

SUPPORTING INFORMATION

Section 1: Optimized geometries of the stationary points (minima and TSs). Cartesian coordinates in Angstrom are given in xyz format.

Contents of Section 1:

1.1) Minimum **A**

1.2) Minimum **B**

1.3) Minimum **C**

1.4) **TS1**

1.5) **TS2**

1.6) **TS3**

1.7) **TS4**

1.1) Geometry of minimum **A**

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Min A

N 3.9286 2.6344 7.9415

O 4.5596 3.6350 7.6596

O 2.7255 2.4543 8.1088

O 4.7873 1.4292 8.1056

H 4.1127 0.7280 8.3076

C 0.0324 0.6875 3.4395

C 0.0325 4.9710 3.4361

C 0.0323 2.1344 3.4368

C 0.0325 6.4179 3.4390

C 1.2689 2.8294 3.4356

C 1.2690 7.1131 3.4407

C 1.2689 -0.0076 3.4407

C 1.2691 4.2762 3.4356

C 2.5057 0.6873 3.4421

C 2.5058 4.9711 3.4407

C 2.5055 2.1344 3.4398

C 2.5058 6.4181 3.4428

C 3.7423 2.8294 3.4436
C 3.7424 7.1130 3.4462
C 3.7424 -0.0077 3.4450
C 3.7425 4.2764 3.4446
C 4.9789 0.6874 3.4451
C 4.9790 4.9711 3.4479
C 4.9787 2.1343 3.4455
C 4.9789 6.4180 3.4478
C 6.2152 2.8292 3.4466
C 6.2154 7.1132 3.4476
C 6.2153 -0.0076 3.4462
C 6.2153 4.2760 3.4478
C 7.4518 0.6874 3.4438
C 7.4518 4.9711 3.4440
C 7.4516 2.1342 3.4430
C 7.4518 6.4181 3.4447
C 8.6881 2.8292 3.4385
C 8.6883 7.1131 3.4411
C 8.6882 -0.0077 3.4414
C 8.6882 4.2760 3.4381

1.2) Geometry of minimum **B**

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Min B

N 3.6076 3.7236 8.0513
O 4.5040 4.4686 7.6096
O 3.1031 2.7582 7.4694
O 6.3826 4.3261 5.4851
H 5.4990 4.2606 5.9486
C 0.0233 0.6888 3.4338
C 0.0288 4.9746 3.4195
C 0.0159 2.1348 3.4592
C 0.0272 6.4187 3.4122
C 1.2629 2.8390 3.4514

C 1.2623 7.1207 3.4165
C 1.2625 -0.0073 3.4248
C 1.2637 4.2738 3.4249
C 2.5020 0.6892 3.4404
C 2.4989 4.9755 3.4427
C 2.5106 2.1343 3.4656
C 2.4991 6.4180 3.4335
C 3.7331 2.8247 3.5148
C 3.7301 7.1111 3.4528
C 3.7330 -0.0102 3.4435
C 3.7318 4.2804 3.5278
C 4.9698 0.6815 3.4688
C 4.9424 4.9880 3.6283
C 4.9807 2.1203 3.5223
C 4.9606 6.4058 3.5275
C 6.2083 2.7992 3.6107
C 6.2094 7.1140 3.5076
C 6.2083 -0.0304 3.4746
C 6.2182 4.2637 3.9753
C 7.4465 0.6827 3.4594
C 7.4781 4.9881 3.5697
C 7.4354 2.1192 3.5163
C 7.4576 6.4048 3.4899
C 8.6848 2.8257 3.5032
C 8.6879 7.1114 3.4242
C 8.6844 -0.0101 3.4286
C 8.6885 4.2799 3.4899

1.3) Geometry of minimum **C**

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Min C

N 4.2283 4.2133 8.5367
O 3.4278 4.6057 7.7316
O 5.5698 4.0463 8.0035

O 5.6092 4.6267 5.1181
H 5.5133 4.2880 7.0241
C 0.0297 0.6866 3.4098
C 0.0329 4.9786 3.3882
C 0.0193 2.1323 3.4132
C 0.0319 6.4131 3.4027
C 1.2644 2.8366 3.4043
C 1.2770 7.1171 3.4193
C 1.2668 -0.0048 3.4128
C 1.2643 4.2709 3.3931
C 2.5009 0.6947 3.4219
C 2.4974 4.9666 3.4509
C 2.4982 2.1398 3.4296
C 2.4993 6.4274 3.4604
C 3.7279 2.8424 3.5026
C 3.7376 7.1291 3.4846
C 3.7342 0.0041 3.4454
C 3.6985 4.2604 3.5520
C 4.9753 0.6990 3.4625
C 4.9470 4.9955 3.8032
C 4.9874 2.1275 3.5068
C 4.9658 6.4510 3.5647
C 6.2224 2.7990 3.5508
C 6.2005 7.1227 3.5105
C 6.2127 -0.0167 3.4617
C 6.2442 4.2540 3.7904
C 7.4539 0.6779 3.4379
C 7.4900 4.9894 3.5328
C 7.4507 2.1206 3.4695
C 7.4603 6.4077 3.4965
C 8.6890 2.8221 3.4451
C 8.6902 7.1099 3.4263
C 8.6876 -0.0128 3.4183
C 8.6913 4.2833 3.4342

