -0.177122 -0.011760
H -4.236189 0.938187 0.043690
H -0.279679 -0.179622 0.207396
O -1.168771 -0.829946 -0.041572
Cl 2.414068 -0.060736 -0.002972
H 0.926876 1.597486 -0.420543
TS355
E= -650.5306900400 ZPE= 28.6185700000
C -0.272144 0.246218 -0.000016
C 0.195626 1.455330 -0.000002
C 2.530789 -0.211608 0.000008
H 3.422465 0.371576 0.000022
H -0.342265 2.394686 0.000018
O 1.610945 -0.912477 -0.000005
Cl -1.882188 -0.350047 0.000004
H 1.303820 1.544716 -0.000010
TS356
E= -650.5285930900 ZPE= 28.7134700000
C 2.489755 0.577650 -0.012678
C -0.616302 -0.557681 0.005636
C 0.597327 -0.115148 0.112066
H 0.907185 0.964558 0.535107
H 3.374446 0.588236 0.611986
O 1.820717 -0.653621 -0.074074
Cl -2.125642 0.180500 -0.016095
H 2.463864 1.178737 -0.911021
TS357
E= -650.5327644000 ZPE= 31.4365500000
C -0.406320 1.576228 -0.069748
C -1.334814 0.630862 -0.040468
C -1.122158 -0.847271 0.134640
H -1.325357 -1.150947 1.165840
H -2.353807 1.003962 -0.096830
O 0.235545 -1.212859 -0.203137
Cl 1.218011 0.184307 0.056269
H -1.731632 -1.442265 -0.547043
TS358
E= -650.5235515900 ZPE= 25.6808600000
C 0.519469 0.527324 0.000000
C 0.718915 1.966950 0.000000
C 1.633381 -0.307555 0.000000
H -0.311484 2.358684 -0.000002
H -0.322017 0.125014 0.721720

O 2.456923 -1.081475 0.000000
Cl -2.113556 -0.416308 0.000000
H -0.322018 0.125013 -0.721719
TS359
E= -650.5276276600 ZPE= 28.5378500000
C 1.468221 -0.114118 -0.052587
C -0.609150 1.166342 0.529637
C 1.579407 1.081019 -0.192647
H 1.868638 2.083951 -0.380892
H -0.675614 1.834773 -0.349334
O 1.258207 -1.365488 0.138517
Cl -1.540052 -0.250598 -0.125695
H 0.291326 -1.534113 0.052494
TS360
E= -650.5245391000 ZPE= 26.6147800000
C 0.689417 0.083470 -0.016880
C -0.509245 0.218892 -0.047980
C -1.891583 0.371015 -0.305821
H -2.314239 1.536534 -0.028759
H -3.519662 -0.581036 -0.251468
O -2.650192 -0.639620 0.161186
Cl 2.322003 -0.094972 0.020355
H -2.170153 1.735717 0.868792
TS361
E= -650.5222568200 ZPE= 25.4087000000
C 0.758333 0.047822 0.000000
C -0.452360 0.077564 0.000000
C -1.818590 0.325178 0.000000
H -3.602029 0.034939 0.000000
H -3.842282 1.194052 0.000000
O -2.657994 -0.610507 0.000000
Cl 2.390481 -0.022551 0.000000
H -2.854215 1.335044 0.000000
TS362
E= -650.5306026900 ZPE= 30.6735600000
C 0.522690 0.840311 -0.109390
C 1.334300 -0.400132 -0.256372
C -0.460865 0.041435 0.716769
H 0.994136 1.638304 0.474029
H 3.067389 -1.037784 -0.016621
O 2.590392 -0.196865 0.034955
Cl -1.961608 -0.182781 -0.103032
H 0.185924 1.191984 -1.091552
TS363
E= -650.5235310000 ZPE= 26.2361100000
C 2.440739 -1.603660 0.000001
C 1.729637 -0.526116 -0.000004
C 1.775524 0.916377 0.000022
H 0.785743 -1.150668 -0.000045
H -1.334351 0.453419 -0.000042
O 0.541023 1.401835 -0.000013
Cl -2.356250 -0.329577 0.000004
H 0.601269 2.365772 0.000006
TS364
E= -650.5294380400 ZPE= 30.0211000000
C -1.501449 0.528856 -0.698448

C 0.353594 0.977829 0.031301
C -1.309381 0.132360 0.582442
H -1.401550 0.321548 1.640737
H 0.426266 1.595341 -0.852641
O -1.371656 -1.002018 -0.100473
Cl 1.544077 -0.311992 -0.024251
H 0.442639 1.568841 0.936184
TS365
E= -650.5292916000 ZPE= 30.2659100000
C 1.006330 1.343658 -0.770306
C 0.389762 0.867431 0.340893
C 1.285911 -0.228369 0.507666
H 2.069887 -0.280284 1.248207
H 0.267966 1.585852 1.150860
O 1.137516 -1.244293 -0.293863
Cl -1.630776 -0.120173 0.005832
H 0.193187 -1.204607 -0.616830
TS366
E= -650.5279251200 ZPE= 30.1773400000
C 0.319462 -0.009337 -0.818913
C -1.277952 1.394978 0.110266
C 1.431303 -0.018927 -0.117663
H -1.340849 1.684005 -0.924289
H -2.211589 1.300187 0.643822
O 2.520870 0.079824 0.309978
Cl -1.117165 -0.802113 0.122855
H -0.459596 1.812857 0.669969
TS367
E= -650.5203417900 ZPE= 25.4420000000
C -0.457433 0.927545 0.456850
C -1.075081 -1.042032 0.405195
C -1.847641 -1.160438 -0.615278
H -1.078834 -1.366726 1.433339
H 0.120320 -1.036776 -0.051946
O -0.778248 1.726582 -0.304800
Cl 1.623413 -0.272639 -0.112373
H -0.132592 0.875272 1.486738
TS368
E= -650.5227441000 ZPE= 27.0220700000
C 2.117613 -0.006860 -0.052508
C 3.089609 -0.728367 0.003877
C 1.151808 0.974291 -0.240027
H -0.988659 0.965903 -0.048344
H 3.930184 -1.376791 0.062942
O -0.039523 0.613692 0.281415
Cl -2.369837 -0.328823 -0.055924
H -0.492285 -0.343037 0.416733
TS369
E= -650.5206149400 ZPE= 25.7176000000
C 1.735347 -0.544957 -0.000001
C 2.129045 -1.771202 0.000001
C 0.712213 0.449170 0.000000
H -1.027845 0.069622 0.000000
H 2.036120 1.864282 0.000000
O 1.074494 1.697186 0.000000
Cl -2.349920 -0.230353 0.000000

H 2.884782 -0.393460 0.000000
 TS370
 E= -650.5230074800 ZPE= 27.3828600000
 C -0.368385 0.475788 0.000127
 C 2.070477 0.895752 -0.000042
 C -1.638133 0.172729 0.000014
 H 0.595773 1.338306 0.000089
 H 2.689093 0.776099 0.892210
 O -2.801584 0.062376 -0.000058
 Cl 0.944420 -0.744423 0.000000
 H 2.688912 0.776171 -0.892430
 TS371
 E= -650.5231576600 ZPE= 28.0029700000
 C -2.069655 -0.622266 0.293479
 C -1.310882 0.032890 -0.652923
 C 0.716880 1.140447 0.225221
 H -2.087414 -0.378052 1.355174
 H -2.764708 -1.371543 -0.066559
 O -0.531245 1.055697 -0.022649
 Cl 1.531936 -0.520960 -0.004744
 H -0.958879 -1.146089 -0.221426
 TS372
 E= -650.5209782400 ZPE= 26.8455800000
 C 1.707783 -0.864281 0.330154
 C 1.047905 -1.253003 -0.706367
 C 1.811024 0.665390 0.253181
 H -0.007170 0.940116 -0.426994
 H 2.357975 -1.326889 1.054913
 O 0.836249 1.382472 -0.193982
 Cl -2.067966 -0.065324 0.056298
 H -1.285660 -0.851130 0.705057
 TS373
 E= -650.5211724300 ZPE= 27.3721200000
 C 2.003935 -0.398497 -0.750611
 C 1.601434 1.111062 0.034324
 C 0.673162 0.150227 0.495844
 H 1.247877 2.048210 -0.379340
 H -1.091332 0.012853 0.242874
 O 1.559536 -1.015643 0.274327
 Cl -2.406579 -0.015537 -0.069522
 H 2.607833 1.151447 0.446381
 TS374
 E= -650.5203306200 ZPE= 26.8649200000
 C -1.142208 -0.494506 0.034655
 C -2.322767 -0.846374 -0.083244
 C -0.203376 0.629574 0.572100
 H -3.336868 -1.169772 -0.081427
 H -0.185909 -1.056619 -0.319462
 O -0.204397 1.735958 -0.115086
 Cl 1.629057 -0.534082 -0.046424
 H -0.525910 1.685958 -1.030284
 TS375
 E= -650.5221223500 ZPE= 28.1313600000
 C -1.192170 -0.127884 -0.608556
 C -2.089966 -0.624208 0.318380
 C 0.734276 1.114378 0.227709

H -2.709117 -1.455201 0.002622
H -2.139330 -0.315669 1.362263
O -0.512020 1.007711 -0.033806
Cl 1.569705 -0.510413 -0.005063
H -2.453210 0.212489 -0.633564
TS376
E= -650.5256960800 ZPE= 30.6005600000
C 1.554256 0.488637 -0.369752
C 2.104432 -0.708509 -0.088223
C 0.404437 0.990423 0.351571
H 3.096899 -0.971607 -0.429864
H 1.586768 -1.416829 0.543207
O -0.372578 -0.100532 0.841527
Cl -1.657497 -0.155813 -0.308675
H 2.095654 1.218208 -0.959662
TS377
E= -650.5132112300 ZPE= 22.9929700000
C 0.941237 0.678898 -0.689091
C 0.875579 1.610356 0.109133
C 2.000235 -1.031421 -0.553978
H 1.762316 0.310917 0.624645
H 0.766587 2.468668 0.731858
O 2.332704 -0.734493 0.573368
Cl -2.516271 -0.269250 0.061903
H -1.316228 0.126610 -0.192188
TS378
E= -650.5177750800 ZPE= 26.1068400000
C -1.987775 -1.645796 -0.232511
C -2.143531 -0.437109 0.181514
C -1.886857 0.988841 0.074412
H -3.162704 -0.780360 0.553700
H 1.291307 0.081204 -0.003373
O -0.588538 1.153494 -0.127236
Cl 2.536143 -0.238997 0.033754
H -0.425748 2.098538 -0.246748
TS379
E= -650.5218463200 ZPE= 28.7273900000
C 1.497259 -1.095949 -0.000071
C 1.772133 0.350906 -0.000145
C -0.673999 1.189486 -0.000562
H 2.447869 -1.622514 -0.000486
H 0.902285 -1.390663 -0.871645
O 0.640278 1.183482 0.000436
Cl -1.467512 -0.454744 0.000080
H 0.902972 -1.390679 0.871949
TS380
E= -650.5199965300 ZPE= 27.7736000000
C 1.875942 0.678945 -0.060611
C 2.123537 -0.696601 0.101934
C -0.226342 -0.129127 -0.426546
H 0.992995 -0.949202 -0.634063
H 3.100275 -1.061991 -0.188363
O 0.462799 0.803994 0.133615
Cl -1.889799 -0.136416 0.065211
H 1.692101 -1.220995 0.956263
TS381

