

SUPPORTING INFORMATION

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

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1.1) Geometry of minimum **A**

59

Min mono-vacancy (C59)

C 12.0997315 1.08098635 3.51478047
C 12.1139483 5.36236315 3.47204253
C 12.0925886 2.50663114 3.48837082
C 12.145963 6.78832756 3.49748167
C 12.1350493 9.65251423 3.55358716
C 12.1198249 11.0798312 3.55731574
C 0.964511263 3.20576742 3.44333625
C 1.01266481 7.49171683 3.48509839
C 0.974332793 0.354264589 3.50389582
C 0.974277229 4.63584671 3.43817466
C 1.00718094 8.92627349 3.52170687

C 0.989378889 11.7791913 3.52797868
C 2.2102215 1.05508365 3.45953066
C 2.19630255 2.48106976 3.41916079
C 2.24578485 9.62613686 3.51374117
C 2.23104938 11.0530575 3.51203722
C 3.45107335 0.332279391 3.45705464
C 3.46973479 11.7547068 3.48418926
C 4.68018594 1.04695761 3.42626023
C 4.71470893 11.0369382 3.48542119
C 5.92783137 0.352903545 3.46119757
C 5.94203237 11.7728312 3.49259101
C 7.15927287 1.0963309 3.48674995
C 7.17807295 11.0610677 3.53446375
C 8.39497213 0.377734658 3.54189022
C 8.40421897 11.7932204 3.55621664
C 9.61325616 1.11625654 3.54292688
C 9.59736708 2.56626042 3.53046846
C 9.66231671 9.64963815 3.57210201
C 9.64739233 11.0814394 3.57322334
C 10.8512214 3.2380123 3.506946
C 10.9175849 7.51634527 3.54090436
C 10.8583922 0.386267641 3.54679569
C 10.8695902 4.65935276 3.49501623
C 10.9044947 8.946106 3.56192276
C 10.8742919 11.8019285 3.5666626
C 2.21257316 5.34283651 3.40823116
C 2.24246532 6.77046306 3.43650722
C 3.43000416 3.1885935 3.3599231
C 3.49719327 7.47053757 3.44407392
C 3.43104611 4.61391707 3.34083356
C 3.48935192 8.90264573 3.49158557
C 4.65634121 2.4676186 3.36448937
C 4.73300894 9.59468257 3.49338954
C 5.98239696 8.86173239 3.51777297

C 7.19135318 9.62023389 3.54570929
 C 8.43126204 8.92622534 3.56221063
 C 9.63736018 5.39767462 3.52428873
 C 9.70554732 6.81965061 3.54782124
 C 4.67650657 5.31979243 3.25959003
 C 4.72512367 6.74624103 3.391216
 C 5.89191188 3.19110339 3.29520525
 C 6.01065767 7.38890087 3.50358943
 C 5.80435209 4.5490754 3.0948344
 C 7.14431197 2.52384474 3.43533244
 C 7.29145341 6.71730721 3.57530882
 C 8.33236093 3.32801477 3.52010664
 C 8.45070402 7.48904502 3.55929169
 C 8.38710114 4.77962205 3.55602137

1.2) Geometry of minimum A (C31 + HNO₃, as separate reactants)

31

C31

C 2.3401 3.8970 0.3525
 C 2.3409 1.0527 0.3721
 C 2.3384 5.3318 0.3723
 C 2.3396 8.1759 0.4158
 C 3.5842 1.7535 0.3549
 C 3.5864 6.0283 0.4144
 C 3.5992 3.1951 0.3372
 C 3.5796 7.4800 0.4340
 C 4.8151 1.0618 0.3965
 C 4.8126 8.1804 0.4453
 C 6.0436 7.4891 0.5154
 C 7.2856 8.1791 0.4947
 C 8.5256 7.4852 0.5161
 C 9.7600 1.0559 0.3947
 C 9.7591 8.1758 0.4469
 C 10.9897 1.7512 0.3531

