New insights into the kinetics of the reaction of vinyl radical with Nitrogen dioxide

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S1. Theoretical and computational approach

S1.1. Electronic structure calculations

Table S1 Geometries, Frequencies, zero-point correction and rotational constants of all stationary points that calculated at M06-2X/aug-cc-pVDZ level.

C2H3NO2,			
Geometry (Å):			
N	0.00000000	-0.56087700	0.00000000
O	0.78019400	-1.49423700	0.00000000
O	-1.21031700	-0.65536600	0.00000000
C	0.60816600	0.77629900	0.00000000
H	1.69209800	0.72667000	0.00000000
C	-0.15888400	1.85585700	0.00000000
H	-1.24266700	1.75973300	0.00000000
H	0.29585600	2.84362900	0.00000000
Rotational constants (GHZ):	11.9805578	4.7135697	3.3826981
Zero-point correction=		0.055805 (Hartree/Particle)	
Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):			
111.7021	324.8630	519.4505	
532.3126	637.3883	808.9326	
877.7017	932.9365	977.9366	
1028.7780	1216.7599	1323.2844	
1412.1195	1607.1252	1663.7521	

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3036.7577 3118.1623 3140.9974

C2H3ONO,

Geometry (Å):

C	2.27230800	-0.18783700	-0.00000100
H	3.16004700	0.43732700	-0.00000100
H	2.38288800	-1.26950700	-0.00000700
C	1.07532200	0.38501500	0.00000400
H	0.89384500	1.45936800	0.00000100
N	-1.21721900	0.43175900	-0.00000500
O	-2.18100900	-0.22254600	0.00000200
O	-0.06924500	-0.38152500	0.00000100

Rotational constants (GHZ): 42.5016497 2.6770792 2.5184481

Zero-point correction= 0.058847 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950(cm^{-1}):

101.9487 204.0962 244.4417

462.1626 617.9026 681.3238

845.3884 877.5298 933.9089

940.9483 1168.5193 1255.6881

1343.1392 1652.1332 1767.6118

3041.4279 3063.9089 3143.9509

cis-C2H3ONO,

Geometry (Å):

C	-2.14995600	0.10898100	-0.00003500
H	-2.83595400	0.95118500	-0.00000100
H	-2.55074300	-0.90201800	-0.00012800
C	-0.84040400	0.33591100	0.00004200
H	-0.38157400	1.32042000	0.00013900
N	1.40790400	-0.48047400	-0.00000300
O	1.70520400	0.65187100	-0.00003600
O	0.02668400	-0.73632400	0.00003100

Rotational constants (GHZ): 21.3654080 3.3120220 2.8675069

Zero-point correction= 0.053609 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950(cm^{-1}):

39.1200 274.3551 276.1906

402.5880 682.8323 735.2088

818.9777 894.4738 938.3378

940.6655 1117.2967 1254.6574

1344.5188 1646.7399 1709.0215

3037.9452 3102.3691 3139.6901

ONCH2CHO,

Geometry (Å):

N	1.05718100	0.01656700	-0.52623100
C	0.05502100	0.94673500	0.05716600
O	-1.47383000	-0.90481500	-0.05081500
C	-1.30787600	0.27608300	0.08818000
H	0.33587900	1.22309300	1.08435800
H	0.00522100	1.83658300	-0.58316800
O	1.71599000	-0.52979500	0.30559600
H	-2.16152200	0.96432600	0.27210000

Rotational constants (GHZ): 12.0357678 3.8876360 3.2040643

Zero-point correction= 0.053470 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950(cm^{-1}):

38.4045 126.5071 241.8928

521.9691 604.7614 750.3945

811.1858 923.0794 1053.2849

1147.7675 1209.6598 1330.1225

1354.2642 1680.6541 1773.0524

2829.7425 2913.3352 2987.0897

CH2OCHNO

Geometry (Å):

