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Automated transition state search using classical trajectories initialized at multiple minima

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TSSCDS calculations

Postprocessing of structures using SPRINT coordinates and the adjacency and Laplacian matrices

To remove duplicates and also TS structures associated to intermolecular interactions (connecting Van der Waals minima), the so-called social permutation invariant (SPRINT) topological coordinates,[1] as well as the adjacency and Laplacian matrices are employed.[2]

In spectral graph theory, a graph (or molecular structure) can be characterized by an adjacency (or contact) matrix A, whose elements a_{ij} are usually defined as:

$$a_{ij}\begin{cases}1 \text{ if } i \text{ and } j \text{ are connected}\\ 0 \quad\quad\quad\quad\quad \text{otherwise}\end{cases}$$

If matrix A represents a connected graph (with only one component), the Perron-Frobenius holds. This theorem states that the eigenvalue of largest modulus λ^{max} is real, positive and non-degenerate. Additionally, its corresponding eigenvector $\mathbf{v}^{max}$ has all components of equal sign. When a molecule dissociates, the corresponding matrix A becomes disconnected (it has at least two fragments or components), and using the above definition of A, the Perron-Frobenius theorem would not hold. This can be avoided by defining the contact matrix elements as:[1]

$$a_{ij} = \frac{1-(\delta_{ij})^n}{1-(\delta_{ij})^m}$$

Where ij represent a pair of vertices (atoms), δ_{ij} is the normalized distance (defined in the text as r_{ij}/r_{ij}^{ref}). In this work, n and m are 6 and 12, respectively, and the reference distances are gathered in Table 1 of the text.

The SPRINT coordinates are thus defined as:

$$S_i = \sqrt{N}\lambda^{max} v_i^{max,sorted} \quad i = 1,\ldots,N$$

Where N is the number of atoms of our system, and the i^{th} component of the eigenvector is taken after sorting from the smallest to the largest value (we adopt the positive sign convention for the components of the eigenvector). The advantage of using these N SPRINT coordinates is that they are invariant with respect to permutation of like atoms, which is very convenient for our purposes.

Besides the above topological coordinates, we also employ the degree d_i of each vertex (or atom) i, which is defined as $d_i = \sum_{j=1}^{N} a_{ij}$, as well as the eigenvalues of the Laplacian matrix. The Laplacian (or Kirchhoff) matrix L is defined as $L = D - A$, where D is the diagonal degree matrix. An important property of this matrix (relevant to our study) is related with the number of zero eigenvalues, which coincides with the number of components of the graph. Since, by construction, the above adjacency matrix is always connected (only one component), a lower threshold value of 0.005 is set for the eigenvalues. This means that when the two lowest eigenvalues of L are below this threshold, the structure is discarded because it corresponds to a Van der Waals structure.

Levels of theory employed in the TSSCDS procedure

For the trajectory calculations, as well as for a first optimization of TS structures the PM7 semiempirical Hamiltonian is employed. This is the so-called LL.

Then, for all stationary structures, single point energies are calculated at the CCSD(T)/6-311+G(3df,2p) level of theory, and the geometries are optimized using B3LYP/6-311G(d,p) (which, overall, represent our HL). Zero-point energy corrections are calculated also at the B3LYP/6-311G(d,p) level of theory.

A total of 66 minima and 276 transition states are found in this study at the above levels of theory using TSSCDS. Their geometries (in Å) are listed below in increasing order of their relative energies (with respect to min1a).

List of minima

Minima are labeled with numbers and letters, so that they can be arranged in ascending order of their relative energies. The small letters are employed to distinguish conformational isomers.

```
min1a
E=  -191.59370087  Eh
H 0.994133 1.957545 0.661677
C 1.406911 0.954223 0.719646
H 2.401936 0.859777 1.137910
C 0.710287 -0.100071 0.292552
H 1.099143 -1.112560 0.339101
C -0.643362 0.055742 -0.273153
O -1.322692 -0.858964 -0.675958
H -1.011184 1.105745 -0.306185

min2
Erel=0.45737 kcal/mol
H 1.434862 1.401348 -1.626259
C 1.100646 1.342319 -0.586182
H 1.879553 0.833160 -0.016082
C -0.223390 0.617353 -0.481823
H 1.020520 2.363222 -0.201110
C -0.401407 -0.481895 0.208364
O -0.557929 -1.459620 0.822779
H -1.098218 1.000368 -0.994694

min1b
Erel=2.10302 kcal/mol
H 1.769882 -0.296065 0.254942
C 1.075329 -0.469124 1.070129
H 1.476277 -0.818625 2.014107
C -0.227986 -0.250834 0.890684
H -0.946847 -0.415230 1.688341
C -0.764891 0.228650 -0.409309
O -0.090649 0.455312 -1.387368
H -1.865392 0.374386 -0.437240

min3
Erel=20.3454 kcal/mol
H 0.778249 0.599445 -1.753962
C 0.941348 0.185588 -0.763414
H 1.949308 0.314488 -0.380710
C 0.187359 -1.144993 -0.396649
H -0.457806 -1.582422 -1.152597
```

C -0.181365 0.154252 0.186846
O -0.898677 0.763819 0.923371
H 0.713123 -1.867029 0.220846

min4a
Erel=25.6933 kcal/mol
C -1.058250 -0.346171 -1.568539
C -0.315138 -0.325747 -0.495723
C 0.429135 -0.310746 0.579011
O 0.943965 0.796724 1.207834
H -0.626310 -0.412872 -2.565299
H -2.144416 -0.302835 -1.515660
H 0.662941 1.580259 0.720980
H 0.717143 -1.221766 1.091059

min4b
Erel=27.3033 kcal/mol
C -1.087368 -0.346379 -1.554607
C -0.265447 -0.292688 -0.544841
C 0.560066 -0.282582 0.467769
O 1.013951 0.874799 1.061339
H -0.732526 -0.348083 -2.583060
H -2.165553 -0.385701 -1.414611
H 1.604557 0.633462 1.779357
H 0.924693 -1.218338 0.884817

min5a
Erel=28.6712 kcal/mol
C 0.371075 -0.033944 -0.782439
C 0.411857 0.013171 1.883269
C 0.410887 0.005681 0.681725
O -0.945239 0.058361 -1.315891
H 0.919711 0.819041 -1.188905
H 0.882261 -0.943450 -1.128807
H 0.420249 0.029919 2.945668
H -1.475467 -0.630036 -0.901300

min5b
Erel=28.6712 kcal/mol
C 0.371107 0.033603 -0.782439
C 0.411844 -0.013549 1.883269
C 0.410882 -0.006058 0.681725
O -0.945290 -0.057494 -1.315892
H 0.883128 0.942641 -1.128806
H 0.918961 -0.819884 -1.188905
H 0.420219 -0.030305 2.945668
H -1.474887 0.631389 -0.901301

min6
Erel=29.0536 kcal/mol
C -0.587016 0.004651 -0.823142
C -0.842843 0.137664 0.660700
C 0.478619 0.019156 0.822373
O 0.853865 -0.114201 -0.505479
H -0.938473 -0.903466 -1.316322
H -0.762501 0.883467 -1.446295
H -1.706193 0.268335 1.289295
H 1.219581 0.003243 1.610337

min5c
Erel=30.0008 kcal/mol
H 0.907243 -1.181941 -0.825151
C 0.785243 -0.245504 -0.261637
H 1.658448 -0.142146 0.398788
C -0.411346 -0.355500 0.566310
H 1.466908 0.914670 -1.662762
C -1.388339 -0.460817 1.255346
O 0.662166 0.873285 -1.136583
H -2.254766 -0.550627 1.863468

min7
Erel=30.2081 kcal/mol
H 1.038832 1.604096 -1.878274
C 1.044683 1.611202 -0.784096
H 2.089411 1.581764 -0.460691
C 0.303692 0.478857 -0.235562
H 0.624631 2.565826 -0.453090
C -0.302822 -0.452784 0.216666
O -0.905766 -1.496232 0.746258
H -1.831564 -1.506630 0.473321

min8
Erel=30.9738 kcal/mol
H 0.401438 1.959451 -1.288298
C 0.525254 0.887039 -1.236371
H 1.023749 0.374408 -2.048525
C 0.071787 0.220655 -0.193564
H -0.035307 0.269452 1.999342
C -0.574227 0.060867 1.080182
O 0.003477 -1.046178 0.276607
H -1.657659 0.040907 1.147882

min9
Erel=41.866 kcal/mol
H 0.430151 -0.542464 -1.558937
C 0.719271 -0.062433 0.970574
H 1.700251 0.005625 1.415013
C -0.417791 -0.697245 0.883775
H -1.035115 -1.521593 1.206040
C -0.241195 0.454403 -0.040632
O -0.042235 0.287347 -1.428237
H -0.774829 1.391297 0.098974

min10
Erel=42.7038 kcal/mol
H -1.970888 -0.301161 -0.359486
C -1.523850 0.086665 0.558300
H -1.392971 -0.719398 1.283365
C 1.484895 -0.802508 -0.726411
H -2.141938 0.877645 0.977096
C 0.643092 -0.091508 -0.249310
O -0.246913 0.701349 0.265586
H 2.239372 -1.416683 -1.148148

min11a
Erel=43.9846 kcal/mol

C -0.603267 -0.040837 -1.158199
C 0.117798 0.009500 0.139210
O 1.318845 0.110469 0.719482
C -1.157588 -0.106398 0.278185
H 1.986016 0.179310 0.027648
H -0.573553 -0.948683 -1.767498
H -0.736709 0.870920 -1.747429
H -2.054605 -0.193567 0.860814

min11b
Erel=44.1955 kcal/mol
6 -0.851666 -0.335997 -0.774977
6 -1.033071 -0.230646 0.753234
6 0.161582 0.042077 -0.067691
8 1.430472 0.436888 0.065716
1 -1.341540 -0.579607 -1.698883
1 -1.606662 0.599847 1.171891
1 1.838228 0.467807 -0.809727
1 -1.083884 -1.141947 1.354023

min12a
Erel=49.5034 kcal/mol
H 1.614559 0.663633 -1.515386
C 1.722602 0.509865 -0.446934
H 2.698458 0.680432 -0.004772
C 0.661735 0.121446 0.271833
H 0.732180 -0.043245 1.349340
C -0.606176 -0.077120 -0.435423
O -1.505785 -0.454692 0.468800
H -2.344123 -0.587413 0.010073

min12b
Erel=53.147 kcal/mol
H 1.700250 0.466573 -1.516074
C 1.730966 0.514191 -0.433296
H 2.660382 0.811944 0.039476
C 0.633301 0.207123 0.266957
H 0.643955 0.249322 1.367894
C -0.586416 -0.186737 -0.444503
O -1.571021 -0.454858 0.380269
H -1.339959 -0.351074 1.334120

min12c
Erel=53.2495 kcal/mol
C -1.364734 -0.247099 -0.719180
C -0.806355 -0.013463 0.477943
C 0.631088 -0.150290 0.734854
O 1.307267 0.340664 -0.294074
H -0.747760 -0.412257 -1.595452
H -2.438456 -0.332555 -0.846272
H -1.428758 0.085999 1.362969
H 2.243173 0.162897 -0.138323

min12d
Erel=53.2495 kcal/mol
H 0.386697 0.001660 -2.572985
C 0.453278 0.072550 -1.492766
H 1.408489 0.369173 -1.074007

C -0.609387 -0.130203 -0.699605
H -1.578915 -0.363177 -1.131208
C -0.623710 0.208791 0.727227
O 0.539408 -0.126487 1.267395
H 0.534969 0.182360 2.181931

min13
Erel=54.9855 kcal/mol
H 0.266310 1.559542 -1.097016
C 0.618914 1.416100 -0.073544
H 1.713068 1.394671 -0.084198
C -1.046646 -0.617788 -0.151956
H 0.303709 2.281002 0.517774
C 0.042626 0.170225 0.530405
O 0.152988 -1.066576 -0.286304
H 0.227221 -0.031933 1.579743

min12e
Erel=55.3751 kcal/mol
H 0.424242 0.529748 -1.831978
C 0.411446 0.164402 -0.808983
H 1.567350 -0.566115 0.818481
C 1.560236 -0.100182 -0.162610
H 2.527644 0.053847 -0.626091
C -0.887970 -0.249770 -0.282463
O -1.076188 0.090575 0.964806
H -0.336360 0.633757 1.330265

min12f
Erel=55.3751 kcal/mol
H 0.424175 -0.530293 -1.831836
C 0.411425 -0.164672 -0.808939
H 1.567422 0.566136 0.818328
C 1.560249 0.099942 -0.162638
H 2.527638 -0.054335 -0.626077
C -0.887938 0.249806 -0.282530
O -1.076200 -0.090182 0.964830
H -0.336441 -0.633359 1.330434

min14
Erel=57.252 kcal/mol
H 0.804651 -0.750501 -1.798569
C 0.824616 -0.310564 -0.803448
H 1.806778 -0.078807 -0.396633
C -0.267791 -0.730827 0.141147
H -0.970261 -1.537596 0.262278
C -0.337105 0.569764 -0.432459
O -0.196396 0.432174 1.004014
H -1.112804 1.137316 -0.917432

min15
Erel=61.2985 kcal/mol
C -0.702517 -0.028407 -0.724647
C -0.738368 -0.049224 0.810110
C 0.798962 0.034431 0.720754
O 0.757776 0.048502 -0.611273
H -0.999995 -0.934491 -1.254188
H -1.095824 0.853443 -1.232131

H -1.194606 0.809966 1.306891
H -1.099160 -0.964381 1.284949

min16a
Erel=64.8284 kcal/mol
H 1.468506 -0.126835 -1.655128
C 0.940324 0.607453 -1.045637
H 1.654817 1.254946 -0.531408
C 0.066872 -0.045374 -0.036199
H 0.327540 1.240000 -1.694761
C -0.499271 -1.281531 0.169341
O -0.571489 0.519080 0.892946
H -0.083921 -1.908702 0.958869

min16b
Erel=64.9239 kcal/mol
H 0.165114 -1.368076 -1.659939
C 0.603588 -1.237153 -0.669017
H 1.668021 -1.016359 -0.793925
C -0.048308 -0.086493 0.009106
H 0.507726 -2.153274 -0.083748
C -0.237478 0.353947 1.300979
O -0.470454 0.970486 -0.529565
H -1.243574 0.265315 1.714083

min17a
Erel=66.3548 kcal/mol
H 1.724539 -1.100183 -0.888125
C 1.684701 -0.513811 0.020901
H 2.580255 -0.416946 0.618865
C 0.567097 0.078120 0.403738
H 0.407146 0.685611 1.286535
C -1.663266 0.557080 0.054472
O -0.586194 -0.054511 -0.378839
H -2.403823 0.290777 -0.734847

min18a
Erel=67.8844 kcal/mol
H -0.437761 -1.679476 -1.611988
C 0.361200 -1.359078 -0.915053
H 1.306662 -1.602262 -1.404113
C 0.116359 0.072415 -0.776356
H 0.230538 -1.934228 0.010367
C -0.604062 0.662987 0.259737
O 0.123346 0.720043 1.266271
H -1.587878 1.152950 0.171619

min18b
Erel=67.8844 kcal/mol
H 0.361412 -1.043819 -2.095289
C 0.526757 -1.227191 -1.015589
H 1.545079 -0.889866 -0.784276
C -0.528045 -0.439280 -0.387148
H 0.422262 -2.304369 -0.870737
C -0.369261 0.849443 0.118101
O 0.193264 0.775279 1.224238
H -0.810546 1.770412 -0.297608

min17b
Erel=69.1417 kcal/mol
H 1.061480 2.179745 -0.856103
C -0.222376 0.832774 0.068619
H 1.613450 0.394106 -0.836950
C 0.886310 1.150498 -0.573035
H -0.996894 1.519545 0.379458
C -0.039653 -1.503615 -0.113038
O -0.547039 -0.470090 0.511594
H -0.445705 -2.345263 0.495485

min17c
Erel=70.1198 kcal/mol
H 1.830324 0.559206 -1.307782
C 1.776506 0.246651 -0.272837
H 2.673421 0.279662 0.330468
C 0.637994 -0.169183 0.250976
H 0.474338 -0.503227 1.272211
C -1.684444 -0.607542 -0.094499
O -0.525367 -0.208708 -0.542956
H -1.526508 -0.884980 0.988446

min19a
Erel=70.1638 kcal/mol
C -0.343557 -0.047389 0.731787
C 0.469038 0.147847 1.863728
C 0.303011 0.047769 -0.476655
O -0.233666 -0.094059 -1.676259
H -1.423092 -0.264611 0.704723
H -1.180495 -0.281497 -1.592056
H -0.162944 0.046920 2.766845
H 1.365945 0.260066 -0.505495

min19b
Erel=71.3984 kcal/mol
H 1.511793 0.052586 -0.590456
C 0.966365 0.664582 1.520364
H 2.042974 0.886563 1.653952
C 0.771949 0.194952 0.203902
H -1.274892 0.023465 0.699597
C -0.531155 -0.114274 -0.083024
O -0.930841 -0.571595 -1.263400
H -1.882269 -0.727624 -1.263137

min17d
Erel=72.1699 kcal/mol
H 1.296058 -0.422265 -1.189548
C 1.511530 -0.064589 -0.190009
H 2.547023 -0.013911 0.118834
C 0.557809 0.312162 0.643104
H 0.706546 0.723529 1.632194
C -1.438798 -0.657869 -0.312734
O -0.816349 0.308807 0.310594
H -0.682654 -1.478702 -0.453790

min19c
Erel=72.3864 kcal/mol
H -0.603063 -0.069832 -1.536111

C -0.723533 -0.016538 -0.449956
H 1.689903 0.122399 -1.038815
C -1.837317 -0.580634 0.183108
H -1.808159 -0.316257 1.260016
C 0.381308 0.277418 0.318086
O 1.649335 0.283461 -0.085230
H 0.302100 0.436800 1.388453

min20
Erel=72.8077 kcal/mol
H -0.428725 -1.108243 -1.571733
C -0.242906 -0.794285 -0.548161
H 1.393567 -0.930183 0.968117
C 1.030193 -0.345042 0.119286
H 1.846977 -0.167430 -0.585172
C 0.187942 0.834625 0.528085
O -0.896789 0.320312 -0.116314
H 0.016560 1.271863 1.508008

min21a
Erel=72.9863 kcal/mol
H -0.126329 -0.359257 -1.787948
C 0.401099 -0.289862 0.798290
H 1.482115 -0.213475 0.901983
C -0.260256 -1.210451 1.426838
H -1.394470 0.554388 -0.066076
C -0.310585 0.675018 -0.157592
O 0.138357 0.516668 -1.487221
H -0.058042 1.695425 0.133446

min19d
Erel=73.1938 kcal/mol
H 0.332266 0.000042 -1.441083
C 1.538489 0.000042 0.728877
H 1.731924 0.000072 -0.377196
C 0.151956 -0.000014 0.968928
H -0.215110 -0.000048 1.993957
C -0.836631 -0.000031 -0.001394
O -0.638823 0.000003 -1.297694
H -1.897743 -0.000075 0.238747

min19e
Erel=73.8678 kcal/mol
C -0.409979 -0.185571 -1.868509
C -0.677770 0.066156 -0.518556
C 0.416252 0.225306 0.299637
O 0.407109 -0.126247 1.589140
H 0.585320 0.229810 -2.130971
H -1.640360 -0.162688 -0.063410
H 1.283821 -0.023281 1.976861
H 1.368604 0.548348 -0.116646

min21b
Erel=74.4823 kcal/mol
C -0.823140 -0.277670 -0.389082
C -1.751411 -0.491786 0.489980
C 0.650298 -0.361558 0.038562
O 1.307316 0.885737 0.009054

H 1.313830 1.208755 -0.897815
H -1.069838 -0.047140 -1.423638
H 0.714971 -0.719511 1.065159
H 1.139194 -1.100662 -0.608081

min21c
Erel=74.6983 kcal/mol
C -0.504430 0.040627 -0.742623
C -0.584203 -0.240279 0.742348
C 0.195309 -0.120074 1.770276
O 0.805860 0.305891 -1.192733
H -0.965589 -0.797545 -1.282497
H -1.090908 0.935104 -0.965613
H -1.511576 -0.666950 1.163173
H 1.338450 -0.482481 -1.043595

min22a
Erel=75.2254 kcal/mol
H 0.892331 0.810896 -1.596672
C 1.059284 0.729886 -0.519190
H 2.053217 0.306920 -0.351496
C -0.013416 -0.141288 0.085217
H 1.020017 1.720728 -0.058651
C 0.504043 -1.204278 0.671078
O -1.293145 0.304288 -0.072122
H -1.899676 -0.318239 0.346490

min21d
Erel=75.5398 kcal/mol
C -1.215498 0.142126 -1.230892
C -0.972720 -0.081689 0.024936
C 0.275449 -0.139972 0.854009
O 1.385746 0.114608 0.011296
H -1.946557 -0.255167 0.506007
H 0.195664 0.604433 1.659680
H 2.182995 0.076455 0.547435
H 0.338324 -1.132895 1.322799

min23a
Erel=76.9198 kcal/mol
H 1.362354 0.527329 -0.781182
C 1.296502 0.982463 1.001227
H 2.274110 0.618728 1.372493
C 0.819739 -0.007951 0.050139
H 1.171242 -1.049177 0.050595
C -0.658200 0.083999 -0.307282
O -1.334358 -0.876240 -0.556390
H -1.060418 1.117710 -0.289633

min23b
Erel=76.9209 kcal/mol
H 0.668497 -1.411415 -0.749150
C 1.476543 -0.115942 0.898730
H 2.169681 -0.963173 1.064906
C 0.767858 -0.396782 -0.338860
H 1.580827 0.121871 -0.923726
C -0.490137 0.428862 -0.576055
O -1.457481 0.002643 -1.144894

H -0.441886 1.452196 -0.150647

min22b
Erel=77.1466 kcal/mol
H 1.552381 -0.692942 -1.229216
C 1.205914 0.169916 -0.654029
H 1.971530 0.397512 0.095916
C -0.478742 -1.348693 -0.285011
H 1.088891 1.011737 -1.343811
C -0.116571 -0.120052 0.030526
O -0.741594 0.827900 0.780219
H -0.117819 1.536919 0.968267

min23c
Erel=77.4799 kcal/mol
H 0.828628 -0.777977 -1.125127
C 0.578916 -0.625273 -0.072143
H 1.544145 -0.613373 0.500974
C 0.107966 -1.801102 0.655896
H -0.343327 -1.422242 1.602498
C -0.106959 0.712539 0.171556
O -0.538632 1.407550 -0.706563
H -0.240880 0.964346 1.248146

min19f
Erel=78.2419 kcal/mol
H 0.398377 0.027227 -2.232362
C 0.158996 0.633263 1.600039
H 0.830273 1.216400 0.938034
C -0.419347 -0.390903 0.801868
H -1.084427 -1.124849 1.258959
C -0.297051 -0.517996 -0.556556
O 0.463832 0.279083 -1.304905
H -0.851509 -1.283595 -1.104615

min19g
Erel=78.2524 kcal/mol
H 0.326582 0.020962 -2.250605
C 0.226919 0.697331 1.468427
H 0.011215 0.589539 2.549886
C -0.364610 -0.408735 0.815412
H -0.931656 -1.222747 1.283631
C -0.257098 -0.541781 -0.548499
O 0.379257 0.312472 -1.333660
H -0.713752 -1.395766 -1.052924

min23d
Erel=78.7591 kcal/mol
H -1.183091 -0.687954 -1.096912
C -1.042176 -1.382233 -0.241804
H 0.829707 -1.375143 -0.112157
C 0.079109 -0.825622 0.513422
H 0.205634 -1.216004 1.528626
C 0.442845 0.663135 0.402379
O 0.321821 1.301007 -0.607570
H 0.814960 1.127833 1.340733

min24

Erel=83.6281 kcal/mol
H 1.080078 -1.897590 -1.290850
C 0.866470 -0.871318 -1.030735
H 1.308969 -0.016620 -1.529374
C -0.698695 0.455236 0.148124
H 0.665900 1.018304 1.667602
C -0.238506 1.250766 1.100921
O -0.071020 -0.694463 -0.177677
H -0.770306 2.158910 1.351687

min25
Erel=89.0469 kcal/mol
C -0.638037 -0.007407 -1.318242
C -0.488836 -0.128576 1.645979
C 0.447068 0.013091 0.732594
O 0.600171 0.090948 -0.598774
H -1.118833 -0.969770 -1.115519
H -0.385984 0.068575 -2.373639
H -1.308285 0.809659 -1.032664
H 1.373764 0.083845 1.331865

min26
Erel=89.8723 kcal/mol
C -0.133511 -0.057346 -1.536073
C -0.203270 -0.021427 -0.215963
O 0.934479 -0.038870 0.683604
C -0.910423 0.140063 1.000723
H 1.211220 0.874495 0.835803
H 0.824930 -0.091000 -2.035683
H -1.038092 -0.070933 -2.128163
H -1.109295 -0.841344 1.454984

min27
Erel=92.4368 kcal/mol
H -0.265484 0.259724 -1.823526
C 0.141568 0.513062 -0.833292
H 0.801344 1.384973 -0.955643
C -0.920588 0.723908 0.200301
H 0.178776 -0.182930 1.845982
C -0.234072 -0.432834 0.857253
O 0.778335 -0.605200 -0.165863
H -0.888598 -1.308692 0.979437

min28
Erel=95.155 kcal/mol
H -1.450227 -0.675869 -0.956829
C -1.443225 0.317942 -0.475677
H 0.782386 -0.196222 -1.509837
C -0.356055 0.367937 0.402516
H -0.237288 1.118250 1.177153
C 0.879224 0.177246 -0.492708
O 0.649027 -0.722344 0.532657
H 1.635261 0.947311 -0.346320

min29
Erel=95.5528 kcal/mol
H 0.818736 0.205341 -1.831328
C 0.659787 0.397901 -0.772895

H 1.522993 0.845291 -0.267605
C -0.751015 0.586537 -0.296804
H 0.464216 0.454152 1.638295
C -0.344651 0.026833 1.035191
O 0.222060 -0.821271 -0.045154
H -1.096452 -0.502182 1.616193

min30
Erel=120.811 kcal/mol
H 0.542080 -1.464363 -1.937130
C -0.533371 -0.456911 -0.427298
H 1.610644 -0.929058 -0.596519
C 0.620006 -1.321470 -0.854198
H 0.484390 -2.314793 -0.413194
C 0.102706 1.752899 0.633270
O -0.138066 0.554311 0.236465
H 0.147629 1.673154 1.740925

min31a
Erel=126.768 kcal/mol
C -0.389280 0.002599 -1.782387
C -0.243781 0.442793 0.640280
C 0.501802 0.260690 -0.648638
O 0.079314 -0.587839 1.406294
H -1.374277 0.430464 -1.487485
H 1.449509 -0.290591 -0.643314
H -0.446464 -0.533468 2.214994
H 0.692706 1.286830 -1.072676

min31b
Erel=129.223 kcal/mol
H -0.848372 0.092287 -2.504635
C -1.154319 0.252394 -1.450467
H 1.043020 -0.052453 -1.114326
C 0.093342 0.334919 -0.705974
H 0.016985 1.445485 -0.941265
C -0.069894 0.241342 0.791889
O 0.803316 -0.665252 1.186368
H 0.708514 -0.773750 2.142115

min31c
Erel=130.137 kcal/mol
C -0.777044 0.271682 0.116780
C -0.963478 0.354748 1.567218
C 0.655224 0.334414 -0.359884
O 0.973148 -0.750214 -1.012784
H -1.449179 -0.439213 -0.403104
H -1.204034 1.300123 -0.017032
H 0.225996 -1.381026 -1.146508
H -0.085032 0.922670 1.941862

min31d
Erel=132.164 kcal/mol
H -0.387795 -0.001430 -1.396790
C -0.260008 0.119402 0.946622
H 0.081097 0.211664 1.978941
C -1.160919 -1.004296 0.711268
H -1.272583 -1.146149 -0.396123

C 0.901219 0.469688 -0.048298
O 0.544515 0.334896 -1.277274
H -0.955370 0.968633 0.768469

min31e
Erel=133.044 kcal/mol
H -0.082276 -0.466323 -1.403476
C 0.307336 -0.597938 -0.360956
H 1.423737 -0.730080 -0.437021
C 0.208273 -1.891542 0.301426
H 0.049974 -2.627229 -0.513529
C 0.149825 0.638848 0.510482
O -0.535097 1.542956 -0.121106
H -0.817686 1.278922 -1.034449

min32a
Erel=140.63 kcal/mol
H -0.926714 1.013257 -0.896016
C -0.250507 0.891008 -0.039722
H 1.698028 0.304262 -0.437896
C 1.063871 1.207148 -0.488883
H -0.599664 1.584737 0.735097
C -0.024398 -1.467974 -0.137850
O -0.580012 -0.506821 0.508126
H -0.381679 -2.379932 0.395766

min32b
Erel=141.929 kcal/mol
C -0.835029 0.153108 -0.247725
C -1.037327 0.150299 1.182139
C 1.444341 0.169944 0.004063
O 0.473261 -0.398446 -0.637633
H -1.611150 -0.522104 -0.657783
H -0.924918 1.105635 -0.778818
H -1.986259 0.703801 1.338031
H 2.348051 -0.373001 -0.359572

min32c
Erel=145.106 kcal/mol
C -0.730459 0.271635 -0.121763
C -1.571469 -0.319971 0.854881
C 1.693679 0.308975 -0.340351
O 0.633018 -0.393642 -0.256518
H -1.256292 -0.000196 -1.059529
H -0.526322 1.361595 -0.137583
H -2.433406 0.362987 0.971805
1 1.397974 1.404827 -0.315077

List of transition states

The different channels obtained in this study (identified with IRC calculations at the B3LYP/6-311G(d,p) level of theory) can be grouped in seven categories (below min*x* and min*y* refer to any of the 66 different minima):

(1) ***Bim/trim* channel:** A+B (+C)↔D+E(+F), where two or three reactants are connected with two or three products.