C 10.9817 6.0260 0.4141
C 10.9738 3.1928 0.3353
C 10.9916 7.4773 0.4352
C 4.8775 3.8969 0.3361
C 4.8176 5.3413 0.4489
C 6.0693 1.7535 0.3788
C 6.0497 6.0470 0.5737
C 6.0820 3.1494 0.2819
C 7.2866 1.0207 0.4122
C 7.2799 5.4378 0.6622
C 8.5079 1.7475 0.3701
C 8.5162 6.0418 0.5740
C 8.4968 3.1384 0.2596
C 9.6952 3.8927 0.3309
C 9.7493 5.3378 0.4472

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HNO₃

N 3.7097971 2.13231972 2.11898446
O 3.22279528 3.24623783 2.11829653
O 3.19326719 1.01871912 2.11813777
O 5.20054233 2.14337953 2.12284745
H 5.4040639 1.17101633 2.11718526

1.3) Geometry of minimum **B**

36

Min B

N 6.8387 3.0820 3.5991
O 5.9701 3.9844 3.4029
O 6.8656 2.3970 4.6561
O 7.7278 2.8438 2.6841
H 7.2732 4.6804 1.3488
C 2.3313 4.0082 0.1755
C 2.3296 1.1702 0.0849
C 2.3324 5.4392 0.2063
C 2.3312 8.2904 0.1467

C 3.5762 1.8706 0.0680
 C 3.5890 6.1406 0.2433
 C 3.5992 3.3099 0.1329
 C 3.5699 7.5929 0.1860
 C 4.7977 1.1661 0.0361
 C 4.7979 8.2929 0.1154
 C 6.0332 7.6102 0.1984
 C 7.2771 8.3034 0.1080
 C 8.5211 7.6093 0.1933
 C 9.7561 1.1654 0.0316
 C 9.7569 8.2917 0.1061
 C 10.9778 1.8694 0.0662
 C 10.9675 6.1407 0.2394
 C 10.9551 3.3114 0.1303
 C 10.9853 7.5923 0.1797
 C 4.8872 4.0108 0.1774
 C 4.8305 5.4642 0.3464
 C 6.0458 1.8570 -0.0220
 C 6.0524 6.2100 0.4852
 C 6.0747 3.2414 0.0047
 C 7.2784 1.1296 -0.0140
 C 7.2765 5.6166 0.8175
 C 8.5081 1.8551 -0.0157
 C 8.5008 6.2084 0.4804
 C 8.4738 3.2401 0.0430
 C 9.6708 4.0114 0.1783
 C 9.7255 5.4636 0.3397

1.4) Geometry of minimum **C**

36

Min C

N 9.5832 3.1398 5.7552
 O 10.6985 3.2606 5.2720
 O 7.9381 3.6597 2.6950

O 8.8611 2.1782 5.9603
H 7.2028 4.4944 0.3226
C 2.2375 4.0152 0.8377
C 2.2301 1.1661 0.9387
C 2.2453 5.4468 0.8206
C 2.2414 8.2882 0.8802
C 3.4728 1.8702 0.8930
C 3.4956 6.1534 0.7729
C 3.4615 3.3040 0.8133
C 3.4773 7.5962 0.8333
C 4.6990 1.1659 0.9301
C 4.7102 8.2944 0.8821
C 5.9488 7.6214 0.8279
C 7.1943 8.3202 0.9321
C 8.4328 7.6007 0.9225
C 9.6713 1.1575 1.0700
C 9.6724 8.2890 0.9562
C 10.9077 1.8579 1.0356
C 10.9000 6.1433 0.8600
C 10.9055 3.3201 0.9940
C 10.8996 7.5920 0.8753
C 4.6985 4.0060 0.7548
C 4.7208 5.4730 0.6941
C 5.9387 1.8673 0.9723
C 5.9632 6.1878 0.6627
C 5.8200 3.2325 0.8391
C 7.2098 1.1705 1.0745
C 7.2027 5.5535 0.5650
C 8.4459 1.8378 1.2346
C 8.4196 6.1805 0.8077
C 8.5815 3.2382 1.7249
C 9.7057 4.0285 1.1347
C 9.6687 5.4418 0.9343