E= -650.5172507300 ZPE= 26.1674800000
C -1.009249 0.818609 0.000000
C 0.199079 1.277468 0.000000
C -1.554289 -0.567934 0.000000
H -3.227935 -1.366190 0.000000
H -1.711673 1.664061 0.000001
O -2.863715 -0.470487 0.000000
Cl 2.380436 -0.381140 0.000000
H 1.568666 0.776545 0.000000

TS382

E= -650.5204871600 ZPE= 28.6200100000
C -0.287859 -0.339293 0.075119
C 0.504111 0.785171 -0.042649
C 2.055563 0.596703 0.009794
H 0.157962 1.799124 -0.235169
H 0.257974 0.221132 1.122578
O 2.337334 -0.661091 -0.059294
Cl -2.015185 -0.103685 -0.033392
H 1.512655 -1.224355 -0.098984

TS383

E= -650.5160579900 ZPE= 26.0482100000
C -0.153498 0.816218 0.000001
C 0.897313 0.062552 0.000002
C 2.318280 0.532271 -0.000002
H 3.988438 -0.275124 -0.000002
H -1.563456 0.687286 0.000000
O 3.061656 -0.550677 0.000000
Cl -2.704461 -0.203659 -0.000001
H 0.685033 -1.010790 0.000005

TS384

E= -650.5200611600 ZPE= 28.8424600000
C 1.411837 0.995669 0.000639
C 2.684566 0.712686 -0.000707
C 0.625082 -0.228499 0.000160
H 1.975344 -1.588433 0.000922
H 0.841989 1.919726 0.000357
O 1.015731 -1.456750 -0.000038
Cl -2.277905 0.148228 -0.000093
H -0.547707 -0.076304 0.000059

TS385

E= -650.5205553500 ZPE= 29.1595400000
C -1.751264 0.053629 -0.500410
C -1.023872 1.102397 -0.034832
C 0.148412 1.458290 0.219380
H 0.895427 2.141686 0.553839
H -0.127163 -0.994552 0.292268
O -1.197732 -1.098786 0.362647
Cl 1.532996 -0.360245 -0.105287
H -1.487000 -1.918583 -0.062228

TS386

E= -650.5196395900 ZPE= 28.6425700000
C -0.265196 -1.450895 -0.543329
C 0.796249 -1.132981 0.172958
C 1.606555 -0.135072 0.384398
H 2.411172 0.082498 1.062810
H 0.010462 0.994459 -0.155774

O 1.140274 1.136505 -0.281135
Cl -1.511031 0.296699 0.146598
H 1.318060 1.100804 -1.234279
TS387
E= -650.5194044000 ZPE= 29.3577800000
C -1.454261 -0.045411 0.369736
C -1.415921 -1.298575 -0.313111
C 0.594315 1.209517 -0.252456
H -1.180992 -0.176336 1.416584
H -0.836008 -1.233298 -1.240577
O -0.664806 1.148866 -0.128880
Cl 1.381025 -0.429099 0.098322
H -2.486769 0.320207 0.358544
TS388
E= -650.5193683700 ZPE= 29.8575600000
C -0.207769 -1.536420 0.688697
C -1.358701 -1.779128 0.000000
C -0.207769 -1.536420 -0.688697
H 0.360227 -1.541528 -1.597621
H -2.430312 -1.837731 0.000000
O -0.207769 0.430702 0.000000
Cl 0.824555 1.799234 0.000000
H 0.360227 -1.541528 1.597621
TS389
E= -650.5085413900 ZPE= 23.1890100000
C -1.019928 0.821850 -0.233234
C -0.542719 1.928357 -0.033530
C -2.174012 -0.408973 0.663877
H 1.279400 0.201255 -0.020335
H -0.127429 2.895081 0.131179
O -2.278269 -1.213766 -0.266164
Cl 2.415994 -0.408951 0.025630
H -1.577774 -0.481437 -0.799915
TS390
E= -650.5136568600 ZPE= 26.7544800000
C -1.416387 -1.096322 0.307578
C -1.550092 -0.103238 -0.640230
C 0.325316 1.449446 0.218340
H -1.297224 -0.932908 1.374842
H -1.851811 -2.043123 0.004661
O -0.836832 1.174648 0.054996
Cl 1.523603 -0.403781 -0.062589
H -0.210572 -1.056190 -0.069590
TS391
E= -650.5078654000 ZPE= 23.1536200000
C 3.852390 -0.084571 -0.000111
C 2.636534 -0.169122 -0.000003
C 1.135099 0.739483 0.000061
H 4.915006 -0.020626 -0.000211
H -1.812319 -0.048365 0.000082
O 0.308077 -0.206964 0.000156
Cl -3.098743 -0.022980 -0.000054
H 1.367189 -0.799377 0.000115
TS392
E= -650.5111235900 ZPE= 25.2783400000
C -0.738866 1.961155 0.043599

C -0.497027 0.674145 -0.032072
C -1.293782 -0.636182 0.212335
H -0.687935 -1.386769 0.740259
H 0.477195 0.711284 0.691160
O -2.402835 -0.790448 -0.174612
Cl 2.014896 -0.317159 -0.033292
H 0.358220 0.396077 -0.811728
TS393
E= -650.5160174100 ZPE= 28.4820900000
C 0.798982 1.132416 0.112631
C -0.624645 1.105435 -0.001778
C -1.460749 0.063990 -0.580261
H -1.551216 -0.870281 1.104323
H -0.092436 1.109202 1.164950
O -1.857583 -0.908068 0.174242
Cl 1.487826 -0.522655 -0.048944
H -1.070259 2.099713 -0.014703
TS394
E= -650.5185889500 ZPE= 30.2247600000
C 0.450719 1.202542 -0.011439
C -1.121078 -1.299399 -0.197420
C -1.043295 1.157187 0.015504
H 0.779222 1.700528 -0.921679
H -1.151893 -1.772008 0.801162
O -1.481572 -0.032527 0.036234
Cl 1.275994 -0.457613 0.008019
H 0.815273 1.749135 0.854448
TS395
E= -650.5114890700 ZPE= 26.2971400000
C 1.556364 1.310920 0.000124
C 1.883766 0.001873 -0.000021
C 0.422714 0.475509 -0.000244
H 0.813619 -0.738425 -0.000378
H 3.715998 -0.357103 0.000302
O 2.881771 -0.856229 0.000040
Cl -2.890736 -0.170703 0.000049
H -1.618346 0.117490 -0.000236
TS396
E= -650.5129434000 ZPE= 27.2114700000
C 0.591103 0.318651 -0.107863
C -0.628433 0.641348 0.300258
C 1.844811 0.724711 -0.414645
H 3.075591 -0.477932 0.877782
H 1.287941 -0.826036 0.075174
O 2.552026 -0.651502 0.080677
Cl -2.045052 -0.298333 -0.071068
H -0.858734 1.479389 0.943272
TS397
E= -650.5110974200 ZPE= 26.1693800000
C 0.583328 0.350797 -0.136898
C -0.312429 1.184272 0.172355
C 1.871808 0.029758 -0.606676
H -0.900293 2.058359 0.341557
H 2.395496 -0.551808 1.162213
O 2.727170 -0.472393 0.247539
Cl -2.101627 -0.389682 0.010151

H -0.441147 -0.491771 -0.229329
 TS398
 E= -650.5130967000 ZPE= 27.5636800000
 C 1.301931 -0.128693 0.460678
 C 2.082831 -0.887066 -0.350354
 C -0.731537 1.144083 -0.242518
 H 0.967784 -0.375272 1.459638
 H 2.470845 0.154310 0.558764
 O 0.511626 1.112462 0.004507
 Cl -1.508165 -0.528605 0.005362
 H 2.187814 -0.462394 -1.352460
 TS399
 E= -650.5136802700 ZPE= 28.4677900000
 C 0.610566 1.054395 0.007757
 C -0.757853 1.050024 0.371212
 C 1.427351 0.003827 -0.628751
 H -0.221015 1.637438 -0.745985
 H 1.172057 1.938860 0.317026
 O 1.949913 -0.844195 0.206304
 Cl -1.525896 -0.515078 -0.051192
 H 1.709501 -0.715877 1.147488
 TS400
 E= -650.5045453100 ZPE= 23.3110600000
 C -0.637319 0.758772 -0.000001
 C -1.012164 1.991237 0.000001
 C -1.323935 -0.443207 0.000000
 H -0.180552 -1.508298 0.000005
 H 0.623449 0.618062 -0.000001
 O -2.328188 -1.017786 -0.000001
 Cl 2.081317 -0.206618 0.000000
 H 0.640720 -1.295771 0.000004
 TS401
 E= -650.5070351400 ZPE= 25.5003800000
 C -0.895358 0.075487 0.000005
 C 0.147857 0.843778 0.000008
 C -2.325356 0.549393 -0.000009
 H 1.573773 0.705206 0.000008
 H -0.653926 -0.993227 0.000013
 O -3.159123 -0.450118 -0.000001
 Cl 2.680539 -0.210035 -0.000003
 H -2.778876 -1.352392 0.000013
 TS402
 E= -650.5088850200 ZPE= 26.7142600000
 C 0.646500 -0.522418 0.705779
 C 1.648616 1.320261 0.030235
 C 1.860952 0.186708 -0.377008
 H 1.539557 2.355925 0.244409
 H -1.027444 -0.214410 0.254799
 O 1.579545 -1.071346 -0.348469
 Cl -2.313480 0.067405 -0.087535
 H 1.244281 -0.623941 1.622605
 TS403
 E= -650.5126262700 ZPE= 29.1998900000
 C 0.660478 1.005215 -0.009556
 C -2.606158 -0.411664 -0.133380
 C -0.800645 1.008092 0.015270

H 0.986935 1.596249 0.850588
 H -2.727511 -1.478001 0.154224
 O -1.287748 -0.242578 0.111831
 Cl 1.621611 -0.550954 -0.014155
 H 0.953114 1.578737 -0.892828
 TS404
 E= -650.5120314000 ZPE= 28.8338600000
 C -0.472320 -0.014341 0.385699
 C 0.660198 0.791714 -0.021619
 C -1.674511 0.453877 -0.207879
 H -3.464725 -0.056817 -0.433913
 H -0.408101 -0.983494 0.890524
 O -2.653401 -0.451927 -0.097110
 Cl 2.067897 -0.218720 -0.088376
 H -1.134417 0.986468 0.885452
 TS405
 E= -650.5105710800 ZPE= 28.1238600000
 C 2.533039 0.145065 0.334748
 C 0.958735 0.631589 0.212042
 C -1.462529 0.938587 -0.459473
 H 0.510829 0.352161 1.156039
 H 0.998371 1.701943 0.069655
 O 3.078803 -0.651742 -0.306813
 Cl -2.286686 -0.424970 0.079310
 H 0.558565 0.092873 -0.643365
 TS406
 E= -650.5059815900 ZPE= 26.3198400000
 C -1.417391 -0.013914 -0.061512
 C -1.494541 -1.223767 0.132277
 C 0.420993 1.373344 0.327625
 H 0.088727 -1.112448 -0.015283
 H -1.979021 -2.129199 0.412128
 O -0.917517 1.119671 -0.333117
 Cl 1.409037 -0.446415 -0.087520
 H 0.222422 1.059344 1.365590
 TS407
 E= -650.5080134100 ZPE= 27.8354800000
 C -0.639795 0.495601 0.000403
 C -2.063645 0.655676 -0.000231
 C -2.513306 -0.602336 -0.000233
 H -1.330334 -1.290112 -0.000159
 H -2.591984 1.596579 -0.000400
 O -0.212675 -0.721663 0.000317
 Cl 2.164379 0.053488 -0.000154
 H 0.129746 1.263902 0.001006
 TS408
 E= -650.5047566900 ZPE= 26.3112200000
 C 0.353344 1.288184 0.554846
 C -1.429902 0.007940 -0.066834
 C -1.518849 -1.203125 0.121337
 H -2.011334 -2.087535 0.451386
 H -0.007988 -1.088121 -0.015864
 O -0.897263 1.116396 -0.322605
 Cl 1.403580 -0.485495 -0.080706
 H 0.909017 1.939894 -0.138780
 TS409