(2) ***CO* channel**: min*x*→CO + C_2H_4 (different isomers of C_2H_4 are found).

(3) ***CH2O* channel:** min*x*→CH_2O + C_2H_2 (C_2H_2 can be either acetylene or vinylidene, and also the higher energy isomer of formaldehyde HOCH was obtained).

(4) ***H2* channel**: min*x*→H_2 + C_3H_2O (different isomers of C_3H_2 are found).

(5) ***H2O* channel:** min*x*→H_2O + C_3H_2 (different isomers of C_3H_2 are found).

(6) ***Iso* channel:** min*x*↔min*y*. Isomerization reaction between minima *x* and *y*.

(7) ***Triple* channel:** min*x*→CO + H_2 + C_2H_2 (C_2H_2 can be either acetylene or vinylidene). Here it is also included the much higher energy triple channel: H_2 + HCO + CCH.

A total of 25, 11, 20, 48, 16, 150, and 6 transition states are found for channels 1-7, respectively. The transition state structures are labeled with numbers plus an additional tag to distinguish the different channels:, _bim/trim, _co, _ch2o, _h2, _h2o, _iso, and _triple. The information of each transition state includes: the relative energy, the mechanism, and the Cartesian coordinates (in Å).

```
ts1_iso
Erel=1.43024 kcal/mol
Mechanism: min2<-->min2
H -0.008192 -0.010706 -0.001092
C 0.021270 0.033409 1.088003
H 1.073127 0.036113 1.386701
C -0.889084 -1.398225 2.928994
H -0.419758 0.987769 1.388539
C -0.736667 -1.156668 1.649695
```

O -1.024498 -1.612837 4.066051
H -1.197296 -1.877994 0.985555

ts2_iso
Erel=6.85163 kcal/mol
Mechanism: min1a<-->min1b
H 0.040683 0.057781 0.017387
C 0.010167 0.022537 1.104845
H 2.103649 -0.001992 1.344118
C 1.129155 -0.015259 1.818489
H 1.114307 -0.051720 2.903076
C -1.362894 0.022678 1.710750
O -1.976590 1.022483 1.982219
H -1.806795 -0.982184 1.889919

ts3_iso
Erel=28.6994 kcal/mol
Mechanism: min4a<-->min4b
C -0.003370 0.002542 0.007905
C 0.004748 -0.022441 1.310238
C 0.026153 -0.030016 2.616235
O -0.466181 -1.079291 3.385284
H -0.813938 0.464946 -0.548994
H 0.800549 -0.441948 -0.572654
H -1.399258 -0.919378 3.560521
H 0.502551 0.775025 3.173124

ts4_iso
Erel=28.9036 kcal/mol
Mechanism: min5a<-->min5a
C -0.022404 0.000006 -0.035101
C -0.005231 0.000000 2.626568
C 0.011201 -0.000008 1.424878
O -1.345355 0.000617 -0.575902
H 0.511129 0.882899 -0.406985
H 0.510313 -0.883380 -0.406984
H -0.007062 0.000001 3.689172
H -1.964088 0.000904 0.159415

ts5_iso
Erel=30.3845 kcal/mol
Mechanism: min5a<-->min5c
C -0.007578 -0.012497 0.015009
C 0.022019 -0.001889 1.215178
C 0.052867 0.043834 2.676292
O 1.385228 -0.116423 3.165064
H -0.353056 1.008483 3.008576
H -0.031911 -0.032291 -1.046923
H 1.356783 -0.737259 3.896763
H -0.612638 -0.737256 3.063674

ts6_iso
Erel=42.2177 kcal/mol
Mechanism: min9<-->min9
C 0.016043 -0.028337 0.008114
C 0.015971 -0.028380 1.310894
C 1.343469 0.047269 0.659581
O 2.013052 1.300785 0.659662

H -0.542789 0.018890 2.231636
H -0.542616 0.018995 -0.912686
H 2.958899 1.131094 0.659680
H 2.032329 -0.799096 0.659592

ts7_iso
Erel=43.8726 kcal/mol
Mechanism: min10<-->min10
C -0.017136 0.000010 -0.018435
C -0.022074 0.000037 2.323001
C 0.608018 -0.000034 3.345451
O -0.737027 0.000119 1.241796
H -0.311566 -0.893625 -0.569139
H -0.311331 0.893710 -0.569159
H 1.058047 -0.000129 0.158585
H 1.153352 -0.000095 4.254626

ts8_iso
Erel=48.3384 kcal/mol
Mechanism: min11a<-->min11b
C -0.023940 0.002802 -0.027159
C -0.013200 0.015353 1.463648
C 1.168537 -0.002078 0.953208
O -0.806588 0.114081 2.553494
H -0.251813 0.916099 -0.580160
H -0.271296 -0.910644 -0.573329
H -0.970342 -0.766652 2.909723
H 2.242398 -0.002411 1.014670

ts9_iso
Erel=53.2392 kcal/mol
Mechanism: min3<-->min3
H 0.096194 0.001803 -0.009863
C 0.014119 0.000241 1.069176
H 3.326927 -0.000552 1.511634
C 2.333257 0.000092 1.073021
H -0.981000 -0.000276 1.504492
C 1.172270 -0.001070 1.926396
O 1.170226 -0.002793 3.159131
H 2.254761 0.001664 -0.006284

ts10_iso
Erel=53.8932 kcal/mol
Mechanism: min12c<-->min12c
H -0.034633 0.000193 0.000110
C 0.006162 -0.000043 1.084567
H 0.989254 -0.000267 1.542787
C -1.100749 -0.000061 1.837480
H -2.078289 0.000165 1.365084
C -1.141288 -0.000372 3.324024
O 0.106846 -0.000627 3.778020
H 0.060344 -0.000826 4.740676

ts11_iso
Erel=55.3605 kcal/mol
Mechanism: min1b<-->min6
C 0.006340 -0.032515 0.000575
C 0.011893 -0.012671 1.436547

C 1.373992 -0.010672 1.588759
O 1.905607 -0.277663 0.428872
H -0.622518 -0.709197 -0.583767
H 0.386404 0.812808 -0.563543
H -0.811441 -0.137050 2.122071
H 2.009137 0.232474 2.440861

ts1_co
Erel=56.7047 kcal/mol
Mechanism: min3--->CO_channel
H -0.031193 -0.052844 -0.024553
C 0.045471 0.145168 1.034784
H 0.985352 -0.052738 1.529493
C -1.178570 0.181844 1.835461
H -1.113305 0.582107 2.851675
C -1.258336 -1.284029 1.887738
O -1.093337 -2.432191 1.779889
H -2.083521 0.582007 1.368456

ts12_iso
Erel=57.9394 kcal/mol
Mechanism: min12e<-->min12b
C 0.572938 0.180892 0.123310
C 0.081674 -0.285481 1.274657
C 0.858968 -0.955126 2.323558
O 1.111946 -0.180627 3.345060
H -0.066620 0.642215 -0.618698
H 1.629230 0.106759 -0.111073
H 0.787027 0.742407 3.229943
H -0.991695 -0.248267 1.477455

ts13_iso
Erel=58.5936 kcal/mol
Mechanism: min12e<-->min12e
H 0.030671 -0.000122 0.032383
C -0.024018 0.000028 1.115986
H 1.127677 0.000200 2.916186
C 1.107073 0.000054 1.826105
H 2.084089 -0.000071 1.356542
C -1.432172 0.000188 1.646708
O -1.504513 0.000369 2.951123
H -0.642216 0.000379 3.429376

ts14_iso
Erel=61.2519 kcal/mol
Mechanism: min3<-->min8
H -0.027270 0.111864 0.001256
C 0.019697 -0.031766 1.073073
H 0.985606 -0.151763 1.547434
C -2.454929 -0.009624 1.276294
H -3.151556 -0.664720 1.784175
C -1.130947 0.050017 1.815091
O -1.335575 0.201013 3.065351
H -2.856934 0.706245 0.561990

ts15_iso
Erel=66.1733 kcal/mol
Mechanism: min4a<-->min4a

H 0.052722 -0.025488 -0.019975
C 0.034250 0.065003 1.069977
H 1.067438 0.002838 1.423788
C -1.732316 -1.455645 2.341343
H -0.390316 1.029327 1.349454
C -0.743435 -1.047346 1.638399
O -0.548653 -2.389944 1.527933
H -2.553902 -1.794955 2.925802

ts16_iso
Erel=66.8513 kcal/mol
Mechanism: min4a<-->min17a
C -0.001364 -0.001244 -0.024810
C -0.003514 -0.003951 1.426835
O 1.217341 0.017005 2.461139
C -0.200443 -0.010558 2.678059
H 0.501832 0.894035 -0.406410
H -1.025074 -0.020130 -0.407573
H 0.535685 -0.875245 -0.409596
H -0.794092 -0.023856 3.573529

ts17_iso
Erel=67.9726 kcal/mol
Mechanism: min2<-->min18a
H -0.146945 0.036083 0.009268
C 0.006107 -0.038792 1.094894
H 1.060364 0.028394 1.368482
C -0.718660 -1.113665 1.757931
H -0.481501 0.856843 1.532352
C -1.994082 -1.534502 1.322129
O -2.284167 -2.436224 0.551203
H -2.771677 -0.963244 1.910422

ts18_iso
Erel=69.3158 kcal/mol
Mechanism: min18a<-->min18a
H -0.365746 -0.193106 0.105555
C 0.066360 0.015490 1.094411
H 1.146613 0.143733 0.955573
C -0.574079 1.202713 1.596252
H -0.120863 -0.864078 1.722082
C -0.988392 2.238183 2.272355
O -0.214373 2.051636 3.306211
H -1.715949 3.032989 2.114562

ts19_iso
Erel=70.1602 kcal/mol
Mechanism: min17b<-->min17a
H -0.012604 -0.017227 -0.007287
C 0.010928 -0.005551 1.075071
H 0.971655 0.019109 1.571644
C -1.098990 -0.012006 1.785657
H -1.166261 -0.007173 2.865319
C -2.987194 1.020294 0.894759
O -2.368133 -0.102315 1.172030
H -3.927598 0.637721 0.428129

ts20_iso

Erel=70.1614 kcal/mol
Mechanism: min2<-->min16b
H -0.574106 -0.312815 0.273319
C 0.019666 -0.004269 1.136626
H 1.048010 0.193677 0.827323
C -0.582747 1.301718 1.670524
H 0.033187 -0.813058 1.877071
C -0.767915 1.192807 3.068470
O -0.769498 2.304551 0.995390
H -1.764663 0.814208 3.345024

ts21_iso
Erel=70.4631 kcal/mol
Mechanism: min9<-->min19c
H -0.142723 0.293828 -0.111609
C -0.090174 0.162166 0.966188
H 2.338716 -0.356679 0.747471
C -0.773498 -0.716423 1.723767
H -0.679123 -0.721221 2.815609
C 0.991821 0.428433 1.829862
O 2.257977 0.017417 1.635000
H 0.868010 0.871591 2.807557

ts22_iso
Erel=70.6511 kcal/mol
Mechanism: min1a<-->min2
H -0.364887 0.074823 0.100002
C -0.079783 0.039457 1.158776
H 0.973005 -0.174127 1.346120
C -0.923970 0.352019 2.208830
H -0.577138 -0.888952 1.901351
C -2.331877 0.566780 1.979546
O -3.182843 -0.301845 1.901643
H -2.595873 1.651611 1.966674

ts23_iso
Erel=71.4209 kcal/mol
Mechanism: min12a<-->min11a
C -0.006071 0.026720 -0.037422
C -0.130172 0.114622 1.860153
C 0.920590 0.100698 1.025929
O -0.211433 -0.677102 2.943966
H -0.747175 0.783854 -0.225730
H 0.103289 -0.742763 -0.805765
H -1.051677 -0.496030 3.377433
H 1.947978 -0.251283 1.073232

ts24_iso
Erel=71.815 kcal/mol
Mechanism: min1b<-->min18a
H 0.008031 -0.065481 0.120031
C -0.253317 -0.327590 1.431358
H 1.834358 0.191872 0.979035
C 0.979419 -0.475577 0.815804
H 1.198636 -1.377696 0.243201
C -0.541520 0.837451 2.235501
O -0.322126 0.880874 3.432463
H -1.082058 1.658223 1.705862

ts25_iso
Erel=72.0038 kcal/mol
Mechanism: min1a<-->min4a
H 0.287296 0.033561 0.056551
C -0.006523 -0.040044 1.100595
H 0.807924 -0.259400 1.795565
C -1.280946 0.158799 1.483179
H -2.741210 0.769357 1.755664
C -1.693365 0.113930 2.845988
O -2.846968 0.646828 2.932560
H -1.239375 -0.285142 3.756064

ts26_iso
Erel=72.4109 kcal/mol
Mechanism: min1a<-->min2
H 0.017398 0.031066 -0.023247
C 0.018610 -0.023659 1.071002
H 1.019460 -0.002406 1.489741
C -1.136381 0.391774 1.819538
H -1.778470 1.251571 1.680531
C -1.238997 -0.670090 2.682404
O -1.906187 -1.387643 3.362853
H -0.079732 -1.194489 2.105381

ts27_iso
Erel=72.8189 kcal/mol
Mechanism: min17c<-->min17d
H -0.161397 -0.137840 0.011599
C -0.087422 -0.081607 1.090750
H 0.890896 -0.168625 1.545186
C -1.154556 0.095433 1.846568
H -1.164191 0.195310 2.924467
C -3.247175 -0.786838 1.111518
O -2.447779 0.237317 1.279256
H -2.692274 -1.684580 1.502420

ts28_iso
Erel=72.8902 kcal/mol
Mechanism: min12a<-->min12b
H -0.126847 0.146286 0.017888
C -0.026686 0.087922 1.096872
H 0.924075 0.366842 1.539288
C -1.082378 -0.315185 1.824504
H -1.033181 -0.404648 2.912490
C -2.311128 -0.599497 1.086677
O -3.306884 -0.934055 1.973793
H -3.812393 -0.176501 2.289470

ts29_iso
Erel=73.0615 kcal/mol
Mechanism: min9<-->min19a
C -0.003510 -0.029129 -0.023189
C -0.160945 -0.041280 2.044350
C 0.815804 -0.140413 1.112424
O 0.224275 0.785479 -1.058583
H -0.935249 -0.563393 -0.110979
H 1.897066 0.038279 1.110518

H 0.104012 0.483458 2.971477
H 1.060841 1.252725 -0.931395

ts30_iso
Erel=73.6559 kcal/mol
Mechanism: min5a<-->min5a
C 0.010756 -0.011193 0.019092
C 0.441982 0.505172 2.681507
C 0.260568 0.109695 1.489991
O 0.404040 -1.262371 -0.515096
H -1.044486 0.207576 -0.184636
H 0.610470 0.747821 -0.486496
H 0.482902 -0.822337 2.182001
H -0.256929 -1.916942 -0.268555

ts31_iso
Erel=74.7063 kcal/mol
Mechanism: min21c<-->min21d
C 0.025611 0.041825 -0.025387
C -0.034710 0.013705 1.500981
C 1.088119 -0.167549 2.125824
O -0.226418 1.326586 -0.570492
H 1.009185 -0.293844 -0.366143
H -0.718273 -0.673676 -0.392993
H -0.986768 0.136087 2.012244
H -0.490548 1.919697 0.137583

ts32_iso
Erel=75.0694 kcal/mol
Mechanism: min12b<-->min11b
C -0.004666 -0.018976 -0.018726
C 0.120637 -0.078757 1.386342
C 1.451885 -0.127493 1.221040
O 2.386508 0.588692 1.848444
H 0.369230 -0.787689 -0.672110
H -0.617190 0.757771 -0.483435
H 1.992035 1.193778 2.501501
H -0.562814 0.289038 2.152588

ts33_iso
Erel=75.5837 kcal/mol
Mechanism: min11b<-->min11b
C 0.245795 -0.192838 -0.228699
C -0.013258 0.010675 2.211486
C 0.726931 0.144813 1.076068
O 1.999624 0.626090 1.169508
H -0.786840 -0.560259 -0.118242
H 0.380109 0.275470 3.188623
H 2.330878 0.636785 0.260230
H -1.022910 -0.368995 2.153927

ts34_iso
Erel=75.6178 kcal/mol
Mechanism: min21b<-->min21b
C -0.041566 -0.032353 -0.048175
C 0.059099 -0.016469 1.471367
C 0.969729 0.131611 2.378089
O -1.277119 -0.531560 -0.519064

H 0.157266 0.977688 -0.425574
H 0.727649 -0.695623 -0.444304
H -0.857563 -0.181426 2.064470
H -1.950162 0.139672 -0.369407

ts35_iso
Erel=76.157 kcal/mol
Mechanism: min1a<-->min14
H -0.076093 0.019548 0.009593
C 0.019120 0.014438 1.094883
H 1.028550 0.036898 1.500992
C -1.113250 -0.502994 1.788537
H -1.417520 -1.236279 2.518776
C -1.200135 0.932079 1.669652
O -1.060729 1.054551 2.958715
H -1.786735 1.571005 1.008288

ts2_co
Erel=76.2709 kcal/mol
Mechanism: min13--->CO_channel
H -0.091452 0.214140 -0.007582
C 0.016463 -0.022207 1.053174
H 1.067250 -0.183478 1.324257
C -1.014409 -0.923266 1.586231
H -0.301973 0.890245 1.607097
C -1.126364 -2.834592 0.414283
O -0.219749 -3.193661 1.010934
H -0.678125 -1.303285 2.569127

ts1_bim
Erel=76.627 kcal/mol
Mechanism: CH2O+HCCH<-->CO+C2H4
H 0.069473 0.060513 -0.031606
C 0.022439 0.013555 1.038078
H 1.453740 0.060520 2.768281
C 0.575233 0.013558 2.156186
H -0.658849 -0.122204 3.052131
C -1.905335 -0.074394 2.686877
O -2.918978 0.172885 3.188022
H -1.438744 -0.122208 1.474676

ts3_co
Erel=76.8833 kcal/mol
Mechanism: min2--->CO_channel
H 0.007835 0.015922 -0.056062
C -0.002138 0.049452 1.027055
H 0.943277 0.071352 1.551139
C -1.209247 -0.273024 1.794962
H -2.152654 -0.211903 1.262596
C -1.248199 -1.264052 2.880753
O -0.958432 -1.390006 4.008156
H -0.819582 0.827735 2.003066

ts36_iso
Erel=77.2956 kcal/mol
Mechanism: min1a<-->min23a
H -0.079607 -0.012366 0.163957
C -0.093389 0.098401 1.567690

H 0.916544 -0.214242 1.876618
C -0.630399 -0.925981 0.761489
H -0.211045 -1.928308 0.604162
C -2.073290 -0.802179 0.318225
O -2.741819 -1.758458 0.029457
H -2.467851 0.233381 0.341401

ts37_iso
Erel=78.1737 kcal/mol
Mechanism: min1b<-->min9
H -0.124377 0.011256 -0.162328
C 0.096307 0.056399 2.187475
H 0.594326 0.029647 3.161390
C -1.207613 -0.241721 2.084802
H -1.984425 -0.604749 2.763344
C -1.406424 0.660993 1.006271
O -0.866992 0.639428 -0.210081
H -2.153266 1.454129 1.068517

ts38_iso
Erel=79.4698 kcal/mol
Mechanism: min1a<-->min12a
H -0.010879 0.004435 -0.005421
C 0.014225 0.001237 1.078955
H 0.985707 0.003584 1.559948
C -1.127555 -0.005355 1.774143
H -1.156403 -0.008785 2.865470
C -2.413393 -0.008316 1.089884
O -3.489251 -0.014836 1.847436
H -3.594438 -0.011682 0.674379

ts39_iso
Erel=79.4953 kcal/mol
Mechanism: min18a<-->min18b
C 0.026329 -0.157402 -0.004151
C -0.065480 -0.235150 1.443277
C 1.316068 0.058767 2.086825
O 2.339062 0.262277 1.474606
H -0.768834 -0.686075 -0.533373
H -0.277436 0.918987 -0.064342
H 1.008015 -0.232871 -0.488112
H 1.317460 0.071438 3.191984

ts40_iso
Erel=79.5513 kcal/mol
Mechanism: min2<-->min2
H -0.392344 -0.122051 0.247508
C 0.081500 0.007533 1.255953
H 1.151857 0.073086 1.055573
C -0.384560 -1.269789 1.768021
H -0.330684 0.945305 1.666242
C -1.758755 -1.084515 2.414474
O -2.390563 -2.020099 2.836622
H -2.170443 -0.046325 2.507058

ts41_iso
Erel=80.2391 kcal/mol
Mechanism: min1b<-->min23d

H 0.571065 -0.184653 0.115188
C 0.073187 0.159929 1.039094
H 0.992830 -0.118161 2.048749
C 0.095847 -0.942814 1.917586
H -0.394261 -0.858279 2.892826
C 0.491417 -2.367537 1.534292
O 1.227046 -2.619171 0.618588
H 0.035588 -3.169043 2.154173

ts42_iso
Erel=80.2512 kcal/mol
Mechanism: min19b<-->min19a
H 0.027140 0.239235 0.125312
C -0.012572 -0.193164 2.956446
H 1.080406 -0.235774 2.911448
C -0.833324 0.214610 4.034571
H -0.195379 0.706702 4.793744
C -0.711554 -0.396954 1.802422
O -0.140012 -0.588536 0.588904
H -1.799522 -0.421713 1.841289

ts43_iso
Erel=80.3745 kcal/mol
Mechanism: min4b<-->min12a
H 0.006329 0.043244 0.014984
C 0.004273 0.009206 1.098024
H 0.955636 -0.033732 1.610244
C -1.142758 -0.004727 1.750995
H -1.315406 0.477617 2.961068
C -2.387071 0.244328 2.196581
O -3.177589 -0.793155 2.572638
H -3.976540 -0.407216 2.943628

ts44_iso
Erel=80.4165 kcal/mol
Mechanism: min3<-->min3
H -0.023370 0.242909 -0.057781
C -0.016141 -0.238674 0.932010
H 0.973018 -0.061482 1.405950
C -0.686092 -1.658102 0.988359
H -1.329479 -1.862445 1.844754
C -1.073424 0.089442 1.786785
O -1.903635 0.437432 2.503200
H 0.055794 -2.450369 0.884008

ts45_iso
Erel=81.1182 kcal/mol
Mechanism: min23a<-->min23a
H 0.293507 0.299600 0.098976
C -0.039478 -0.229867 1.935262
H 1.031278 -0.280695 2.222938
C -0.127099 0.868335 0.965037
H 0.560960 1.724754 1.077211
C -1.521239 1.386853 0.632135
O -2.305602 1.717752 1.478969
H -1.768199 1.479369 -0.448501

ts46_iso

Erel=81.1222 kcal/mol
Mechanism: min9<-->min21a
H -0.121221 -0.082135 0.028176
C -0.017787 0.017482 2.505796
H 1.011845 0.026828 2.817282
C -1.107360 -0.709307 2.708003
H -1.878053 0.155911 1.894610
C -0.844722 0.793214 1.580357
O -0.649056 0.704841 0.205539
H -1.135711 1.805575 1.855497

ts47_iso
Erel=81.1284 kcal/mol
Mechanism: min1b<-->min23a
H 0.108307 -0.004958 0.191244
C -0.100829 -0.070766 1.393268
H 0.780766 -0.200870 2.041009
C -0.691463 -1.087125 0.613239
H 0.018107 -1.931593 0.610929
C -0.865525 1.208986 1.666124
O -1.191668 2.008199 0.832301
H -1.112650 1.348675 2.741502

ts48_iso
Erel=81.1691 kcal/mol
Mechanism: min1a<-->min23a
H 0.205676 -0.008860 -0.024261
C 0.063964 -0.336726 1.021140
H 1.177146 0.039111 2.799794
C 0.812947 0.533218 1.889762
H 1.503795 1.303806 1.530799
C -0.537933 1.183909 2.440733
O -0.919661 2.251153 2.064849
H -1.034930 0.574859 3.209652

ts49_iso
Erel=81.2576 kcal/mol
Mechanism: min11a<-->min11a
C 0.215227 0.232373 -0.252526
C 0.007407 0.009888 2.189528
C 0.746067 -0.091271 1.051658
O 2.047789 -0.507152 1.046660
H 0.396879 -0.230993 3.178219
H -0.828532 0.543134 -0.067516
H -1.018733 0.343816 2.139433
H 2.333558 -0.704771 1.946092

ts50_iso
Erel=81.2789 kcal/mol
Mechanism: min9<-->min19f
H 0.031377 -0.014405 0.067939
C -0.056608 0.049555 3.615518
H 0.855767 0.112407 3.012548
C -1.205988 -0.325329 2.987753
H -2.172208 -0.430896 3.474713
C -1.053446 0.010552 1.631086
O -0.135973 -0.569760 0.837536
H -1.640379 0.801587 1.159123

ts51_iso
Erel=81.4908 kcal/mol
Mechanism: min1a<-->min23d
H 0.015287 0.177370 0.108413
C -0.040506 -0.036703 1.195789
H 2.133790 0.015532 1.049121
C 1.304093 0.308631 1.707762
H 1.479360 -0.017395 2.736907
C 1.337702 1.874504 1.691379
O 1.526447 2.519799 0.703794
H 1.174962 2.337695 2.682265

ts52_iso
Erel=81.84 kcal/mol
Mechanism: min1b<-->min12c
H -0.288872 -0.203565 0.032669
C -0.097901 -0.073476 1.093367
H 0.934972 -0.021663 1.417824
C -1.124059 0.029220 1.943617
H -0.980569 0.188593 3.006455
C -2.509319 0.036119 1.445589
O -2.722030 -0.413067 0.225884
H -3.617833 -0.000768 0.856102

ts53_iso
Erel=82.242 kcal/mol
Mechanism: min9<-->min21a
H -0.116201 -0.047321 0.012796
C -0.026536 0.000301 3.233359
H 0.835666 0.004039 3.874630
C -1.273236 -0.439498 3.242087
H -1.531131 0.073472 1.987284
C -0.315411 0.440119 1.870443
O 0.310820 -0.264053 0.849223
H -0.433256 1.512664 1.695137

ts54_iso
Erel=82.6171 kcal/mol
Mechanism: min12e<-->min2
H 0.020585 0.011219 -0.010051
C 0.029973 -0.027858 1.075291
H 1.036617 0.059609 1.476178
C -1.037016 0.505255 1.838644
H -0.927287 1.006423 2.789652
C -2.243846 0.109035 1.257111
O -2.205317 -1.008941 0.720007
H -0.889342 -1.220421 0.901692

ts55_iso
Erel=82.9424 kcal/mol
Mechanism: min5a<-->min21c
C 0.021987 0.048607 0.047678
C 0.035536 -0.026688 1.933821
C 1.177454 0.010935 1.419705
O 0.099980 1.299383 -0.528496
H 0.513896 -0.754751 -0.497961
H -1.039612 -0.204727 0.127335