1.5) Geometry of minimum **D**

36

Min D

N	9.73120448	2.22344881	4.65732866
O	10.1479353	1.13994887	4.22164009
O	7.20276383	3.93019731	1.2036925
O	9.13662886	3.09969331	4.00510553
H	7.20658608	4.80024197	-0.78556098
C	2.25770563	4.09290873	0.522877923
C	2.25693515	1.25542063	0.605591502
C	2.25789137	5.53125324	0.506040561
C	2.25752412	8.37655676	0.52911216
C	3.49690804	1.95646989	0.625827769
C	3.51227535	6.22897927	0.4575584
C	3.51630768	3.40174504	0.575459091
C	3.49552265	7.67977743	0.486315479
C	4.72198988	1.25008759	0.641040028
C	4.72345782	8.3792635	0.54410481
C	5.96361222	7.70250136	0.434928135
C	7.20494034	8.39837844	0.526314929
C	8.44500531	7.70050266	0.441662974
C	9.68589685	1.24884772	0.646414352
C	9.68538355	8.37901796	0.548768449
C	10.9100701	1.95593595	0.631540767
C	10.896548	6.22854852	0.46018259
C	10.8919579	3.40182706	0.582862281
C	10.912109	7.67959275	0.48898412
C	4.78399252	4.09995579	0.596469016
C	4.75758287	5.55062166	0.369386887
C	5.96062872	1.92990308	0.751072382
C	5.97409046	6.30219782	0.143709195
C	5.96980095	3.33319383	0.85254212
C	7.20618496	1.22678632	0.716874303
C	7.20511973	5.73329894	-0.236153285

C 8.44838834 1.92788479 0.760154651
 C 8.4340905 6.30090186 0.150866846
 C 8.44072426 3.33257469 0.879629645
 C 9.62625699 4.10064266 0.612021535
 C 9.65125902 5.54808954 0.377174788

1.6) Geometry of minimum **E**

36

Min E

N 8.7937 4.2197 4.3124
 O 7.8694 5.0498 4.2855
 O 10.0008 4.4470 4.4286
 O 6.5325 3.3308 2.0597
 H 6.4082 4.2706 2.3438
 C 2.2573 3.8421 0.1002
 C 2.2398 0.9933 0.1239
 C 2.2850 5.2814 0.1264
 C 2.2618 8.1227 0.1109
 C 3.4675 1.6628 0.2229
 C 3.5306 5.9546 0.2066
 C 3.4743 3.1139 0.2394
 C 3.5077 7.3993 0.1469
 C 4.7036 0.9499 0.2817
 C 4.7464 8.0666 0.1940
 C 6.0040 7.3617 0.2134
 C 7.2070 8.1389 0.2166
 C 8.4489 7.4518 0.1225
 C 9.6283 1.0788 0.1191
 C 9.6601 8.1685 0.1172
 C 10.8856 1.7222 0.0806
 C 10.9373 6.0138 0.0717
 C 10.9105 3.1557 0.0458
 C 10.9116 7.4604 0.0950
 C 4.6746 3.7978 0.5204

C 4.7581 5.2329 0.3506
 C 5.9018 1.6481 0.5335
 C 6.0490 5.8731 0.2223
 C 5.7446 2.9940 1.0159
 C 7.1706 1.0215 0.3416
 C 7.3337 5.2186 0.1164
 C 8.3684 1.8190 0.1826
 C 8.4787 5.9923 0.0637
 C 8.4373 3.2899 0.0737
 C 9.6797 3.8856 0.0229
 C 9.7345 5.3322 0.0279