1.4) Geometry of **TS1**

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TS1

N	0.6723	5.6445	6.4085
O	1.5742	6.4388	6.6476
O	-0.4168	5.4950	6.9575
O	0.7616	4.8259	4.2198
H	0.5580	3.9151	4.5512
C	-2.9717	2.5400	2.0884
C	-2.9644	6.8240	2.1091
C	-2.9723	3.9852	2.0961
C	-2.9696	8.2701	2.0896
C	-1.7386	4.6804	2.1471
C	-1.7365	8.9679	2.0817
C	-1.7390	1.8466	2.0911
C	-1.7365	6.1316	2.1396
C	-0.5056	2.5494	2.1344
C	-0.4920	6.8339	2.1258
C	-0.5181	3.9778	2.2094
C	-0.4993	8.2751	2.0861
C	0.7383	4.6956	2.4593
C	0.7387	8.9806	2.0919
C	0.7390	1.8451	2.1224
C	0.7382	6.1538	2.1842
C	1.9831	2.5496	2.1344
C	1.9683	6.8338	2.1289
C	1.9948	3.9772	2.2100
C	1.9761	8.2751	2.0886
C	3.2157	4.6802	2.1481
C	3.2134	8.9680	2.0844
C	3.2162	1.8467	2.0924
C	3.2132	6.1310	2.1427
C	4.4489	2.5400	2.0896

C 4.4408 6.8237 2.1117
C 4.4489 3.9853 2.0974
C 4.4460 8.2700 2.0920
C 5.6843 4.6840 2.0917
C 5.6841 8.9656 2.0851
C 5.6843 1.8406 2.0828
C 5.6841 6.1234 2.1052

1.5) Geometry of **TS2**

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TS2

N 4.5305 4.6556 7.8360
O 5.6947 4.5918 8.2032
O 4.2963 4.5163 6.5156
O 6.3392 4.2166 5.1386
H 5.2780 4.3847 5.9029
C -0.0924 0.5102 3.2120
C -0.0912 4.7926 3.2185
C -0.0998 1.9566 3.2323
C -0.0904 6.2419 3.2094
C 1.1452 2.6615 3.2243
C 1.1406 6.9390 3.1981
C 1.1444 -0.1866 3.2022
C 1.1448 4.0932 3.2065
C 2.3828 0.5079 3.2099
C 2.3801 4.7967 3.2084
C 2.3942 1.9536 3.2350
C 2.3801 6.2358 3.1997
C 3.6157 2.6441 3.2757
C 3.6101 6.9293 3.2031
C 3.6144 -0.1925 3.2008
C 3.6116 4.1018 3.2694
C 4.8494 0.4980 3.2227
C 4.8210 4.8086 3.3472

C 4.8626 1.9366 3.2782
C 4.8397 6.2232 3.2578
C 6.0877 2.6170 3.3543
C 6.0938 6.9344 3.2422
C 6.0901 -0.2132 3.2212
C 6.0928 4.0828 3.6942
C 7.3308 0.5046 3.2240
C 7.3550 4.8113 3.3515
C 7.3146 1.9371 3.2782
C 7.3399 6.2327 3.2569
C 8.5681 2.6501 3.2737
C 8.5710 6.9347 3.2135
C 8.5689 -0.1881 3.2070
C 8.5782 4.0957 3.2803

1.6) Geometry of **TS3**

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TS3

O 6.1273 4.3324 5.3015
C -0.0522 0.6916 3.4469
C -0.0516 4.9766 3.4699
C -0.0625 2.1381 3.4696
C -0.0500 6.4226 3.4569
C 1.1853 2.8460 3.4694
C 1.1852 7.1215 3.4497
C 1.1852 -0.0041 3.4457
C 1.1851 4.2748 3.4629
C 2.4228 0.6914 3.4474
C 2.4221 4.9766 3.4690
C 2.4335 2.1379 3.4687
C 2.4203 6.4224 3.4572
C 3.6551 2.8316 3.4953
C 3.6500 7.1137 3.4447
C 3.6531 -0.0088 3.4319