H -0.890776 -0.010850 2.468486
H 1.029886 1.557477 -0.526642

ts56_iso
Erel=83.2595 kcal/mol
Mechanism: min4a<-->min12b
H -0.025184 -0.044907 0.014545
C -0.019844 0.003513 1.097079
H 0.934578 0.075295 1.600443
C -1.162324 -0.018833 1.763912
H -1.324809 -0.510782 2.964731
C -2.404876 -0.290485 2.199197
O -3.284623 0.655046 2.583731
H -2.966518 1.546194 2.360252

ts57_iso
Erel=84.0519 kcal/mol
Mechanism: min4a<-->min18a
H -0.186168 0.058289 0.034203
C -0.002533 -0.022072 1.111802
H 1.047367 -0.020460 1.391206
C -0.968835 -0.452532 2.000182
H -0.806209 1.094666 1.404540
C -2.244938 0.068257 1.766968
O -2.236901 1.324868 1.567069
H -3.182236 -0.486995 1.833077

ts1_triple
Erel=84.1716 kcal/mol
Mechanism: min1a--->triple_channel
H 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.642981
H 1.049564 0.000000 1.837623
C -1.208238 0.000152 1.910525
H -2.009042 0.000177 2.619675
C -2.262259 -0.000187 0.198948
O -3.394833 -0.001286 0.049346
H -0.652619 0.000016 -0.524764

ts58_iso
Erel=84.955 kcal/mol
Mechanism: min19d<-->min19f
C -0.194016 0.082811 -0.014132
C -0.078416 0.078996 1.399287
C 1.125372 0.013034 2.044687
O 2.335243 0.204412 1.447016
H 2.623811 1.119422 1.550719
H 0.699304 0.571593 -0.444237
H -0.947590 -0.161563 2.011906
H 1.190773 -0.361342 3.068979

ts59_iso
Erel=85.8126 kcal/mol
Mechanism: min11a<-->min22b
H 0.008767 -0.040408 0.020488
C 0.002678 -0.010766 1.110656
H 0.979469 0.091347 1.584823
C -1.082693 -0.676833 1.840266

H -0.589068 1.140135 1.380943
C -1.556016 0.538569 2.031574
O -1.415822 -1.940408 2.153013
H -0.752946 -2.537382 1.793610

ts60_iso
Erel=86.1686 kcal/mol
Mechanism: min7<-->min22a
H 0.141649 -0.063659 0.043327
C -0.028413 -0.008202 1.113080
H 0.910378 0.076941 1.654114
C -0.548197 -1.855179 1.166214
H -0.666191 0.862546 1.295551
C -1.170994 -1.058754 1.934465
O -2.038722 -0.546064 2.793924
H -1.696540 -0.635394 3.693557

ts61_iso
Erel=86.4115 kcal/mol
Mechanism: min12e<-->min11a
C -0.019571 0.032367 0.004769
C -0.014182 0.024463 1.423268
C 1.306230 -0.063778 1.511001
O 2.536458 0.265520 1.227135
H 0.424758 0.867891 -0.527527
H -0.348984 -0.810781 -0.595756
H -0.759188 -0.238311 2.170230
H 2.581773 0.996121 0.583937

ts62_iso
Erel=86.5122 kcal/mol
Mechanism: min5a<-->min21b
C 0.004129 -0.054493 0.054279
C -0.020187 0.229864 1.275445
C 1.725492 0.063173 0.869979
O 2.314850 1.311118 0.929326
H 2.083027 1.807123 0.137656
H -0.069836 -0.300118 -0.985046
H 1.968651 -0.491203 1.768908
H 2.062365 -0.530488 0.009665

ts63_iso
Erel=86.5942 kcal/mol
Mechanism: min23d<-->min20
H 0.074412 0.114302 -0.007135
C 0.050543 -0.207829 1.050006
H 1.595025 0.073018 2.644987
C 1.169942 0.584353 1.772523
H 2.002771 0.967994 1.165037
C 0.263745 1.677790 2.172138
O -0.833588 1.574872 1.631235
H 0.478166 2.478574 2.899417

ts64_iso
Erel=86.6036 kcal/mol
Mechanism: min1b<-->min23c
H -0.073846 -0.053014 -0.022996
C -0.079957 -0.072232 1.065891

H 0.909657 0.130720 1.503519
C -1.100387 -0.835837 1.697732
H -0.849004 -0.923513 2.772872
C -1.111952 1.210524 1.386154
O -1.536880 1.850364 0.477708
H -1.204016 1.508236 2.442249

ts65_iso
Erel=87.0223 kcal/mol
Mechanism: min14<-->min23c
C 0.192658 0.141796 -0.071679
C 0.183056 0.047482 1.413108
C 1.634263 -0.275768 0.152517
O 1.007339 0.748256 2.011228
H -0.454047 -0.604411 -0.541932
H 0.092117 1.135868 -0.501821
H -0.335680 -0.794159 1.901801
H 1.649563 -1.287996 0.604570

ts4_co
Erel=87.5489 kcal/mol
Mechanism: min1a--->CO_channel
H -0.120653 -0.096493 0.038010
C -0.003011 -0.056463 1.125599
H 1.031690 -0.070872 1.468910
C -1.061089 0.013442 1.923232
H -1.007391 0.077867 3.009257
C -2.743416 0.618897 0.850181
O -3.158199 1.653093 1.175419
H -2.260412 -0.371787 0.840590

ts1_h2
Erel=87.5687 kcal/mol
Mechanism: min12b--->H2_channel
H -0.069222 -0.000075 -0.020002
C 0.015718 0.000006 1.060278
H 1.010990 -0.000024 1.489081
C -1.050144 0.000138 1.845208
H -1.128800 0.000250 3.188807
C -2.458494 0.000214 1.664064
O -3.165000 0.000337 2.634063
H -2.015080 0.000352 3.740474

ts5_co
Erel=87.6 kcal/mol
Mechanism: min1b--->CO_channel
H 0.084858 0.029866 -0.038368
C 0.077462 0.131233 1.039299
H 0.947917 -0.219236 1.576520
C -1.136469 -0.002352 1.745089
H -1.101428 0.124336 2.833091
C -2.466799 0.358884 1.324944
O -3.574830 0.455102 1.010431
H -1.831949 -1.050910 1.685434

ts2_h2
Erel=87.6456 kcal/mol
Mechanism: min1a--->H2_channel

H -0.124713 -0.000008 -0.327991
C 0.175458 -0.000148 1.594506
H 0.658388 -0.000334 2.582582
C -1.186098 0.000324 1.745068
H -1.751423 0.000504 2.682106
C -2.119289 0.000668 0.711624
O -3.127713 0.001029 0.168067
H -0.677700 0.000194 -0.881647

ts1_ch2o
Erel=87.8851 kcal/mol
Mechanism: min8--->CH2O_channel
H -0.090768 0.000091 -0.021701
C 0.033443 -0.000033 1.051941
H 1.043100 0.000089 1.468308
C -0.887781 -0.000322 1.967340
H -3.191543 -0.931677 2.242868
C -2.998271 -0.000658 1.682696
O -2.799170 -0.000457 0.472617
H -3.191874 0.930138 2.243123

ts2_ch2o
Erel=87.959 kcal/mol
Mechanism: min24--->CH2O_channel
H -0.028538 0.002511 0.000658
C 0.048944 0.041691 1.082187
H 1.033378 0.230088 1.503767
C -1.079344 -0.168069 1.762934
H -1.761209 -1.662178 3.755231
C -1.147852 -0.828556 4.104333
O -0.672243 -0.034268 3.288958
H -0.953955 -0.656339 5.162121

ts66_iso
Erel=88.0196 kcal/mol
Mechanism: min2<-->min7
H -0.067699 -0.033048 0.004514
C -0.020937 0.001148 1.097385
H 1.038883 0.042410 1.373864
C -0.629751 -1.169441 1.711392
H -0.479860 0.934045 1.439137
C -1.259934 -2.124115 2.172962
O -1.941678 -3.124671 2.650503
H -2.377081 -2.068472 1.808301

ts67_iso
Erel=89.5258 kcal/mol
Mechanism: min6<-->min20
C 0.010487 0.029088 -0.002952
C -0.004689 -0.028832 1.480132
C 1.415025 -0.165359 1.381199
O 1.364008 -0.012094 -0.010018
H -0.612395 -0.240592 -0.841004
H -0.237713 1.088301 1.037563
H -0.763894 -0.332548 2.185291
H 2.261764 0.244491 1.912974

ts68_iso

Erel=89.6742 kcal/mol
Mechanism: min1b<-->min19d
H -0.820156 0.000006 -0.217674
C 0.080619 0.000007 1.396060
H 0.923365 0.000050 0.740339
C -1.192279 -0.000048 1.827041
H -1.510712 -0.000080 2.874303
C -2.233619 -0.000066 0.841377
O -1.897031 -0.000030 -0.385766
H -3.302598 -0.000109 1.046202

ts69_iso
Erel=89.8509 kcal/mol
Mechanism: min11a<-->min26
C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.331130
O 1.168547 0.000000 2.139546
C -0.919133 0.166536 2.410831
H 1.575409 0.870985 2.053569
H 0.921879 -0.138103 -0.549438
H -0.929804 0.080332 -0.546320
H -0.883565 -0.757622 3.012275

ts3_h2
Erel=90.2011 kcal/mol
Mechanism: min2--->H2_channel
H 0.015213 0.243676 0.086635
C -0.066610 -0.067568 1.134463
H 1.847252 -0.060353 1.190608
C -0.526103 0.958831 2.014648
H -0.746906 0.795383 3.063647
C -0.735778 2.163249 1.471780
O -0.924524 3.152286 0.908208
H 1.175068 -0.572331 1.383657

ts2_bim
Erel=90.2207 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
C 0.157158 -0.000003 -0.020376
C -0.027704 -0.000013 1.235606
C 1.005632 -0.000007 2.218629
O 1.163803 -0.000012 3.389445
H 1.515678 0.000013 -0.183236
H 2.322524 0.000020 0.355643
H -0.386224 -0.000004 -0.948066
H 2.023921 0.000009 1.423620

ts3_ch2o
Erel=90.3313 kcal/mol
Mechanism: min1a--->CH2O_channel
H -0.234561 -0.622126 0.151990
C -0.046021 -0.205425 1.149814
H 0.981813 -0.283074 1.494780
C -0.929980 0.362608 1.940149
H -2.068235 0.502502 1.675087
C -2.668717 0.063589 0.422995
O -3.814231 0.298379 0.359327
H -2.017241 -0.436768 -0.336239

ts70_iso
Erel=90.6089 kcal/mol
Mechanism: min19f<-->min19g
H 0.006204 -0.490244 -0.469866
C -0.042076 0.015319 3.387850
H 0.961467 -0.216237 3.804910
C -0.478055 -1.060342 2.552327
H -1.054387 -1.765249 3.165575
C -0.419717 -1.268826 1.235453
O 0.323047 -0.424343 0.434678
H -0.905576 -2.113278 0.761680

ts71_iso
Erel=90.9384 kcal/mol
Mechanism: min25<-->min25
C 0.004328 0.000470 -0.064728
C 0.187453 -0.009977 3.043917
C 1.033354 -0.000525 2.045833
O 1.213094 0.005657 0.723078
H 0.015243 -0.889466 -0.695366
H 0.003214 0.895186 -0.688660
H -0.882918 -0.007895 0.569929
H 1.957422 0.003350 2.671603

ts72_iso
Erel=91.0196 kcal/mol
Mechanism: min1b<-->min17a
H 0.060744 -0.078852 -0.000616
C -0.020259 -0.083923 1.074749
H 2.019145 0.084523 1.602242
C 1.002206 -0.031258 1.952050
H 0.820860 -0.108582 3.015386
C -1.535347 0.822528 1.457197
O -1.301872 -0.490004 1.578694
H -1.981821 1.172546 2.421257

ts4_ch2o
Erel=91.2916 kcal/mol
Mechanism: min1b--->CH2O_channel
H -0.190593 0.006134 0.019149
C -0.042129 -0.001092 1.104931
H 0.982759 -0.004025 1.465824
C -1.027657 -0.006195 1.964052
H -2.158699 -0.004065 1.769452
C -2.731575 0.005288 0.322188
O -2.247769 0.012316 -0.750108
H -3.828640 0.004042 0.520235

ts4_h2
Erel=91.3794 kcal/mol
Mechanism: min2--->H2_channel
H -0.062824 0.162409 -0.217117
C -0.024252 0.086594 1.702481
H 1.027769 -0.182971 1.559572
C -0.817446 -1.042955 2.066662
H -0.562062 -2.101721 2.097762
C -2.043203 -0.697730 2.489226

O -3.085532 -0.378742 2.850400
H -0.284759 0.650592 0.433590

ts5_h2
Erel=91.3858 kcal/mol
Mechanism: min1b--->H2_channel
H -0.105224 0.114964 0.027243
C -0.008541 -0.005351 1.101279
H 0.995114 -0.015255 1.509563
C -1.046911 -0.102048 1.922226
H -1.500341 0.775585 2.953490
C -2.446115 -0.059623 1.768151
O -3.470757 -0.609127 1.757811
H -2.345910 1.286963 2.693045

ts73_iso
Erel=91.4477 kcal/mol
Mechanism: min1b<-->min19d
C -0.053067 0.028238 -0.002778
C 0.054714 -0.029084 2.585318
C 0.478691 0.020297 1.222815
O -1.387426 0.115824 -0.315469
H 0.556451 -0.046364 -0.891546
H 1.569655 -0.141347 1.290703
H 0.022859 1.002703 2.998897
H -1.918056 -0.001385 0.478997

ts74_iso
Erel=91.8343 kcal/mol
Mechanism: min6<-->min15
C 0.033596 -0.003333 -0.006644
C 0.016294 0.031603 1.493264
C 1.429636 0.023728 1.500568
O 1.483172 -0.068404 0.092677
H -0.369457 -0.888867 -0.502878
H -0.322146 0.902234 -0.507080
H -0.724667 0.143896 2.273934
H 0.847717 -1.006253 1.940919

ts75_iso
Erel=92.2907 kcal/mol
Mechanism: min1a<-->min1a
H -0.163250 0.197288 0.018846
C 0.011346 0.026841 1.080785
H 1.048583 0.007343 1.413943
C -0.964766 -0.156946 1.903652
H -1.589558 0.401197 3.636929
C -2.056479 -0.280692 2.832799
O -2.674495 -1.315401 3.227455
H -2.682544 0.573033 2.375921

ts76_iso
Erel=92.3925 kcal/mol
Mechanism: min9<-->min12a
C 0.042846 0.237816 -0.137208
C 0.125399 0.056862 1.195760
C 1.552819 -0.115761 1.163602
O 2.048468 -1.215374 1.749000

H -0.780948 -0.122436 -0.757221
H 1.504754 0.288307 -0.086820
H 2.994683 -1.246617 1.566519
H -0.579537 -0.196254 1.976760

ts5_ch2o
Erel=92.6324 kcal/mol
Mechanism: min17b--->CH2O_channel
H -0.012129 0.000063 0.134424
C 0.037390 -0.000034 1.368627
H 0.993926 -0.000053 1.864669
C -1.166096 -0.000089 1.748178
H -1.996765 -0.000159 2.419870
C -1.308169 0.000113 -0.844508
O -2.144075 0.000026 0.034236
H -1.734430 0.000184 -1.867031

ts77_iso
Erel=92.863 kcal/mol
Mechanism: min19b<-->min19e
C -0.088792 -0.085595 -0.037598
C 0.101903 -0.003839 1.364115
C 1.073516 0.051408 2.275952
O 0.780507 0.073866 3.625662
H -0.260589 0.930212 -0.453260
H -0.933291 -0.139311 1.741632
H 1.492559 -0.363375 4.101190
H 2.119706 0.127127 1.997166

ts78_iso
Erel=92.9387 kcal/mol
Mechanism: min19b<-->min19e
C 0.064828 0.112591 -0.104328
C 0.126124 -0.004111 1.308493
C 1.009077 -0.036732 2.306917
O 0.597359 0.091348 3.619628
H -0.940192 0.126095 1.590008
H -0.039635 -0.896283 -0.558588
H 1.274711 -0.280524 4.190112
H 2.078079 -0.085672 2.128939

ts79_iso
Erel=93.1262 kcal/mol
Mechanism: min19a<-->min19c
C -0.005396 -0.011416 -0.047366
C 0.042851 -0.041905 2.536009
C 0.514151 -0.012839 1.183060
O 0.680085 -0.127110 -1.230891
H -1.069527 0.068334 -0.224543
H 1.605241 -0.157572 1.312746
H 0.021848 0.996414 2.934606
H 1.623091 -0.204910 -1.051689

ts6_h2
Erel=93.2102 kcal/mol
Mechanism: min1a--->H2_channel
H -0.220177 -0.000821 -0.191265
C 0.080616 -0.000098 1.679288

H 0.422091 -0.000783 0.333888
C -1.211333 0.000404 1.952076
H -1.454538 0.000938 3.013560
C -2.362452 0.000335 1.006717
O -3.519796 0.000812 1.313870
H -2.024146 -0.000230 -0.061605

ts80_iso
Erel=93.3775 kcal/mol
Mechanism: min3<-->min23a
H 0.014949 0.161531 0.037502
C 0.037395 -0.219213 1.079450
H 1.490939 0.054977 2.727977
C 1.183964 0.515938 1.786206
H 2.056305 0.860287 1.222373
C 0.173697 1.591800 1.944459
O 0.195519 2.723521 2.344558
H -0.848470 1.155265 1.576080

ts81_iso
Erel=93.7782 kcal/mol
Mechanism: min1b<-->min4a
H -0.088278 -0.024286 -0.076003
C -0.095345 -0.249552 3.211811
H 0.713271 0.268198 3.760170
C -0.626445 0.572052 2.260269
H -1.174594 0.754750 3.307251
C -1.149498 1.032061 1.128574
O -0.688804 0.726841 -0.132343
H -1.956084 1.749248 1.111306

ts82_iso
Erel=93.9929 kcal/mol
Mechanism: min4a<-->min4b
C 0.332845 0.077236 -0.021629
C -0.297644 -0.200058 1.303750
C 1.176174 -0.022327 1.226783
O 1.701208 1.041053 1.973893
H 0.574068 -0.704357 -0.735374
H -0.079384 0.969740 -0.491149
H 1.753017 1.808937 1.398297
H 1.810960 -0.905783 1.203459

ts83_iso
Erel=94.3109 kcal/mol
Mechanism: min4b<-->min19b
H -0.043882 -0.048346 0.090004
C -0.072850 0.346692 1.581517
H 0.705708 -0.337111 1.965988
C -0.954037 -0.323384 0.786214
H -2.959810 -0.922350 0.867348
C -2.089778 -0.750030 0.243018
O -2.216163 -0.931207 -1.121621
H -2.733764 -1.726575 -1.278454

ts84_iso
Erel=94.3416 kcal/mol
Mechanism: min6<-->min27

C 0.038629 -0.014102 0.013188
C -0.081859 0.096943 1.530731
C 1.347222 -0.069753 1.427365
O 1.509126 -0.089310 0.031987
H -0.423516 -0.860235 -0.498626
H -0.290546 0.928499 -0.439039
H 0.943091 -1.110475 1.805106
H 2.187466 0.205583 2.062885

ts85_iso
Erel=94.6398 kcal/mol
Mechanism: min1b<-->min5a
C 0.078755 0.058082 -0.007259
C -0.354496 -0.028237 2.587976
C 0.108141 -0.078964 1.380329
O -0.243045 1.193517 -0.643196
H 1.268940 -0.086029 1.005831
H 0.412621 -0.719578 -0.682910
H 0.307201 0.120752 3.438272
H -0.675329 1.781736 -0.006127

ts86_iso
Erel=94.8956 kcal/mol
Mechanism: min9<-->min12b
H 0.116469 0.712163 0.344175
C -0.044189 0.021271 1.174173
H 1.127038 0.587150 4.313835
C 0.911875 -0.383839 2.032606
H 1.995957 -0.381432 2.016791
C -0.005236 -0.447442 3.148659
O 0.238544 0.194635 4.289577
H -0.965480 -0.283489 2.248396

ts87_iso
Erel=94.956 kcal/mol
Mechanism: min8<-->min8
H -0.136095 -0.211906 0.102526
C 0.046829 0.348815 1.036847
H 0.878216 -0.211938 1.500719
C -1.056659 0.132138 1.837361
H -2.994147 -0.993920 2.096666
C -2.099956 -0.636746 2.594197
O -1.913931 0.862649 2.459281
H -1.904548 -0.993954 3.598641

ts88_iso
Erel=95.1752 kcal/mol
Mechanism: min4a<-->min19a
C 0.044736 0.023091 0.038106
C 0.061287 0.292014 1.380443
C 0.382622 0.009518 -1.246879
O -0.451563 -0.006205 -2.339917
H -1.073146 0.223905 0.404855
H -1.362969 0.121451 -2.057354
H -0.125331 -0.635025 1.954964
H 1.424726 -0.054969 -1.527876

ts7_h2

Erel=95.527 kcal/mol
Mechanism: min4a--->H2_channel
H -0.012287 0.003876 -0.060356
C -0.046248 -0.022205 1.408008
H 0.995606 -0.038414 1.666942
C -1.238776 0.142412 1.806147
H -3.270670 -0.096027 0.976023
C -2.277859 0.345175 0.847794
O -2.014592 0.956219 -0.209447
H -0.700929 0.535959 -0.400414

ts89_iso
Erel=95.7619 kcal/mol
Mechanism: min1b<-->min19a
C -0.025809 0.009072 -0.189770
C 0.220828 -0.012153 1.120021
C 1.211938 -0.051040 2.130794
O 1.496928 -1.149484 2.821418
H -1.089509 0.106643 -0.443076
H -0.665400 -0.018888 1.802998
H 1.151755 -1.913760 2.331758
H 1.655728 0.830042 2.586465

ts8_h2
Erel=96.2256 kcal/mol
Mechanism: min1a--->H2_channel
H 0.031872 0.000298 0.130686
C -0.183036 -0.000185 2.304263
H 1.656506 0.000057 1.952981
C -0.561481 0.000051 1.035189
H 1.202949 -0.000127 2.623723
C -2.041033 -0.000038 0.822057
O -2.530333 0.000153 -0.281098
H -2.660310 -0.000289 1.736509

ts2_triple
Erel=96.3645 kcal/mol
Mechanism: min17d--->triple_channel
H -0.081408 -0.000018 0.175892
C 0.061777 0.000036 1.457058
H 1.120468 -0.000019 1.658245
C -1.028743 0.000134 2.054529
H -1.849814 0.000218 2.730547
C -1.991972 0.000054 -0.756266
O -2.476126 0.000137 0.309735
H -0.670728 -0.000025 -0.702052

ts90_iso
Erel=96.6433 kcal/mol
Mechanism: min9<-->min9
C -0.016837 0.124808 -0.027955
C 0.003729 0.020633 1.344047
C 1.186331 0.020614 0.631738
O 0.879095 -1.768079 1.459556
H -0.553950 -0.148927 -0.919684
H 1.375305 -1.902536 2.283387
H -0.466186 0.201647 2.293929
H 2.245707 0.201603 0.660493

ts3_triple
Erel=96.9589 kcal/mol
Mechanism: min12e--->triple_channel
H -0.048673 0.000021 0.038506
C 0.023506 -0.000041 1.472986
H 1.076806 -0.000145 1.673169
C -1.127823 0.000044 1.989216
H -1.574597 0.000047 2.965326
C -2.412042 0.000207 0.813029
O -2.211699 0.000234 -0.341009
H -0.571954 0.000096 -0.661665

ts6_ch2o
Erel=97.0121 kcal/mol
Mechanism: min1a--->CH2O_channel
H -0.087320 0.089886 -0.013263
C -0.036690 0.054175 1.517493
H 1.017255 -0.098647 1.668471
C -1.261440 0.046150 1.801988
H -1.999303 -0.013021 2.578701
C -1.318166 -0.268983 -0.040910
O -1.642673 -1.356160 -0.449735
H -1.711033 0.730116 -0.231494

ts91_iso
Erel=97.0714 kcal/mol
Mechanism: min2<-->min11a
H -0.089076 0.146970 0.107044
C 0.022171 -0.036479 1.674491
H 1.093726 -0.017310 1.867167
C -0.695479 1.143369 0.783226
H -0.487458 -0.979357 1.866794
C -0.767640 1.261476 2.054319
O -0.683512 1.124200 -0.502724
H -1.078758 1.772474 2.944216

ts7_ch2o
Erel=97.0808 kcal/mol
Mechanism: min6--->CH2O_channel
C -0.206367 -0.071314 -0.026025
O 0.034449 -0.001694 1.223597
C 1.466999 0.109994 1.468617
C 2.123204 0.788508 0.538456
H -1.231926 0.122570 -0.325081
H 0.562931 -0.378402 -0.719125
H 3.210361 0.817871 0.650561
H 1.667180 -0.297995 2.453387

ts92_iso
Erel=97.3364 kcal/mol
Mechanism: min8<-->min26
C -0.002940 0.004770 0.024541
C -0.047865 -0.034099 1.342082
C 0.633919 -0.101932 2.610042
O -1.143935 0.089454 2.206537
H -0.911594 0.072229 -0.557703
H 0.948847 -0.025957 -0.486987