C	0.34802700	1.02893900	0.00001000
H	0.18730700	2.09773500	-0.00036500
C	1.43206400	-0.00122600	0.00008300
H	2.03850400	-0.08281600	0.90790100
H	2.03955000	-0.08227400	-0.90711800
N	-0.55856600	0.08490900	-0.00002800
O	0.37284500	-1.00555800	-0.00016400

O	-1.75233800	-0.08110400	0.00006700

Rotational constants (GHZ): 14.3809987 5.5170840 4.0946370

Zero-point correction= 0.056477 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

268.6635 471.0074 594.1462

664.6377 729.1171 876.6685

926.4279 966.5398 1015.9699

1057.5041 1149.9219 1261.9914

1298.3422 1419.2964 1720.8243

2954.5597 3016.9797 3158.4593

W,

Geometry (Å):

C	0.18109400	-0.12056700	0.41687800
H	-0.04808700	-0.36946000	1.45536200
C	1.36353100	0.66205500	0.00540000
H	2.05539900	0.98735200	0.78175400
H	1.29636900	1.26199500	-0.90216900
N	-0.96905200	0.01914500	-0.47293600
O	1.28035000	-0.73779800	-0.19756800
O	-2.00385700	0.07994500	0.12780900

Rotational constants (GHZ): 19.1041807 3.5645429 3.3887438

Zero-point correction= 0.055061 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

129.3448 332.8639 396.5927

522.4933 804.2698 876.8006

903.2681 1019.3220 1083.0665

1088.0613 1096.3354 1184.2263

1330.2865 1435.7825 1662.5180

2986.0702 3018.7224 3090.5960

CH2OCNOH,

Geometry (Å):

C	0.25613100	-0.20044900	0.00002500
H	-1.19942600	-1.49978600	0.00000300
C	1.67455900	-0.40992500	-0.00001200
H	2.18949600	-0.63733800	-0.93239500
H	2.18954400	-0.63734500	0.93234300

N	-0.98807700	-0.49549800	0.00000500
O	0.99135700	0.90798100	0.00000300
O	-1.97225900	0.33016900	-0.00001100

Rotational constants (GHZ): 19.7483533 3.6414626 3.1415150

Zero-point correction= 0.056151 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

167.9079 216.6871 439.1394

547.1558 781.4693 796.8752

943.5390 1002.8839 1027.8306

1060.3010 1154.0392 1228.3908

1400.5429 1443.2067 1861.8736

2997.1160 3100.4858 3245.6123

CH2CNOOH,

Geometry (Å):

N	0.42899900	0.11153000	-0.00003200
O	1.10617800	-1.11072400	-0.00002700
O	1.15675000	1.13511800	0.00001200
C	-0.82932500	0.02137300	-0.00013900
H	2.02723500	-0.79795000	0.00045800
C	-2.13010100	-0.03257400	0.00006400
H	-2.68838000	-0.05529900	0.93686000
H	-2.68871700	-0.05540000	-0.93652500

Rotational constants (GHZ): 11.7746790 3.9918851 3.0447199

Zero-point correction= 0.053660 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

108.1144 179.7811 282.4664

501.1876 557.8711 595.9901

630.8638 794.3376 903.2524

946.4607 1088.7641 1207.0396

1360.5615 1517.1112 2058.4590

2989.7425 3077.9428 3576.4906

IRCP,

Geometry (Å):

N	0.94913400	-0.28240600	0.00000100
O	1.08904900	1.06994500	-0.00000200
O	1.98648700	-0.83614200	0.00000000

C	-1.71537900	0.53596500	0.00000300
H	0.15379500	1.36862300	0.00000000
C	-2.55161100	-0.45561500	-0.00000100
H	-2.17240700	-1.48077100	-0.00000500
H	-3.62768100	-0.26354200	-0.00000100

Rotational constants (GHZ): 12.4445415 2.2375682 1.8965606

Zero-point correction= 0.047431 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