E= -650.5086427300 ZPE= 28.8182600000
C -0.616876 0.470792 0.162208
C 0.450604 -0.540685 -0.041290
C -2.924114 0.391102 -0.171036
H 0.389741 -1.295459 0.747183
H 0.306136 -1.051718 -0.997585
O -1.772884 -0.245692 0.104708
Cl 2.099334 0.164841 -0.018776
H -3.659161 -0.416850 0.032634
TS410
E= -650.5089226200 ZPE= 29.2453600000
C 2.054926 -0.778766 0.416310
C -0.517386 1.013105 0.129656
C 0.937783 0.965769 -0.099376
H -0.716997 1.477032 1.094404
H -0.869192 1.721397 -0.631153
O 1.350092 -0.275967 -0.569009
Cl -1.544770 -0.484910 0.013879
H 2.194617 0.052120 1.173337
TS411
E= -650.5073121600 ZPE= 28.8369700000
C -1.604176 0.946397 0.165339
C -1.900241 -0.817131 -0.483453
C -0.821529 -0.284661 0.060563
H -2.025922 1.239702 1.121830
H -2.619838 0.265143 -0.388291
O 0.351313 -0.735214 0.504212
Cl 1.718748 0.210174 -0.156736
H -1.427784 1.736275 -0.557418
TS412
E= -650.5053909200 ZPE= 27.7088300000
C -0.417321 0.878116 0.161835
C 0.985074 0.967303 -0.179097
C -0.746801 -0.390593 0.120403
H -3.060801 -1.220032 -0.108171
H -0.999120 1.785672 0.216583
O -3.239809 -0.284240 0.028272
Cl 2.035840 -0.416062 -0.008095
H -3.556588 0.052379 -0.815810
TS413
E= -650.5038020600 ZPE= 26.7979800000
C -1.740972 0.020570 0.000032
C -2.866704 -0.670632 -0.000020
C -0.717945 0.748496 0.000029
H -3.342994 -0.972854 0.925407
H -3.343087 -0.972572 -0.925490
O 0.541249 1.082573 0.000047
Cl 2.029079 -0.548351 -0.000015
H -0.184532 2.016204 -0.000284
TS414
E= -650.5017786900 ZPE= 25.5344800000
C 1.663229 -1.675801 0.000006
C 1.065361 -0.617137 -0.000006
C 0.636688 1.919067 0.000001
H -0.444699 1.704373 0.000002
H 2.058384 -2.663448 0.000014

O 1.425208 0.991208 0.000002
Cl -1.917607 -0.242644 0.000004
H -0.607703 -0.602419 -0.000099
TS415
E= -650.5060373200 ZPE= 28.4053700000
C -1.622081 0.861177 0.177913
C -2.160268 -0.181327 -0.455438
C -1.256297 -0.426705 0.563238
H -0.337746 -1.016582 0.876307
H -2.796801 -0.574109 -1.228375
O 0.868843 -1.100149 -0.024821
Cl 1.642901 0.408919 -0.086738
H -1.513645 1.921392 0.310900
TS416
E= -650.5069120600 ZPE= 29.2129500000
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C 0.561863 0.995810 0.106675
C -2.514589 -0.315058 0.215076
H 0.942647 1.724306 -0.609777
H 0.684078 1.434119 1.098380
O -1.265694 -0.382706 -0.342057
Cl 1.651132 -0.473810 0.018831
H -2.551128 -1.278059 0.771182
TS417
E= -650.5019979600 ZPE= 26.1608300000
C 1.664498 -1.238283 0.237376
C 2.649092 0.792038 0.260936
C 1.588716 0.511912 -0.277342
H 3.552635 1.194201 0.648525
H -1.380650 -0.068659 -0.221378
O 0.690844 -0.350693 -0.597985
Cl -2.607406 0.139511 0.105564
H 1.213335 -1.085677 1.236331
TS418
E= -650.4984134000 ZPE= 24.2514500000
C 0.538105 0.187638 0.000001
C -0.692254 0.140131 0.000000
C 1.826004 -0.703224 0.000000
H 1.266157 1.304872 0.000001
H 2.097609 1.854431 0.000000
O 2.907457 -0.127558 -0.000001
Cl -2.315975 -0.056056 0.000000
H 2.717017 1.066852 -0.000001
TS419
E= -650.5072346200 ZPE= 29.8180800000
C -0.456520 0.625405 0.000003
C 0.378626 -0.593212 0.000006
C -2.429755 -0.751666 -0.000001
H -3.516353 -0.512901 -0.000005
H -0.245478 1.238935 0.880815
O -1.910902 0.440214 -0.000003
Cl 2.020024 -0.068815 -0.000002
H -0.245470 1.238944 -0.880800
TS420
E= -650.5031212600 ZPE= 27.3205000000
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C -1.357184 -1.567607 -0.429564
C -0.035074 -0.162339 0.717963
H 2.456004 0.641551 0.609005
H 0.560850 -2.232868 0.365668
O 2.471651 0.091605 -0.179514
Cl -0.940126 1.141402 -0.059780
H 2.560750 0.705697 -0.914420
TS421
E= -650.4991920200 ZPE= 25.2833700000
C 2.256928 -0.524632 -0.330631
C -0.158460 0.335710 0.566645
C 1.150122 0.095240 0.004025
H 1.567613 -2.465092 0.685988
H 2.145430 -2.155950 0.287466
O 0.535826 1.338219 -0.158537
Cl -1.600516 -0.355233 -0.162991
H -0.282422 0.516354 1.625466
TS422
E= -650.5033384600 ZPE= 27.9513600000
C -1.905071 0.504864 -0.635530
C -2.041821 -0.768219 -0.040788
C -0.766909 -0.745438 0.427853
H -0.260630 1.514641 -0.006601
H -2.672911 -1.599795 -0.299976
O -0.972809 0.990120 0.404137
Cl 2.231823 -0.068159 -0.096950
H 1.057819 -0.624347 0.212424
TS423
E= -650.5066908400 ZPE= 30.0813600000
C -0.549514 -0.266186 -0.000001
C 0.524808 0.493785 0.000001
C -2.905102 -0.263040 0.000002
H 0.468142 1.571067 0.000003
H -3.811192 -0.813365 0.000001
O -1.850696 0.420622 -0.000002
Cl 2.139747 -0.151066 0.000000
H -0.648223 -1.341921 -0.000003
TS424
E= -650.5067428300 ZPE= 30.3921200000
C -0.684155 0.924333 0.000000
C 0.633545 0.861445 0.000000
C 2.574291 -0.444862 0.000000
H 3.633308 -0.493030 0.000002
H 1.315434 1.700616 0.000000
O 1.311807 -0.413050 -0.000001
Cl -1.728743 -0.460059 0.000000
H -1.196655 1.872322 0.000000
TS425
E= -650.5018494000 ZPE= 27.4364200000
C 2.310505 -1.038558 -0.053554
C 1.636415 -0.023353 0.060210
C 0.640289 1.028349 0.294581
H 0.862650 1.694397 1.125805
H 1.827600 1.031300 -0.561582
O -0.408775 1.087807 -0.384902
Cl -1.757727 -0.549579 0.053400

H 2.938062 -1.883930 -0.200240
TS426
E= -650.5055336900 ZPE= 29.7984400000
C -0.140825 1.606546 -0.048584
C -0.035228 0.216905 0.402933
C -1.068914 -0.635033 -0.319689
H -2.917222 -0.809734 -0.368077
H -0.089571 0.072233 1.481792
O -2.257787 -0.260303 0.079516
Cl 1.672647 -0.347934 -0.049031
H 0.103887 1.604291 -1.124269
TS427
E= -650.5036874900 ZPE= 29.1430800000
C -0.452947 0.748201 0.236334
C 0.324426 -0.439614 0.043993
C -2.477465 -0.721544 0.014800
H -1.773928 -1.361111 0.606158
H -0.705137 0.937243 1.276717
O -1.976275 0.369776 -0.296899
Cl 2.005986 -0.101173 -0.058420
H -0.176573 1.663342 -0.285315
TS428
E= -650.4998171200 ZPE= 27.4634600000
C -1.005161 1.090268 0.025211
C 0.314844 1.455550 -0.002343
C -1.801194 -0.080022 -0.051308
H -1.447053 -2.034448 -0.125279
H -1.607940 2.000142 0.015298
O -0.974180 -1.213306 0.048562
Cl 1.506343 -0.235181 -0.006960
H 0.189670 -1.055953 0.010448
TS429
E= -650.4955118100 ZPE= 25.7078200000
C 0.744340 0.966637 -0.031949
C -2.282568 -0.745653 0.144416
C -1.438531 0.073840 -0.063550
H -3.017921 -1.486789 0.328796
H 1.052363 1.619409 0.963599
O -0.587157 1.042489 -0.313377
Cl 1.402668 -0.669061 -0.044347
H 0.678013 1.132567 1.675025
TS430
E= -650.5029270900 ZPE= 30.3887200000
C -0.097653 0.132478 0.645683
C 0.375678 1.419957 0.079556
C -1.222568 -0.786904 0.184295
H -0.040202 1.495714 -0.943374
H -2.066338 0.859962 -0.386262
O -2.211734 -0.110991 -0.314057
Cl 1.493765 -0.355219 -0.195641
H 0.073669 -0.022206 1.710793
TS431
E= -650.5013545900 ZPE= 29.6509600000
C -1.529687 0.647411 0.775051
C -0.739121 0.485098 -0.407739
C 0.215854 -0.440570 0.089618

H -0.558184 1.138086 -1.254573
H -2.018952 -1.303057 -0.019595
O -2.163542 -0.369240 -0.272902
Cl 1.895687 0.007759 -0.007886
H -0.023485 -1.164663 0.849869
TS432
E= -650.4940802200 ZPE= 28.2331000000
C -0.778004 1.122654 -0.373112
C 0.556915 1.320482 0.090784
C 1.764788 0.765253 0.166867
H 1.041646 -1.653086 0.667874
H 0.849378 2.389463 0.118534
O 1.529760 -1.373168 -0.115402
Cl -1.430679 -0.438411 0.098858
H 0.930250 -1.548378 -0.851007
TS433
E= -650.4937060800 ZPE= 29.0742600000
C -1.414579 -0.316221 -0.000036
C -0.652433 0.956108 0.000026
C 1.811343 -1.256925 0.000043
H -0.733159 1.545843 -0.907698
H -0.733185 1.545766 0.907797
O -2.620494 -0.408443 0.000013
Cl 1.456061 0.300883 -0.000016
H -0.788739 -1.236846 -0.000124
TS434
E= -650.4877515700 ZPE= 25.5152200000
C -0.752085 -0.309388 -0.227467
C -2.019998 -0.315984 -0.011792
C -3.254905 -0.645133 0.131499
H -0.396103 1.966026 0.748667
H 0.842548 1.343002 0.010357
O -0.106478 1.587382 -0.091846
Cl 2.113628 -0.457525 0.048267
H 0.635639 -0.607134 -0.198242
TS435
E= -650.4887599900 ZPE= 26.1896800000
C 3.194783 -0.103175 0.016608
C 1.916210 -0.234452 -0.002236
C 0.715741 -0.700128 -0.012770
H -0.875483 -1.484052 -0.041645
H -2.283935 -1.642356 0.732920
O -1.886646 -1.335875 -0.092363
Cl -0.881687 1.188375 0.004986
H -1.719142 -0.162439 -0.046750
TS436
E= -650.4838394500 ZPE= 23.4463400000
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C -2.321116 -1.225291 0.000295
C -0.506775 0.668654 0.042867
H 1.345390 0.083912 1.064790
H -3.001018 -2.040748 -0.006095
O -0.552022 1.868312 -0.042079
Cl 1.731759 -0.421445 -0.062753
H 3.201025 -0.955448 0.100490
TS437