H -0.622337 -0.501870 3.039330
H 1.015850 0.878353 2.924429

ts93_iso
Erel=97.597 kcal/mol
Mechanism: min2<-->min10
H -0.051622 0.287042 0.103315
C -0.231071 0.025521 1.127048
H 0.560923 -0.153278 1.826690
C 2.475841 -0.460363 0.061670
H -1.252485 -0.181581 1.436851
C 2.137333 0.671399 0.450121
O 1.569381 1.640466 0.901376
H 2.968075 -1.285153 -0.390468

ts94_iso
Erel=98.0932 kcal/mol
Mechanism: min19g<-->min5c
C 0.336079 0.004493 -0.116442
C 0.241284 -0.059034 1.171556
C 0.636607 0.057980 2.503328
O 1.045876 1.234127 3.012532
H 1.019377 1.203084 3.976502
H -0.544410 0.085130 -0.749523
H 0.551278 -0.781000 3.187765
H -0.771170 -0.202070 1.809372

ts95_iso
Erel=98.1707 kcal/mol
Mechanism: min4a<-->min9
C 0.043460 0.079700 -0.037080
C -0.064827 -0.034287 1.516118
C 1.180904 0.025754 0.853151
O -0.230650 1.254681 -0.745013
H -0.240873 -0.846652 -0.531573
H 0.915998 0.952146 1.590798
H 2.245119 -0.162165 0.932282
H -1.182883 1.401037 -0.708442

ts96_iso
Erel=98.2275 kcal/mol
Mechanism: min6<-->min19g
C -0.159012 -0.183437 -0.062846
C 0.017676 -0.001792 1.377336
C 1.349026 0.042483 1.435656
O 1.744687 0.008535 0.074662
H 1.214543 -0.804227 -0.352515
H -0.424139 0.701889 -0.649098
H -0.732605 -0.063500 2.152225
H 2.109697 -0.040148 2.196751

ts8_ch2o
Erel=98.4721 kcal/mol
Mechanism: min28--->CH2O_channel
H 0.044830 -0.155868 0.128322
C -0.031953 -0.011794 1.213899
H 0.942397 -0.058067 1.712683
C -0.690391 -1.733016 2.730673

H -0.163581 -1.243297 3.550079
C -1.185108 -0.981265 1.754807
O -0.976972 0.769040 1.710690
H -1.945716 -1.157643 1.012377

ts97_iso
Erel=98.6627 kcal/mol
Mechanism: min5a<-->min4b
C 0.156979 -0.020415 0.088565
C -0.204498 0.155145 1.459934
C 0.977972 -0.001012 1.959049
O 1.856655 -0.347913 0.515351
H -0.113551 -0.938795 -0.428591
H 0.210174 0.845614 -0.571182
H 2.423378 0.402632 0.275094
H 1.629936 -0.095302 2.808431

ts98_iso
Erel=99.0237 kcal/mol
Mechanism: min7<-->min22a
H -0.106889 0.103595 0.017729
C 0.039676 0.063247 1.100349
H 1.086701 -0.209634 1.287584
C -0.756508 -0.954332 1.744566
H -0.124679 1.049995 1.543244
C -1.385034 -1.836458 2.428525
O -2.641143 -0.932377 2.059221
H -3.072501 -1.473469 1.385333

ts99
Erel=99.0937 kcal/mol
Mechanism: min8<-->min24
H 0.124844 0.066642 0.096649
C -0.033972 0.072867 1.169702
H 0.732721 0.390590 1.864369
C -1.587398 1.024274 2.196385
H 0.081603 2.188679 2.987122
C -0.978703 2.018074 2.827242
O -1.229905 -0.237746 1.630547
H -1.642573 2.770418 3.242583

ts9_ch2o
Erel=99.1559 kcal/mol
Mechanism: min9--->CH2O_channel
H -0.161467 -0.064399 -0.069100
C -0.195707 0.034678 0.988657
H 2.974840 -0.196269 2.852295
C -0.154645 0.082711 2.200688
H -0.360601 0.316732 3.217702
C 1.537572 -1.300687 2.383220
O 2.707629 -0.736608 2.097541
H 1.310850 -1.927335 1.496033

ts100_iso
Erel=99.2623 kcal/mol
Mechanism: min11a<-->min11b
C -0.051266 -0.182963 -0.090347
C -0.040121 -0.219960 1.836904

C 0.951042 -0.145466 0.863561
O 2.230237 0.203174 0.808525
H -0.881716 -0.575328 0.871582
H -0.161052 0.714639 -0.710002
H 2.592508 0.239454 1.702879
H -0.134980 0.661097 2.486664

ts101_iso
Erel=99.5275 kcal/mol
Mechanism: min5a<-->min19d
C -0.449990 -0.169846 0.055178
C 0.116136 0.135711 1.184377
C 0.836078 -0.013469 2.365321
O 1.217441 -1.192315 2.886688
H 1.098427 -1.877770 2.214155
H 0.158571 -0.298909 -0.840399
H -0.616120 0.500068 2.081184
H 1.026913 0.809387 3.042687

ts10_ch2o
Erel=99.9044 kcal/mol
Mechanism: min1b--->CH2O_channel
H 0.250288 0.000173 0.020635
C 0.254630 0.000007 1.083319
H 1.166102 -0.000280 3.126584
C 0.510094 -0.000172 2.282388
H -1.082089 -0.000302 2.732808
C -2.153024 -0.000107 1.239815
O -2.122862 -0.000303 2.499310
H -3.220352 -0.000097 0.933298

ts102_iso
Erel=100.324 kcal/mol
Mechanism: min4a<-->min11b
H -0.054708 -0.173707 -0.029271
C -0.017511 0.012145 1.036914
H 0.982171 0.043169 1.462993
C -1.003177 -0.677782 2.109330
H -2.024313 0.125195 1.247832
C -1.099486 0.675612 1.749329
O -1.348581 1.910129 2.261593
H -1.821100 1.797224 3.098810

ts103_iso
Erel=100.476 kcal/mol
Mechanism: min12a<-->min7
H -0.022493 -0.235568 0.019130
C 0.014826 0.004006 1.076795
H 0.990301 -0.047397 1.559726
C -1.142957 0.350967 1.761079
H -1.215603 -0.783825 1.364127
C -1.866992 0.934313 2.669418
O -2.706446 0.373989 3.546287
H -3.220281 1.078984 3.953188

ts9_h2
Erel=100.591 kcal/mol
Mechanism: min19a--->H2_channel

H 0.017000 -0.000080 0.113050
C -0.111167 -0.000173 3.306000
H 0.834861 0.000226 3.830352
C -0.310148 -0.000244 2.032891
H 0.598430 0.000158 0.974463
C -1.453583 -0.000723 1.174572
O -1.259700 -0.000626 -0.055989
H -2.466706 -0.001162 1.567711

ts3_bim
Erel=100.699 kcal/mol
Mechanism: C2H4+CO<-->HOCH+C2H2
H 0.242012 0.000024 0.121960
C -0.148451 -0.000003 2.280693
H 0.308433 0.000007 3.243216
C -0.873908 -0.000021 1.297901
H -1.793415 -0.000048 0.750530
C 2.141232 0.000084 0.482300
O 1.205079 0.000058 -0.350333
H 1.672790 0.000062 1.544613

ts104_iso
Erel=100.715 kcal/mol
Mechanism: min16b<-->min22a
H 0.000766 -0.009941 0.010212
C -0.008351 -0.001866 1.104076
H 1.016356 -0.070012 1.470732
C -0.809536 -1.122640 1.611798
H -0.442495 0.948820 1.427183
C -0.851178 -2.213012 2.336261
O -2.164131 -1.342906 1.337493
H -2.084958 -2.428332 2.096365

ts105_iso
Erel=100.853 kcal/mol
Mechanism: min4a<-->min9
H 0.007618 0.131551 0.130257
C -0.010448 -0.060397 1.200792
H 2.003327 -0.115290 1.556904
C 1.031900 0.543461 2.205410
H -1.623885 0.726697 1.896430
C 1.026097 -0.815868 1.884462
O -1.285347 -0.167392 1.767761
H 1.384577 -1.793225 2.187181

ts106_iso
Erel=100.895 kcal/mol
Mechanism: min4b<-->min11a
C 0.050214 0.000743 -0.135524
C 0.127749 0.292172 1.450875
C 1.228898 0.453470 0.602910
O 2.297881 1.286893 0.469632
H -0.017649 -0.990714 -0.567363
H -0.607391 0.742285 -0.581732
H 2.708989 1.111547 -0.384707
H 1.434318 -0.515495 1.255343

ts1_h2o

Erel=101.049 kcal/mol
Mechanism: min4a--->H2O_channel
H -0.001743 0.193101 0.035996
C -0.013133 -0.013611 1.102088
H 0.946349 -0.136343 1.595729
C -1.141688 -0.105331 1.772928
H -3.162543 0.073780 3.054568
C -2.227639 -0.332140 2.397255
O -2.965784 1.296665 3.207446
H -3.347497 1.683934 2.406344

ts107_iso
Erel=101.537 kcal/mol
Mechanism: min2<-->min10
C 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.402171
C 1.365541 0.000000 1.508730
C 2.004818 -0.208823 0.332721
H 0.075819 0.987840 -0.444594
H 1.176729 -0.697521 -0.406143
H -0.755061 -0.651291 -0.442061
H 1.793705 0.224254 2.476840

ts108_iso
Erel=101.656 kcal/mol
Mechanism: min4a<-->min21c
C -0.011798 -0.066003 0.018476
C 0.078398 0.000412 1.327792
C 1.489681 0.036687 0.770912
O 2.208509 1.191952 0.900227
H 1.225552 -0.194047 -0.516444
H -0.560529 0.184373 -0.878412
H 1.640008 1.821250 1.367155
H 2.105396 -0.855320 0.836668

ts10_h2
Erel=101.714 kcal/mol
Mechanism: min18a--->H2_channel
H 0.335808 -0.198939 -0.004813
C -0.169994 0.055030 0.911450
H 0.822631 0.173468 1.806553
C -1.283026 0.608397 1.281664
H 0.514391 -0.659671 1.838923
C -1.852393 0.964904 2.535095
O -1.601068 1.983509 3.160233
H -2.615316 0.233985 2.888853

ts109_iso
Erel=101.796 kcal/mol
Mechanism: min4b<-->min26
C 0.019314 -0.007705 -0.058238
C 0.142887 0.053376 1.254442
C 0.345866 0.134477 2.589918
O -1.184655 0.229125 2.313803
H -0.812895 0.452201 -0.572315
H 0.829934 -0.431837 -0.637869
H -1.589927 -0.657096 2.266509
H 0.657793 -0.642085 3.275448

ts2_ch2o
Erel=101.808 kcal/mol
Mechanism: min9--->H2O_channel
C -0.448483 0.584289 0.211375
C -0.287804 0.007439 1.389260
C 0.719852 -0.188710 0.414402
O 0.714141 -2.098095 -0.359180
H -1.040950 1.190975 -0.453094
H 1.475057 -0.951684 0.005606
H -0.647203 -0.200418 2.382616
H 0.555731 -1.936942 -1.299618

ts110_iso
Erel=101.829 kcal/mol
Mechanism: min12a<-->min7
C 0.000550 0.032497 0.022960
C -0.072836 0.038437 1.409274
C 0.510489 -0.167215 2.567013
O 0.760123 0.755870 3.498464
H -0.472823 -0.998960 0.896415
H 0.940610 0.146113 -0.516230
H 1.139891 0.307351 4.260820
H -0.899077 -0.055085 -0.576451

ts11_ch2o
Erel=102.08 kcal/mol
Mechanism: min9--->CH2O_channel
C 0.033459 -0.011479 -0.286729
C 0.065689 0.045494 2.358311
C 1.077920 0.032914 1.692923
O -0.233742 -1.258715 -0.633146
H -0.905762 0.493862 0.045859
H 2.080271 0.013543 1.339183
H -0.845770 0.067339 2.904410
H -1.157367 -1.530577 -0.499311

ts111_iso
Erel=102.914 kcal/mol
Mechanism: min2<-->min2
H -0.172811 0.631219 0.174289
C 0.001676 0.149056 1.135578
H 0.978497 -0.357185 1.052705
C 0.236155 -2.201865 1.134012
H 0.042803 0.843461 1.975947
C 0.418236 -2.262781 2.474630
O 0.593526 -2.544330 3.595921
H -0.846153 -0.539338 1.292525

ts112_iso
Erel=103.03 kcal/mol
Mechanism: min5a<-->min8
C -0.073959 0.001367 0.004016
C -0.030972 0.003905 2.622111
C 0.323385 0.009614 1.424364
O -1.416765 -0.022866 0.328774
H 0.292705 0.903441 -0.517568
H 0.325358 -0.887498 -0.516269

H 0.153312 0.007964 3.673663
H -1.085111 -0.015859 1.890202

ts113_iso
Erel=103.108 kcal/mol
Mechanism: min17d<-->min6
H 0.018434 0.002827 -0.028185
C -0.056317 -0.040310 2.918410
H 1.028766 0.068155 2.776472
C -0.272735 0.302907 0.965866
H -0.586334 -0.569012 1.747059
C -0.616870 1.472315 1.544498
O -0.601996 1.289222 2.863441
H -0.877064 2.449870 1.152580

ts3_h2o
Erel=103.121 kcal/mol
Mechanism: min5a--->H2O_channel
H -0.007735 -0.118066 -0.047224
C -0.037732 -0.019720 1.010435
H 2.170128 0.183964 3.616104
C -0.084133 0.068594 2.221210
H 0.814739 0.874390 4.267395
C -0.186255 0.299471 3.585783
O 1.604868 0.075929 4.394179
H -0.675325 -0.482863 4.161754

ts114_iso
Erel=103.391 kcal/mol
Mechanism: min16a<-->min13
H 0.513061 -0.660117 0.617692
C 0.015951 0.029224 1.301589
H 0.756719 0.654190 1.804700
C -0.809190 -0.698392 2.288855
H -0.652241 0.684601 0.736495
C -1.627940 -1.712606 2.677898
O -1.648200 -0.231489 3.266081
H -0.197992 -1.662172 2.905337

ts115_iso
Erel=103.826 kcal/mol
Mechanism: min12b<-->min7
H -0.063914 0.043803 -0.014894
C -0.018459 -0.004264 1.072123
H 0.927525 0.246321 1.539205
C -1.112918 -0.370879 1.855104
H -0.785857 0.762075 2.101869
C -2.217874 -0.987994 2.137379
O -3.413711 -0.630442 2.578471
H -3.557810 0.329013 2.506769

ts11_h2
Erel=103.896 kcal/mol
Mechanism: min3--->H2_channel
H 0.058138 -0.193483 -0.065186
C 0.063260 -0.016582 1.003171
H 1.017580 0.102578 1.499529
C -1.128698 -0.022363 1.730113

H -1.603008 -1.030911 2.657411
C -1.554402 1.177905 2.101517
O -1.894671 2.253682 2.373675
H -2.017161 -0.900637 1.771838

ts116_iso
Erel=103.979 kcal/mol
Mechanism: min8<-->min28
C 0.025118 0.005602 0.063318
C -0.232628 0.020211 2.760395
C 0.352578 0.164842 1.476028
O 1.176575 -0.654669 0.659926
H -0.789774 -0.656594 -0.217349
H 0.257965 0.791977 -0.649333
H 0.431007 -0.639224 3.355593
H 0.784637 1.164483 1.800747

ts117_iso
Erel=104.277 kcal/mol
Mechanism: min8<-->min28
C 0.010214 -0.018817 0.081438
C 0.010930 0.255887 2.832989
C 0.401368 0.004420 1.497964
O 1.063398 0.840782 0.589804
H -0.895877 0.495941 -0.226438
H 0.338106 -0.827094 -0.566802
H -0.703142 -0.554305 3.079199
H 1.014135 -0.873203 1.904679

ts4_h2o
Erel=104.33 kcal/mol
Mechanism: min5c--->H2O_channel
H -0.027030 0.107909 0.296952
C -0.018242 -0.231865 1.574568
H 0.879514 0.062007 2.118115
C -1.191694 -0.162278 2.306377
H 0.824997 1.537150 0.208559
C -2.235990 -0.224859 2.922373
O -0.098613 1.249428 0.218326
H -3.146721 -0.272858 3.467726

ts6_co
Erel=104.532 kcal/mol
Mechanism: min12e--->CO_channel
H -0.013378 -0.080969 0.033667
C -0.015892 -0.024744 1.118167
H 0.957233 -0.027704 1.602900
C -1.147723 0.057436 1.847503
H -0.838233 -0.654855 2.980145
C -1.123073 0.707357 3.409037
O -0.663973 -0.216365 4.149162
H -2.124710 0.090803 1.374186

ts118_iso
Erel=104.653 kcal/mol
Mechanism: min12b<-->min7
H -0.054596 0.038518 0.023955
C -0.018286 -0.051654 1.103662

H 0.965783 -0.015303 1.568835
C -1.189340 -0.227511 1.836852
H -1.154816 0.823728 1.217968
C -1.821803 -0.127908 2.978897
O -2.358495 -1.035619 3.780070
H -2.195380 -1.939916 3.461124

ts12_h2
Erel=105.138 kcal/mol
Mechanism: min23a--->H2_channel
H 0.244069 0.058023 -0.053878
C -0.086639 -0.020546 0.982314
H 2.097247 0.031173 1.684739
C 0.823041 0.195403 1.925887
H 1.887413 0.914918 1.684780
C 0.772643 0.183369 3.405061
O 1.719463 0.408147 4.119210
H -0.234742 -0.055839 3.790161

ts4_bim
Erel=105.322 kcal/mol
Mechanism: CH2O+C2H2<-->HOCH+C2H2
C 0.003049 0.000523 0.015347
C 0.001171 -0.000206 1.230375
C 0.284243 -0.000343 -2.558555
O -0.941200 0.010175 -2.320836
H -0.935257 0.009430 -1.191113
H 0.648303 -0.004402 -1.107813
H -0.017581 -0.000696 2.294787
H 0.493963 -0.001504 -3.639758

ts5_bim
Erel=105.923 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
H 0.494513 0.000264 0.205921
C -0.125106 -0.000091 2.351442
H -0.085092 -0.000105 3.441658
C -1.268307 -0.000609 1.631529
H 0.674238 0.000317 1.302209
C -2.477613 -0.001197 2.218415
O -3.546396 -0.001714 2.645972
H -0.956425 -0.000429 0.494351

ts6_trim
Erel=106.26 kcal/mol
Mechanism: CH2O+C2H2<-->H2+CO+C2H2
H 0.117479 0.015407 0.289782
C -0.033987 0.005104 2.534312
H 0.200320 0.005475 3.572353
C -0.361243 0.003667 1.350475
H -1.498923 -0.013765 0.838416
C -0.825300 0.004830 -1.260684
O -1.044475 0.004969 -2.390592
H -1.743471 -0.014003 -0.287959

ts119_iso
Erel=107.282 kcal/mol
Mechanism: min3<-->min11b

C 0.232371 0.128400 0.479156
C -0.342863 -0.530243 1.682050
C 0.746537 0.225461 1.927725
O -1.380036 -1.027504 2.286315
H 0.816370 -0.499544 -0.192390
H -0.270658 0.964490 -0.007359
H -0.704806 0.131361 2.671883
H 1.535008 0.608671 2.550803

ts12_ch2o
Erel=107.483 kcal/mol
Mechanism: min23d--->CH2O_channel
H -0.402604 -0.130229 0.200497
C 0.276743 0.093732 1.025114
H 0.394706 -0.090822 3.213672
C -0.096521 -0.225790 2.254699
H -1.281606 -0.424841 2.551296
C -1.014858 -1.795573 2.467613
O -1.537981 -2.396189 1.590899
H -0.674428 -2.170196 3.446259

ts120_iso
Erel=107.92 kcal/mol
Mechanism: min17c<-->min8
H 0.191913 -0.170153 0.046937
C -0.091402 0.093432 1.093729
H 1.224043 -0.203423 1.815406
C 1.607154 -2.314138 2.184458
H 2.668203 -2.153899 2.306580
C 0.803427 -1.307059 1.874121
O -0.507542 -1.199730 1.659630
H 1.194559 -3.297765 2.374307

ts13_h2
Erel=107.929 kcal/mol
Mechanism: min2--->H2_channel
H -0.074116 0.233134 0.090686
C -0.078261 0.016041 1.163349
H 1.327486 0.172276 1.293718
C -0.887772 0.805268 2.062467
H -0.007560 -1.048024 1.386644
C -1.306526 2.016752 2.078239
O -1.768107 3.088680 2.238807
H 0.693362 0.689517 1.871054

ts13_ch2o
Erel=108.041 kcal/mol
Mechanism: min5a--->CH2O_channel
H 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.089516
H 3.200646 0.000000 1.062950
C 2.435118 -0.201335 1.778812
H 0.133407 0.936400 1.614457
C 1.650671 -0.443552 2.706984
O -0.484311 -1.031924 1.670789
H 0.080924 -0.983395 2.581066

ts14_h2

Erel=108.407 kcal/mol
Mechanism: min23a--->H2_channel
H 0.044733 0.076132 0.046717
C -0.042868 -0.069307 1.386971
H 0.840607 0.076082 0.375320
C -0.192956 -1.326459 1.750298
H -0.607129 -1.458213 2.753406
C -0.212260 1.337651 1.797445
O 0.069236 2.293030 1.115803
H -0.633199 1.433444 2.816976

ts121_iso
Erel=108.533 kcal/mol
Mechanism: min8<-->min24
H -0.389507 0.454918 0.143466
C -0.171711 0.100536 1.144270
H 0.863826 -0.081486 1.417944
C -1.113991 -0.099703 2.014730
H -2.523495 1.491979 3.714252
C -2.958745 0.857440 2.932766
O -1.912354 -0.380447 2.883380
H -2.836904 1.309053 1.936040

ts14_ch2o
Erel=108.79 kcal/mol
Mechanism: min17a--->CH2O_channel
H 0.004777 -0.000217 -0.014646
C 0.019640 -0.000022 1.069066
H 0.982067 0.000045 1.569768
C -1.136439 0.000120 1.707078
H -2.516165 0.000255 2.278386
C -2.222748 0.000487 3.606339
O -1.003769 0.000401 3.289431
H -2.381719 0.000687 4.696694

ts15_ch2o
Erel=109.442 kcal/mol
Mechanism: min5a--->CH2O_channel
C -0.457506 0.106717 -0.204030
C 0.468282 -0.492137 1.994329
C 1.596390 0.005835 2.108458
O 0.163441 1.171232 0.049141
H 0.028215 -0.859717 -0.181178
H -1.479941 0.198457 -0.572086
H 2.567410 0.337957 2.406350
H 0.906002 0.834035 0.784515

ts7_trim
Erel=109.52 kcal/mol
Mechanism: H2+C3H2O<-->H2+CO+C2H2
H -0.419185 -0.000525 0.089289
C 0.288799 0.000232 2.119348
H 0.593228 -0.000056 -0.053506
C 0.498981 0.000586 3.331444
H 0.634042 0.000872 4.387384
C -1.129991 -0.000650 1.244520
O -2.242940 -0.001147 1.564386
H 0.930123 0.000335 1.068510

ts122_iso
Erel=109.69 kcal/mol
Mechanism: min12c<-->min21c
C -0.070599 0.036872 -0.024265
C 0.028292 0.036487 1.410038
C 1.373990 0.045428 1.688365
O 1.712038 0.473929 0.243108
H 0.217666 -0.836335 -0.602317
H -0.750071 0.697072 -0.575528
H -0.795741 0.131915 2.104013
H 2.481813 -0.022067 -0.093798

ts15_h2
Erel=110.643 kcal/mol
Mechanism: min7--->H2_channel
H -0.071616 0.045173 -0.037884
C -0.045277 -0.032411 1.390198
H 1.034370 -0.118111 1.528282
C -0.876265 -1.161258 1.560930
H -0.421802 0.954397 1.662475
C -1.044058 -1.862434 0.547920
O -0.987359 -1.857608 -0.688293
H -0.421897 -0.628654 -0.724055

ts16_h2
Erel=111.053 kcal/mol
Mechanism: min23a--->H2_channel
H -0.063219 0.179769 0.087289
C 0.077541 -0.123041 2.339528
H 1.155783 0.023636 2.277432
C -0.644351 0.179552 1.267329
H -0.162357 1.039840 0.396785
C -2.090942 0.138679 0.917465
O -2.960705 -0.227655 1.656247
H -2.302324 0.488327 -0.121308

ts17_h2
Erel=111.207 kcal/mol
Mechanism: min4a--->H2_channel
H 0.010629 0.016469 0.020895
C -0.106794 -0.012407 3.411553
H 1.517274 -0.004016 3.868845
C -0.034906 0.721695 2.365077
H 0.725285 -0.383939 4.209496
C -0.243761 1.429350 1.266974
O -0.182113 0.962617 -0.005132
H -0.478639 2.487261 1.291113

ts123_iso
Erel=111.236 kcal/mol
Mechanism: min6<-->min28
C 0.011408 -0.016825 0.013028
C 0.051449 0.092780 1.475679
C 1.433477 0.059941 1.764578
O 0.873638 -1.071033 0.536956
H -0.886244 -0.418867 -0.454398
H 0.550312 0.725912 -0.572280