38.0337 83.0044 149.7903

160.3893 182.7790 225.3599

389.9987 703.3371 755.8704

767.8138 944.4367 1145.9774

1378.8233 1664.9576 1737.6963

2993.3947 3084.1291 3372.8135

IRCP3,

Geometry (Å):

N	1.10599300	-0.10935600	0.00005100
O	2.26148200	-0.45864100	-0.00012600
O	0.68883500	1.03414300	0.00006500
C	-1.72378900	-0.75442800	0.00013100
H	0.35321100	-0.84601700	0.00020600
C	-2.69309800	0.05142400	-0.00010000
H	-3.60014500	0.63446800	-0.00039700
H	-1.59622300	0.59105200	0.00014000

Rotational constants (GHZ): 17.4756582 2.0652094 1.8469443

Zero-point correction= 0.047787 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

60.1075 83.4196 146.4814

209.1819 210.2161 286.6321

592.3181 595.2070 766.8077

1072.3514 1108.8790 1383.9058

1450.0892 1653.1442 1813.3277

2317.3180 2949.0181 3229.0158

NOCH2CHO

Geometry (Å):

C	-0.02730500	0.75954200	0.15839200

H	0.23262800	1.66512900	-0.39797300
H	-0.13019500	0.95964800	1.22864300
C	0.97530600	-0.35098400	-0.08233300
H	0.54174500	-1.33999900	-0.34394500
N	-1.80713900	-0.70773100	0.21347500
O	-1.36837200	0.31687000	-0.31572800
O	2.15809600	-0.16462100	0.01105200

Rotational constants (GHZ): 18.4609204 3.0385282 2.7321230

Zero-point correction= 0.053009 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950(cm^{-1}):

53.4902 176.0650 281.1468

425.8245 583.6975 716.4890

772.4984 994.9559 1047.2097

1146.0184 1189.8226 1319.4692

1347.4307 1419.2616 1775.8169

2847.1075 2966.6297 3041.9561

TS1

Geometry (Å):

C	1.70283300	-0.52634100	-0.22969700
H	2.73673000	-0.58172700	0.10029600
H	1.35814600	-1.15910200	-1.04202200
C	0.88356400	0.28915500	0.43000500
H	1.07637100	0.94611900	1.26762300
N	-0.72890600	0.04432800	0.31221500
O	-1.53713100	-0.77755500	0.01006700
O	-0.41128000	1.01599600	-0.47422300

Rotational constants (GHZ): 11.5930266 4.4847464 3.7248140

Zero-point correction= 0.051834 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-812.8284 162.2771 299.6946

469.1226 532.0735 559.7191

759.5644 792.2235 918.6585

934.0316 1169.2289 1236.6017

1297.0618 1547.1372 1594.9398

3043.3407 3143.8398 3155.2074

TS2

Geometry (Å):

C	2.13492300	-0.19871200	-0.20946700
H	2.90468500	-0.81415000	0.24675900
H	2.36390200	0.35955300	-1.11394900
C	0.93852900	-0.12249400	0.36470800
H	0.67565600	-0.66908200	1.27290800
N	-1.37552300	0.26644600	0.34424600
O	-1.80140600	-0.55585900	-0.34401000
O	-0.04313100	0.70408200	-0.12435100

Rotational constants (GHZ): 20.5601415 3.0367598 2.9068268

Zero-point correction= 0.052369 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-238.1417 36.8138 271.2450

404.2994 601.0988 676.3487

773.8219 860.1579 910.0382

925.2349 1113.1787 1271.7992

1342.4859 1641.8263 1793.0100

3027.9224 3045.7262 3142.9648

TS3,

Geometry (Å):

O	0.05507100	-0.59843400	0.00000000
H	-0.88113500	-0.86768100	0.00000000
O	0.05507100	0.70689500	0.00000000

Rotational constants (GHZ): 16.5784651 3.0223595 2.7440957

Zero-point correction= 0.044114 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1603.2886 89.3196 181.2495