C 3.6462 4.2821 3.5054
C 4.8887 0.6831 3.4332
C 4.8698 4.9929 3.5517
C 4.9058 2.1149 3.4761
C 4.8812 6.4095 3.4710
C 6.1312 2.7949 3.5241
C 6.1312 7.1200 3.4424
C 6.1312 -0.0344 3.4249
C 6.1303 4.2515 3.8741
C 7.3740 0.6833 3.4328
C 7.3919 4.9929 3.5547
C 7.3568 2.1151 3.4768
C 7.3810 6.4094 3.4716
C 8.6077 2.8318 3.4978
C 8.6126 7.1136 3.4446
C 8.6095 -0.0088 3.4314
C 8.6163 4.2819 3.5092

1.7) Geometry of **TS4**

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TS4

N 4.3549 4.7150 6.4418
O 3.2133 5.1072 6.3513
O 4.4716 3.2886 7.0414
O 5.3597 4.7227 5.0914
H 3.5197 3.0984 7.2566
C 0.0299 0.5875 3.0764
C 0.0303 4.8750 3.0737
C 0.0260 2.0318 3.0742
C 0.0306 6.3124 3.0887
C 1.2660 2.7327 3.0789
C 1.2754 7.0142 3.0989
C 1.2679 -0.1070 3.0823
C 1.2659 4.1739 3.0811

C 2.5016 0.5911 3.0794
C 2.4997 4.8689 3.1403
C 2.4988 2.0379 3.0873
C 2.5019 6.3228 3.1346
C 3.7314 2.7400 3.1382
C 3.7448 7.0242 3.1352
C 3.7374 -0.1011 3.0919
C 3.7159 4.1638 3.2178
C 4.9760 0.6034 3.0917
C 4.9781 4.8829 3.4443
C 4.9797 2.0334 3.1157
C 4.9742 6.3418 3.1996
C 6.2195 2.7303 3.1278
C 6.2047 7.0243 3.1304
C 6.2141 -0.1071 3.0880
C 6.2325 4.1635 3.2158
C 7.4522 0.5874 3.0763
C 7.4600 4.8748 3.1346
C 7.4522 2.0330 3.0843
C 7.4531 6.3176 3.1262
C 8.6863 2.7277 3.0799
C 8.6817 7.0122 3.0937
C 8.6851 -0.1087 3.0803
C 8.6862 4.1776 3.0822

Section 2: Normal modes of vibration (NMV) with the imaginary frequency for each transition state. The x (first row), y (second row) and z (third row) displacements of each atom are given (same order of atoms as in the geometry specification).

Contents of Section 2:

2.1) **TS1**

2.1.1) Frequency (cm^{-1})

2.1.2) Normal mode

2.2) **TS2**

2.2.1) Frequency (cm^{-1})

2.2.2) Normal mode

2.3) **TS3**

2.3.1) Frequency (cm^{-1})

2.3.2) Normal mode

2.4) **TS4**

2.4.1) Frequency (cm^{-1})

2.4.2) Normal mode

2.1) NMV with the imaginary frequency for **TS1**.

2.1.1) Frequency: $515i \text{ cm}^{-1}$

2.1.2) NMV

-0.044402

-0.005278

-0.213000

0.044787

-0.071182

0.000439

0.008121

-0.002095

0.067444

-0.017545

0.156399

0.667732

-0.017033

0.045570

0.207749

-0.014441

-0.024065

0.010814

-0.006337

-0.024028

-0.002432

0.004417
-0.021267
0.020771
0.015677
-0.023300
0.005322
-0.002588
0.016842
-0.007824
0.000807
0.008806
0.012536
0.010409
0.009543
0.027254
0.013128
0.006589
-0.010643
0.001064
-0.001891
-0.010809
0.000955
0.000430
0.003265
0.027797
0.030923
-0.083506
0.011058
0.009921
0.024562
-0.008060
-0.036994
-0.622380
-0.000483
-0.014030
0.004915
0.003665
0.011636
-0.006175
0.005132
-0.033930
-0.058539
-0.018873
-0.020655
-0.006082
0.018871
-0.019818
0.004483
-0.048132
0.016284

-0.061958
0.009506
-0.010109
0.024502
-0.009275
-0.005441
-0.007523
-0.003512
-0.016839
0.006111
-0.004484
-0.014959
0.021803
0.000168
-0.018043
-0.015501
-0.011306
-0.010596
0.005786
0.017254
-0.011326
-0.005398
-0.012566
-0.006834
0.014802
0.013641
-0.011035
0.001818
-0.013754
0.023117
0.017887
-0.009674
0.024467
-0.001735
0.009158
0.031983
0.012951
0.012844
0.031180
0.001751

2.2) NMV with the imaginary frequency for **TS2**.