H -0.813432 -0.109512 2.113858
H 1.623977 -0.557851 2.651934

ts124_iso
Erel=111.404 kcal/mol
Mechanism: min18a<-->min13
H -0.124984 -0.004532 0.060100
C 0.012624 -0.028226 1.137941
H 1.086780 -0.124998 1.321216
C -1.332279 -1.397256 1.193141
H -0.431498 0.823016 1.648170
C -0.282605 -1.574169 2.035223
O -0.072434 -2.516354 1.109039
H 0.089917 -1.480173 3.047617

ts18_h2
Erel=111.959 kcal/mol
Mechanism: min23d--->H2_channel
H 0.065822 -0.111996 -0.006030
C -0.130854 0.095285 2.185073
H 0.368205 -0.002679 3.151304
C 0.432439 -0.592426 1.215626
H -0.436177 -0.791558 0.184364
C 1.536144 -1.509455 0.852553
O 2.355580 -1.893338 1.642887
H 1.546918 -1.817882 -0.219883

ts5_h2o
Erel=111.98 kcal/mol
Mechanism: min5a--->H2O_channel
C 0.013886 0.017543 -0.052275
C 0.206496 -0.020711 1.379886
C -0.217165 -0.017001 2.558325
O -1.549491 0.146794 0.013819
H 0.343159 0.909110 -0.584387
H 0.246993 -0.885646 -0.620186
H -1.329851 0.113971 1.184975
H -1.972795 -0.672633 -0.290317

ts19_h2
Erel=112.408 kcal/mol
Mechanism: min5c--->H2_channel
C -0.011034 0.017648 0.004498
C 0.019947 -0.029006 1.210407
C 0.284927 -0.063421 2.604904
O 0.000809 -1.242277 3.184496
H -0.143768 0.967168 3.202492
H -0.059902 0.056971 -1.056068
H 0.415604 -1.252057 4.056141
H -1.072812 1.065079 3.092708

ts125_iso
Erel=112.745 kcal/mol
Mechanism: min8<-->min29
H 0.056902 0.151462 0.022110
C -0.030697 -0.003849 1.097667
H 0.916988 -0.088825 1.632832
C -1.338839 -0.125941 1.682561

H -0.275902 -0.191100 3.707918
C -1.061703 -0.621287 3.081296
O -0.579396 -1.512763 2.101613
H -1.939053 -0.976927 3.613293

ts20_h2
Erel=112.955 kcal/mol
Mechanism: min5a--->H2_channel
C -0.010856 -0.050409 0.065834
C 0.018132 -0.015818 1.273609
C 0.269798 -0.021354 2.673376
O -0.022408 -1.142578 3.337583
H -0.578829 -1.740307 2.813074
H -0.036235 -0.062530 -0.996579
H -0.179544 1.039309 3.254913
H -1.077303 1.175967 3.127026

ts8_bim
Erel=113.184 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
C -0.111719 -0.000131 -0.129695
C -0.024443 -0.000004 2.467920
C 0.028800 -0.000023 1.259152
O 0.890694 0.000272 -0.885046
H -0.805744 -0.000499 -2.220079
H -1.036047 -0.000564 -1.252946
H -0.034686 0.000028 3.531277
H 0.331382 -0.000001 -1.880360

ts21_h2
Erel=113.613 kcal/mol
Mechanism: min4b--->H2_channel
H 0.044722 0.062042 0.104951
C -0.095681 0.023928 1.320273
H 0.964932 0.034684 -0.009448
C 0.768175 -0.040330 2.262390
H 2.259205 -0.996390 4.840883
C 1.432543 -0.056793 3.404761
O 1.806740 -1.210945 4.019403
H 1.719449 0.871616 3.893061

ts16_ch2o
Erel=114.572 kcal/mol
Mechanism: min5a--->CH2O_channel
H -0.001631 0.006462 -0.044094
C 0.045153 -0.060456 4.123794
H 0.649420 -0.115612 4.998561
C -0.686616 -0.011841 3.157977
H -1.391651 -0.184129 1.950884
C -1.346678 0.686478 1.071711
O -0.302075 0.861687 0.296385
H -1.683440 1.658845 1.447637

ts126_iso
Erel=114.95 kcal/mol
Mechanism: min6<-->min28
C 0.024761 -0.011437 0.040729
C -0.036686 0.069208 1.501334

C 1.315746 -0.135726 1.939543
O 0.956299 -1.023326 0.585596
H -0.798382 -0.454416 -0.525333
H 0.549418 0.779862 -0.496633
H -0.929031 -0.149009 2.088850
H 2.069532 0.578130 1.592816

ts22_h2
Erel=115.073 kcal/mol
Mechanism: min4b--->H2_channel
H 0.022564 0.103704 0.155497
C -0.001321 0.007702 3.355872
H 0.948651 0.037147 3.888461
C -0.106365 -0.496228 2.153012
H -0.859456 0.418910 3.886418
C -0.210168 -0.994418 0.956801
O -0.424864 -2.015274 0.211557
H -0.155505 -0.742157 -0.310225

ts23_h2
Erel=115.132 kcal/mol
Mechanism: min2--->H2_channel
H -0.264528 0.152456 -0.048221
C -0.019988 -0.095942 0.978016
H 1.342415 0.012493 1.596516
C 0.540816 -1.455676 2.734665
H 0.147203 0.806719 1.596857
C -0.414975 -1.234124 1.612879
O 0.796118 -2.335892 3.473848
H 1.372233 -0.454904 2.640402

ts127_iso
Erel=115.668 kcal/mol
Mechanism: min12e<-->min21c
C -0.012768 -0.038787 -0.034091
C -0.002860 0.010506 2.243148
C 0.807617 -0.059240 1.137718
O -1.321163 -0.298752 1.405736
H -0.633648 0.815713 -0.273341
H 0.189759 -0.677607 -0.902839
H 1.885665 -0.176048 1.135533
H -1.356627 -1.263431 1.411330

ts128_iso
Erel=115.89 kcal/mol
Mechanism: min4a<-->min7
C -0.002025 -0.020789 0.014299
C -0.011934 0.055383 1.521944
C 1.267331 0.096733 1.173955
O 2.359394 0.853936 1.426223
H -0.022519 -0.981268 -0.495280
H -0.487126 0.792553 -0.531874
H 2.076112 1.578416 2.001286
H 1.373119 -0.135965 -0.114794

ts129_iso
Erel=116.191 kcal/mol
Mechanism: min5a<-->min11b

C 0.017385 -0.005779 0.036882
C -0.289624 -0.044677 2.521712
C 0.301019 -0.014924 1.396690
O 1.910304 -0.255593 0.904439
H -0.561331 -0.794504 -0.439563
H 0.304082 0.838191 -0.582174
H -0.031104 0.060349 3.560046
H 2.366273 0.602540 0.904060

ts17_ch2o
Erel=116.318 kcal/mol
Mechanism: min5a--->CH2O_channel
H 0.000000 0.000000 0.000000
C 0.000000 0.000000 4.178764
H 0.677051 0.000000 5.000221
C -0.804700 0.002683 3.273630
H -1.749179 -0.217225 2.310212
C -1.525044 0.201089 1.141995
O -0.747779 -0.504832 0.355320
H -1.282029 1.273766 1.178686

ts130_iso
Erel=117.312 kcal/mol
Mechanism: min4b<-->min7
C -0.031893 -0.013575 0.016203
C -0.001902 0.082504 1.509215
C 1.284187 0.109855 1.157278
O 2.303397 0.954193 1.439127
H -0.043372 -0.972628 -0.496389
H -0.529185 0.795655 -0.524071
H 3.136100 0.528386 1.203655
H 1.373363 -0.142089 -0.126881

ts9_bim
Erel=117.47 kcal/mol
Mechanism: H2+C3H2O<-->H2O+C3H2
C -0.094095 -0.068105 0.047732
C 0.024701 0.018153 1.252254
C 0.163346 0.079233 2.628788
O 0.159454 -1.014041 3.388743
H 0.181671 -1.833356 2.864082
H -0.192451 -0.134135 -1.008291
H -1.270536 -1.979776 3.673288
H 0.005655 0.990316 3.186747

ts131_iso
Erel=118.039 kcal/mol
Mechanism: min17c<-->min8
H -0.232261 -0.061311 0.069611
C 0.014673 0.082340 1.110202
H 1.029835 0.316967 1.397779
C -0.915606 -0.041456 2.048571
H -2.128888 0.278763 1.588669
C -2.294950 -0.641975 2.485885
O -1.112139 0.054841 3.332148
H -3.145419 0.035771 2.685582

ts6_h2o

Erel=118.419 kcal/mol
Mechanism: min9--->H2O_channel
C -0.233529 -0.062490 0.108310
C -0.224899 -0.087951 1.521745
C 0.973410 0.102626 0.956383
O -0.019645 1.441203 -0.587025
H 1.051004 1.168999 0.066955
H -0.487568 -0.691664 -0.730684
H -0.820494 -0.027468 2.420482
H -0.510762 2.102126 -0.077342

ts7_h2o
Erel=119.045 kcal/mol
Mechanism: min4b--->H2O_channel
C -0.298356 0.154946 0.343140
C 0.517690 -0.044431 1.311829
C 0.402401 -0.150947 2.645357
O -1.100166 -0.123598 2.793061
H -1.209934 0.270246 1.611287
H -0.507568 -0.408959 -0.555104
H -1.452252 -1.022886 2.836107
H 0.873592 0.437874 3.415067

ts132_iso
Erel=119.295 kcal/mol
Mechanism: min4b<-->min11a
C -0.026331 0.015342 -0.024837
C 0.058793 -0.052879 1.628072
C 1.163259 0.008356 0.746037
O 0.707718 1.391720 1.868793
H -0.275603 0.848980 -0.681400
H -0.472350 -0.935764 -0.291098
H 0.197865 1.990773 1.307930
H 2.238472 0.118589 0.750290

ts10_bim
Erel=119.445 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
H -0.123251 0.035943 0.070989
C -0.008611 -0.008800 1.372937
H 1.059635 -0.036813 1.594366
C -1.012767 -0.020504 2.330332
H 0.034335 0.969223 0.655581
C -2.256129 -0.005355 2.559546
O -3.399424 0.005445 2.869640
H -0.002769 -0.938898 0.593322

ts24_h2
Erel=119.484 kcal/mol
Mechanism: min8--->H2_channel
C 0.006083 0.023808 0.039623
C -0.030703 -0.044177 1.352336
C 0.406795 -0.141388 2.709525
O -0.968874 -0.181790 2.358552
H 0.951267 0.154341 -0.468200
H -0.902807 -0.045510 -0.543295
H 0.825070 0.709856 3.451296
H 0.657632 1.441878 2.861867

ts25_h2
Erel=119.922 kcal/mol
Mechanism: min6--->H2_channel
H 0.231279 0.013495 -0.226802
C -0.042933 0.017705 1.587624
H 0.726155 -0.027981 0.456041
C -1.306999 -0.697423 1.743097
H -1.581138 -1.727191 1.891842
C -1.777109 0.508406 2.146652
O -0.716228 1.293765 1.699820
H -2.501562 0.908742 2.846895

ts8_h2o
Erel=120.543 kcal/mol
Mechanism: min4b--->H2O_channel
C 0.063167 -0.213173 -0.000662
C -0.077525 0.014613 1.259329
C 0.800591 0.220131 2.241712
O 2.083642 0.358324 1.428757
H 1.588995 -0.203151 0.486005
H -0.329908 0.330492 -0.850875
H 2.844861 -0.057075 1.870242
H 0.949144 -0.297402 3.175858

ts26_h2
Erel=120.703 kcal/mol
Mechanism: min5a--->H2_channel
C -0.067879 -0.077706 -0.024463
C 0.003927 0.002959 2.630360
C 0.018310 -0.045170 1.429992
O -0.927917 -0.881753 -0.627687
H 0.154662 0.906998 -0.470007
H 1.269366 -0.628266 -0.338042
H -0.003759 0.038911 3.693145
H 0.445717 -1.059954 -0.716012

ts133_iso
Erel=123.314 kcal/mol
Mechanism: min7<-->min13
H -0.180125 -0.020488 0.024208
C -0.045045 0.016696 1.108402
H 1.029594 -0.149902 1.296377
C -0.987841 -2.268712 1.079740
H -0.301522 1.000526 1.500014
C -0.663996 -1.097838 1.889691
O -2.235943 -1.836131 1.223164
H -2.069534 -1.074402 2.115455

ts11_bim
Erel=123.316 kcal/mol
Mechanism: H2+C3H2O<-->CH2O+C2H2
H 0.091764 0.048431 -0.004589
C -0.002249 0.013597 1.055470
H 0.630749 -0.087205 3.431703
C -0.096437 -0.048245 2.264217
H -1.200131 -0.780472 4.038055
C -0.818657 0.227957 3.874796

O -1.292647 1.303682 4.095728
H 0.438659 -0.037706 4.450634

ts27_h2
Erel=123.716 kcal/mol
Mechanism: min9--->H2_channel
H -0.039825 -0.054698 0.146611
C 0.009863 0.000184 2.858258
H 0.759089 0.011943 3.636585
C -1.278280 0.125432 2.553329
H -2.279098 0.307351 2.917385
C -0.388224 -0.307691 1.514477
O -0.264990 -1.243885 0.609351
H -0.045013 0.887935 0.555708

ts7_co
Erel=124.121 kcal/mol
Mechanism: min17d--->CO_channel
H -0.500697 -0.901093 0.592312
C 0.343596 0.180500 1.874241
H 0.758955 0.298626 2.864880
C -0.798045 -0.078880 1.270738
H -1.858420 0.008766 1.507250
C 0.397251 0.283681 -1.143912
O 1.381044 -0.051859 -0.644388
H -0.621583 0.224640 -0.243761

ts9_h2o
Erel=124.208 kcal/mol
Mechanism: min12b--->H2O_channel
H 0.026556 -0.055538 0.056436
C -0.046658 0.122078 1.123463
H 0.833268 0.504982 1.629805
C -1.169730 -0.096985 1.786296
H -2.508984 0.118207 1.378186
C -2.152981 -0.538912 2.566739
O -3.332365 0.565300 2.323457
H -2.982780 1.427705 2.599164

ts28_h2
Erel=124.222 kcal/mol
Mechanism: min11a--->H2_channel
H -0.019482 -0.013964 -0.073357
C -0.023958 -0.026973 2.347489
H 0.786579 -0.083373 3.117163
C -0.299592 0.190934 0.943792
H 1.351898 1.039234 3.038633
C -1.037431 0.819795 1.839616
O -2.014724 1.669654 2.074428
H -2.095555 1.801712 3.028192

ts4_triple
Erel=124.282 kcal/mol
Mechanism: min12b--->triple_channel
C -0.015553 -0.000909 -0.088666
C -0.192470 -0.002171 1.206730
O 1.297546 0.004577 2.157435
C 1.195897 0.004994 3.338882

H 0.950159 0.003471 -0.578251
H -0.914245 -0.004642 -0.699162
H -0.761467 -0.003734 2.673551
H -0.422614 -0.001701 3.505072

ts29_h2
Erel=125.683 kcal/mol
Mechanism: min7--->H2_channel
H 0.089839 -0.120623 0.113957
C -0.343176 -0.025457 1.488296
H 0.908069 -0.048352 0.005024
C -0.223882 1.215408 2.027306
H 0.272080 -0.812409 1.929982
C -0.407050 2.379024 2.400034
O -0.172705 3.482017 3.046343
H -0.849485 4.142313 2.839471

ts12_bim
Erel=126.015 kcal/mol
Mechanism: CO+C2H4<-->CO+C2H4
H 0.015846 -0.437310 -0.094392
C 0.136582 0.033362 1.723897
H 0.429948 0.364669 2.730918
C -1.247685 -0.407864 1.703644
H -1.424711 -1.194875 2.462596
C -1.777096 -0.905012 0.312549
O -0.816551 -0.806005 -0.542472
H -1.920011 0.385148 2.085969

ts134_iso
Erel=127.483 kcal/mol
Mechanism: min12a<-->min31e
C -0.052187 0.016140 -0.013404
C -0.082954 0.109760 1.404087
C 1.278152 -0.011488 -0.652753
O 1.438107 1.155505 -1.255335
H -0.293003 -1.012998 0.625142
H -0.964941 0.173271 -0.595326
H 2.338860 1.192646 -1.602518
H 0.953807 -0.080869 1.749059

ts30_h2
Erel=127.914 kcal/mol
Mechanism: min4b--->H2_channel
C -0.046728 -0.000026 0.022862
C 0.052462 0.000032 1.306654
C 1.333544 0.000006 1.825628
O 1.651032 0.000053 3.085210
H 1.478627 -0.000107 -0.392691
H -0.796857 -0.000034 -0.752504
H 2.615917 0.000019 3.165666
H 2.086440 -0.000098 0.305185

ts13_trim
Erel=128.086 kcal/mol
Mechanism: H2+CO+C2H2<-->H2+C3H2O
H -0.297964 -0.000119 0.014801
C 0.048770 0.000046 2.359484

H 0.689083 0.000010 0.165396
C 0.638704 0.000177 3.438537
H 1.161366 0.000292 4.364868
C -1.372199 -0.000165 1.686972
O -1.428433 -0.000235 0.464960
H 0.639685 0.000055 1.161238

ts14_bim
Erel=128.109 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
H -0.088614 -0.051181 -0.004979
C 0.057028 0.054805 1.350022
H 1.415158 -0.051036 1.237248
C -0.238918 -1.321924 1.708429
H 0.915946 0.030106 0.310270
C -0.546069 -2.419871 2.080438
O -0.360065 1.078938 1.854798
H -0.810901 -3.398105 2.401201

ts15_bim
Erel=128.281 kcal/mol
Mechanism: H2+C3H2O<-->H2O+C3H2
H 0.061799 0.340571 0.043517
C 0.031965 -0.012344 1.069114
H 0.964200 -0.350823 1.509200
C -1.095505 -0.012699 1.765788
H -3.004594 2.055604 3.705707
C -2.189358 -0.118405 2.373343
O -3.026586 0.404259 3.227807
H -3.717658 0.963500 2.807474

ts135_iso
Erel=128.303 kcal/mol
Mechanism: min30<-->min30
H -0.385151 -0.156649 0.146247
C 0.031824 -0.010363 1.147807
H 1.110286 0.139975 0.963439
C -0.405706 1.321930 1.610315
H -0.108601 -0.867225 1.807581
C -0.584907 0.323756 3.786957
O -0.710210 1.382352 2.980867
H -0.852228 0.774214 4.768960

ts136_iso
Erel=130.292 kcal/mol
Mechanism: min5a<-->min27
H 0.005684 -0.005997 -0.007940
C 0.008232 0.026696 1.072929
H 1.101966 0.046523 1.562469
C -0.834860 0.132268 2.130295
H 0.230287 -0.804296 3.839851
C -0.137723 -0.977913 2.824518
O 0.942293 -1.293061 1.854536
H -0.809744 -1.846802 2.831935

ts16_bim
Erel=130.72 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O

C 0.066936 0.000011 -0.042928
C -0.162220 -0.000016 1.211328
C 0.175410 -0.000010 2.581277
O -0.697683 -0.000071 3.479959
H -2.343833 -0.000151 2.004324
H -1.750216 -0.000125 2.805878
H -1.512703 -0.000095 1.347415
H 1.224060 0.000047 2.891543

ts10_h2o
Erel=131.385 kcal/mol
Mechanism: min4b--->H2O_channel
H 0.040644 -0.033844 -0.103319
C 0.047914 0.052021 2.238510
H 1.690467 -0.009150 1.420193
C 0.301675 -0.253481 0.924313
H 2.688497 -1.597312 1.289894
C 0.731469 -1.293591 1.828967
O 2.226574 -1.080997 1.970265
H 0.414800 -2.292103 2.094204

ts137_iso
Erel=131.577 kcal/mol
Mechanism: min18a<-->min31c
C 0.046305 -0.076909 0.053618
C -0.113270 -0.044020 1.466369
C 1.408186 0.027264 -0.509362
O 1.819986 -1.129486 -0.974079
H -0.792506 -0.391763 -0.582436
H -0.376913 0.966213 0.555199
H 1.155752 -1.853819 -0.948293
H 0.856348 0.299769 1.877271

ts31_h2
Erel=132.944 kcal/mol
Mechanism: min8--->H2_channel
C 0.006438 0.001577 0.062293
C 0.362290 -0.002249 2.771567
C 0.408357 -0.000472 1.455494
O 1.389498 0.000485 0.480882
H -0.342753 -0.926173 -0.382070
H -0.342051 0.930798 -0.379540
H -1.829192 -0.001511 2.834843
H -1.184771 -0.002331 3.273444

ts32_h2
Erel=135.24 kcal/mol
Mechanism: min10--->H2_channel
H 0.217768 0.066498 -0.108122
C -0.004945 0.042524 4.090673
H 0.521826 0.120795 5.008409
C -0.892442 -0.996512 0.978121
H -1.623579 -0.834061 0.167336
C -0.593036 -0.065224 3.054077
O -1.285159 -0.104815 1.939552
H 0.321032 -0.608226 0.380036

ts138_iso

Erel=135.453 kcal/mol
Mechanism: min17b<-->min30
H 0.269704 0.189349 0.148994
C -0.028564 -0.072024 1.379704
H 2.140147 -0.158581 1.076087
C 1.149465 -0.561617 0.845336
H 1.096760 -1.449350 0.222455
C 0.528854 2.217263 1.675415
O 0.224628 1.054784 2.186264
H 0.643079 2.849882 2.585317

ts11_h2o
Erel=135.593 kcal/mol
Mechanism: min21a--->H2O_channel
H 0.127716 0.224667 0.084186
C -0.153623 -0.216425 1.029588
H 0.760081 -0.006724 1.833178
C -1.222704 -0.067412 2.047817
H -1.369591 0.541530 2.922782
C -1.500782 -0.991667 1.163835
O 1.237330 -1.130759 1.407869
H 0.849486 -1.832654 1.954281

ts33_h2
Erel=135.688 kcal/mol
Mechanism: min21c--->H2_channel
H -0.026382 -0.147327 0.125095
C 0.227961 -0.049396 1.456895
H 0.812896 -0.010494 0.193690
C -0.556868 -1.271795 2.013000
H -0.825235 1.475457 1.845504
C 0.766713 -1.148741 2.152404
O 0.115784 1.291772 1.713443
H 1.691483 -1.481856 2.593935

ts18_ch2o
Erel=136.916 kcal/mol
Mechanism: min12a--->CH2O_channel
H -0.075642 0.004419 -0.050529
C -0.020657 -0.068027 1.033574
H 0.980109 -0.232462 1.451596
C -1.136865 0.053875 1.731977
H -1.121477 -0.026308 2.904411
C 0.182265 0.273583 3.497606
O -0.105975 1.448338 3.919874
H 0.624736 1.807746 4.455616

ts139_iso
Erel=137.077 kcal/mol
Mechanism: min12b<-->min31d
H -0.114300 0.151486 0.252899
C -0.090376 0.013431 2.667076
H 0.397252 0.092602 3.639274
C -0.562520 -1.294202 2.313713
H -1.317570 -1.192523 1.504260
C 1.217002 -0.073750 1.652064
O 0.848921 0.094045 0.423781
H -0.634568 0.941035 2.412680

ts140_iso
Erel=137.19 kcal/mol
Mechanism: min12c<-->min11a
H -0.124069 0.193398 0.088198
C -0.094545 -0.044570 1.180697
H 0.950942 -0.046754 1.508579
C -1.045181 0.897621 1.810885
H -0.586661 1.891773 1.973944
C -0.954911 -1.153893 1.704303
O -1.691020 -1.664048 0.724698
H -2.335046 -2.265601 1.118652

ts141_iso
Erel=137.631 kcal/mol
Mechanism: min12b<-->min31e
H -0.290614 0.220830 0.112359
C -0.094046 0.043493 1.188159
H 0.982612 -0.003317 1.389909
C -0.853813 -0.869690 1.986750
H -1.673778 -1.306757 1.386319
C -0.440961 1.322891 2.132196
O -1.479556 1.938766 1.645833
H -1.886603 1.544506 0.845949

ts34_h2
Erel=138.039 kcal/mol
Mechanism: min22b--->H2_channel
H 0.041190 0.077906 0.122539
C -0.069832 -0.015600 1.451169
H 0.976575 -0.038752 1.727143
C -1.254776 -1.105992 1.628249
H 0.013736 0.903830 0.386312
C -1.300233 0.120298 2.123441
O -1.975719 1.033956 2.843898
H -1.379374 1.753395 3.078079

ts12_h2o
Erel=138.61 kcal/mol
Mechanism: min12c--->H2O_channel
H -0.216234 -0.022284 -0.030652
C 0.141306 0.064658 0.994756
H 1.534156 -0.026608 1.886195
C -0.620015 0.505989 2.007467
H -1.613155 0.941960 2.105195
C -0.038266 -0.457649 2.880505
O 1.650922 -0.035700 2.930367
H 2.059172 -0.877675 3.176556

ts19_ch2o
Erel=138.713 kcal/mol
Mechanism: min21b--->CH2O_channel
C -0.136121 -0.088823 -0.203357
C -0.028868 0.137448 2.442674
C 1.242681 0.073940 2.321945
O -0.295472 -1.270090 -0.724894
H -0.833963 0.072233 3.156274
H 0.946233 0.145377 -0.281104

H -1.227470 -1.530770 -0.664564
H -0.389292 0.307407 1.295195

ts17_bim
Erel=138.823 kcal/mol
Mechanism: H2+C3H2O<-->H2O+C3H2
H -0.105543 -0.192698 0.011357
C -0.032043 -0.127636 1.084745
H 1.888541 -0.552196 3.568001
C -0.307345 0.538181 2.196643
H -0.784686 1.379306 2.671387
C 0.447668 -0.682985 2.308540
O 1.719005 -0.905991 2.676472
H 2.820366 0.423368 2.505322

ts142_iso
Erel=139.88 kcal/mol
Mechanism: min17b<-->min32a
H -0.093618 0.101656 0.142577
C -0.015489 0.057630 1.316450
H 1.848610 -0.413376 0.683699
C 1.215486 0.476672 0.835675
H -0.776977 0.724788 1.712686
C 0.064822 -2.302798 1.144467
O -0.331531 -1.290193 1.854036
H -0.246453 -3.168590 1.773506

ts13_h2o
Erel=139.896 kcal/mol
Mechanism: min21c--->H2O_channel
C 0.080710 0.033159 0.063313
C -0.189808 -0.044318 1.949557
C 0.903353 0.078127 1.242690
O 0.242137 -1.701807 -0.802612
H -0.987425 0.210227 0.064281
H 0.513574 -0.439755 -0.956531
H 1.979082 0.114717 1.286122
H -0.623066 -1.811409 -1.223381

ts8_co
Erel=140.771 kcal/mol
Mechanism: min21a--->CO_channel
H 0.039529 0.137835 0.595700
C 0.647252 -0.132199 1.449074
H 3.816777 0.535696 2.566547
C 0.716611 0.310229 2.662139
H 1.461669 -0.954235 1.224661
C 2.819170 -1.023472 2.085679
O 3.761250 -0.158954 1.884504
H 2.260010 -0.842865 3.051973

ts9_co
Erel=140.915 kcal/mol
Mechanism: min31d--->CO_channel
H -0.333346 -0.388517 0.183914
C 0.041238 0.384374 1.997030
H 0.533141 0.015018 1.028299
C -1.294231 0.133363 2.134265