236.3158 342.4559 473.2681

663.9491 668.7792 694.1137

811.3370 849.0677 970.4715

1060.8513 1549.2940 1630.0366

1752.2682 3178.1046 3244.5825

TS4,

Geometry (Å):

C	-1.87248500	-0.67522800	0.02247700
H	-2.66580100	-1.40014100	0.11939900

H	-0.60608300	-0.66129800	-0.51663400
C	-1.57075000	0.52242600	0.25984500
H	-1.52101400	1.56253100	0.53903400
N	1.25572600	0.42116200	0.22005900
O	1.91779000	-0.56113000	0.15326700
O	0.16498900	0.36957900	-0.57528500

Rotational constants (GHZ): 16.2828556 2.9679409 2.7174795

Zero-point correction= 0.044151 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1600.6207 74.4583 201.9947

223.9757 337.5646 512.4357

644.3386 668.7961 701.2254

752.1680 885.5151 974.6240

1077.3902 1545.8201 1651.4847

1743.8460 3176.3858 3239.0497

TS5,

Geometry (Å):

C	-1.62360600	-0.44439100	0.00025500
H	-1.90830600	-1.48159400	0.00031900
H	-0.26731100	0.94773900	-0.00038100
C	-1.63568500	0.80637800	-0.00007100
H	-2.29997000	1.65643600	-0.00008500
N	0.80637000	0.17358000	-0.00016300
O	1.98783900	0.39057400	0.00022000
O	0.31050300	-0.95426900	-0.00019700

Rotational constants (GHZ): 15.1079355 3.4518231 2.8098384

Zero-point correction= 0.047669 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-977.8993 213.4192 345.8000

411.2837 495.2214 571.9494

675.3724 701.1856 714.9063

809.8039 954.3334 1131.6961

1378.5446 1603.8579 1642.0759

1786.4409 3182.2228 3259.8556

TS6,

Geometry (Å):

N	-0.80646800	-0.17378600	-0.00003600
O	-0.31040800	0.95402500	0.00071400
O	-1.98800800	-0.39037100	-0.00038300
C	1.62338100	0.44450000	-0.00069300
H	1.90805500	1.48183600	-0.00135900
C	1.63589400	-0.80625800	0.00040900
H	0.26772800	-0.94842000	0.00036200
H	2.30117100	-1.65559500	0.00030600

Rotational constants (GHZ): 12.3685900 3.9599714 2.9996067

Zero-point correction= 0.048237 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-759.7795 208.6867 287.9193

384.8459 530.4416 618.1308

667.1135 672.8804 724.9022

915.5559 984.9494 1081.3194

1348.8419 1590.2260 1738.7261

1962.6416 3169.4464 3228.1646

TS7,

Geometry (Å):

C	0.50804100	-0.92341600	-0.04578300
H	0.41807200	-1.96565600	-0.31686600
C	1.58664300	-0.02571800	0.11023600
H	2.49697300	-0.11586800	-0.49340000
H	1.68348000	0.58103500	1.00982800
N	-0.52471200	-0.04681800	-0.01790200
O	0.03403400	1.13731000	-0.14990400
O	-1.72074000	-0.19693200	0.09228300

Rotational constants (GHZ): 13.3554596 5.2879532 3.9050160

Zero-point correction= 0.054124 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-884.6389 252.4228 527.5502

565.8445 703.6988 732.2315

843.2253 960.1377 997.0402

1033.3435 1122.7912 1250.5810

1320.6733 1466.5234 1598.1308

2973.1128 3068.2228 3154.1976

TS8,

Geometry (Å):

C	0.08391600	1.03930800	-0.06746600
H	-0.19174900	2.09785900	-0.14579700
C	1.39828700	0.17732300	0.05668100
H	1.74580500	0.52135500	1.06484800
H	2.13924900	0.55885600	-0.68435100
N	-0.86500800	0.22262900	0.02465700
O	0.99561600	-1.07637000	-0.05948100
O	-1.81204900	-0.42816300	0.01665800