E= -650.4893443600 ZPE= 26.9511400000
C -0.608223 0.193604 0.150318
C -1.832867 0.934814 0.175481
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H 1.220668 0.039833 0.084360
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Cl 2.553108 -0.005677 -0.025868
H -2.337676 1.821513 0.536419
TS438
E= -650.4906155300 ZPE= 28.0252400000
C -0.745856 1.018272 0.072199
C 0.613700 1.048403 0.347800
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H -1.038994 -1.086282 1.179355
H -1.369925 1.848826 0.384643
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Cl 1.477007 -0.414576 -0.082668
H 0.026449 1.647231 -0.723265
TS439
E= -650.4931821500 ZPE= 29.8160900000
C 0.956462 -0.290422 0.000004
C 2.102813 0.142446 -0.000026
C -0.106122 -1.416850 0.000045
H 0.067212 -2.013678 -0.900776
H 3.127691 0.421320 -0.000061
O -1.376955 -0.875354 -0.000064
Cl -0.586195 1.176334 0.000013
H 0.067134 -2.013531 0.900980
TS440
E= -650.4924308700 ZPE= 29.3638500000
C 2.040687 -0.780388 0.428973
C -0.415763 0.786466 0.641069
C 0.505661 0.906921 -0.539101
H -0.090417 0.382456 1.595590
H -0.977670 1.704258 0.762244
O 1.604938 0.039685 -0.528505
Cl -1.522554 -0.421479 -0.152786
H 1.328481 -0.717047 1.281926
TS441
E= -650.4913729800 ZPE= 28.9405300000
C 0.037115 1.630174 -0.035498
C 0.019030 0.247430 0.491599
C 1.052934 -0.879639 0.194689
H 0.962536 1.803027 -0.641942
H -0.066223 0.277939 1.584140
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Cl -1.589706 -0.327712 -0.155651
H 2.160641 0.600586 -0.361826
TS442
E= -650.4910793100 ZPE= 29.0233700000
C 1.173184 1.160097 0.018913
C -0.652875 -1.288810 -0.142765
C -1.529398 -0.216458 0.121834
H -2.380907 -0.627608 0.709762
H 0.625369 1.723457 -0.706563

O -1.440828 1.000102 -0.099644
Cl 1.037372 -0.505670 -0.003311
H 1.701376 1.570759 0.862356
TS443
E= -650.4921564100 ZPE= 29.7140500000
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C -0.184069 0.144781 0.758968
C -2.247093 0.063852 -0.226939
H -2.963080 -0.683786 -0.617361
H 0.852628 1.984535 0.319547
O -1.216859 -0.638324 0.107553
Cl 1.515780 -0.374618 -0.138501
H -0.369835 1.467531 -0.984956
TS444
E= -650.4887406600 ZPE= 27.6719300000
C 0.455033 0.444750 0.013129
C -2.972618 -0.193618 -0.104439
C -0.621470 -0.430374 0.063822
H 0.001899 -0.020226 1.151484
H -2.772451 -1.288318 -0.083017
O -1.805676 0.391384 0.007491
Cl 2.098718 -0.133291 -0.048589
H 0.372086 1.518869 -0.137455
TS445
E= -650.4915256500 ZPE= 29.5856500000
C -1.770297 1.155219 0.000034
C 0.476628 -0.669589 0.000018
C 1.415480 0.396220 -0.000017
H 1.000816 1.415992 -0.000072
H 0.695749 -1.723736 0.000060
O 2.625705 0.197177 0.000006
Cl -1.210976 -0.439314 -0.000013
H -2.846479 0.907565 -0.000027
TS446
E= -650.4868701600 ZPE= 27.1006700000
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C -1.349829 -0.038674 -0.508991
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H -0.837617 2.046789 -0.494897
O -2.034215 -0.748290 0.338779
Cl 1.521908 -0.545442 -0.003231
H -0.817516 1.284041 1.090044
TS447
E= -650.4856599500 ZPE= 26.3827600000
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C -1.660152 -0.034023 0.120899
C 0.423426 1.109323 -0.557093
H 0.925600 1.817106 0.121955
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Cl 1.773624 -0.460128 -0.044661
H -3.624025 -0.894736 -0.575003
TS448
E= -650.4858797800 ZPE= 26.7032400000
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C 0.161478 0.357280 0.310891
C -1.324502 -1.027924 -0.207968
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Cl 1.784472 -0.290152 -0.049202
H -2.019780 0.669644 0.238572
TS449
E= -650.4818882800 ZPE= 25.2429800000
C 0.578584 0.782871 0.265557
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C 1.331445 -0.490767 0.445443
H 2.305885 0.640138 -0.878512
H 1.475196 1.267293 -0.665577
O 2.330917 -0.560556 -0.232231
Cl -1.779119 -0.377584 -0.031134
H 0.788566 1.467107 1.092662
TS450
E= -650.4872808500 ZPE= 28.6518400000
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C -1.782285 -0.840240 0.427973
C -1.110888 -0.018688 -0.254321
H -0.905985 1.944000 0.706364
H -2.362888 -1.291939 1.201640
O -0.591606 1.593208 -0.140298
Cl 1.582606 -0.198376 0.157796
H 0.386558 1.283603 0.000800
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E= -650.4865506800 ZPE= 28.2667700000
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C 0.255505 -0.759926 -0.106569
C 3.353032 0.493984 -0.390275
H 0.058048 -1.775512 -0.418723
H 2.525341 -0.417754 1.135780
O 2.484930 -0.093832 0.219891
Cl -2.381277 0.114036 -0.031670
H -0.305527 1.240564 0.386429
TS452
E= -650.4758891500 ZPE= 21.7052000000
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C -2.389165 -0.052582 -0.000029
C -3.398102 -0.816479 -0.000012
H -1.348228 -1.130214 0.000109
H -0.373843 -0.817791 0.000135
O -0.345757 1.274534 0.000000
Cl 2.575859 -0.338974 -0.000012
H 1.831004 0.708285 0.000089
TS453
E= -650.4862913100 ZPE= 28.9484700000
C 0.244488 -1.007564 0.370736
C 1.466937 -0.372076 0.085743
C -0.862411 1.227735 0.731891
H -0.690108 1.983350 -0.061050
H 2.327018 -1.043583 0.271390
O 1.651843 0.761617 -0.351830
Cl -1.176820 -0.247600 -0.320351

H 0.060197 -1.912080 0.920042
TS454
E= -650.4857031300 ZPE= 28.8580800000
C 0.403437 -1.044443 0.225770
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C 1.681683 -0.369537 0.109014
H -1.546437 0.454728 1.633957
H -2.889573 -0.321455 0.542482
O 1.942786 0.825073 0.155159
Cl -0.839210 0.088743 -0.557503
H 2.486311 -1.132521 0.016761
TS455
E= -650.4853501300 ZPE= 28.8651200000
C -0.909546 -0.937474 -0.499534
C -1.845776 -0.408736 0.440736
C -0.970599 0.605973 -0.398481
H -1.403166 1.132755 -1.244630
H -2.874006 -0.406332 0.081098
O 0.064396 1.068880 0.238803
Cl 1.637202 -0.255083 0.028467
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TS456
E= -650.4822897600 ZPE= 27.1502200000
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C -2.364365 0.759110 -0.137078
C -1.031621 -1.440127 -0.040556
H -0.740473 -1.868987 0.919570
H -2.900061 1.645022 0.111520
O 1.061481 1.296561 0.142418
Cl 1.506917 -0.337047 -0.077307
H 0.103768 1.275776 -0.035548
TS457
E= -650.4772669000 ZPE= 24.7424000000
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C 1.284991 0.175178 -0.010276
C 2.521655 -0.439343 0.000149
H 1.277799 -1.110056 -0.012158
H 4.385751 -0.323753 0.018182
O 3.623396 0.270880 0.011746
Cl -3.271677 -0.007333 0.006313
H -1.960307 0.070543 -0.012936
TS458
E= -650.4829726500 ZPE= 29.1170200000
C -1.948716 -1.066547 -0.260145
C 0.524155 -0.022928 0.037469
C -2.197842 0.028345 0.479340
H -2.606329 0.338399 1.435129
H 0.030164 -0.435967 -0.817133
O -1.679454 0.799066 -0.442026
Cl 2.216431 -0.010897 0.024506
H 0.066893 0.257067 0.961623
TS459
E= -650.4821408000 ZPE= 28.8383200000
C 0.502214 -0.914013 0.369803
C -1.408907 1.151600 0.205131
C 1.294121 0.206383 -0.171483

H -1.671615 1.791364 -0.619036
H -0.949680 1.473772 1.122478
O 2.498068 0.209802 0.005532
Cl -1.206049 -0.503173 -0.124897
H 0.815023 0.946567 -0.845157
TS460
E= -650.4779424500 ZPE= 26.4664500000
C 2.647312 -0.408945 0.000859
C 1.346285 1.346447 0.000053
C 0.608350 0.306553 -0.000966
H 1.559530 2.394561 0.000656
H -1.188808 0.110319 -0.000824
O 1.428118 -0.847535 -0.000569
Cl -2.515157 -0.112966 0.000230
H 3.350303 -1.268514 0.001135
TS461
E= -650.4807526700 ZPE= 28.8824600000
C -0.298379 -1.011212 0.204692
C 1.795552 -0.051604 0.497080
C 1.358456 0.970626 -0.125862
H 0.846823 1.901105 -0.252933
H 2.385694 -0.694064 1.112771
O 0.915896 -0.421357 -0.637566
Cl -1.591867 0.264426 0.075713
H -0.631731 -1.778289 -0.501898
TS462
E= -650.4812644300 ZPE= 29.4780800000
C -0.159363 0.575111 0.361109
C 1.755340 0.846946 -0.111050
C 0.753495 -0.822409 0.161923
H 1.669436 1.018592 -1.200244
H -0.167933 0.685842 1.440291
O 1.977284 -0.604007 -0.057709
Cl -1.833649 -0.118529 -0.125523
H -0.244579 1.544722 -0.116377
TS463
E= -650.4789518600 ZPE= 28.2245400000
C -0.060304 -0.430777 -0.000014
C -0.346031 0.811676 0.000005
C 2.304912 0.603186 -0.000012
H 3.277309 1.133756 0.000007
H -0.376788 1.877409 0.000018
O 2.579779 -0.651331 0.000009
Cl -2.154929 -0.151436 0.000001
H 1.703571 -1.130601 0.000005
TS464
E= -650.4795689100 ZPE= 28.7077500000
C 0.462761 0.519435 -0.423338
C -2.175130 -0.939327 -0.145084
C 1.467712 -0.173342 0.301022
H 1.150185 -0.587985 1.281079
H 0.505524 0.829698 -1.453606
O 2.625640 -0.286630 -0.077853
Cl -1.156339 0.421789 0.188167
H -1.535122 -1.559680 -0.799089
TS465