H -1.692298 -0.870272 1.948532
C -2.145933 0.253911 0.259445
O -1.248098 -0.206759 -0.421530
H -1.868299 0.666347 2.887290

ts143_iso
Erel=141.97 kcal/mol
Mechanism: min6<-->min32a
C 0.015358 0.001939 0.041852
C -0.215080 -0.045834 1.480581
C 2.170913 0.070814 0.629675
O 1.419949 -0.334576 -0.337726
H -0.685620 -0.722573 -0.410965
H -0.154777 0.967778 -0.434260
H 0.428888 -0.833658 1.897992
H 3.213302 -0.179561 0.332032

ts14_h2o
Erel=142.35 kcal/mol
Mechanism: min12e--->H2O_channel
H -0.256525 -0.138537 -0.011619
C 0.175484 -0.066914 0.986372
H 1.603271 0.240669 1.765381
C -0.522993 -0.369229 2.096129
H -1.500545 -0.807882 2.297521
C 0.030020 0.736583 2.802955
O 1.801951 0.489772 2.762389
H 1.981652 -0.321419 3.262697

ts144_iso
Erel=142.41 kcal/mol
Mechanism: min6<-->min32b
C 0.064539 0.013554 0.097992
C -0.076702 -0.002575 1.541282
C 2.305858 0.023712 0.423782
O 1.379559 -0.517779 -0.299299
H -0.718301 -0.665425 -0.290768
H -0.032153 0.961809 -0.438155
H -0.978636 0.606536 1.759608
H 3.243356 -0.476704 0.088304

ts145_iso
Erel=142.851 kcal/mol
Mechanism: min1b<-->min28
H 0.306664 -0.535185 0.129524
C 0.043048 -0.157953 1.130836
H 2.085165 0.566071 -0.259805
C 1.170553 0.543001 1.767576
H 1.102353 1.277846 2.562415
C 2.237098 0.367917 0.796341
O 1.368448 -0.840046 2.055607
H 3.182095 -0.072903 1.096506

ts15_h2o
Erel=144.34 kcal/mol
Mechanism: min22a--->H2O_channel
H -0.065484 -0.128967 -0.010403
C 0.024997 0.018881 1.062670

H 1.573691 -0.092396 1.613110
C -0.656335 -2.009279 2.166881
H -0.567548 0.837771 1.460375
C 0.262230 -1.132121 1.900759
O 1.728274 -0.997264 2.331624
H 2.283231 -1.717443 1.976824

ts18_trim
Erel=144.665 kcal/mol
Mechanism: H2+CO+C2H2<-->H2+CO+C2H2
H 0.269987 -0.021840 0.097514
C 0.229279 0.413521 1.113330
H 1.239323 -0.384354 2.724624
C 0.374698 -0.620504 2.085229
H -0.502565 -0.605664 2.750291
C 0.687538 -3.039684 2.436280
O 0.550704 -2.061301 1.608758
H 0.648412 -2.608132 3.482749

ts35_h2
Erel=144.736 kcal/mol
Mechanism: min12a--->H2_channel
H -0.038524 -0.000452 0.087759
C 0.032796 0.000737 1.952104
H 2.112493 0.000515 2.813034
C 0.351532 0.002051 4.152739
H 1.788869 0.002117 5.083293
C 1.038651 0.001039 2.996788
O 0.643203 -0.000263 0.771039
H 0.985334 0.002579 5.327587

ts146_iso
Erel=144.773 kcal/mol
Mechanism: min9<-->min9
H 0.011274 0.041516 0.064085
C 0.108181 -0.021059 1.983063
H 0.921357 -0.089848 2.693883
C -1.043035 -0.803958 1.719246
H -1.546106 -1.124060 2.645826
C -0.847080 1.110030 1.985979
O 0.507515 0.595858 0.702345
H -1.830469 0.810945 1.537215

ts10_co
Erel=144.884 kcal/mol
Mechanism: min32c--->CO_channel
C 0.284088 -0.168931 0.315157
C -0.315005 -0.490085 1.579432
C 2.714073 -0.021944 0.473698
O 1.661289 -0.685955 0.127198
H -0.275820 -0.484280 -0.576251
H 0.330548 0.942191 0.310115
H -1.345601 -0.089511 1.515992
H 2.362524 0.974865 0.880387

ts36_h2
Erel=144.986 kcal/mol
Mechanism: min12d--->H2_channel

H -0.006742 0.020629 -0.028077
C -0.210202 0.018934 1.977379
H 1.214492 0.016951 3.127415
C 0.570359 0.017378 0.896298
H 0.388428 -0.048107 3.205838
C 2.041556 -0.085883 0.691857
O 2.655383 0.084190 1.849663
H 3.604109 -0.024856 1.710407

ts11_co
Erel=145.028 kcal/mol
Mechanism: min17d--->CO_channel
H 0.142479 -0.094729 0.066258
C -0.254393 0.117104 1.510332
H 1.872341 0.006769 0.750076
C 0.883312 0.468084 0.805360
H -0.008503 2.511743 1.773773
C 0.530284 2.881869 0.863420
O 1.040063 1.835662 0.277117
H -0.142950 -0.936109 1.809412

ts37_h2
Erel=147.641 kcal/mol
Mechanism: min12d--->H2_channel
C 0.165235 -0.190501 -0.005848
C -0.016371 -0.086954 1.310507
C 1.200115 -0.170195 2.154849
O 2.055746 -1.044961 1.660053
H -1.437756 0.260687 -0.431404
H -0.902738 0.230149 1.844783
H -0.751509 0.098902 -0.902503
H 2.848891 -1.014422 2.210238

ts38_h2
Erel=148.935 kcal/mol
Mechanism: min12e--->H2_channel
C 0.196514 0.091660 -0.064313
C 0.066014 -0.042104 1.247004
C 1.350101 0.186939 1.983478
O 2.406272 -0.324334 1.412159
H -1.535308 0.022710 -0.471740
H -0.862806 0.186384 -0.922856
H -0.817004 -0.114058 1.868109
H 2.213572 -0.815915 0.583780

ts39_h2
Erel=149.663 kcal/mol
Mechanism: min5a--->H2_channel
C -0.048647 0.043767 0.019398
C 0.173290 0.059756 2.686987
C -0.051437 -0.044773 1.456269
O -0.535549 1.149978 -0.585277
H 1.297953 0.021811 -0.355708
H -0.266624 -0.855930 -0.556598
H 1.207573 -0.060519 0.612050
H -0.642286 1.828767 0.098157

ts147_iso

Erel=149.834 kcal/mol
Mechanism: min31c<-->min31a
C -0.020068 -0.340081 0.228542
C 0.207523 0.174272 2.546927
C 0.964173 -0.064755 1.271039
O 0.463044 -0.875882 3.385960
H -0.970775 0.140190 0.560599
H 1.896951 -0.637275 1.247676
H -0.073353 -1.666029 3.251759
H 1.119446 0.941816 0.783928

ts40_h2
Erel=150.891 kcal/mol
Mechanism: min22b--->H2_channel
H -0.079011 0.151758 -0.053684
C 0.047431 0.107705 1.025210
H 1.401277 -0.171510 1.550162
C -0.315464 -2.351066 1.909694
H 0.008065 1.069534 1.527179
C -0.407394 -1.020474 1.703763
O 0.281214 -1.324509 2.908186
H 1.459848 -0.722522 2.379772

ts41_h2
Erel=151.26 kcal/mol
Mechanism: min19f--->H2_channel
C 0.067450 0.000430 0.008330
C -0.032383 0.000159 1.397476
C 1.189799 -0.001400 2.029267
O 0.937806 -0.000304 -0.890422
H -0.360512 0.001287 -1.346854
H -1.114260 0.001943 -0.649942
H -1.007515 0.001129 1.874220
H 2.038673 -0.002164 1.327490

ts42_h2
Erel=151.27 kcal/mol
Mechanism: min4a--->H2_channel
C 0.010662 -0.024963 -0.086304
C -0.040956 -0.058822 1.223212
C 1.390818 0.086324 -0.009302
O 1.995322 1.311316 -0.131728
H -0.892935 0.532318 -0.932308
H -0.892486 -0.338933 -1.073607
H 2.887996 1.256395 0.226166
H 2.047161 -0.778198 -0.053632

ts19_bim
Erel=152.116 kcal/mol
Mechanism: CO+C2H4<-->H2+C3H2O
C -0.070002 0.000409 -0.082059
C 0.041154 0.000487 2.492320
C 0.533534 -0.001018 1.094811
O -1.262515 0.004001 2.462810
H 0.492369 -0.001253 -1.012626
H 1.786027 -0.443704 1.196871
H -1.593496 0.004773 1.526488
H 1.788368 0.434979 1.196749

ts148_iso
Erel=152.207 kcal/mol
Mechanism: min8<-->min27
C 0.184651 0.465820 0.300675
C -0.072988 0.103660 1.532623
C 1.508914 -0.018457 1.260524
O 1.440293 0.460485 -0.200033
H -0.834970 0.524542 -0.803212
H -0.732936 1.294408 -0.555537
H 2.098160 0.700358 1.821428
H 1.867083 -1.043266 1.260521

ts43_h2
Erel=152.923 kcal/mol
Mechanism: min31b--->H2_channel
H -0.042390 -0.000012 0.081694
C -0.099891 -0.000018 4.496629
H 0.993643 0.000020 4.614181
C -0.369581 -0.000026 3.167398
H -1.579424 0.448153 2.957976
C 0.324496 -0.000001 1.916735
O -0.538679 -0.000030 0.908659
H -1.579393 -0.448288 2.957976

ts20_bim
Erel=154.969 kcal/mol
Mechanism: H2+C3H2O<-->CH2O+C2H2
H 0.171844 0.001243 0.089379
C -0.261073 -0.000427 3.274364
H 0.293319 0.000884 4.182742
C -0.449324 -0.000926 2.063525
H 0.530659 0.000909 0.883895
C -1.455249 -0.001265 -0.077480
O -1.611544 -0.003337 1.170604
H -2.463000 -0.003791 -0.522136

ts44_h2
Erel=155.546 kcal/mol
Mechanism: min14--->H2_channel
C 0.007855 0.032965 0.034700
C -0.022035 0.193537 1.533448
C 1.246473 0.032954 0.734685
O 0.889197 1.188907 -0.078955
H -0.435563 -0.489756 -0.794275
H -0.431328 -0.805412 2.257674
H -0.231640 -1.580865 1.904316
H 2.185368 -0.489778 0.686902

ts45_h2
Erel=156.486 kcal/mol
Mechanism: min21d--->H2_channel
C -0.223145 0.267303 0.011887
C 0.046989 -0.015512 1.262502
C 1.279924 0.177856 2.015659
O 2.381627 0.129748 1.259666
H -0.855940 -0.296957 1.817176
H 1.284311 -0.435942 3.086448

H 3.125836 0.459978 1.778851
H 1.158716 -1.406949 2.965599

ts21_bim
Erel=156.894 kcal/mol
Mechanism: H2+C3H2O<-->H2O+C3H2
C -0.247602 0.351978 0.041257
C 0.206252 -0.752762 0.515626
C 1.059263 -0.171073 -0.617110
O 0.878531 -0.599940 -1.886811
H -0.898077 1.182481 -0.162396
H 2.069641 0.157144 -0.386702
H 1.231610 -2.265105 -2.170517
H 1.706441 -0.982341 -2.310397

ts22_bim
Erel=157.012 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
H -0.066138 0.021940 0.161631
C 0.085930 -0.063397 2.649287
H 0.967933 -0.057311 0.319595
C 0.563278 0.222078 3.862016
H 1.371561 0.300842 4.575530
C -0.822817 0.401701 3.642207
O 0.258585 -0.474346 1.430274
H 0.582044 0.208711 -0.522963

ts46_h2
Erel=157.784 kcal/mol
Mechanism: min21c--->H2_channel
C 0.099745 -0.074717 -0.092579
C 0.052927 0.010892 1.371758
C 1.031854 0.142787 2.230154
O 0.998429 0.665876 -0.726446
H -1.055020 -0.043810 -0.597749
H -1.550471 0.725217 -0.347224
H -0.898619 -0.214889 1.867921
H 1.359619 1.377603 -0.174184

ts149_iso
Erel=158.407 kcal/mol
Mechanism: min23a<-->min31b
H 0.207260 0.124873 -0.102224
C -0.100709 0.252147 0.955539
H 2.077972 -0.178269 1.329018
C 1.144356 0.272437 1.716352
H 1.217461 1.388306 1.584378
C 1.043407 0.056844 3.207183
O 1.984814 -0.693166 3.707896
H 1.143847 -0.280477 4.415691

ts47_h2
Erel=159.214 kcal/mol
Mechanism: min31d--->H2_channel
H 0.057895 -0.047118 -0.018159
C -0.083781 0.069100 1.061938
H 0.758828 -0.085012 3.092647
C 0.744579 -0.620808 1.828715

H 0.218913 -0.734613 3.091743
C 1.870220 -1.556223 1.927358
O 2.285280 -1.900169 0.733446
H 1.778738 -1.478792 0.001413

ts16_h2o
Erel=162.449 kcal/mol
Mechanism: min19d--->H2O_channel
H 0.323385 -0.287156 -0.085637
C -0.019408 0.034100 2.850839
H 0.296739 -0.036177 3.895408
C 0.943973 0.458403 2.021125
H 1.431144 0.626806 0.889944
C -1.176429 -0.655859 2.394507
O 0.412747 0.624456 0.228119
H -1.501108 -0.198546 1.443253

ts150_iso
Erel=165.582 kcal/mol
Mechanism: min16b<-->min16b
H 0.080901 0.058607 0.056819
C -0.061614 0.366448 1.093439
H 0.564131 -0.126243 2.022805
C -1.287174 -0.010683 1.695632
H 1.032596 -0.121685 1.293893
C -1.850700 -0.463269 2.894429
O -2.432822 -0.067510 1.148671
H -2.285657 0.365350 3.464164

ts23_bim
Erel=165.963 kcal/mol
Mechanism: H2O+C3H2<-->H2+C3H2O
C -0.191229 -0.025739 -0.017158
C 0.123083 -0.007812 2.576577
C -0.051358 -0.024266 1.326258
O -1.639281 0.034500 -0.594853
H -1.734551 0.824061 -1.148897
H 0.470034 0.535807 -0.673874
H -0.042320 -1.248842 -0.580237
H -0.914198 -1.016745 -0.972733

ts24_bim
Erel=167.143 kcal/mol
Mechanism: H2+C3H2O<-->HOCH+C2H2
H 0.165868 -0.000729 -0.053039
C -0.036047 -0.000922 1.411053
H 0.709985 -0.000172 3.561420
C 0.346292 -0.000596 2.561111
H 0.089599 -0.001242 -0.909572
C -3.035076 -0.008232 0.619017
O -1.954403 -0.004819 0.201754
H -3.984217 -0.010810 0.054790

ts25_bim
Erel=172.367 kcal/mol
Mechanism: H2+C3H2O<-->H2+C3H2O
H -0.107255 -0.005997 0.131141
C 0.030590 -0.019468 3.684309

H 0.653641 -0.020313 4.545572
C -0.646516 -0.028301 2.671991
H 0.671172 -0.600785 0.042240
C -1.758984 0.054413 1.767363
O -1.545253 -0.145436 0.505266
H -0.258741 -0.853615 0.239636

ts48_h2
Erel=173.188 kcal/mol
Mechanism: min17b--->H2_channel
H 0.271616 -0.240363 0.067365
C -0.019195 0.056206 1.061887
H 2.076603 0.070783 1.913308
C 0.692790 0.284184 2.182100
H 2.310531 -0.154762 1.162073
C -1.702719 0.587298 2.401028
O -1.418070 0.231174 1.181959
H -2.807437 0.704069 2.416537

ts5_triple
Erel=176.136 kcal/mol
Mechanism: min12f--->H2+HCO+CCH triple_channel
C 0.063947 0.079685 -0.219073
C -0.096457 0.581634 2.803871
C 0.888114 0.099194 2.080032
O 0.848614 0.570779 0.664919
H -0.589152 -0.694380 0.246041
H -0.066450 0.155010 4.238547
H 0.488763 -0.348392 4.511767
H 1.760838 -0.506799 2.253824

ts20_ch2o
Erel=181.259 kcal/mol
Mechanism: min10--->CH2O_channel
C 0.174891 0.033141 -0.051120
C -0.201754 0.138628 2.919726
C 1.006813 0.526442 2.885402
O 0.225041 -0.696868 1.096849
H 1.074304 0.565660 -0.352302
H -0.794163 0.403580 -0.378925
H -1.214680 -0.143100 3.111766
H 0.595988 -1.280356 0.218952

ts6_triple
Erel=182.276 kcal/mol
Mechanism: min10--->H2+HCO+CCH triple_channel
C -0.008486 0.238748 -0.071093
C 0.286199 0.057812 3.501062
C 0.603207 0.059345 2.224127
O -0.102523 0.672944 1.182778
H 0.798339 -0.510332 -0.188451
H -1.128266 -0.474101 -0.446786
H -1.084254 -1.262183 -0.125426
H 1.534360 -0.462313 1.986945

Tables 1-7S display graphically the 12 (or a lower number) lowest energy transition states of each type.

Table 1S. Lowest energy bim/trim TSs

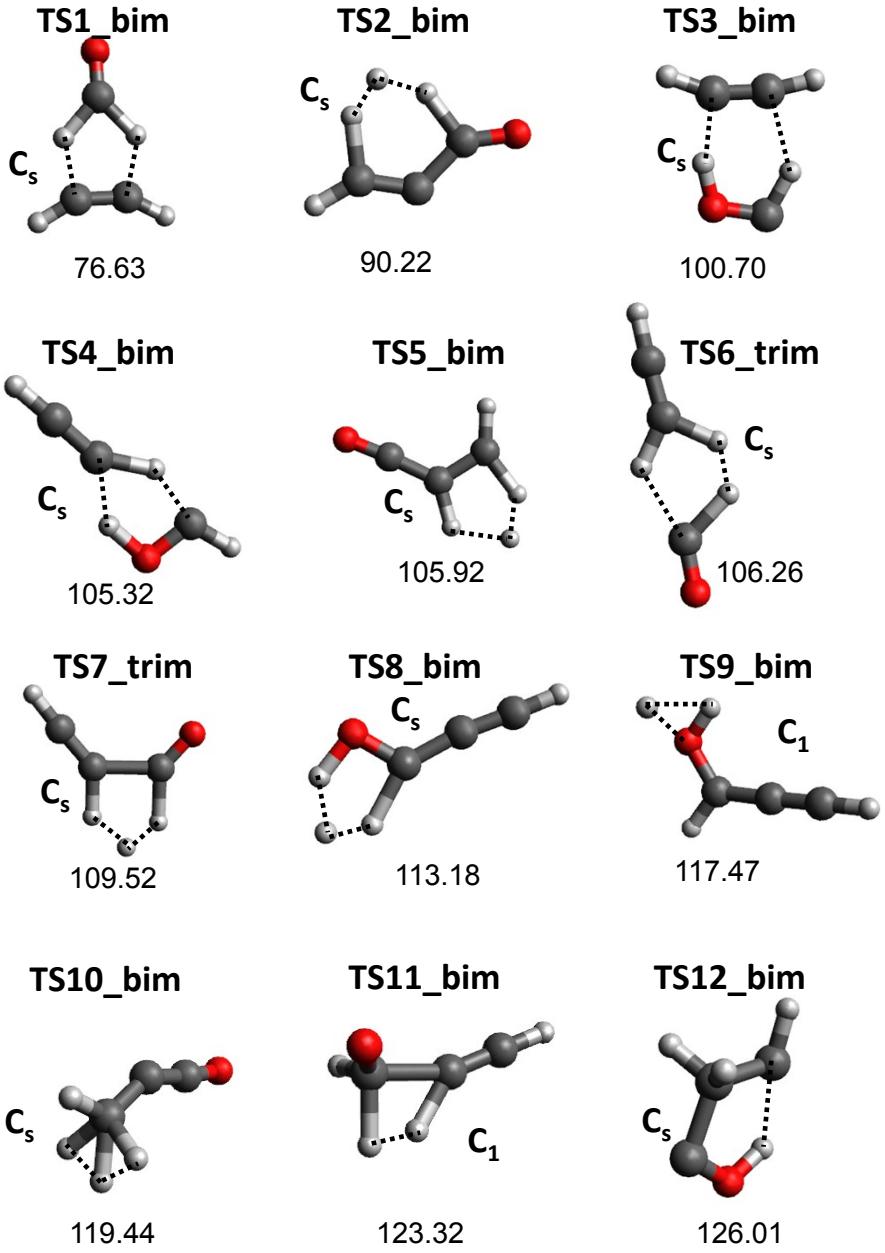


Table 2S. Lowest energy CO TSs

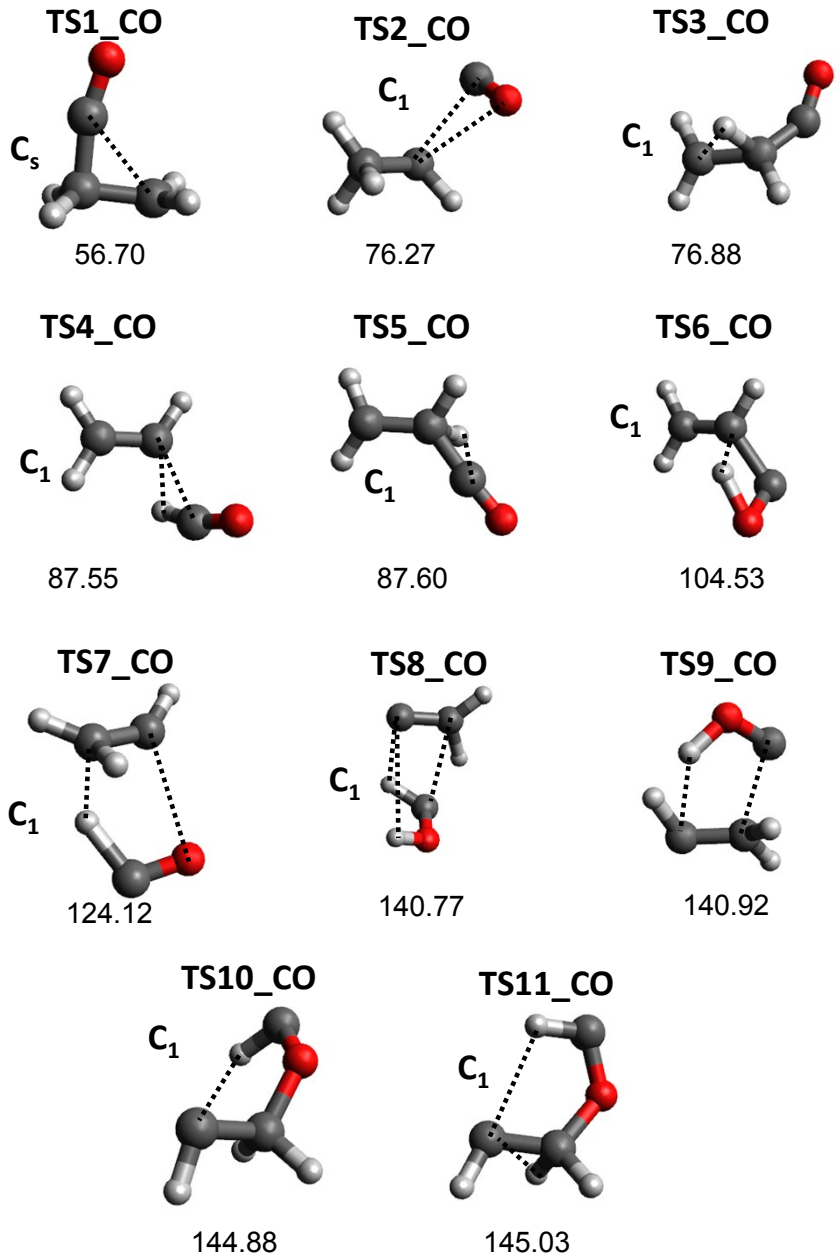


Table 3S. Lowest energy CH_2O TSs

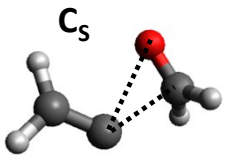
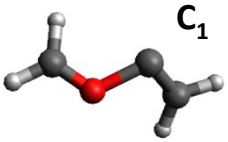
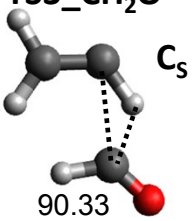
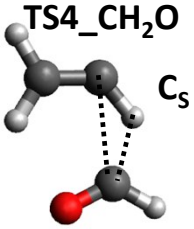
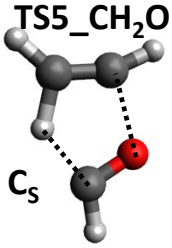
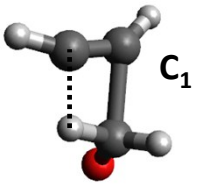
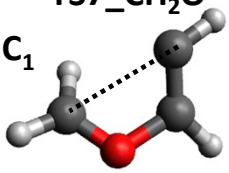
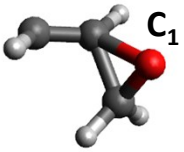
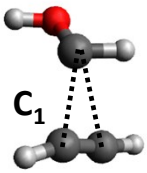
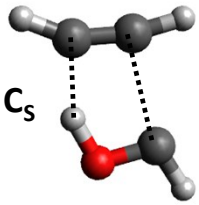
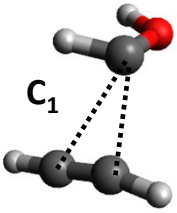
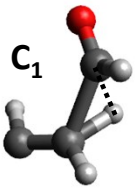
TS1_CH_2O  87.89	TS2_CH_2O  87.96	TS3_CH_2O  90.33
TS4_CH_2O  91.29	TS5_CH_2O  92.63	TS6_CH_2O  97.01
TS7_CH_2O  97.08	TS8_CH_2O  98.47	TS9_CH_2O  99.16
TS10_CH_2O  99.90	TS11_CH_2O  102.08	TS12_CH_2O  107.48