2.2.1) Frequency: $1613i \text{ cm}^{-1}$

2.2.2) NMV

-0.150751
-0.022854
-0.196219
0.148091

-0.025195
0.082940
-0.021117
0.030911
0.082384
-0.102828
-0.007915
0.130126
0.700880
-0.115708
-0.593574
-0.033616
-0.029131
0.010535
-0.005790
-0.022422
-0.000122
0.000476
-0.026278
0.005110
0.020319
-0.027007
-0.003498
-0.002018
0.014195
-0.004331
-0.002091
0.014635
-0.005847
-0.003155
0.014564
-0.003455
0.000763
0.017377
-0.009270
-0.011388
0.011899
-0.001293
0.003298
0.010379
-0.002779
-0.011223
0.008395
-0.002319
0.011896
0.013003
-0.005389
-0.003566
0.004829
0.001804

-0.005387
0.006670
0.000887
0.006975
0.006880
-0.000190
0.004596
0.002139
0.004620
-0.019205
-0.003256
0.002854
-0.000135
-0.002645
0.011746
-0.011725
-0.001097
0.006128
0.014903
0.003901
0.001221
-0.003783
-0.011243
0.012409
-0.010237
-0.012840
0.009554
0.000782
-0.003285
0.005850
-0.008785
0.004134
0.004294
-0.017590
-0.015491
0.011346
0.027911
-0.011598
-0.019946
-0.005578
-0.005656
0.014751
0.012222
-0.022213
0.003446
-0.015272
0.022951
0.001979
-0.017736
0.029654

-0.005249
0.013660
0.031182
0.001253
0.002369
0.038115
-0.003248

2.3) NMV with the imaginary frequency for **TS3**.

2.3.1) Frequency: $397i \text{ cm}^{-1}$

2.3.2) NMV

-0.958735
-0.013828
-0.060395
0.029973
0.002229
0.040203
0.040413
0.009423
0.051512
0.027086
0.002064
0.046384
0.042153
-0.000906
0.045889
0.033116
0.006909
0.038127
0.053248
0.006782
0.051223
0.034574
0.006277
0.047336
0.040363
0.005955
0.044192
0.032172
0.009475
0.024326
0.042502
0.000164
0.017348
0.028070
0.007512
0.008889
0.040196

0.010886
0.031901
0.029562
0.009095
-0.032042
0.040418
0.009731
0.003235
0.028654
0.008396
0.005986
0.027094
-0.006409
-0.029531
0.033174
0.006978
-0.022710
0.044870
0.005261
-0.042142
0.034069
-0.001478
-0.044595
0.043141
0.017072
-0.037184
0.034420
-0.004736
-0.043846
0.028786
-0.003166
-0.030639
0.030995
-0.005220
-0.025556
0.002840
-0.004068
-0.052527
0.031630
-0.013107
-0.014671
0.044867
-0.009614
-0.015999
0.032350
-0.007015
-0.011567
0.044434
-0.019444
-0.010150

0.026525
-0.013436
0.015792
0.044377
-0.011566
-0.001713
0.032224
-0.008636
-0.003091
0.028221
0.000550
0.015323

2.4) NMV with the imaginary frequency for **TS4**.

2.4.1) Frequency: $525i \text{ cm}^{-1}$

2.4.2) NMV

-0.140469
0.096471
0.408775
-0.061617
0.000538
0.024658
-0.087195
0.010824
0.051899
0.328194
0.144195
-0.732562
-0.013194
0.000535
-0.015715
-0.011960
-0.015278
-0.032844
0.004487
-0.009349
-0.015535
-0.016838
-0.012255
-0.014344
0.013100
-0.023073
0.007828
-0.013646
-0.005282
-0.009775
0.015945
-0.006599

0.009434
-0.003109
-0.003619
-0.022356
-0.005463
-0.018947
-0.002817
-0.008249
-0.004074
-0.012786
-0.005009
-0.031185
0.006216
-0.015444
-0.007162
-0.008482
0.001832
-0.012744
0.020089
-0.013555
-0.009304
0.001596
0.002415
0.003450
0.013704
-0.005038
0.001345
0.010283
-0.038277
-0.040649
0.019632
-0.006381
0.009346
-0.012074
-0.014954
-0.021361
0.313319
0.008045
-0.019972
-0.009768
-0.000710
0.027473
0.031392
0.007712
-0.020175
0.005666
-0.001595
0.008642
0.001550
0.004161

-0.001576
-0.022983
0.017597
-0.029797
0.082810
0.002843
-0.008182
-0.017515
0.014197
-0.002558
-0.000852
0.001597
-0.007886
-0.005103
0.013467
-0.015488
-0.004185
-0.007383
0.005249
-0.004495
0.002494
-0.011870
0.008855
0.002888
-0.007847
-0.005988
0.003311
0.006858
-0.010228