E= -650.4757984500 ZPE= 26.5394800000
C 0.437632 -0.535464 -0.000007
C -0.496540 0.421554 -0.000009
C -1.906373 0.605782 0.000007
H -0.013627 1.658821 0.422702
H -0.013632 1.658814 -0.422715
O -2.529539 -0.557768 0.000000
Cl 2.090156 -0.083822 0.000003
H -3.477394 -0.381743 0.000013
TS466
E= -650.4783077000 ZPE= 28.1857600000
C -0.370199 -1.121240 -0.057258
C 1.009289 1.302292 -0.003317
C -1.234554 -0.006381 0.179998
H 1.895354 1.795939 0.372426
H 0.582124 1.651764 -0.930137
O -2.371129 0.278920 -0.098614
Cl 1.215563 -0.438522 -0.013950
H -0.600244 0.727796 0.867238
TS467
E= -650.4697735800 ZPE= 23.4207400000
C -1.575737 -0.611243 0.000073
C -2.553439 -1.469592 -0.000050
C -1.586492 0.850261 -0.000102
H -1.429335 2.109976 -0.000249
H -0.606564 -1.133283 0.000346
O -0.437500 1.474312 0.000090
Cl 2.262674 -0.351057 -0.000026
H 1.364450 0.580230 0.000097
TS468
E= -650.4745372400 ZPE= 27.2407100000
C -0.444566 1.926833 -0.199626
C -0.101638 0.641686 0.100960
C 1.930353 -0.814144 -0.106840
H -1.529170 2.048948 -0.239362
H -0.216630 1.180550 1.134384
O 1.409897 0.325821 0.073008
Cl -1.116557 -0.868906 -0.002709
H 1.143201 -1.590904 -0.200008
TS469
E= -650.4766649600 ZPE= 28.8849700000
C 0.495205 0.819186 0.311779
C 0.123395 1.650363 -0.648936
C -1.580427 0.089874 0.605208
H -2.066130 1.066003 0.407804
H -1.583152 -1.588246 -0.219877
O -1.979086 -0.716318 -0.354365
Cl 1.458571 -0.604736 -0.017506
H 0.457235 1.176760 1.336284
TS470
E= -650.4777820800 ZPE= 29.6551900000
C -1.521766 0.774743 -0.586108
C 0.263005 0.616924 0.568399
C -0.807815 -0.755332 0.537666
H 0.258379 1.643637 0.219865
H -2.042766 1.349660 0.206613

O -1.840644 -0.602746 -0.167305
Cl 1.675133 -0.153516 -0.226496
H 0.431738 0.620441 1.642649
TS471
E= -650.4705867900 ZPE= 25.2488100000
C -0.504372 -0.156198 0.000000
C 0.694520 -0.819021 0.000000
C -1.840899 -0.596306 0.000000
H -2.457507 1.250679 0.000000
H -0.427776 1.087945 0.455811
O -2.775012 0.312539 0.000000
Cl 2.083392 0.206016 0.000000
H -0.427776 1.087946 -0.455811
TS472
E= -650.4748610200 ZPE= 27.9764900000
C 0.870438 -1.470426 0.289146
C -0.005790 1.356312 0.314385
C -1.859013 0.386731 -0.080295
H 0.225177 2.287257 -0.191763
H -0.040428 1.389618 1.395755
O -1.645780 -0.747969 -0.153958
Cl 1.093284 0.119876 -0.257050
H 0.361855 -1.366712 1.258099
TS473
E= -650.4706886100 ZPE= 25.7279500000
C -0.825547 0.808350 -0.000022
C -0.122932 1.842374 0.000029
C -1.533938 -1.532057 0.000077
H -0.435355 -1.716014 0.000055
H 0.948895 1.207961 0.000001
O -1.609161 -0.188281 -0.000071
Cl 1.618276 -0.447421 -0.000008
H -0.256434 2.908457 0.000144
TS474
E= -650.4709247600 ZPE= 26.0716800000
C 1.533400 1.089553 0.238935
C -0.020359 -1.060284 0.155234
C 0.986857 -0.172369 0.080528
H -0.266249 -1.786893 -0.602821
H -1.899838 0.866084 -1.038189
O 2.297371 -0.310052 -0.144834
Cl -1.924782 0.148923 0.035186
H 1.509030 1.728145 -0.646650
TS475
E= -650.4660292900 ZPE= 23.0164600000
C 0.025793 0.054970 0.001399
C -1.231149 0.023519 0.000778
C -2.542225 -0.194985 -0.000073
H -2.739089 -1.497438 -0.000382
H -3.618265 -0.998902 -0.000876
O -3.651259 0.377665 -0.000690
Cl 3.298284 0.007235 -0.000374
H 1.982083 0.051006 0.000517
TS476
E= -650.4686598500 ZPE= 25.2182700000
C -0.416736 1.478464 -0.025984

C 0.021774 0.238327 -0.024463
C -1.075745 -0.723577 -0.319896
H -2.342833 0.393118 0.611899
H 0.528902 2.585556 -0.134790
O -2.269874 -0.443822 0.111717
Cl 1.618860 -0.452504 0.055053
H 1.276546 2.305192 -0.084686
TS477
E= -650.4690994600 ZPE= 26.1516200000
C 0.022064 0.837584 0.000000
C -0.974832 -0.014046 0.000000
C -3.170222 -0.656745 0.000000
H -4.135258 -0.112411 0.000000
H -0.738585 -1.078473 0.000000
O -2.307453 0.341853 0.000000
Cl 2.728023 -0.189215 0.000000
H 1.695024 0.671954 0.000000
TS478
E= -650.4706290600 ZPE= 27.1617900000
C 0.666027 1.259173 -0.015187
C -0.753023 1.206101 -0.025115
C -1.714506 0.242972 0.021117
H -2.173659 -0.947219 0.499948
H -1.186528 2.202916 0.036704
O -1.265894 -1.217779 -0.105906
Cl 1.448885 -0.377926 0.012027
H -0.334698 -1.338199 0.221258
TS479
E= -650.4676755400 ZPE= 25.3474900000
C 3.301497 0.669407 0.342227
C 2.782842 -0.410861 -0.127056
C 0.327062 0.264101 -0.432895
H 0.697346 0.864120 -1.276402
H 2.952826 -1.355838 -0.602028
O 1.119333 -0.351447 0.254463
Cl -2.909981 0.004585 0.070983
H -1.603565 0.089465 -0.057652
TS480
E= -650.4713755800 ZPE= 28.7112600000
C 0.847796 -0.037161 0.590033
C 2.036132 -0.152771 -0.374156
C 1.730085 1.061289 -0.088315
H -1.948946 1.362696 0.294102
H 2.532950 -0.993352 -0.816504
O -2.240387 0.577716 -0.193335
Cl -0.658723 -0.594650 -0.021401
H 0.853300 -0.110156 1.667529
TS481
E= -650.4655256200 ZPE= 26.2907300000
C 0.041519 1.677924 0.118435
C -2.267335 -0.802618 0.515813
C -0.672617 0.679139 -0.130917
H -0.180620 2.727481 0.219834
H -2.787088 -1.580340 -0.074342
O -1.451284 -0.280153 -0.466575
Cl 1.815192 -0.552436 0.020448

H 1.110312 1.158825 0.219508
 TS482
 E= -650.4643272900 ZPE= 25.7354400000
 C 0.029738 -1.582112 0.236110
 C 1.145053 -0.996364 -0.112812
 C 1.934314 1.228593 0.316056
 H 2.248891 0.703733 1.243257
 H 2.049801 -1.585396 -0.198089
 O 1.331869 0.417998 -0.467350
 Cl -1.833061 0.371401 -0.019650
 H -2.446243 -0.676837 0.391550
 TS483
 E= -650.4665963900 ZPE= 27.4736600000
 C 2.519329 -0.895915 0.056493
 C 1.935634 0.218808 0.065270
 C 0.751935 1.038543 0.007533
 H 0.427708 1.503127 0.934903
 H 0.629620 1.689263 -0.853141
 O -0.095860 -0.214993 -0.224338
 Cl -1.903787 -0.160711 0.052904
 H 0.832546 -0.908967 0.037802
 TS484
 E= -650.4627226300 ZPE= 25.4667500000
 C 0.446798 1.284612 0.132458
 C 0.460225 -1.245960 -0.162227
 C 1.096377 0.021688 -0.004262
 H 0.322955 -1.771934 0.788962
 H -1.888998 0.569201 1.064725
 O 2.345671 -0.020528 0.021483
 Cl -1.736265 -0.045962 -0.058295
 H 0.296787 1.786284 -0.830344
 TS485
 E= -650.4621276900 ZPE= 25.4123100000
 C 2.332741 -0.630222 -0.336835
 C 1.397774 0.183442 -0.003891
 C 0.465651 1.109161 0.018775
 H 0.677370 2.172168 0.039217
 H 3.063928 -1.306230 0.434953
 O -0.892934 0.959670 0.042844
 Cl -1.444564 -0.673533 -0.007504
 H 2.782766 -1.067515 1.242365
 TS486
 E= -650.4602349500 ZPE= 24.5878700000
 C -1.663094 -0.581375 0.000004
 C -2.712783 0.182119 0.000000
 C 0.604715 -0.815886 -0.000006
 H -2.459626 1.544787 -0.419656
 H -2.459626 1.544821 0.419634
 O -0.418630 0.014934 0.000002
 Cl 2.039660 0.234515 0.000001
 H -3.778952 0.095014 0.000005
 TS487
 E= -650.4661693000 ZPE= 28.4007500000
 C -0.710643 -0.951760 -0.448848
 C 2.346471 0.098692 -0.357583
 C -1.864092 -0.376187 0.119885

H 3.028233 -0.679306 -0.056971
H 2.388052 0.537593 -1.340373
O -2.063404 0.798467 -0.234707
Cl 0.883563 0.122823 0.391007
H -2.560036 -0.958493 0.747150
TS488
E= -650.4661595800 ZPE= 28.5762400000
C -1.290539 1.509300 0.000114
C 0.222232 -0.061980 -0.000123
C 1.434081 -0.235674 0.000230
H 3.300919 -0.470776 -0.000247
H -1.926789 1.606480 -0.888430
O 2.662759 0.250222 -0.000027
Cl -1.349581 -0.706695 -0.000015
H -1.927959 1.606449 0.887825
TS489
E= -650.4598629200 ZPE= 24.6432800000
C 1.730782 0.470107 0.000000
C 2.147430 -0.800875 0.000000
C -0.298956 -0.426931 0.000002
H 4.112020 -0.141427 -0.000001
H 3.681071 -0.804459 -0.000001
O 0.335683 0.707642 0.000000
Cl -2.014379 -0.091567 0.000000
H 2.290358 1.387579 0.000000
TS490
E= -650.4598968400 ZPE= 24.9755100000
C 1.554528 0.000738 -0.180934
C 1.836576 -1.339226 -0.263415
C 1.831862 1.341749 -0.262282
H 1.048485 1.932215 -0.739855
H 1.055308 -1.932023 -0.741553
O 0.760689 -0.001107 0.887573
Cl -2.261662 -0.000558 -0.106521
H -1.078846 -0.001418 0.431468
TS491
E= -650.4610697900 ZPE= 25.8281100000
C -0.462536 1.536465 0.002039
C -1.266599 0.561984 -0.007496
C -1.066406 -1.382593 0.015063
H -0.025772 -0.849113 0.128134
H 0.674411 1.133720 -0.117336
O -2.104572 -0.453580 -0.017437
Cl 1.978059 -0.208429 -0.002642
H -0.665826 2.592190 0.115971
TS492
E= -650.4651004800 ZPE= 28.7077100000
C -0.638004 -0.949806 0.354337
C -1.657919 -0.017636 -0.011596
C -1.476766 1.262525 -0.299940
H 1.472337 1.727411 -0.447029
H -2.717288 -0.264910 0.090810
O 1.272381 1.287788 0.391460
Cl 0.848517 -0.703025 -0.250375
H -0.722756 -1.583892 1.224108
TS493