Rotational constants (GHZ): 11.9948672 4.5210587 3.3619307

Zero-point correction= 0.050239 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1097.3339 155.8968 224.1952

360.5366 559.9455 585.1468

668.3500 871.8546 1021.0629

1055.6662 1120.2407 1193.6826

1272.3155 1381.7350 2037.2085

2690.4896 2757.1320 2994.2604

TS9,

Geometry (Å):

C	-0.12827900	0.84312600	-0.12269000
H	0.17857100	1.69234300	-0.74989300
C	-1.45165700	0.25370700	0.14197500
H	-2.17317700	0.63583100	-0.60118100
H	-1.84954100	0.33741600	1.16278200
N	0.78247900	-0.03260100	0.35227100
O	-0.91622400	-0.97080800	-0.21020500
O	1.89702500	-0.15648900	-0.08895900

Rotational constants (GHZ): 15.1602802 4.2703292 3.5776425

Zero-point correction= 0.052447 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-792.6315 228.8495 283.4952

443.1246 594.0265 831.5378

874.1567 995.9889 1052.8242

1096.2024 1139.0429 1203.6956

1352.3471 1377.5288 1614.5839

2872.6598 2942.9832 2967.5976

TS10,

Geometry (Å):

C	0.24404300	-0.18642300	-0.17056300
H	-0.59023900	-1.00640000	-1.02101000
C	1.63280600	-0.40981500	0.14854300
H	2.32822800	-0.70451400	-0.63437200
H	1.92393900	-0.57726700	1.18422100
N	-1.04055200	-0.55111000	0.06930700
O	0.98945000	0.90906700	-0.07989000
O	-1.94434400	0.30635600	0.09465600

Rotational constants (GHZ): 18.7706565 3.6843459 3.2272421

Zero-point correction= 0.049750 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1466.6165 194.8562 220.3810

479.2635 556.1282 782.5188

885.7012 965.7769 1010.4000

1046.3845 1059.4475 1176.9977

1350.3750 1404.9049 1594.0933

1897.9223 3006.4509 3114.3252

TS11,

Geometry (Å):

C	-0.71430800	0.03747800	0.70794300
H	1.61997000	-0.98285000	0.92408000
C	-1.67396800	-0.57284500	-0.27847200
H	-2.68224300	-0.82304400	0.04085900
H	-1.28837900	-0.99686300	-1.20165400
N	1.36572600	-0.46629900	0.03913900
O	-1.32967700	0.83224200	-0.09614300
O	2.21970500	0.32763900	-0.23061800

Rotational constants (GHZ): 15.5233168 2.5950440 2.4431799

Zero-point correction= 0.049920 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-163.5044 45.9901 124.0757

192.0064 246.7792 520.0842

838.6974 862.4160 876.9659

1062.9820 1071.8910 1355.8571

1465.5610 1471.7276 1647.4406

2892.1508 3013.5860 3128.3158

TS12,

Geometry (Å):

N	0.94123900	0.00076600	-0.50008200
C	-0.90401000	1.11266700	0.12281500
O	-0.50195800	-1.15991200	0.21905800
C	-1.29569100	-0.21368800	-0.06984100
H	-0.24843400	1.37055200	0.94960300
H	-1.46903900	1.92197600	-0.33630600
O	1.81969000	0.12939300	0.18121900
H	-2.21484900	-0.44760300	-0.63278300

Rotational constants (GHZ): 10.2615738 4.4783912 3.3855597

Zero-point correction= 0.052090 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-373.6542 234.2742 330.8774

382.5389 426.0745 545.5508

730.5521 807.6917 926.1721

982.6005 1180.4049 1282.6757

1406.2090 1475.2986 1942.9571

2909.1394 3031.6007 3126.9886

TS13,

Geometry (Å):

N	-1.09154100	-0.02568600	-0.50622700
C	0.02859600	1.02757900	0.11986800
O	2.02964500	-0.51251200	0.10017000
C	0.99811800	0.01023500	-0.06903700
H	0.09513100	1.89661600	-0.53669700
H	-0.24684700	1.24653500	1.15262900
O	-1.80001400	-0.54637400	0.34423300
H	-0.20482200	-0.71914400	-0.93255200