Table 4S. Lowest energy H_2 TSs

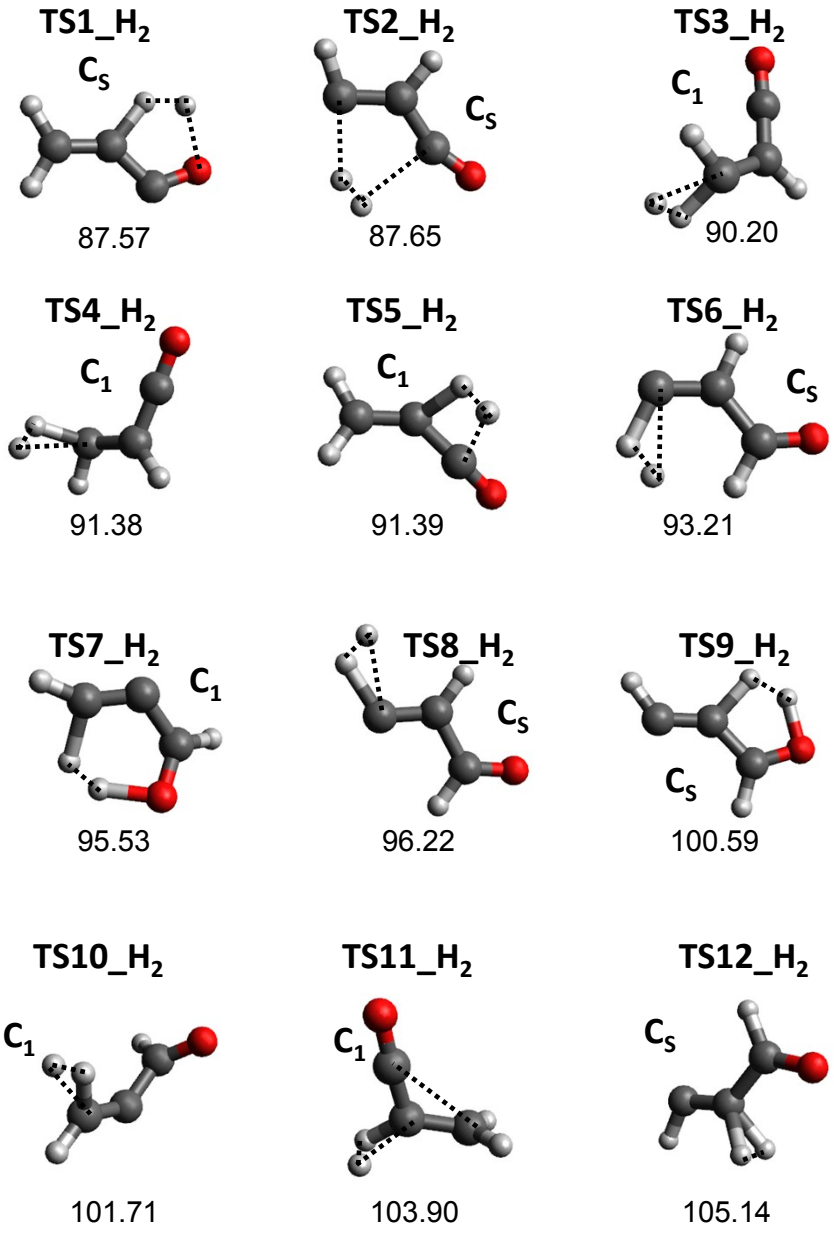


Table 5S. Lowest energy H_2O TSs

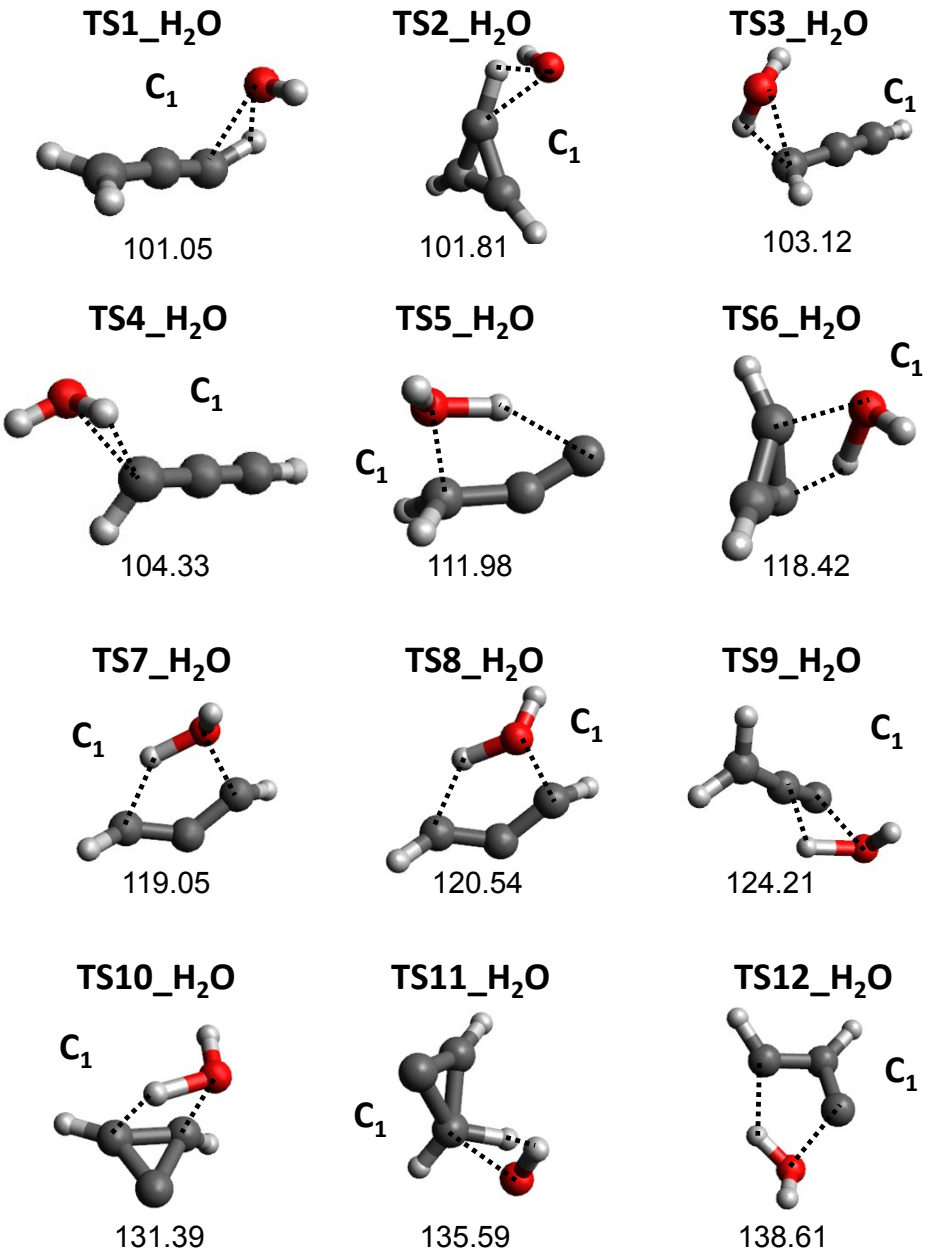


Table 6S. Lowest energy iso TSs

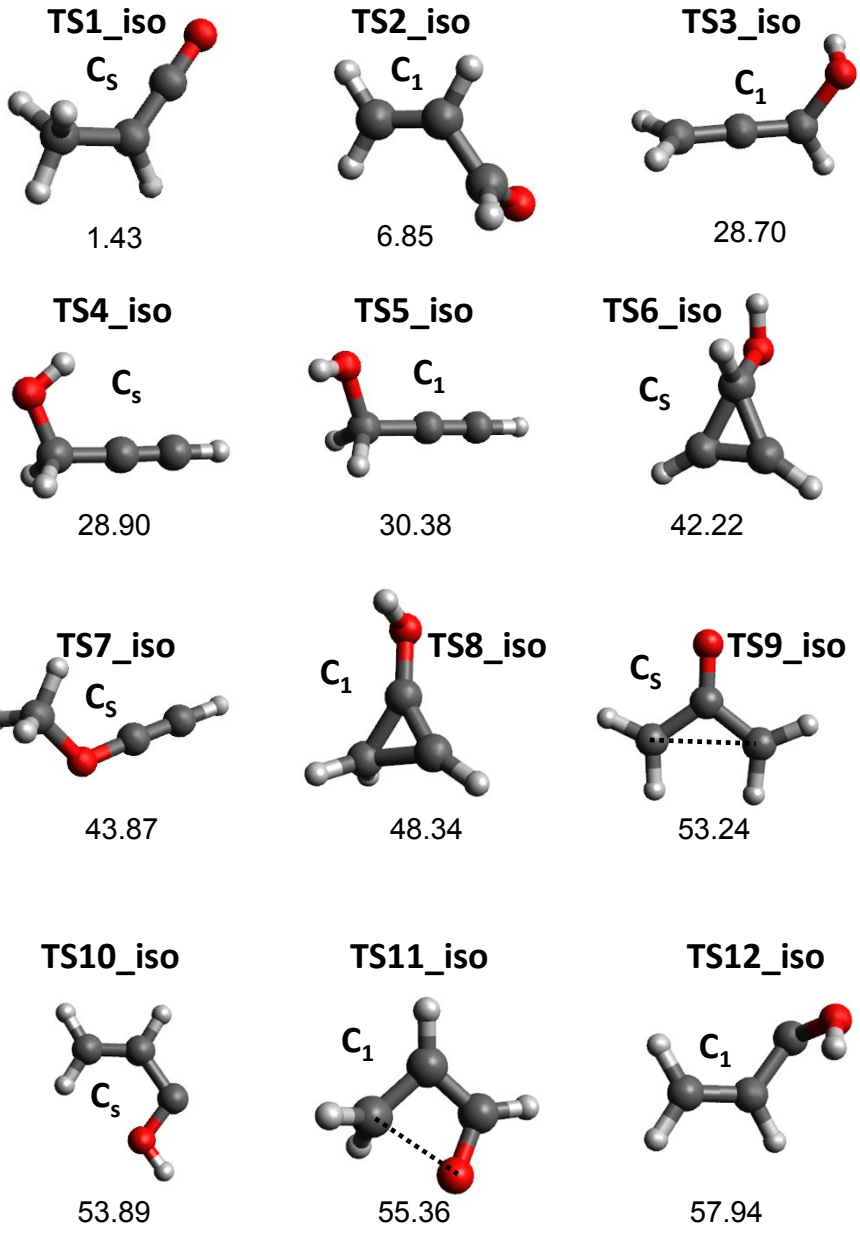
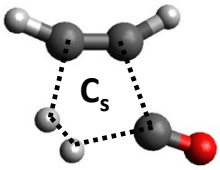
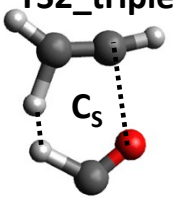
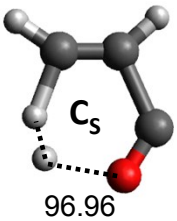
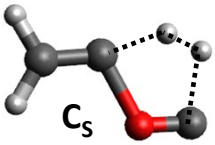
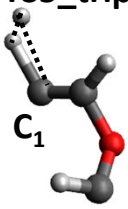
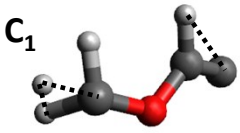


Table 7S. Lowest energy triple TSs

TS1_triple	TS2_triple	TS3_triple
		
84.16	96.36	96.96
TS4_triple	**TS5_triple**	**TS6_triple**
		
124.28	176.14	182.28

Kinetic calculations

The kinetic calculations consist of RRKM and KMC calculations. The RRKM rate coefficients for a given process *i* are computed according to the following expression:

$$k_i(E) = \sigma_i \frac{W_i^{TS}(E)}{h\rho_i(E)}$$

Where σ_i is the reaction path degeneracy, $W_i^{TS}(E)$ is the sum of states at the TS, $\rho_i(E)$ is the density of states at the reactant, and E is the excitation (vibrational) energy of the system. Two different excitation energies are employed: 148 and 182 kcal/mol. The reaction path degeneracy is calculated as $\sigma_i = \frac{m_i^{TS}}{m_i}$, where m_i and m_i^{TS} are the number of optical isomers of the reactant and transition states, respectively.[3] The sums and densities of states were evaluated by direct count of the harmonic vibrational states using the Beyer-Swinehart algorithm.

Isomerizations between different conformers are not taken into account. This means that the different conformers of a given minimum form a microcanonical ensemble and are in equilibrium. Thus, the total sum of states of minimum MINx $\rho_{MINx}(E)$ can be expressed as:[4]

$$\rho_{MINx}(E) = \sum_{j=a}^{N} \rho_{MINxj}(E)$$

Where N is the number of conformational isomers of MINx and $\rho_{MINxj}(E)$ is the density of states of conformer j.

To simplify even more the calculation, all conformers of a given minimum are considered degenerate, and their vibrational frequencies equal to those of the most stable one (denoted as above with the letter a). These two approximations are quite

reasonable taken into account the small energy differences of the conformational isomers (see above) and their similar vibrational frequencies.

With this approach, the density of states of a given minimum can be simply computed as $\rho_{MINx}(E) = N\rho_{MINxa}(E)$.

Transition energies with energies greater than 150 kcal/mol are not considered. The frequencies, calculated at the B3LYP/6-311G(d,p) level of theory, of the 32 minima and 192 transition states considered in the KMC simulations are listed below.

The total number of chemical processes is 297 including 210 isomerizations, 37 H_2 eliminations, 19 CH_2O eliminations, 15 H_2O eliminations, 12 CO eliminations, and 4 three-body dissociations. We also included the barrierless process MIN2→ CO + CH_3CH, using the variational RRKM rate coefficients computed by Lee and co-workers.[5]

Frequencies (in cm^{-1}) of the minima considered in the KMC simulations

```
min1
173 319 572 613 919 997 1029 1041 1166 1295 1389 1453 1680 1785
2865 3130 3170 3222
min2
144 213 520 563 655 901 1057 1082 1156 1413 1420 1486 1513 2220
3022 3070 3106 3176
min3
320 509 640 709 722 950 1015 1054 1063 1106 1163 1417 1435 1940
3104 3105 3182 3195
min4
216 267 432 627 636 903 926 990 1036 1199 1287 1419 1502 2056 3086
3151 3180 3810
min5
201 283 357 557 658 702 913 993 1053 1220 1361 1420 1493 2219 2984
3075 3475 3825
min6
439 686 882 888 924 953 1009 1044 1115 1169 1237 1315 1487 1622
3062 3120 3216 3280
min7
49 211 227 401 434 759 1055 1060 1229 1305 1423 1482 1487 2414 3019
3071 3076 3782
min8
378 395 721 729 813 896 1008 1038 1097 1127 1199 1436 1503 1872
3101 3160 3193 3253
min9
```

328 442 448 658 820 904 904 976 1059 1064 1228 1277 1426 1681 3122
3215 3258 3808
min10
160 220 459 546 585 653 900 1137 1166 1227 1472 1486 1498 2272 3036
3110 3157 3494
min11
305 411 421 685 698 956 1002 1031 1060 1104 1190 1344 1523 1907
3003 3059 3307 3822
min12
139 328 560 606 833 930 1021 1030 1098 1253 1305 1368 1429 1664
3081 3135 3227 3787
min13
153 365 412 764 812 962 1015 1116 1178 1337 1416 1472 1488 1512
3026 3084 3106 3158
min14
486 671 675 781 919 948 995 1069 1069 1105 1133 1254 1378 1495 3075
3169 3251 3271
min15
242 711 821 917 928 935 993 1147 1173 1212 1233 1334 1436 1509 3061
3065 3107 3130
min16
30 297 394 414 687 788 846 1010 1053 1388 1403 1466 1496 1630 3038
3103 3130 3137
min17
153 350 574 643 811 864 925 998 1123 1289 1324 1408 1441 1712 2859
3162 3197 3259
min18
158 180 291 372 756 925 983 1062 1278 1328 1404 1461 1501 1569 2942
2970 3016 3087
min19
154 327 575 590 747 911 1036 1038 1166 1244 1303 1347 1406 1587
2934 2975 3208 3746
min20
297 506 687 816 950 967 1001 1059 1087 1191 1194 1266 1347 1400
3063 3110 3146 3149
min21
124 177 354 416 713 858 914 1041 1088 1217 1378 1405 1504 1726 3033
3102 3145 3820
min22
224 261 363 387 496 844 994 1031 1135 1332 1386 1461 1466 1724 3023
3099 3101 3805
min23
125 340 410 542 666 796 942 1073 1118 1186 1298 1335 1402 1826 2795
2914 2952 3008
min24
149 359 457 607 761 783 866 870 996 1231 1383 1443 1516 1666 3060
3129 3210 3281
min25
155 186 264 459 683 920 977 1170 1213 1226 1473 1486 1501 1743 2990
3014 3076 3151
min26
274 378 411 560 660 784 831 879 955 1025 1105 1215 1424 1786 3029
3164 3256 3789
min27
173 339 814 834 880 913 1013 1052 1089 1157 1229 1297 1374 1417
2977 2994 3018 3022
min28

253 458 633 714 836 937 1042 1057 1136 1151 1224 1294 1352 1515
2995 3074 3159 3167
min29
411 600 764 786 926 1068 1089 1094 1107 1174 1219 1254 1501 1530
3016 3016 3151 3151
min30
71 200 293 528 689 863 981 1075 1100 1267 1371 1451 1469 1532 2888
2997 3076 3083
min31
111 380 413 506 715 782 942 944 1063 1184 1252 1300 1343 1368 2810
2898 3028 3766
min32
163 198 331 545 585 732 852 1009 1155 1175 1234 1327 1384 1411 2842
3000 3030 3066

Frequencies (in cm^{-1}) of the transition states considered in the KMC simulations

ts11_iso
469 627 826 848 973 1014 1045 1100 1172 1258 1384 1484 1534 3070 3118 3170 3239
ts1_co
301 324 453 468 819 839 1089 1149 1249 1266 1402 1460 2035 3017 3071 3160 3262
ts14_iso
350 395 645 658 793 899 979 984 1044 1350 1442 1478 1566 3118 3151 3245 3253
ts16_iso
190 213 283 695 879 929 1048 1065 1123 1407 1454 1480 1986 3009 3057 3096 3304
ts17_iso
149 299 348 716 831 945 1067 1230 1309 1379 1406 1503 1680 2693 2934 3000 3095
ts20_iso
151 401 502 657 771 785 888 1032 1226 1357 1452 1464 1668 3013 3041 3091 3126
ts21_iso
436 492 554 680 807 824 989 1084 1224 1269 1360 1474 1511 3074 3119 3228 3780
ts14_iso
184 329 379 789 931 1001 1064 1112 1305 1387 1467 1541 1729 2180 2829 3005 3115
ts23_iso
310 455 668 758 853 918 996 1062 1172 1286 1365 1495 1605 3067 3133 3266 3805
ts15_iso
162 327 381 736 957 999 1058 1114 1306 1398 1468 1537 1722 2192 2821 3005 3113
ts21_iso
70 313 572 752 969 1002 1038 1154 1173 1269 1459 1507 1654 2025 3055 3110 3157
ts9_iso
327 475 643 682 815 982 1023 1076 1188 1320 1386 1539 1628 1936 3039 3151 3200
ts29_iso
434 543 585 654 853 869 997 1109 1208 1266 1350 1486 1525 3008 3047 3273 3778
ts32_iso
307 440 631 762 848 916 999 1036 1181 1306 1369 1499 1598 3067 3089 3270 3588
ts35_iso
401 579 677 849 952 986 989 1021 1142 1206 1333 1369 1473 3070 3089 3161 3245
ts2_co
78 198 236 279 659 762 940 1099 1252 1327 1384 1504 2066 2901 2966 3010 3090
ts4_iso
149 343 537 574 720 787 808 1080 1143 1277 1389 1456 1956 2455 3130 3166 3248
ts36_iso
144 345 534 737 942 1030 1095 1137 1172 1258 1351 1423 1815 2276 2927 2993 3027
ts6_iso

371 479 635 680 928 952 983 1064 1234 1288 1375 1522 1549 3035 3074
3114 3660
ts33_iso
156 296 524 555 690 931 1017 1021 1162 1281 1373 1433 1669 2643
3095 3141 3231
ts1_iso
115 292 526 768 842 1003 1084 1129 1264 1351 1401 1410 1814 2278
2886 2980 3061
ts43_iso
247 342 602 640 668 797 931 977 1098 1210 1367 1461 1866 2143 3148
3236 3832
ts46_iso
315 380 495 715 770 962 1061 1126 1208 1259 1334 1396 1612 2146
3122 3279 3812
ts5_iso
140 323 467 785 918 1008 1070 1148 1178 1266 1402 1415 1824 2288
2878 2954 2995
ts9_iso
279 439 524 774 841 919 1055 1133 1195 1244 1365 1490 1800 2971
2997 3008 3062
ts50_iso
348 474 526 714 831 921 999 1079 1254 1288 1325 1456 1542 3075 3081
3116 3814
ts51_iso
132 348 559 792 884 963 1049 1100 1198 1300 1387 1494 1820 2927
2938 2986 3065
ts3_iso
119 297 497 627 701 947 1015 1023 1066 1311 1360 1424 1649 2650
3134 3178 3226
ts53_iso
371 377 484 714 778 979 1076 1088 1189 1233 1323 1391 1620 2134
3059 3294 3806
ts54_iso
469 554 625 774 881 960 1005 1109 1189 1254 1340 1497 1528 1683
3117 3182 3229
ts55_iso
242 369 487 524 597 873 938 1115 1197 1296 1400 1494 1849 3045 3107
3386 3796
ts3_iso
239 341 602 626 674 802 920 975 1104 1264 1327 1457 1857 2154 3147
3236 3629
ts19_iso
352 470 619 766 940 988 1058 1086 1142 1292 1435 1511 1537 1642
3026 3114 3151
ts13_iso
51 180 481 496 592 702 728 732 816 912 999 1032 1830 2080 2893 3343
3418
ts59_iso
212 447 450 671 765 929 1010 1085 1113 1206 1356 1478 1798 2189
3042 3128 3850
ts60_iso
141 255 387 405 623 924 971 1007 1264 1317 1452 1490 2010 3034 3132
3185 3756
ts61_iso
253 416 566 709 743 757 979 1033 1214 1266 1325 1474 1785 3093 3105
3176 3564
ts62_iso

223 244 408 537 577 850 940 1107 1176 1322 1383 1495 1836 2985 3173
3376 3831
ts63_iso
259 663 714 813 905 914 967 1125 1219 1253 1365 1445 1687 2965 2976
2996 3038
ts39_iso
175 468 501 638 875 952 1089 1152 1244 1276 1374 1529 1812 2927
2961 2984 3115
ts65_iso
374 522 829 884 931 955 1001 1081 1148 1239 1367 1477 1605 2947
2971 3048 3135
ts8_iso
103 160 231 437 692 883 961 992 1014 1182 1421 1624 1897 3022 3037
3102 3130
ts1_h2
188 352 704 742 755 790 928 980 1098 1211 1319 1420 1724 1781 1797
3148 3235
ts20_iso
158 212 372 549 637 804 841 1033 1161 1218 1354 1459 1812 2116 3054
3144 3238
ts2_h2
197 337 445 508 642 705 832 879 932 978 1117 1233 1403 2152 3026
3066 3713
ts1_ch2o
94 211 345 438 632 634 813 1165 1247 1261 1510 1678 1712 2926 2982
3103 3239
ts2_ch2o
137 317 352 622 779 884 972 1091 1241 1361 1453 1602 1640 3052 3105
3185 3197
ts66_iso
90 170 220 367 441 760 1029 1056 1269 1412 1467 1482 2204 2655 3010
3061 3070
ts67_iso
489 601 698 824 943 996 1038 1087 1178 1238 1304 1319 1382 2194
3216 3234 3250
ts40_iso
267 354 751 755 886 950 969 1046 1146 1295 1346 1468 1581 2125 3024
3161 3400
ts7_iso
319 415 498 605 706 804 882 943 1044 1142 1267 1422 1706 3000 3160
3253 3804
ts10_iso
185 253 540 598 633 684 914 971 1112 1194 1226 1346 1441 2194 2607
3073 3159
ts29_iso
40 312 347 498 610 760 879 901 959 1196 1372 1626 1913 2422 2771
2998 3161
ts72_iso
344 472 605 695 837 861 951 1051 1237 1303 1322 1393 1583 2802 3164
3242 3264
ts4_ch2o
155 258 410 446 497 718 860 934 940 1186 1354 1643 1870 2650 2824
3022 3165
ts4_h2
174 224 508 598 608 740 927 946 1063 1136 1195 1381 1394 2223 2870
3070 3098
ts62_iso

231 308 405 600 673 772 850 910 1030 1170 1360 1454 1677 1876 2046
3129 3214
ts73_iso
159 279 465 551 605 847 922 976 1063 1176 1319 1427 1707 2891 2986
3222 3831
ts74_iso
432 780 884 922 967 989 1009 1122 1151 1224 1293 1375 1472 2163
3042 3104 3215
ts76_iso
163 488 624 650 763 906 943 1044 1135 1201 1251 1409 1516 2080 3102
3206 3807
ts32_iso
320 389 628 637 728 775 785 936 1083 1128 1217 1643 1784 1807 2916
3258 3390
ts10_iso
150 318 475 554 664 678 810 982 1005 1112 1270 1389 1676 1813 2770
3069 3145
ts80_iso
183 515 719 742 894 944 1069 1085 1159 1239 1369 1486 1836 2368
2938 3031 3082
ts81_iso
243 295 342 542 718 825 954 989 1047 1180 1305 1431 1839 2420 2947
3229 3823
ts83_iso
240 276 373 568 609 808 924 1001 1084 1172 1267 1410 1842 2502 2959
3164 3830
ts84_iso
364 824 859 910 928 1028 1067 1111 1171 1219 1328 1364 1433 2409
3039 3110 3138
ts85_iso
196 455 551 602 654 825 925 992 1038 1233 1320 1455 1786 2161 3157
3203 3747
ts2_ch2o
153 493 613 630 770 899 941 1030 1145 1204 1293 1359 1515 2077 3105
3182 3651
ts88_iso
220 283 339 536 633 824 933 1015 1077 1206 1284 1413 1843 2411 2940
3213 3829
ts7_h2
423 512 606 712 769 898 954 1049 1144 1209 1303 1383 1581 1779 2082
3071 3325
ts89_iso
244 365 590 659 775 860 924 939 1031 1229 1330 1454 1615 2846 3038
3163 3711
ts7_iso
162 288 368 532 565 573 856 982 1018 1127 1222 1418 1614 1773 2951
3204 3366
ts83_iso
262 324 483 485 610 665 737 762 945 1112 1343 1396 1672 1886 1919
3256 3456
ts25_iso
236 285 438 558 667 735 753 834 983 1039 1110 1195 1698 1897 2471
3284 3344
ts6_ch2o
147 299 549 627 645 772 814 917 1111 1138 1324 1676 1801 1839 3102
3272 3344
ts51_iso

414 425 555 664 692 802 913 1025 1055 1085 1160 1474 1948 2122 3051
3148 3316
ts7_ch2o
412 486 632 714 763 873 942 961 1181 1231 1402 1498 1571 3092 3130
3171 3280
ts92_iso
375 440 541 707 817 849 935 974 1056 1123 1200 1431 1798 2292 3045
3166 3258
ts93_iso
39 255 382 506 556 588 609 652 949 1281 1441 1463 2079 3114 3303
3408 3469
ts94_iso
204 437 505 560 632 806 902 958 1029 1233 1280 1473 1793 2240 3154
3160 3797
ts95_iso
286 437 456 702 834 923 996 1088 1192 1224 1324 1343 1492 2352 3115
3180 3798
ts96_iso
206 526 677 759 822 906 1002 1022 1060 1134 1303 1362 1611 2464
3082 3216 3245
ts8_ch2o
262 410 600 781 853 948 988 1166 1178 1234 1307 1492 1548 2990 3051
3140 3256
ts97_iso
370 415 619 656 731 899 983 1020 1095 1154 1213 1476 1639 3087 3166
3301 3726
ts98_iso
128 238 307 503 713 874 1003 1056 1145 1379 1433 1485 1855 3012
3072 3089 3789
ts99
189 367 543 633 764 804 854 980 1189 1289 1426 1512 1639 3101 3112
3170 3247
ts42_iso
158 232 297 571 620 673 770 795 1038 1204 1249 1467 1976 2913 3410
3499 3756
ts101_iso
223 457 541 633 666 759 906 1005 1134 1233 1317 1462 1765 2208 3126
3204 3766
ts33_iso
258 348 499 572 597 709 742 761 1166 1256 1449 1536 1876 2173 2899
3359 3469
ts102_iso
366 458 546 710 899 943 992 1062 1139 1258 1379 1465 1571 2380 3107
3194 3745
ts4_iso
183 274 507 624 648 834 919 1040 1085 1237 1379 1497 1801 2318 3077
3178 3804
ts76_iso
210 412 693 733 773 851 989 1013 1165 1259 1301 1537 1683 1757 1849
3179 3233
ts104_iso
177 347 352 606 623 932 957 1061 1150 1413 1468 1483 1811 2305 3032
3086 3126
ts105_iso
279 418 451 773 857 886 1015 1067 1173 1218 1305 1382 1462 2276
3103 3176 3784
ts106_iso