E= -650.4570686600 ZPE= 23.8171100000
C -2.547481 0.041633 -0.000046
C -1.245536 -0.177127 0.000030
C 0.842675 1.079280 0.000003
H -3.369015 -1.460603 -0.000012
H -0.712479 -1.112507 0.000106
O -0.441452 1.001293 0.000015
Cl 1.668614 -0.525816 -0.000010
H -3.051273 -2.161073 0.000039

TS494

E= -650.4630410200 ZPE= 27.6875400000
C 0.657971 -1.023635 -0.049485
C -1.852641 1.052995 0.052086
C 1.567944 -0.002385 0.305865
H -1.505521 1.640228 0.889636
H -1.954550 1.538142 -0.908631
O 2.452154 0.587567 -0.286548
Cl -1.164129 -0.481205 -0.056115
H 1.393393 0.139729 1.414544

TS495

E= -650.4564428600 ZPE= 23.5811600000
C 2.405274 -1.224562 -0.120526
C 1.640652 -0.230821 0.160934
C 0.516602 1.344848 0.446131
H 0.918390 0.015799 1.146892
H 2.526768 -2.069300 0.543136
O 1.293822 0.968335 -0.488377
Cl -2.258373 -0.340219 -0.062152
H -2.778564 0.753764 0.354328

TS496

E= -650.4614399100 ZPE= 27.2238400000
C 0.710117 1.243158 0.000000
C -0.581415 1.290933 0.000000
C 2.391816 -0.568130 0.000000
H 0.136234 -0.736457 0.000000
H -1.371604 2.011675 0.000000
O 1.140802 -0.141400 0.000000
Cl -1.486080 -0.604173 0.000000
H 2.249207 -1.668834 0.000000

TS497

E= -650.4564133300 ZPE= 24.1560100000
C 0.836962 0.893817 0.139670
C -2.318120 -0.572244 -0.274817
C -1.373911 0.202240 -0.115440
H -3.078953 -1.238634 0.235110
H -3.006261 -1.209344 1.417056
O -0.464047 1.087949 0.016925
Cl 1.499164 -0.657278 -0.019571
H 1.442217 1.775238 0.048669

TS498

E= -650.4607271300 ZPE= 27.0994500000
C 2.868341 1.082145 -0.000258
C 2.496876 -0.165275 -0.000074
C -0.900060 0.572218 0.000409
H 3.529792 -0.587892 -0.000172
H 0.627614 -0.503077 0.000312

O 1.473756 -1.026564 0.000173
Cl -2.452599 -0.076092 -0.000169
H -1.044210 1.662512 0.000878
TS499
E= -650.4588038300 ZPE= 25.9578100000
C 0.957678 1.020596 0.078588
C -2.392552 0.278870 -0.506536
C -1.833054 0.288349 0.628760
H -1.579532 0.717312 1.578381
H -2.964985 0.405306 -1.395402
O -1.513752 -0.957069 0.030782
Cl 2.090283 -0.248951 -0.038443
H 0.727293 1.239215 -0.980581
TS500
E= -650.4564829900 ZPE= 24.5862700000
C 1.146804 -0.254549 -0.514841
C 2.269072 -0.563289 0.058175
C -0.772775 1.087821 0.085282
H 3.023012 -1.320452 -0.002593
H 2.868129 0.493756 0.796596
O 0.492725 0.908509 -0.139811
Cl -1.656281 -0.475718 0.069550
H 2.465229 0.025939 1.370439
TS501
E= -650.4607924600 ZPE= 27.9498700000
C -0.982475 1.217791 0.321946
C 2.057661 -0.514136 0.187522
C -0.196639 0.712490 -0.773909
H -1.853500 1.836218 0.104350
H 1.419129 -1.436483 0.057248
O 1.516340 0.554230 -0.011352
Cl -0.957738 -0.853119 0.008769
H -0.686093 1.172573 1.366783
TS502
E= -650.4533848500 ZPE= 23.4837800000
C 1.480901 -0.915007 -0.024965
C 2.008318 0.206282 0.332797
C 0.905481 -2.049721 -0.167107
H 0.150304 1.478916 -0.000250
H 1.940126 1.387061 0.563204
O 1.054834 1.714972 -0.268314
Cl -2.087781 0.056371 0.057750
H -1.405026 -0.993384 -0.242548
TS503
E= -650.4567832000 ZPE= 25.9293800000
C 1.454355 -0.158423 -0.151155
C 2.510054 -0.898129 0.017805
C 0.473410 0.479097 0.696857
H -0.538873 2.196960 0.398405
H 1.507526 -0.024019 -1.253960
O -0.171651 1.552966 -0.224700
Cl -1.483235 -0.702911 -0.016651
H -1.007370 0.817541 -0.444821
TS504
E= -650.4631259300 ZPE= 30.0474000000
C 1.253112 0.193222 -0.278050

C 2.568064 0.064026 0.010173
C 0.424923 -0.618981 0.546448
H 3.335168 0.500780 -0.615771
H 2.880202 -0.509823 0.872130
O -1.302316 1.119464 0.288777
Cl -1.304445 -0.445547 -0.184323
H 0.902133 0.798032 -1.104507
TS505
E= -650.4575997900 ZPE= 26.6088400000
C 1.751813 -0.042215 -0.000011
C 3.063778 0.030681 0.000081
C 0.532006 0.653656 -0.000122
H 3.703076 -0.841582 0.000116
H 3.542906 1.007236 0.000124
O -0.233443 -0.501854 -0.000128
Cl -2.245037 0.071739 0.000057
H 0.701604 -1.223121 0.000124
TS506
E= -650.4533853800 ZPE= 24.3509000000
C 2.750594 -0.501737 0.027488
C 1.650709 -0.980965 0.069556
C 0.427650 1.504185 -0.487679
H 3.733804 -0.103069 -0.019740
H 0.651934 -1.370618 0.104315
O -0.469633 1.338917 0.301891
Cl -1.742080 -0.689334 -0.041920
H 0.012968 2.352133 0.556743
TS507
E= -650.4566824800 ZPE= 28.5893500000
C -0.430414 -0.748457 0.756006
C 1.247760 1.220322 0.042620
C -1.374056 0.340097 0.401049
H 1.956980 1.268748 0.860386
H 1.608041 1.598416 -0.907879
O -1.986393 0.099977 -0.620770
Cl 1.018284 -0.569319 -0.193102
H -1.644446 1.139662 1.098336
TS508
E= -650.4526801200 ZPE= 26.8392300000
C -0.459720 1.137785 -0.303575
C 0.927447 1.067379 -0.004169
C 1.521084 -0.049166 0.671645
H 1.442844 2.017467 -0.092408
H 0.665649 -0.141510 -0.975684
O 1.304920 -0.999495 -0.343716
Cl -1.505632 -0.288766 0.098659
H 1.115027 -1.906971 -0.042788
TS509
E= -650.4565258400 ZPE= 29.9991800000
C 1.575564 -0.489320 0.136745
C 1.870485 0.804239 -0.110995
C 0.282037 -1.071852 0.332515
H 2.889482 1.162717 -0.055703
H 1.094362 1.534983 -0.288057
O -1.466465 0.493064 0.902055
Cl -0.999803 -0.054884 -0.555616

H 2.376002 -1.167589 0.423202
TS510
E= -650.4459325600 ZPE= 24.0549000000
C -1.710914 1.988328 0.059878
C -0.859958 1.073617 -0.044368
C 1.855008 0.689978 -0.047371
H 2.430308 1.627695 -0.173305
H 0.688936 0.854289 -0.050610
O 2.336186 -0.388661 0.079572
Cl -0.904881 -1.230286 -0.028317
H -2.130575 -0.969362 0.259890
TS511
E= -650.4398068600 ZPE= 24.9990600000
C 2.208440 -0.511150 0.438824
C -0.768731 0.897118 0.112297
C 1.408018 0.131062 -0.352612
H -1.361290 1.793457 0.122303
H 3.044686 -1.299987 -0.823517
O 0.498606 1.037499 -0.040459
Cl -1.521303 -0.623021 -0.013140
H 3.103554 -1.304286 0.057210
TS512
E= -650.4392886000 ZPE= 24.7232500000
C 1.047491 -1.610353 -0.130078
C -0.231989 -1.556788 -0.122395
C 1.527349 0.417129 0.405801
H 1.209067 0.388904 1.452750
H 2.142471 -0.556068 0.084122
O 1.335391 1.299989 -0.370430
Cl -1.610259 0.299053 0.045296
H -0.717369 1.183430 -0.263436
TS513
E= -650.4382751300 ZPE= 25.0920600000
C -1.201696 0.033527 -0.436556
C -2.179068 -0.358190 0.290893
C 0.900520 1.085602 0.114338
H -3.159165 -1.079896 -0.595946
H -2.777655 -0.354012 1.180104
O -0.372847 1.085930 -0.057932
Cl 1.556811 -0.598578 0.020058
H -2.664727 -1.643329 -0.273734
TS514
E= -650.4435153800 ZPE= 28.6210700000
C 1.021067 0.056868 0.085402
C 1.318988 -1.261256 0.112130
C 1.863540 1.030699 -0.340281
H 2.354745 -1.564952 0.051459
H 0.541738 -2.015550 0.098783
O -1.758083 -0.400930 -0.706804
Cl -0.909304 0.349596 0.423413
H 1.404771 1.886940 -0.837349
TS515
E= -650.4362476300 ZPE= 26.5189100000
C -3.544286 -1.037891 -0.010074
C -2.720340 -0.031046 -0.027329
C -1.831043 0.885557 -0.067534