1.7) Geometry of minimum **F**

36

Min F

N 8.0081 5.8054 3.7308
 O 6.6455 5.3005 4.0413
 O 8.3166 6.6945 4.4633
 O 6.4572 3.1491 2.1352
 H 6.5405 4.5707 3.3573
 C 2.4024 3.7072 0.1484
 C 2.4041 0.8573 0.1750
 C 2.4335 5.1400 0.1320
 C 2.4175 7.9831 0.1276
 C 3.6241 1.5228 0.2887
 C 3.6783 5.8113 0.1678
 C 3.6212 2.9873 0.2973
 C 3.6596 7.2570 0.1377
 C 4.8670 0.8016 0.3018
 C 4.8989 7.9199 0.1878
 C 6.1572 7.2110 0.1808
 C 7.3606 7.9950 0.1682
 C 8.6051 7.3111 0.0977
 C 9.7840 0.9395 0.1357

C 9.8136 8.0296 0.1142
 C 11.0413 1.5868 0.1320
 C 11.0854 5.8750 0.0824
 C 11.0561 3.0141 0.1012
 C 11.0677 7.3230 0.1011
 C 4.8209 3.6796 0.4778
 C 4.9091 5.0816 0.2886
 C 6.0729 1.4940 0.4779
 C 6.2081 5.7332 0.1874
 C 5.9108 2.8521 1.0616
 C 7.3180 0.8746 0.2815
 C 7.4850 5.0787 0.1041
 C 8.5275 1.6812 0.1706
 C 8.6329 5.8485 0.0595
 C 8.5874 3.1442 0.0866
 C 9.8273 3.7430 0.0605
 C 9.8844 5.1922 0.0481

1.8) Geometry of minimum **G**

36

Min G

N 8.6880199 3.18924809 4.08604054
 O 7.22337264 2.78943404 3.86207632
 O 8.94906145 3.163311 5.23675658
 O 7.57675403 3.08481126 0.430807432
 H 7.15892255 2.86738979 2.87669801
 C 2.62944841 3.0594716 0.113208476
 C 2.62946429 0.202925187 0.102692666
 C 2.62920182 4.49471672 0.135218546
 C 2.62933464 7.33240114 0.121813957
 C 3.8644645 0.905547159 0.0996287298
 C 3.86839946 5.18897081 0.151363214
 C 3.8597834 2.35087416 0.105011521
 C 3.86978009 6.63680241 0.135013225

C 5.09921759 0.211694183 0.113359292
 C 5.10367115 7.32995634 0.125882801
 C 6.34401922 6.632297 0.13843171
 C 7.57513263 7.34370807 0.146530768
 C 8.80676622 6.63316591 0.134513682
 C 10.0514155 0.212348776 0.112330042
 C 10.0470534 7.33046912 0.122108179
 C 11.28634 0.906011776 0.0999150147
 C 11.282024 5.18951481 0.148810463
 C 11.2914418 2.35055031 0.104990354
 C 11.2807185 6.63700562 0.132053537
 C 5.09648174 3.0542862 0.144698756
 C 5.09097089 4.49763566 0.176445158
 C 6.3455422 0.910720396 0.144592921
 C 6.33712246 5.19392074 0.169615067
 C 7.57502627 0.191529355 0.164143374
 C 8.80511889 0.911337946 0.14436855
 C 8.81438902 5.1944642 0.165945223
 C 10.0600797 4.49818707 0.173162142
 C 10.0547445 3.05386021 0.144019822
 C 8.8854861 2.30750914 0.149278785
 C 7.57596238 4.5598685 0.197117996
 C 6.26627197 2.30690006 0.1494042

1.9) Geometry of **TS1**

36

TS1

N 7.6583 4.4833 4.1935
 O 7.8757 5.7080 4.1276
 O 7.7759 3.7635 5.1942
 O 7.2458 3.8356 3.0440
 H 7.2846 4.5686 2.0681
 C 2.3392 3.8906 0.3609
 C 2.3391 1.0528 0.3445