Rotational constants (GHZ): 14.1683367 3.2648761 2.9073757

Zero-point correction= 0.047663 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1074.1003 106.1025 290.5119

378.7398 441.8750 534.0235

606.0915 833.0339 896.5188

949.0634 1066.4710 1209.7908

1318.9062 1404.8655 1810.0464

1974.1515 2981.6756 3073.8694

TS14,

Geometry (Å):

N	0.47038500	0.11924200	-0.00008200
O	1.40589300	-0.77559200	0.00014300
O	0.69491100	1.28136500	-0.00003200
C	-0.77306100	-0.70930000	-0.00024000
H	0.54679600	-1.53610500	0.00001900
C	-1.88330000	0.03721400	0.00009500
H	-1.84767200	1.13050700	0.00032500
H	-2.86008600	-0.44276400	0.00021100

Rotational constants (GHZ): 10.9993314 4.8609044 3.3711163

Zero-point correction= 0.050104 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1196.1523 93.5998 305.5067

480.6182 554.4877 715.7015

811.5781 812.5128 956.8125

1020.5001 1056.3076 1266.7120

1327.5208 1567.8623 1660.1317

2171.8292 2990.3196 3101.5676

TS15,

Geometry (Å):

N	-0.65604100	-0.04127500	0.37492800
O	-1.41553400	0.95349100	-0.12613000
O	-1.26883800	-0.84977800	0.96517800
C	1.30850000	0.79240100	-0.43129500
H	-0.73407900	1.50342800	-0.56660500
C	2.22238600	-0.06059000	-0.04607300
H	2.06927400	-0.96760500	0.53388000
H	3.23385300	0.21350200	-0.36690200

Rotational constants (GHZ): 10.5879577 3.0752529 2.3830912

Zero-point correction= 0.048984 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-103.9823 90.1681 165.4710

191.0672 269.9362 466.8129

581.9353 699.4366 725.2737

798.0926 980.1606 1187.7593

1356.6856 1629.1036 1748.9509

2989.6559 3111.7554 3434.1949

TS16,

Geometry (Å):

N	0.83316600	-0.02995600	-0.00023000
O	1.88490600	-0.61732000	0.00043500
O	0.65542200	1.16183400	-0.00023500
C	-1.40280400	-0.90398000	-0.00041000
H	-0.19183500	-0.99866200	-0.00093700
C	-2.13142800	0.16390400	0.00036000
H	-3.21971000	0.19304400	0.00065400
H	-1.53784600	1.09964500	0.00058900

Rotational constants (GHZ): 12.6183512 3.0792273 2.4752082

Zero-point correction= 0.045078 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-1069.0895 85.7299 198.3267

263.7914 351.3943 379.5041

466.7874 680.2104 794.2808

834.5603 910.5525 1173.3099

1356.6762 1624.7064 1632.9683

2095.7336 2858.0470 3091.1594

TS17,

Geometry (Å):

C	1.35505200	-0.48608500	-0.06334300
O	0.10712500	-0.34952400	0.25087600
N	-2.25400000	0.09495800	0.41848700
O	-1.73769100	0.20387100	-0.54178200
H	1.68620300	-1.47792100	-0.41633200
C	2.28199600	0.51126800	0.01460300
H	1.99513100	1.50257600	0.36295300

H	3.31890100	0.32477300	-0.25634000

Rotational constants (GHZ): 23.1189428 2.1989413 2.1505885

Zero-point correction= 0.051046 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-119.9312 69.6664 98.0200

289.3212 395.2902 497.5292

685.4065 837.2506 950.1301

965.5454 1222.9969 1251.2117

1363.6840 1515.1871 2094.9134

2900.1221 3023.8782 3126.0938

TS18,

Geometry (Å):