363 437 550 701 899 936 978 1061 1138 1251 1338 1473 1591 2394 3105
3189 3806
ts60_iso
159 271 331 343 537 620 779 939 1034 1165 1201 1472 1990 2290 3118
3197 3780
ts107_iso
419 578 641 828 897 971 1040 1083 1175 1201 1241 1476 1588 2324
3077 3185 3215
ts108_iso
383 431 486 553 772 938 954 1096 1164 1272 1396 1458 1654 1868 3149
3230 3748
ts15_iso
121 279 353 620 691 884 931 953 1013 1360 1380 1417 1695 1768 2782
2845 3262
ts109_iso
350 399 517 628 687 746 826 952 1020 1094 1226 1399 1862 3155 3203
3243 3607
ts2_ch2o
222 247 351 544 682 783 922 943 955 1117 1183 1263 1658 2561 3252
3294 3772
ts110_iso
198 311 503 666 684 841 934 1070 1234 1255 1387 1510 1745 2289 3076
3181 3803
ts11_ch2o
155 214 291 579 598 670 767 784 988 1191 1265 1433 1988 2813 3417
3507 3610
ts112_iso
145 317 487 621 649 708 847 1050 1096 1151 1311 1506 1895 1959 2911
2922 3394
ts113_iso
449 646 759 812 877 933 985 1088 1170 1229 1289 1349 1598 2126 3018
3173 3253
ts3_h2o
156 314 340 450 493 532 780 816 913 1064 1111 1487 2042 2121 3150
3471 3786
ts114_iso
213 323 409 615 855 961 1076 1187 1235 1404 1465 1483 1674 1866
3042 3109 3128
ts16_iso
184 280 472 620 625 813 896 1046 1089 1296 1320 1493 1823 2295 3084
3189 3594
ts23_iso
133 271 404 490 587 679 842 997 1067 1170 1265 1440 1501 2184 2335
3132 3226
ts116_iso
392 579 759 814 853 947 1001 1104 1116 1134 1183 1464 1552 2706
2954 3090 3179
ts117_iso
399 627 716 822 842 981 1002 1111 1115 1166 1185 1457 1544 2637
2962 3088 3179
ts4_h2o
161 315 332 469 490 512 782 785 927 1074 1132 1488 1989 2121 3123
3472 3790
ts6_co
161 351 413 468 734 913 987 1048 1115 1255 1377 1486 1564 1823 3112
3156 3197
ts118_iso

198 306 486 648 687 827 915 1067 1233 1310 1318 1507 1766 2301 3081
3188 3604
ts12_iso
160 344 463 581 696 859 968 975 1027 1150 1366 1538 1606 1788 2697
2968 3134
ts119_iso
331 407 497 654 757 913 991 1052 1081 1098 1222 1489 1743 2289 3049
3126 3279
ts12_ch2o
197 277 395 557 643 924 952 981 1109 1263 1378 1560 1818 2016 2976
3120 3156
ts120_iso
248 493 714 717 842 871 967 1008 1106 1206 1353 1438 1752 2391 2848
3156 3258
ts63_iso
169 187 599 611 767 851 945 1041 1267 1369 1468 1518 1743 2201 2262
3020 3110
ts104_iso
175 212 334 651 657 702 776 1065 1165 1311 1407 1577 1931 2239 3106
3238 3411
ts44_iso
143 345 491 568 679 850 984 1011 1015 1060 1371 1485 1631 1783 2937
3018 3115
ts121_iso
163 249 372 530 582 727 936 1028 1130 1153 1405 1415 2042 2963 3098
3116 3198
ts113_iso
138 334 541 727 733 783 879 1019 1209 1294 1367 1543 1684 1994 3002
3135 3223
ts15_ch2o
164 234 380 574 653 675 749 1040 1161 1317 1445 1580 1814 1956 3101
3248 3392
ts122_iso
427 580 658 772 824 898 1004 1096 1113 1132 1216 1476 1522 3037
3149 3210 3641
ts15_h2
141 455 561 645 948 1015 1029 1120 1218 1258 1343 1435 1501 1694
2115 3061 3124
ts70_iso
224 297 404 647 687 849 963 1013 1032 1079 1421 1487 1607 1833 2608
2834 3140
ts17_h2
204 262 452 534 551 617 722 892 1012 1232 1317 1461 1679 2043 2440
3186 3791
ts123_iso
456 511 838 936 982 1032 1069 1125 1153 1205 1283 1423 1496 3025
3068 3080 3163
ts124_iso
207 343 454 530 775 944 966 1063 1231 1246 1428 1454 1543 3037 3135
3195 3199
ts11_iso
241 282 394 694 728 848 868 1009 1044 1056 1406 1442 1631 1817 2836
2956 3131
ts5_h2o
195 232 333 708 732 903 990 1081 1154 1263 1330 1503 1672 2008 3061
3124 3732
ts19_h2

216 313 492 574 596 633 662 735 932 1187 1241 1388 1551 2167 2228
3475 3778
ts125_iso
384 558 769 840 953 1072 1095 1121 1148 1194 1278 1505 1532 3038
3042 3144 3161
ts20_h2
203 308 540 569 584 645 697 738 921 1160 1291 1341 1540 2154 2286
3471 3663
ts21_h2
210 261 322 492 545 617 711 855 1017 1242 1277 1481 1692 2057 2439
3134 3843
ts16_ch2o
73 99 232 337 681 700 744 1017 1129 1269 1391 1476 2017 2107 3086
3449 3743
ts126_iso
402 527 782 879 957 1027 1065 1127 1157 1223 1281 1363 1512 3040
3058 3105 3120
ts17_iso
115 218 378 541 656 767 933 968 977 1045 1441 1568 1953 2142 2212
3074 3138
ts23_h2
176 400 511 644 679 783 868 1019 1119 1181 1289 1378 1502 1683 1915
2950 3197
ts127_iso
343 527 648 750 780 859 978 1014 1085 1130 1210 1472 1528 3031 3179
3189 3811
ts128_iso
323 392 495 678 846 969 978 1020 1091 1318 1398 1545 1631 1888 3041
3150 3753
ts129_iso
187 311 367 408 618 662 712 865 1000 1043 1105 1479 1867 3111 3210
3303 3717
ts17_ch2o
82 114 234 435 679 682 704 1010 1115 1296 1338 1466 1969 2113 3016
3450 3686
ts130_iso
318 426 514 671 850 964 987 1011 1087 1293 1385 1528 1608 1835 3048
3152 3787
ts131_iso
258 430 479 669 689 780 988 1008 1083 1189 1301 1436 1793 1976 2986
3177 3278
ts6_h2o
261 405 536 657 751 834 913 931 1025 1173 1199 1326 1589 1734 3211
3224 3770
ts7_h2o
332 438 523 605 691 778 834 865 1075 1189 1306 1363 1521 1828 3219
3237 3780
ts132_iso
377 474 571 654 850 869 933 959 1021 1145 1228 1311 1454 3077 3189
3210 3785
ts24_h2
348 382 542 644 734 770 825 878 1006 1071 1152 1436 1718 1868 2501
3162 3255
ts105_iso
357 422 604 670 745 819 918 969 986 1073 1170 1279 1374 1528 2919
3189 3281
ts8_h2o

332 405 536 581 678 798 808 869 1073 1200 1316 1380 1551 1804 3196
3228 3689
ts26_h2
216 278 580 676 705 752 817 912 1036 1226 1350 1372 1857 2117 2214
2942 3471
ts133_iso
130 266 384 630 833 961 986 1050 1145 1288 1355 1424 1491 2026 2979
3062 3126
ts27_h2
341 430 485 623 762 875 890 963 1053 1075 1138 1503 1598 1782 1975
3210 3247
ts7_co
143 199 290 452 495 569 770 784 974 1004 1269 1438 1606 2001 2981
3088 3232
ts73_iso
187 237 317 585 609 656 872 904 1021 1066 1124 1460 1853 1881 3129
3211 3721
ts28_h2
320 416 463 550 633 744 820 962 1015 1062 1197 1239 1402 1856 2863
3297 3791
ts4_triple
70 181 451 497 625 679 780 855 940 1217 1306 1357 1657 1797 2276
3140 3233
ts5_iso
128 188 351 473 507 593 833 876 885 1021 1265 1293 1437 2122 3035
3108 3720
ts134_iso
172 361 425 759 820 935 1081 1107 1235 1265 1289 1345 1394 2256
2929 3062 3762
ts30_h2
126 464 599 669 727 737 859 864 1083 1177 1215 1315 1526 1703 2075
3275 3750
ts127_iso
333 364 665 780 852 883 1029 1057 1134 1262 1276 1412 1425 2366
3023 3078 3230
ts10_h2o
298 464 623 718 799 822 877 933 1053 1168 1190 1235 1481 1713 3182
3206 3714
ts137_iso
169 343 405 751 816 924 1078 1105 1229 1272 1304 1342 1390 2261
2946 3007 3428
ts31_h2
267 280 355 389 447 741 818 917 992 1077 1112 1171 1502 1772 3094
3195 3756
ts32_h2
197 255 474 550 600 623 665 853 952 1036 1167 1393 1401 2276 2950
3005 3492
ts138_iso
117 329 486 751 763 825 1046 1081 1258 1312 1354 1421 1511 2141
2857 3048 3196
ts11_h2o
301 333 378 520 663 719 848 990 1045 1097 1240 1282 1636 2210 3197
3280 3740
ts33_h2
302 459 505 540 732 843 922 971 1011 1076 1250 1390 1447 1603 3054
3253 3733
ts18_ch2o

126 228 283 546 640 686 898 946 1010 1208 1357 1370 1605 2393 2996
3146 3632
ts139_iso
106 371 442 669 763 927 1034 1106 1171 1250 1268 1360 1527 2871
2919 3091 3488
ts140_iso
149 380 475 656 746 872 951 1023 1093 1276 1303 1344 1398 2803 2951
3022 3777
ts141_iso
234 362 414 689 736 879 952 1104 1162 1217 1273 1325 1474 2868 2956
3046 3482
ts34_h2
268 393 432 532 614 709 854 938 998 1198 1338 1380 1497 1815 2924
3174 3822
ts88_iso
260 419 467 542 690 806 867 941 1021 1081 1323 1487 1518 2297 3101
3127 3790
ts19_ch2o
101 131 190 254 516 677 872 1050 1202 1329 1360 1436 1643 1767 2933
3272 3717
ts81_iso
101 348 522 708 738 813 1024 1075 1228 1255 1375 1396 1426 2503
2856 3018 3157
ts13_h2o
162 286 373 386 481 697 801 818 1037 1091 1183 1370 1659 2230 3215
3261 3774
ts8_co
92 248 279 455 505 735 869 987 1188 1343 1371 1402 1702 2055 2681
3225 3606
ts9_co
272 401 432 673 774 807 869 1041 1082 1116 1267 1386 1481 1815 2587
3038 3152
ts143_iso
342 573 640 727 752 816 970 1146 1242 1257 1369 1401 1450 2878 2970
3035 3106
ts14_h2o
204 368 430 542 690 805 896 935 1022 1072 1314 1484 1506 2330 3091
3122 3745
ts144_iso
353 583 622 719 726 795 1012 1106 1199 1240 1359 1381 1420 2860
2940 2957 3060
ts145_iso
424 488 759 829 904 957 1020 1080 1139 1153 1246 1298 1491 2978
3109 3154 3220
ts15_h2o
210 321 380 491 545 702 854 953 1058 1117 1329 1470 1676 1888 3104
3183 3651
ts35_h2
152 236 482 544 575 670 781 913 1072 1133 1278 1335 1443 1622 3053
3102 3779
ts146_iso
413 512 586 733 752 814 946 1008 1065 1148 1185 1225 1374 2886 3018
3188 3552
ts10_co
187 382 473 687 724 772 1050 1096 1173 1257 1301 1393 1434 2653
2874 2968 3018
ts36_h2

66 372 387 600 725 730 801 867 929 1125 1267 1307 1342 1615 3072
3123 3798
ts11_co
145 339 609 638 732 862 1042 1083 1170 1240 1297 1414 1447 2431
2782 3030 3080
ts37_h2
220 301 339 531 636 681 792 890 970 1183 1292 1351 1439 1631 2963
3183 3772

Rate coefficients of the 297 elementary processes considered in KMC

The format of the three columns listed below is the following: 1st column in k(E) in ps^{-1}, second and third columns are the labels for the reactant, and product, respectively.

The labels are the same as those employed above for the minima (1-32):

1-32 are the minima (in the same order as above)

33-43 are the CO channels (in the same order as above)

44-47 are the triple channels (in the same order as above)

48-84 are the H2 channels (in the same order as above)

85-103 are the CH2O channels (in the same order as above)

104-118 are the H2O channels (in the same order as above)

119 is the MIN2→ CO+CH3CH barrierless channel.

Rates for excitation energy=148 kcal/mol

```
0.001058 2 50
0.001033 2 10
5.337e-06 2 10
0.007224 2 1
0.01723 2 18
0.005643 2 35
1.681e-06 2 70
0.01133 2 16
2.274e-05 2 11
0.0002722 2 12
1.109e-05 2 60
0.001073 2 51
0.004094 2 7
0.002317 2 1
0.0005342 18 13
0.02323 18 57
3.588 18 2
0.06013 18 4
1.467 18 1
6.362e-07 18 31
0.001985 4 1
7.672e-05 4 64
5.634e-05 4 68
1.765e-05 4 69
0.002001 4 19
0.01209 4 12
0.0003095 4 54
```

0.001953 4 18
0.08716 4 1
0.001874 4 19
0.08949 4 17
0.0001534 4 5
1.137e-06 4 111
0.007639 4 12
0.0001505 4 26
1.715e-06 4 110
7.757e-08 4 77
0.0002271 4 9
7.942e-05 4 11
1.532e-06 4 7
9.56e-05 4 21
2.432e-06 4 7
7.535e-05 4 11
0.001948 4 104
8.151e-07 4 11
0.0001302 4 9
1.307e-08 4 113
0.002784 17 98
0.0005507 17 39
0.002467 17 6
4.83e-07 17 30
10.01 17 4
0.001964 17 8
0.06489 17 89
5.587e-10 17 43
0.0002438 17 8
0.06575 17 1
4.39e-08 17 32
0.1446 17 45
0.2391 9 19
0.07554 9 21
0.1309 9 19
3.178e-05 9 109
0.01747 9 95
0.003196 9 4
0.00874 9 105
0.01738 9 12
0.001832 9 4
0.01156 9 12
0.05701 9 1
0.05678 9 21
0.04554 9 19
2.414e-06 9 74
0.02766 9 93
0.0002281 1 90
0.0003437 1 4
0.0004404 1 53
0.001368 1 23
0.00156 1 49
0.03384 1 44
0.008453 1 2
0.002631 1 23
0.002623 1 37

0.0007801 1 14
1.629e-12 1 28
0.01508 1 4
0.008696 1 6
0.0006754 1 23
0.008243 1 18
4.141e-05 1 94
9.312e-05 1 19
0.0003864 1 23
0.003437 1 12
0.001898 1 23
0.0001601 1 5
0.0007249 1 19
0.002863 1 87
0.003072 1 23
8.635e-05 1 19
0.002075 1 12
0.000841 1 52
0.0007007 1 9
0.0001019 1 17
0.0003695 1 55
0.006885 1 36
0.0008629 1 88
0.002712 1 2
0.01707 12 48
0.0007783 12 7
1.466e-08 12 31
0.001433 12 38
0.001418 12 7
3.939e-10 12 117
0.08484 12 4
1.094e-08 12 11
1.589e-05 12 47
4.072e-05 12 21
0.008501 12 46
0.05359 12 4
0.001371 12 7
0.1393 12 1
0.09895 12 11
1.26e-05 12 21
0.01629 12 11
1.158e-12 12 84
0.002777 12 7
9.847e-11 12 83
6.209e-09 12 31
4.637e-08 12 102
0.01291 12 2
0.008658 12 9
0.062 12 11
0.0841 12 1
7.042e-07 12 31
0.005765 12 9
4.113e-11 12 82
1.082e-05 12 112
3.775e-09 12 115
3.438 14 1

0.4431 14 23
0.09064 23 20
0.001371 23 65
0.009619 23 96
0.8241 23 1
1.586 23 1
0.4071 23 1
0.2327 23 1
1.144 23 1
0.004617 23 61
1.853 23 1
0.06062 23 14
0.01915 23 59
0.001814 23 63
0.04468 23 3
1.188e-07 21 114
2.248e-08 21 40
0.2025 21 5
0.1545 21 9
0.000167 21 12
2.993e-07 21 103
0.2013 21 5
5.164e-05 21 12
2.647e-08 21 116
0.002753 21 4
6.431e-08 21 80
0.1161 21 9
2.519e-05 7 12
4.592e-05 7 12
4.438e-05 7 12
8.994e-05 7 12
0.0002449 7 22
0.002822 7 22
4.467e-06 7 62
2.262e-07 7 13
3.463e-07 7 4
5.533e-07 7 76
5.495e-07 7 4
0.006316 7 2
1.796 20 23
0.7611 20 6
0.2346 8 85
3.187e-05 8 29
0.0003237 8 17
1.818 8 3
0.004624 8 26
3.037e-05 8 71
0.003263 8 5
3.729e-07 8 78
0.0003616 8 28
0.000415 8 28
0.005995 8 24
4.025e-05 8 17
0.002118 8 24
2.925e-08 11 12
0.0005707 11 3

0.2663 11 12
0.0004084 11 5
0.0438 11 12
0.002904 11 2
0.03434 11 26
0.001497 11 4
0.03382 11 22
9.072e-06 11 75
0.1668 11 12
0.001421 11 4
1.536e-05 11 4
1.578 26 8
0.9438 26 4
11.38 26 11
4.151e-05 5 97
4.452e-09 5 27
0.0004279 5 106
0.0003185 5 107
8.523e-05 5 100
3.479e-05 5 101
0.002262 5 21
8.821e-05 5 19
4.931e-05 5 4
0.0001772 5 19
1.401e-05 5 67
1.67e-05 5 66
0.002249 5 21
3.185e-05 5 99
8.835e-06 5 108
0.0002974 5 1
5.523e-07 5 73
6.963e-06 5 11
5.711e-05 5 8
0.2058 19 4
1.749 19 9
0.02822 19 5
0.1928 19 4
0.0567 19 5
0.05535 19 1
0.4311 19 1
0.9579 19 9
0.02146 19 6
0.05137 19 1
0.3331 19 9
0.009932 19 56
0.05724 10 2
0.0002958 10 2
8.981e-08 10 79
0.1399 32 6
0.1927 32 6
0.03854 32 42
2.019 32 17
0.0009609 13 18
24.65 13 34
0.006037 13 16
5.56e-05 13 7

0.8965 29 8
0.0007907 27 5
5.9 27 6
0.01189 30 17
6.807e-07 28 1
1.458 28 8
0.07347 28 6
1.673 28 8
0.1632 28 6
10.83 28 92
0.02111 31 12
0.2109 31 18
0.00893 31 12
1.021 31 12
0.001046 31 41
0.2114 15 6
0.3678 22 7
4.234 22 7
3.157e-07 22 81
0.06219 22 16
0.6138 22 11
4.238e-09 22 118
0.4558 16 2
0.000646 16 13
0.001079 16 22
0.6847 24 8
10.67 24 86
0.2416 24 8
4.967e-05 6 72
0.0009309 6 17
0.006209 6 91
2.123 6 1
0.01555 6 20
0.004316 6 27
0.006709 6 15
4.172e-05 6 28
6.888e-10 6 32
0.008784 6 19
9.269e-05 6 28
9.559e-10 6 32
0.7867 3 33
0.003442 3 58
0.4701 3 8
0.0001435 3 11
0.002037 3 23
0.0459 2 119

Rates for excitation energy=182 kcal/mol

0.01788 2 50
0.02611 2 10
0.0001551 2 10
0.04166 2 1
0.08923 2 18

0.04297 2 35
0.0002432 2 70
0.06403 2 16
0.000531 2 11
0.002638 2 12
0.0006325 2 60
0.01954 2 51
0.05602 2 7
0.0143 2 1
0.007605 18 13
0.1698 18 57
3.712 18 2
0.1266 18 4
1.774 18 1
0.0001921 18 31
0.02423 4 1
0.004434 4 64
0.004362 4 68
0.001546 4 69
0.02548 4 19
0.06902 4 12
0.004424 4 54
0.01331 4 18
0.3451 4 1
0.02529 4 19
0.2823 4 17
0.002341 4 5
0.0001784 4 111
0.05054 4 12
0.003048 4 26
0.0002171 4 110
4.756e-05 4 77
0.003506 4 9
0.001368 4 11
0.0001359 4 7
0.001918 4 21
0.0001813 4 7
0.001357 4 11
0.04305 4 104
9e-05 4 11
0.002451 4 9
1.361e-05 4 113
0.0367 17 98
0.07118 17 39
0.01779 17 6
0.0004332 17 30
10.66 17 4
0.02203 17 8
0.256 17 89
3.283e-05 17 43
0.008828 17 8
0.2112 17 1
0.0001751 17 32
0.8511 17 45
0.5891 9 19
0.3048 9 21

0.3552 9 19
0.002608 9 109
0.2748 9 95
0.03463 9 4
0.1375 9 105
0.1338 9 12
0.0242 9 4
0.1053 9 12
0.1913 9 1
0.2424 9 21
0.1776 9 19
0.0004788 9 74
0.3406 9 93
0.0056 1 90
0.006544 1 4
0.009222 1 53
0.01239 1 23
0.02334 1 49
0.4433 1 44
0.04918 1 2
0.02323 1 23
0.03637 1 37
0.005407 1 14
6.592e-08 1 28
0.09317 1 4
0.02792 1 6
0.005973 1 23
0.05034 1 18
0.001228 1 94
0.001917 1 19
0.004482 1 23
0.03321 1 12
0.01759 1 23
0.003163 1 5
0.01182 1 19
0.04762 1 87
0.02371 1 23
0.001221 1 19
0.0179 1 12
0.01575 1 52
0.005227 1 9
0.001511 1 17
0.009535 1 55
0.0921 1 36
0.01511 1 88
0.01688 1 2
0.0911 12 48
0.0116 12 7
3.409e-05 12 31
0.02325 12 38
0.02041 12 7
1.059e-05 12 117
0.2802 12 4
2.851e-05 12 11
0.003491 12 47
0.0008338 12 21

0.08827 12 46
0.2052 12 4
0.01611 12 7
0.4994 12 1
0.206 12 11
0.0004909 12 21
0.06904 12 11
5.688e-06 12 84
0.0303 12 7
2.534e-05 12 83
1.791e-05 12 31
0.0001574 12 102
0.04683 12 2
0.05497 12 9
0.1511 12 11
0.2692 12 1
0.0001679 12 31
0.0433 12 9
8.808e-06 12 82
0.001961 12 112
1.821e-05 12 115
7.138 14 1
1.525 14 23
0.1392 23 20
0.01727 23 65
0.07244 23 96
1.008 23 1
1.891 23 1
0.4862 23 1
0.3647 23 1
1.432 23 1
0.04063 23 61
1.931 23 1
0.09406 23 14
0.1263 23 59
0.02114 23 63
0.1043 23 3
0.000107 21 114
0.0001642 21 40
0.3919 21 5
0.2301 21 9
0.001531 21 12
0.001137 21 103
0.3193 21 5
0.0009011 21 12
0.0001558 21 116
0.01431 21 4
5.82e-05 21 80
0.183 21 9
0.00059 7 12
0.001038 7 12
0.0008193 7 12
0.001541 7 12
0.003637 7 22
0.01886 7 22
0.0001988 7 62

4.808e-05 7 13
2.801e-05 7 4
0.000246 7 76
3.737e-05 7 4
0.0507 7 2
3.517 20 23
1.779 20 6
1.847 8 85
0.001314 8 29
0.009756 8 17
4.259 8 3
0.0636 8 26
0.00408 8 71
0.07471 8 5
0.0008126 8 78
0.007656 8 28
0.008605 8 28
0.08945 8 24
0.00391 8 17
0.07268 8 24
8.845e-05 11 12
0.01255 11 3
0.6405 11 12
0.025 11 5
0.2146 11 12
0.02932 11 2
0.2111 11 26
0.01726 11 4
0.1667 11 22
0.001888 11 75
0.4695 11 12
0.01713 11 4
0.001135 11 4
2.71 26 8
2.167 26 4
11.86 26 11
0.001423 5 97
2.799e-06 5 27
0.01083 5 106
0.008972 5 107
0.006251 5 100
0.00317 5 101
0.01593 5 21
0.001455 5 19
0.0007095 5 4
0.002703 5 19
0.0009546 5 67
0.001072 5 66
0.01298 5 21
0.001298 5 99
0.0004376 5 108
0.00355 5 1
8.891e-05 5 73
0.0006007 5 11
0.001357 5 8
0.7738 19 4

1.812 19 9
0.1458 19 5
0.7681 19 4
0.2709 19 5
0.2157 19 1
1.33 19 1
1.093 19 9
0.09918 19 6
0.1375 19 1
0.5463 19 9
0.06085 19 56
0.64 10 2
0.003803 10 2
0.0002641 10 79
0.2926 32 6
0.2964 32 6
0.5275 32 42
2.594 32 17
0.0218 13 18
59.93 13 34
0.06948 13 16
0.006364 13 7
3.762 29 8
0.05406 27 5
6.726 27 6
0.2472 30 17
0.001592 28 1
3.008 28 8
0.3772 28 6
3.381 28 8
0.5635 28 6
14.44 28 92
0.262 31 12
0.6323 31 18
0.1376 31 12
1.293 31 12
0.07493 31 41
0.8558 15 6
1.434 22 7
7.434 22 7
0.0006345 22 81
0.2884 22 16
1.077 22 11
0.0002178 22 118
0.572 16 2
0.005196 16 13
0.007218 16 22
1.819 24 8
14.05 24 86
1.477 24 8
0.007549 6 72
0.01908 6 17
0.08147 6 91
4.191 6 1
0.1298 6 20
0.04634 6 27

```
0.06261 6 15
0.002326 6 28
1.758e-05 6 32
0.1321 6 19
0.003475 6 28
1.781e-05 6 32
1.951 3 33
0.1154 3 58
1.348 3 8
0.005249 3 11
0.02509 3 23
0.162 2 119
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