C 2.3394 5.3354 0.3811
 C 2.3394 8.1755 0.3998
 C 3.5829 1.7499 0.3217
 C 3.5888 6.0298 0.4275
 C 3.5954 3.1916 0.3300
 C 3.5786 7.4794 0.4264
 C 4.8131 1.0522 0.3429
 C 4.8144 8.1736 0.4134
 C 6.0472 7.4839 0.5107
 C 7.2857 8.1748 0.4550
 C 8.5242 7.4838 0.5100
 C 9.7575 1.0527 0.3403
 C 9.7565 8.1739 0.4121
 C 10.9877 1.7499 0.3199
 C 10.9825 6.0300 0.4254
 C 10.9752 3.1920 0.3289
 C 10.9924 7.4796 0.4254
 C 4.8797 3.8961 0.3374
 C 4.8299 5.3467 0.5044
 C 6.0628 1.7455 0.3041
 C 6.0571 6.0452 0.6804
 C 6.0623 3.1438 0.2242
 C 7.2857 1.0235 0.3301
 C 7.2862 5.4168 0.9605
 C 8.5075 1.7459 0.3002
 C 8.5145 6.0453 0.6789
 C 8.5085 3.1448 0.2147
 C 9.6910 3.8970 0.3349
 C 9.7412 5.3469 0.5007

1.10) Geometry of **TS2**

36

TS2

N 8.7291 3.3147 4.2302

O 9.7299 4.0437 4.1129
O 7.9368 3.0598 3.1275
O 8.3272 2.7762 5.2746
H 7.3148 4.7108 2.2334
C 2.4188 4.0049 1.0781
C 2.4122 1.1666 0.9777
C 2.4144 5.4360 1.1037
C 2.4155 8.2835 1.0190
C 3.6623 1.8715 0.9632
C 3.6705 6.1415 1.1171
C 3.6791 3.3060 1.0391
C 3.6524 7.5920 1.0547
C 4.8846 1.1692 0.9205
C 4.8822 8.2969 0.9835
C 6.1140 7.6167 1.0502
C 7.3647 8.2961 0.9720
C 8.6043 7.5939 1.0557
C 9.8475 1.1475 0.9421
C 9.8461 8.2751 0.9701
C 11.0719 1.8579 0.9871
C 11.0581 6.1314 1.1399
C 11.0485 3.3081 1.0587
C 11.0724 7.5804 1.0480
C 4.9637 4.0072 1.0933
C 4.9077 5.4698 1.2262
C 6.1349 1.8613 0.8942
C 6.1241 6.2174 1.3426
C 6.1416 3.2466 0.9263
C 7.3747 1.1324 0.9106
C 7.3420 5.6300 1.6860
C 8.6070 1.8279 0.9783
C 8.5811 6.1994 1.3614
C 8.5814 3.2068 1.2584
C 9.7932 4.0038 1.1888

C 9.8163 5.4470 1.2771

1.11) Geometry of **TS3**

36

TS3

N 7.7619 3.7793 4.1100

O 7.1469 4.3290 5.0183

O 8.9366 3.4622 4.0308

O 6.7930 3.4591 2.5168

H 5.9253 3.6859 2.9375

C 2.3373 3.8919 0.1603

C 2.3281 1.0442 0.1493

C 2.3637 5.3325 0.1687

C 2.3464 8.1737 0.1314

C 3.5627 1.7218 0.2202

C 3.6127 6.0128 0.1947

C 3.5591 3.1688 0.2422

C 3.5910 7.4567 0.1460

C 4.7992 1.0118 0.2389

C 4.8319 8.1262 0.1646

C 6.0843 7.4235 0.1517

C 7.2946 8.1816 0.1590

C 8.5333 7.4910 0.1116

C 9.7239 1.1131 0.1168

C 9.7485 8.2056 0.1214

C 10.9766 1.7650 0.1201

C 11.0175 6.0563 0.1222

C 10.9914 3.2026 0.1181

C 10.9971 7.5042 0.1215

C 4.7934 3.8580 0.3994

C 4.8404 5.3011 0.2626

C 6.0181 1.7208 0.3902

C 6.1193 5.9377 0.1466

C 5.9105 3.0883 0.6963

C 7.2694 1.0585 0.2413
C 7.3922 5.2907 0.0805
C 8.4652 1.8443 0.1347
C 8.5564 6.0321 0.0789
C 8.5218 3.3059 0.0684
C 9.7573 3.9270 0.0997
C 9.8112 5.3704 0.0903