C	-1.20108900	0.20572000	-0.40113200
H	-1.87919700	1.00361900	-0.71108200
H	-1.40171000	-0.77756500	-0.82768500
C	-0.89523000	0.15963900	1.05676700
H	-0.86746800	1.13180200	1.59266900
N	1.02387700	-0.23442500	-1.23928800
O	0.21353400	0.63187200	-1.08881800
O	-0.61155600	-0.87111200	1.61857800

Rotational constants (GHZ): 11.7836789 3.6458920 3.0793754

Zero-point correction= 0.051425 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-165.4072 102.0042 148.8659

303.2083 465.6921 530.8790

871.7849 957.1457 1033.2827

1082.5106 1116.6476 1333.2386

1369.7168 1475.6513 1740.5501

2841.1393 2984.5311 3087.5646

TS19,

Geometry (Å):

C	1.29093800	1.02508100	-0.14909300
H	0.65105800	1.40819200	-0.94301300
H	1.99691000	1.70512400	0.32203800
C	1.29497700	-0.32217200	0.16250200
H	2.02875400	-0.67827900	0.90829500

N	-2.08704300	0.23024800	-0.15755900
O	-1.12985700	0.11593200	0.36807600
O	0.43199300	-1.14896000	-0.27618300

Rotational constants (GHZ): 10.6941447 3.6352491 2.9022038

Zero-point correction= 0.051210 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

-93.8207 146.5590 253.1503

283.0293 383.6523 509.1154

650.6460 784.1629 943.4155

966.1227 1199.0547 1274.8278

1391.0199 1469.7415 2076.2791

2883.0281 3019.4621 3121.2753

C2H3,

Geometry (Å):

C	0.05027400	-0.58843500	0.00000000
H	0.97945600	-1.16207700	0.00000000
H	-0.88410400	-1.16169200	0.00000000
C	0.05027400	0.72383000	0.00000000
H	-0.69864400	1.51139800	0.00000000

Rotational constants (GHZ): 229.6686185 32.5318039 28.4955088

Zero-point correction= 0.036896 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

680.8507 801.7926 902.1903

1003.4532 1312.4594 1594.9018

2948.4748 3041.4441 3100.3317

NO2,

Geometry (Å):

N	0.00000000	0.00000000	0.31821200
O	0.00000000	1.09413100	-0.13921800
O	0.00000000	-1.09413100	-0.13921800

Rotational constants (GHZ): 247.9838677 13.1967389 12.5299439

Zero-point correction= 0.009222 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

735.0660 1402.6203 1708.0344

C2H2,

Geometry (Å):

O	-1.05226700	0.59856300	-0.23953000
C	-1.31472000	-0.72229200	0.02680400
C	0.18208400	1.00587400	0.30073700
H	-1.53159200	-0.93417900	1.07702300
H	-2.00996000	-1.13905800	-0.69376700
H	-0.08533500	-1.25292100	-0.07815700
H	0.33028600	2.04971700	0.03923400
H	0.21048700	0.82544100	1.38046900
O	1.18877100	0.27709300	-0.33271300
O	1.09873800	-1.03196800	0.11098700

Rotational constants (GHZ): 35.1431498 35.1431274

Zero-point correction= 0.025183 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

584.4096 585.2118 714.6745

1993.9341 3260.1722 3363.0038

HONO,

Geometry (Å):

H	1.71227700	0.41688300	0.00000100
O	1.01652600	-0.25681800	-0.00000100
N	-0.15884000	0.48433800	0.00000200
O	-1.09157600	-0.21908800	-0.00000100

Rotational constants (GHZ): 96.0142134 13.0088740 11.4566266

Zero-point correction= 0.021032 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

555.1843 668.0000 871.0246

1282.6071 1757.3695 3636.2941

cis-HONO,

Geometry (Å):

H	0.91321000	1.03682800	-0.00010900
N	-0.15665800	-0.51905300	-0.00002100
O	-1.04741000	0.25352500	0.00001200
O	1.07033400	0.07104300	0.00002000