H -1.788986 1.960547 0.005635
H -0.251241 0.354312 -0.471222
O 0.538189 0.393850 0.159540
Cl 2.699278 -0.235234 -0.054768
H 0.421003 -0.366401 0.749948
TS516
E= -650.4332182100 ZPE= 25.7073800000
C -0.583838 0.409694 0.000032
C 0.302365 -0.568099 -0.000048
C 3.076982 -0.347103 0.000025
H -0.410270 1.473512 0.000112
H 2.802776 -1.418560 0.000128
O 2.039965 0.435980 -0.000020
Cl -2.266699 -0.087355 -0.000002
H 3.048600 0.975282 -0.000108
TS517
E= -650.4266359900 ZPE= 22.9989700000
C 1.140211 0.938588 0.000021
C -0.024672 1.530946 -0.000095
C -2.725564 -0.015286 0.000245
H -3.813745 -1.285884 -0.000120
H 1.915248 1.711325 0.000126
O -1.631591 -0.404834 -0.000307
Cl 1.672629 -0.700566 0.000049
H -3.823322 -0.002628 0.000590
TS518
E= -650.4326577500 ZPE= 27.8919000000
C 0.440197 0.930497 0.133605
C 1.632969 0.330664 0.214988
C 2.227737 -0.863678 -0.165683
H 2.227350 -1.645673 0.604756
H 2.487079 0.953981 0.544094
O -1.892464 -0.433961 0.701218
Cl -0.917328 -0.009787 -0.486276
H 0.214449 1.944866 0.410646
TS519
E= -650.4206833900 ZPE= 24.9064200000
C -0.024315 0.857213 -0.047052
C 0.707893 -0.247287 -0.148063
C 3.167159 -0.019752 0.410558
H 0.432346 -1.295271 -0.151218
H -2.569888 1.080479 0.252493
O 2.037044 0.081379 -0.287102
Cl -2.403754 -0.175185 0.049354
H 3.600582 -0.999134 0.063870
TS520
E= -650.4204488100 ZPE= 24.8505800000
C 0.460849 0.673737 -0.062172
C -2.348812 0.108029 -0.330670
C 1.669822 0.189830 -0.020345
H -2.505599 1.403221 1.062530
H -2.154617 1.010860 -0.921529
O 2.815375 -0.056976 0.004713
Cl -0.802710 -0.500486 0.083145
H -2.907872 0.720413 0.886955
TS521

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E= -650.4174268400 ZPE= 24.3158500000
C 0.664993 -0.459840 -0.000002
C -0.465347 0.191398 0.000000
C 3.023474 -0.151714 0.000002
H 2.902610 -1.255666 0.000004
H -0.267220 1.559565 0.420475
O 1.810192 0.349053 -0.000002
Cl -2.128731 -0.125586 0.000000
H -0.267222 1.559566 -0.420471
TS522
E= -650.4231551300 ZPE= 27.9211400000
C 1.475034 -0.908332 0.115215
C 2.333245 -0.033408 0.084064
C -1.513355 0.361532 0.590974
H -0.264912 2.454798 0.402976
H 3.205859 0.577749 0.085164
O -0.256883 1.772573 -0.278318
Cl -0.897183 -0.882977 -0.166298
H 0.596679 1.278722 -0.176041
TS523
E= -650.4132648100 ZPE= 25.4151300000
C -2.765159 -0.685073 -0.042608
C -1.679390 -0.015963 0.253859
C 0.410673 1.224754 0.300347
H 0.882635 1.750421 -0.541238
H -1.670300 0.255357 1.317229
O -0.613266 0.389649 -0.515820
Cl 1.738669 -0.460162 0.048891
H 0.339680 -0.442534 -0.550161
TS524
E= -650.3861157400 ZPE= 26.9233200000
C -2.621274 0.203231 -0.000012
C 1.739754 1.040980 0.000023
C -0.641512 -0.908693 0.000010
H 2.813133 1.050322 0.000126
H 1.066418 1.874852 -0.000219
O -1.285899 0.299046 0.000012
Cl 1.085488 -0.506170 -0.000011
H -2.907473 1.274235 0.000057
TS525
E= -650.3665009000 ZPE= 22.3763100000
C -1.949063 -1.350857 -0.000034
C -1.571871 -0.218386 0.000000
C -0.039260 1.567694 -0.000031
H 1.922607 0.924294 -0.000441
H -2.266720 -2.363041 -0.000068
O -1.253605 1.075580 0.000055
Cl 1.683858 -0.347330 0.000024
H 3.108527 -1.251988 0.000056
TS526
E= -650.3715087000 ZPE= 25.8207700000
C -2.410978 -1.123469 -0.084780
C 0.973879 0.150978 0.887639
C -1.671833 1.266610 -0.324636
H -0.619583 1.331086 0.051583
H 1.520370 0.797724 1.599458

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O -2.032758 0.088118 -0.066742
Cl 2.171866 -0.194016 -0.286579
H -2.906843 -1.300195 0.885407

Reaction mechanisms employed in the KMC simulation(the dominant pathways at 148 kcal/mol are highlighted in red)

TS	12	Path:	MIN	1 <-->	MIN	6
TS	13	Path:	MIN	1 <-->	HCl + C3H2O	
TS	14	Path:	MIN	6 <-->	HCl + C3H2O	
TS	17	Path:	MIN	1 <-->	MIN	12
TS	18	Path:	MIN	39 <-->	ClCHO + C2H2	
TS	19	Path:	MIN	1 <-->	HCl + C3H2O	
TS	20	Path:	MIN	1 <-->	CO + C2H3Cl	
TS	22	Path:	MIN	11 <-->	CO + C2H3Cl	
TS	25	Path:	MIN	4 <-->	MIN	20
TS	28	Path:	MIN	1 <-->	MIN	11
TS	30	Path:	MIN	1 <-->	MIN	11
TS	31	Path:	MIN	13 <-->	HCl + C3H2O	
TS	32	Path:	MIN	3 <-->	MIN	17
TS	34	Path:	MIN	1 <-->	HCl + CO + C2H2	
TS	40	Path:	MIN	11 <-->	MIN	55
TS	41	Path:	MIN	37 <-->	HCl + C3H2O	
TS	42	Path:	MIN	1 <-->	CO + C2H3Cl	
TS	43	Path:	MIN	3 <-->	MIN	6
TS	44	Path:	MIN	12 <-->	CO + C2H3Cl	
TS	46	Path:	MIN	27 <-->	MIN	36
TS	47	Path:	MIN	16 <-->	HCl + C3H2O	
TS	49	Path:	MIN	3 <-->	HCl + CO + C2H2	
TS	50	Path:	MIN	1 <-->	HCl + CO + C2H2	
TS	51	Path:	MIN	27 <-->	HCl + C3H2O	
TS	52	Path:	MIN	3 <-->	MIN	13
TS	54	Path:	MIN	4 <-->	MIN	65
TS	56	Path:	MIN	47 <-->	CO + C2H3Cl	
TS	57	Path:	MIN	35 <-->	MIN	37
TS	58	Path:	MIN	1 <-->	MIN	71
TS	59	Path:	MIN	15 <-->	HCl + C3H2O	
TS	61	Path:	MIN	3 <-->	MIN	84
TS	65	Path:	MIN	1 <-->	MIN	71
TS	67	Path:	MIN	6 <-->	MIN	84
TS	69	Path:	MIN	3 <-->	MIN	84
TS	70	Path:	MIN	16 <-->	MIN	91
TS	73	Path:	MIN	4 <-->	MIN	30
TS	75	Path:	MIN	40 <-->	HCl + C3H2O	
TS	76	Path:	MIN	3 <-->	HCl + C3H2O	
TS	81	Path:	MIN	4 <-->	MIN	65
TS	84	Path:	MIN	3 <-->	ClCHO + C2H2	
TS	87	Path:	MIN	13 <-->	MIN	16
TS	88	Path:	MIN	3 <-->	MIN	65
TS	91	Path:	MIN	1 <-->	MIN	26
TS	93	Path:	MIN	22 <-->	MIN	80
TS	94	Path:	MIN	12 <-->	CO + C2H3Cl	
TS	95	Path:	MIN	16 <-->	HCl + C3H2O	
TS	96	Path:	MIN	3 <-->	MIN	65
TS	97	Path:	MIN	3 <-->	HCl + C3H2O	
TS	98	Path:	MIN	40 <-->	HCl + C3H2O	
TS	99	Path:	MIN	6 <-->	CO + C2H3Cl	
TS	100	Path:	MIN	12 <-->	MIN	55
TS	102	Path:	MIN	13 <-->	HCl + C3H2O	
TS	103	Path:	MIN	13 <-->	MIN	16
TS	104	Path:	MIN	12 <-->	MIN	71

TS 105	Path:	MIN	4	<-->	MIN	21
TS 106	Path:	MIN	6	<-->	MIN	3
TS 107	Path:	MIN	1	<-->	MIN	39
TS 110	Path:	MIN	6	<-->	MIN	83
TS 113	Path:	MIN	4	<-->	HCl + C3H2O	
TS 114	Path:	MIN	4	<-->	MIN	16
TS 115	Path:	MIN	6	<-->	MIN	83
TS 116	Path:	MIN	3	<-->	HCl + C3H2O	
TS 117	Path:	MIN	4	<-->	HCl + C3H2O	
TS 118	Path:	MIN	23	<-->	HCl + C3H2O	
TS 120	Path:	MIN	58	<-->	CO + C2H3Cl	
TS 122	Path:	MIN	4	<-->	MIN	37
TS 123	Path:	MIN	6	<-->	CO + C2H3Cl	
TS 125	Path:	MIN	3	<-->	HCl + C3H2O	
TS 128	Path:	MIN	58	<-->	CO + C2H3Cl	
TS 129	Path:	MIN	13	<-->	HCl + C3H2O	
TS 131	Path:	MIN	1	<-->	MIN	85
TS 132	Path:	MIN	6	<-->	MIN	84
TS 133	Path:	MIN	4	<-->	HCl + C3H2O	
TS 134	Path:	MIN	3	<-->	MIN	110
TS 135	Path:	MIN	3	<-->	MIN	106
TS 136	Path:	MIN	3	<-->	H2 + C3HOCl	
TS 138	Path:	MIN	58	<-->	CO + C2H3Cl	
TS 139	Path:	MIN	4	<-->	MIN	110
TS 140	Path:	MIN	3	<-->	MIN	36
TS 141	Path:	MIN	3	<-->	MIN	36
TS 142	Path:	MIN	4	<-->	MIN	110
TS 143	Path:	MIN	11	<-->	CO + C2H3Cl	
TS 144	Path:	MIN	4	<-->	ClCHO + C2H2	
TS 145	Path:	MIN	4	<-->	MIN	37
TS 146	Path:	MIN	1	<-->	MIN	85
TS 147	Path:	MIN	3	<-->	CO + C2H3Cl	
TS 149	Path:	MIN	4	<-->	MIN	110
TS 150	Path:	MIN	4	<-->	HCl + CO + C2H2	
TS 151	Path:	MIN	6	<-->	MIN	36
TS 153	Path:	MIN	12	<-->	CO + C2H3Cl	
TS 154	Path:	MIN	27	<-->	MIN	36
TS 157	Path:	MIN	1	<-->	MIN	4
TS 158	Path:	MIN	4	<-->	CO + C2H3Cl	
TS 159	Path:	MIN	1	<-->	ClCHO + C2H2	
TS 160	Path:	MIN	119	<-->	ClCHO + C2H2	
TS 162	Path:	MIN	16	<-->	MIN	95
TS 163	Path:	MIN	3	<-->	CO + C2H3Cl	
TS 164	Path:	MIN	11	<-->	MIN	37
TS 165	Path:	MIN	39	<-->	HCl + CO + C2H2	
TS 166	Path:	MIN	3	<-->	MIN	106
TS 168	Path:	MIN	47	<-->	MIN	55
TS 169	Path:	MIN	4	<-->	Cl + C3H3O	
TS 171	Path:	MIN	13	<-->	MIN	36
TS 172	Path:	MIN	39	<-->	MIN	63
TS 176	Path:	MIN	4	<-->	MIN	21
TS 177	Path:	MIN	106	<-->	MIN	110
TS 178	Path:	MIN	39	<-->	ClCHO + C2H2	
TS 179	Path:	MIN	3	<-->	CO + C2H3Cl	
TS 180	Path:	MIN	3	<-->	CO + C2H3Cl	
TS 181	Path:	MIN	21	<-->	ClCH + C2H2O	