1.12) Geometry of **TS4**

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TS4

N 7.5643 3.9424 3.2134
O 7.5716 5.1792 3.1495
O 8.4040 3.1225 2.5479
O 6.1652 3.2661 3.3040
H 5.6458 4.0057 3.7118
C 2.5364 3.7771 0.1800
C 2.5520 0.9271 0.1983
C 2.5156 5.2194 0.2140
C 2.5343 8.0572 0.1938
C 3.7958 1.6479 0.1691
C 3.7552 5.9399 0.1676
C 3.7745 3.0868 0.1461
C 3.7758 7.3870 0.1843
C 5.0486 0.9948 0.1980
C 5.0245 8.0882 0.2020
C 6.2407 7.3748 0.2111
C 7.4797 8.0636 0.2811
C 8.6893 7.3070 0.2621
C 9.9746 0.8969 0.3170
C 9.9399 8.0111 0.2484
C 11.2100 1.6044 0.2617
C 11.1625 5.8983 0.2793
C 11.2064 3.0516 0.2690

C	11.1812	7.3418	0.2199
C	5.0112	3.8097	0.1416
C	4.9629	5.2541	0.1329
C	6.3083	1.7238	0.2590
C	6.2175	5.9153	0.1626
C	6.2390	3.1801	0.1894
C	7.5052	0.9420	0.3878
C	7.3857	5.1804	0.2063
C	8.7615	1.5996	0.5406
C	8.6589	5.8209	0.2753
C	8.9032	2.9567	0.9014
C	9.9891	3.7434	0.5233
C	9.9375	5.1854	0.3942

1.13) Geometry of **TS** for bimolecular dehydration in gas phase (Gaussian 98)

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TS (HNO₃)₂

N	2.49397	-0.09351	1.93467
N	2.62494	-2.35358	-0.30453
O	2.00517	0.631	2.79462
O	2.01925	-1.26018	1.67215
O	3.54459	0.31408	1.24238
O	2.09487	-1.66797	-1.10841
O	2.62407	-3.46762	0.10422
O	4.40126	-1.58306	-0.06122
H	4.03414	-0.6824	0.54859
H	4.82289	-2.20143	0.57039

Section 2: Normal modes of vibration (NMV) with the imaginary frequency for each transition state. The x (first column), y (second column) and z (third column) 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

2.5) **TS** gas-phase $(\text{HNO}_3)_2$ (Gaussian 98)

2.5.1) Frequency (cm^{-1})

2.5.2) Normal mode

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

2.1.1) Frequency: $1537i \text{ cm}^{-1}$

2.1.2) NMV

-5.074E-02	-5.624E-02	-1.275E-01
-1.875E-02	-1.553E-02	2.576E-02
1.800E-02	4.913E-03	2.610E-02
7.795E-02	3.902E-02	1.283E-01
-1.690E-01	3.807E-01	-8.503E-01
3.860E-05	-2.129E-02	1.586E-02
1.641E-02	-1.588E-02	4.328E-03
1.881E-03	-1.105E-02	1.193E-02
-9.761E-03	-1.743E-02	1.311E-02
9.148E-03	-9.503E-04	4.472E-04

4.090E-03	1.515E-03	-5.735E-04
-7.700E-04	-6.054E-03	3.925E-03
7.609E-04	-5.025E-04	1.948E-03
4.983E-03	-4.773E-04	2.317E-03
-2.643E-03	-3.228E-03	-1.060E-03
-2.818E-03	-1.128E-02	-1.840E-02
8.563E-04	1.138E-02	-1.935E-03
6.897E-04	-2.944E-03	-2.036E-02
6.598E-03	8.115E-04	3.257E-03
-2.246E-03	1.047E-02	4.768E-03
-6.360E-03	1.317E-02	-1.424E-03
2.978E-03	1.024E-02	-5.138E-03
1.476E-02	1.497E-02	-6.220E-03
8.516E-03	1.596E-02	-9.103E-03
1.271E-02	-7.243E-03	9.846E-03
1.684E-02	9.747E-03	1.601E-02
-4.733E-03	-6.294E-04	-3.593E-03
-1.767E-04	2.256E-02	2.659E-03
-8.195E-03	-4.756E-03	1.531E-04
1.058E-02	-4.853E-03	7.406E-03
3.009E-02	-7.812E-02	1.976E-01
7.476E-03	1.811E-03	-8.962E-03
1.048E-02	3.376E-02	-8.776E-03
1.017E-02	-1.658E-02	1.105E-02
7.996E-04	-6.067E-04	4.413E-03
-1.443E-02	9.212E-03	1.557E-02

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

2.2.1) Frequency: 152i cm⁻¹

2.2.2) NMV

-7.244E-02	-7.437E-02	9.334E-02
-1.768E-02	-2.758E-02	-1.156E-01
-5.252E-02	-1.166E-01	5.234E-01
3.450E-01	-1.319E-01	2.377E-01

1.504E-02	-1.281E-02	-8.539E-03
7.012E-03	3.137E-02	-1.970E-02
-1.201E-02	2.322E-02	1.722E-02
-2.692E-03	2.846E-02	-1.357E-03
1.439E-03	2.608E-02	2.269E-02
-8.880E-03	1.710E-02	-3.334E-04
3.766E-03	2.013E-02	9.168E-03
5.445E-03	1.879E-02	-1.827E-02
2.122E-03	1.690E-02	9.011E-03
-1.533E-02	1.531E-02	2.226E-03
1.269E-03	7.380E-03	-1.253E-02
1.680E-03	8.385E-03	9.561E-03
2.020E-04	1.811E-02	3.846E-03
2.264E-03	2.177E-02	2.698E-02
-1.036E-02	1.482E-02	-9.368E-03
5.412E-03	1.562E-02	3.775E-02
-1.506E-02	6.473E-03	-2.787E-02
-7.591E-03	5.964E-03	2.357E-02
-1.616E-02	-3.120E-03	-5.991E-02
-1.403E-03	7.202E-03	5.722E-02
1.342E-02	2.080E-02	-4.831E-02
4.609E-03	1.215E-02	-1.363E-02
-1.407E-02	5.781E-03	-4.764E-02
9.094E-03	5.132E-03	4.866E-03
1.105E-02	4.906E-03	-6.023E-02
-2.598E-02	5.805E-03	-4.076E-02
8.477E-03	-6.777E-03	5.355E-03
-1.665E-02	4.307E-02	-1.534E-01
-1.473E-03	1.920E-02	7.101E-03
-2.589E-02	7.827E-02	-6.032E-01
-4.390E-02	1.402E-02	-2.186E-01
-9.676E-03	2.226E-02	-5.518E-02