TS 182	Path:	MIN	1 <-->	MIN	4
TS 185	Path:	MIN	1 <-->	H2 + C3HOC1	
TS 187	Path:	MIN	84 <-->	HCl + C3H2O	
TS 188	Path:	MIN	4 <-->	MIN	75
TS 189	Path:	MIN	6 <-->	HCl + C3H2O	
TS 190	Path:	MIN	12 <-->	HCl + C3H2O	
TS 191	Path:	MIN	36 <-->	HCl + CO + C2H2	
TS 192	Path:	MIN	1 <-->	ClCHO + C2H2	
TS 193	Path:	MIN	1 <-->	H2 + C3HOC1	
TS 194	Path:	MIN	39 <-->	ClCHO + C2H2	
TS 195	Path:	MIN	6 <-->	H2 + C3HOC1	
TS 197	Path:	MIN	6 <-->	CO + C2H3Cl	
TS 198	Path:	MIN	4 <-->	ClCHO + C2H2	
TS 199	Path:	MIN	1 <-->	H2 + C3HOC1	
TS 200	Path:	MIN	3 <-->	MIN	59
TS 201	Path:	MIN	6 <-->	MIN	36
TS 203	Path:	MIN	6 <-->	HCl + C3H2O	
TS 204	Path:	MIN	13 <-->	MIN	40
TS 205	Path:	MIN	39 <-->	CO + C2H3Cl	
TS 206	Path:	MIN	6 <-->	H2 + C3HOC1	
TS 207	Path:	MIN	4 <-->	HCl + C3H2O	
TS 209	Path:	MIN	26 <-->	ClCHO + C2H2	
TS 211	Path:	MIN	110 <-->	HCl + C3H2O	
TS 212	Path:	MIN	6 <-->	MIN	23
TS 213	Path:	MIN	3 <-->	MIN	76
TS 214	Path:	MIN	4 <-->	MIN	81
TS 215	Path:	MIN	6 <-->	MIN	32
TS 216	Path:	MIN	110 <-->	ClCHO + C2H2	
TS 217	Path:	MIN	4 <-->	H2 + C3HOC1	
TS 218	Path:	MIN	62 <-->	CO + C2H3Cl	
TS 219	Path:	MIN	4 <-->	HCl + C3H2O	
TS 220	Path:	MIN	3 <-->	MIN	106
TS 221	Path:	MIN	11 <-->	H2 + C3HOC1	
TS 222	Path:	MIN	6 <-->	MIN	129
TS 225	Path:	MIN	70 <-->	MIN	81
TS 226	Path:	MIN	11 <-->	H2 + C3HOC1	
TS 227	Path:	MIN	1 <-->	MIN	63
TS 228	Path:	MIN	23 <-->	MIN	37
TS 230	Path:	MIN	3 <-->	MIN	76
TS 231	Path:	MIN	20 <-->	COH2 + C2HCl	
TS 232	Path:	MIN	15 <-->	MIN	85
TS 233	Path:	MIN	6 <-->	MIN	32
TS 235	Path:	MIN	15 <-->	MIN	85
TS 236	Path:	MIN	23 <-->	HCl + C3H2O	
TS 237	Path:	MIN	6 <-->	CO + C2H3Cl	
TS 239	Path:	MIN	22 <-->	COH2 + C2HCl	
TS 241	Path:	MIN	3 <-->	COH2 + C2HCl	
TS 242	Path:	MIN	22 <-->	MIN	124
TS 243	Path:	MIN	22 <-->	MIN	118
TS 245	Path:	MIN	39 <-->	CO + C2H3Cl	
TS 247	Path:	MIN	6 <-->	MIN	27
TS 248	Path:	MIN	3 <-->	HCl + C3H2O	
TS 250	Path:	MIN	36 <-->	MIN	85
TS 252	Path:	MIN	6 <-->	MIN	71
TS 253	Path:	MIN	6 <-->	HCl + C3H2O	
TS 254	Path:	MIN	37 <-->	H2 + C3HOC1	

TS 255	Path:	MIN 21 <-->	MIN 39
TS 256	Path:	MIN 17 <-->	MIN 59
TS 257	Path:	MIN 59 <-->	MIN 76
TS 259	Path:	MIN 22 <-->	MIN 118
TS 260	Path:	MIN 71 <-->	HCl + C3H2O
TS 261	Path:	MIN 20 <-->	MIN 132
TS 262	Path:	MIN 62 <-->	MIN 63
TS 263	Path:	MIN 39 <-->	ClCHO + C2H2
TS 264	Path:	MIN 4 <-->	H2 + C3HOC1
TS 266	Path:	MIN 65 <-->	COH2 + C2HCl
TS 267	Path:	MIN 65 <-->	H2 + C3HOC1
TS 268	Path:	MIN 36 <-->	H2 + C3HOC1
TS 269	Path:	MIN 4 <-->	MIN 3
TS 271	Path:	MIN 11 <-->	MIN 126
TS 272	Path:	MIN 71 <-->	H2 + C3HOC1
TS 273	Path:	MIN 1 <-->	ClCHO + C2H2
TS 274	Path:	MIN 71 <-->	H2 + C3HOC1
TS 275	Path:	MIN 124 <-->	COH2 + C2HCl
TS 277	Path:	MIN 16 <-->	H2O + C3HCl
TS 278	Path:	MIN 12 <-->	H2 + C3HOC1
TS 279	Path:	MIN 13 <-->	H2O + C3HCl
TS 280	Path:	MIN 12 <-->	H2 + C3HOC1
TS 281	Path:	MIN 65 <-->	COH2 + C2HCl
TS 283	Path:	MIN 71 <-->	H2 + C3HOC1
TS 284	Path:	MIN 91 <-->	ClCHO + C2H2
TS 285	Path:	MIN 36 <-->	CO + C2H3Cl
TS 286	Path:	MIN 30 <-->	H2O + C3HCl
TS 287	Path:	MIN 4 <-->	H2 + C3HOC1
TS 288	Path:	MIN 6 <-->	HCl + C3H2O
TS 289	Path:	MIN 135 <-->	ClCHO + C2H2
TS 290	Path:	MIN 37 <-->	CO + C2H3Cl
TS 291	Path:	MIN 35 <-->	HCl + C3H2O
TS 292	Path:	MIN 12 <-->	MIN 27
TS 294	Path:	MIN 30 <-->	COH2 + C2HCl
TS 295	Path:	MIN 23 <-->	MIN 111
TS 296	Path:	MIN 91 <-->	HCl + C3H2O
TS 297	Path:	MIN 4 <-->	COH2 + C2HCl
TS 298	Path:	MIN 65 <-->	H2 + C3HOC1
TS 299	Path:	MIN 23 <-->	MIN 111
TS 300	Path:	MIN 40 <-->	MIN 65
TS 301	Path:	MIN 36 <-->	CO + C2H3Cl
TS 303	Path:	MIN 13 <-->	MIN 115
TS 304	Path:	MIN 32 <-->	HCl + C3H2O
TS 306	Path:	MIN 76 <-->	MIN 108
TS 309	Path:	MIN 116 <-->	Cl + C3H3O
TS 312	Path:	MIN 30 <-->	COH2 + C2HCl
TS 314	Path:	MIN 32 <-->	HCl + C3H2O
TS 315	Path:	MIN 23 <-->	MIN 36
TS 317	Path:	MIN 20 <-->	MIN 118
TS 318	Path:	MIN 40 <-->	H2 + C3HOC1
TS 320	Path:	MIN 55 <-->	MIN 136
TS 322	Path:	MIN 58 <-->	MIN 83
TS 324	Path:	MIN 6 <-->	H2 + C3HOC1
TS 325	Path:	MIN 76 <-->	HCl + CO + C2H2
TS 327	Path:	MIN 65 <-->	H2 + C3HOC1
TS 329	Path:	MIN 1 <-->	ClCHO + C2H2

TS 330	Path:	MIN 6	<-->	H2 + C3HOC1
TS 331	Path:	MIN 6	<-->	MIN 32
TS 335	Path:	MIN 136	<-->	CO + C2H3C1
TS 336	Path:	MIN 55	<-->	HCl + C3H2O
TS 340	Path:	MIN 64	<-->	HCl + C3H2O
TS 341	Path:	MIN 12	<-->	MIN 80
TS 344	Path:	MIN 81	<-->	ClCHO + C2H2
TS 345	Path:	MIN 35	<-->	MIN 55
TS 347	Path:	MIN 138	<-->	HCl + CO + C2H2
TS 349	Path:	MIN 11	<-->	MIN 136
TS 350	Path:	MIN 13	<-->	H2 + C3HOC1
TS 353	Path:	MIN 81	<-->	ClCH + C2H2O
TS 354	Path:	MIN 32	<-->	ClCH + C2H2O
TS 355	Path:	MIN 81	<-->	COH2 + C2HCl
TS 356	Path:	MIN 41	<-->	MIN 133
TS 357	Path:	MIN 144	<-->	COH2 + C2HCl
TS 359	Path:	MIN 27	<-->	MIN 36
TS 360	Path:	MIN 25	<-->	H2 + C3HOC1
TS 362	Path:	MIN 35	<-->	MIN 138
TS 364	Path:	MIN 58	<-->	MIN 84
TS 365	Path:	MIN 13	<-->	MIN 40
TS 366	Path:	MIN 11	<-->	MIN 126
TS 369	Path:	MIN 40	<-->	HCl + C3H2O
TS 370	Path:	MIN 126	<-->	MIN 129
TS 371	Path:	MIN 39	<-->	MIN 136
TS 374	Path:	MIN 85	<-->	HCl + C3H2O
TS 375	Path:	MIN 39	<-->	MIN 136
TS 380	Path:	MIN 119	<-->	MIN 136
TS 381	Path:	MIN 36	<-->	HCl + C3H2O
TS 382	Path:	MIN 36	<-->	MIN 138
TS 383	Path:	MIN 36	<-->	HCl + C3H2O
TS 390	Path:	MIN 136	<-->	HCl + CO + C2H2
TS 393	Path:	MIN 36	<-->	MIN 138
TS 394	Path:	MIN 149	<-->	ClCH + C2H2O
TS 396	Path:	MIN 36	<-->	H2O + C3HCl
TS 397	Path:	MIN 36	<-->	HCl + C3H2O
TS 398	Path:	MIN 39	<-->	CO + C2H3C1
TS 399	Path:	MIN 36	<-->	MIN 138
TS 401	Path:	MIN 36	<-->	HCl + C3H2O
TS 404	Path:	MIN 40	<-->	MIN 138
TS 410	Path:	MIN 58	<-->	MIN 149
TS 411	Path:	MIN 130	<-->	MIN 148
TS 413	Path:	MIN 75	<-->	HCl + C3H2O
TS 415	Path:	MIN 116	<-->	HOCl + C3H2
TS 416	Path:	MIN 83	<-->	MIN 149
TS 421	Path:	MIN 21	<-->	H2 + C3HOC1
TS 425	Path:	MIN 3	<-->	MIN 78
TS 426	Path:	MIN 37	<-->	MIN 151
TS 427	Path:	MIN 156	<-->	CO + C2H3C1
TS 428	Path:	MIN 159	<-->	HCl + C3H2O
TS 429	Path:	MIN 32	<-->	H2 + C3HOC1
TS 430	Path:	MIN 27	<-->	MIN 36
TS 431	Path:	MIN 36	<-->	MIN 134