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

2.3.1) Frequency: 360i cm⁻¹

2.3.2) NMV

-1.517E-01	5.005E-02	-3.278E-02
-1.486E-01	1.599E-03	-9.012E-02
-1.087E-01	-1.980E-02	1.324E-02
3.401E-01	7.909E-02	7.682E-01
3.487E-02	4.343E-02	8.500E-02
-2.637E-02	-3.509E-02	-1.065E-02
-1.948E-02	-3.432E-02	-1.230E-02
-2.024E-02	-3.274E-02	-2.643E-02
-2.317E-02	-3.237E-02	-1.202E-02
-1.493E-02	-3.095E-02	-2.338E-02
-2.164E-02	-3.153E-02	-3.470E-02
-2.795E-02	-3.555E-02	-2.168E-02
-2.507E-02	-3.184E-02	-1.348E-02
-2.168E-02	-3.606E-02	-1.875E-02
-2.555E-02	-3.497E-02	-8.078E-03
-2.180E-02	-2.560E-02	-2.404E-02
-2.362E-02	-3.256E-02	-2.477E-02
-2.419E-02	-3.022E-02	-2.059E-02
-1.683E-02	-2.845E-02	-1.212E-02
-2.313E-02	-2.786E-02	-1.717E-02
-1.756E-02	-2.649E-02	-6.578E-03
-2.263E-02	-2.308E-02	-1.899E-02
-2.133E-02	-2.260E-02	-6.265E-03
-2.321E-02	-2.482E-02	-1.652E-02
-1.012E-02	-3.471E-02	-1.205E-01
-2.102E-02	-2.207E-02	-7.605E-02
-1.538E-02	-2.067E-02	-1.054E-01
-2.515E-02	-2.939E-02	-4.167E-02
-8.431E-03	-1.260E-02	-3.474E-01
-1.013E-02	-3.164E-02	-5.572E-02
-2.456E-02	-2.576E-02	-3.643E-02
-2.041E-02	-3.531E-02	-3.605E-02

-2.217E-02	-2.738E-02	-1.911E-02
-3.099E-02	-2.420E-02	-2.014E-02
-2.482E-02	-2.351E-02	-3.415E-03
-2.201E-02	-2.655E-02	-1.525E-02

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

2.4.1) Frequency: 581i cm⁻¹

2.4.2) NMV

-8.672E-03	-1.254E-01	-2.695E-01
-1.034E-01	3.437E-02	1.492E-02
-2.167E-01	2.403E-01	6.959E-01
-3.944E-02	-2.194E-02	6.370E-02
-4.623E-02	-7.834E-02	1.156E-01
8.738E-04	-7.184E-03	1.540E-02
-5.136E-04	-3.096E-03	2.655E-03
-1.622E-03	-3.018E-03	6.141E-03
-1.624E-02	-6.338E-03	-1.186E-02
-8.307E-03	5.511E-03	-2.548E-03
-1.176E-02	9.077E-03	6.352E-03
-3.127E-03	7.355E-03	7.835E-03
-1.344E-02	1.017E-02	1.839E-03
-9.566E-03	4.708E-03	2.782E-03
-1.323E-02	3.602E-03	-1.305E-02
-9.399E-03	4.296E-03	-9.834E-03
-1.580E-02	1.782E-03	-2.173E-02
-8.477E-03	1.271E-02	-4.101E-03
1.204E-03	-1.509E-03	1.206E-02
-1.461E-02	1.315E-03	-2.578E-03
-1.614E-02	2.044E-02	-2.872E-03
-1.341E-02	2.214E-02	-3.279E-03
1.802E-02	1.776E-02	6.741E-03
-5.925E-04	2.302E-02	5.108E-03
-3.613E-03	1.194E-02	1.607E-02
-7.290E-03	9.976E-03	7.040E-03

-1.290E-02	-1.876E-03	-1.903E-02
-1.145E-02	5.409E-03	-3.691E-03
-6.756E-03	-3.820E-03	-1.737E-02
-1.813E-02	5.452E-03	-3.038E-02
1.291E-03	2.174E-02	-2.065E-02
-2.352E-02	1.393E-03	-8.890E-02
-2.120E-03	9.533E-03	-2.153E-02
-2.447E-02	5.083E-03	-4.998E-01
-1.560E-02	1.226E-02	-1.017E-01
-1.160E-02	2.352E-02	-4.174E-02

2.5) NMV with the imaginary frequency for **TS** (HNO₃)₂ (Gaussian 98)

2.5.1) Frequency: 670i cm⁻¹

2.5.2) NMV

-0.07	-0.07	0.04
0.16	-0.01	-0.08
0.04	0.03	-0.03
0.00	0.00	0.02
0.08	-0.05	-0.06
0.00	0.01	0.03
-0.01	0.03	0.02
-0.14	0.01	0.02
-0.50	0.63	0.50
-0.12	-0.05	-0.03