Rotational constants (GHZ): 85.4731489 13.6339545 11.7583602

Zero-point correction= 0.020991 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

658.8506 671.3542 936.7171

1311.9489 1703.5772 3470.8668

HNO2,

Geometry (Å):

H	0.00017800	1.35203600	0.00001800
N	-0.00002600	0.30909200	-0.00000800
O	1.08658600	-0.21974000	0.00000200
O	-1.08658500	-0.21971900	0.00000200

Rotational constants (GHZ): 107.8365300 13.3806536 11.9036197

Zero-point correction= 0.022548 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.944(cm^{-1}):

768.3296 1033.2560 1413.0784

1438.3168 1667.8811 3081.7040

CH2O,

Geometry (Å):

C	0.52835500	0.00000000	0.00000100
H	1.10993900	-0.94567600	-0.00000100
H	1.10994900	0.94567200	-0.00000100
O	-0.67375200	0.00000100	0.00000000

Rotational constants (GHZ): 280.3619787 39.0774172 34.2970283

Zero-point correction= 0.026949 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

1150.7705 1193.4630 1446.2771

1768.7477 2801.3901 2876.9467

ONCH,

Geometry (Å):

C	-1.17759800	-0.00042100	-0.02499600
H	-2.24514100	-0.00140600	-0.04764400
N	-0.01984500	-0.00012600	-0.00041800
O	1.18120600	0.00060200	0.02506900

Rotational constants (GHZ): 11.4993814 11.4993812

Zero-point correction= 0.019701 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

325.5452 488.8221 543.5700

1254.7799 2254.5936 3348.0337

CH2(O)C,

Geometry (Å):

C	0.55301000	0.72075500	-0.00001400
C	-0.80330900	0.05033600	-0.00000400
H	-1.34153400	-0.07278700	-0.93618500
H	-1.34146600	-0.07268400	0.93623600
O	0.52309900	-0.56013400	0.00000700

Rotational constants (GHZ): 38.7132635 24.0414970 16.5469472

Zero-point correction= 0.032688 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

811.9485 842.0727 872.9607

1058.5485 1066.2696 1366.6120

1479.0126 3009.6981 3123.6788

HNO,

Geometry (Å):

H	-0.94388800	0.90874400	0.00000000
N	0.06292600	0.57700300	0.00000000
O	0.06292600	-0.61847100	0.00000000

Rotational constants (GHZ): 559.2559437 43.3009288 40.1892384

Zero-point correction= 0.014439 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

1500.1005 1682.4430 2838.4261

CH2CO,

Geometry (Å):

C	-1.21233500	0.00002800	-0.00002000
O	1.26533200	0.00004500	-0.00004300
C	0.10471100	-0.00015000	0.00009800
H	-1.73819500	0.94782200	-0.00006400
H	-1.73871900	-0.94744700	-0.00006400

Rotational constants (GHZ): 279.2029910 10.2746257 9.9099415

Zero-point correction= 0.031933 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

419.4754 534.7753 586.5015

931.2574 1122.3523 1335.8301

2143.7886 3067.6794 3174.3680

CH2CHO,

Geometry (Å):

C	-1.16989000	-0.17091700	0.00000200

H	-2.06044400	0.45368400	0.00000100
H	-1.26510500	-1.25476300	0.00000500
C	0.13868600	0.40939800	-0.00000100
H	0.20135300	1.51672600	-0.00000300
O	1.16392800	-0.26831600	-0.00000100

Rotational constants (GHZ): 66.5654335 11.4714347 9.7851316

Zero-point correction= 0.042900 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

421.8496 477.4042 735.1005

928.3551 933.3477 1111.5095

1320.2524 1395.0820 1544.0939

2857.1528 3023.8982 3141.5198

NO,

Geometry (Å):

O	0.00000000	0.00000000	0.53374700
N	0.00000000	0.00000000	-0.60999700

Rotational constants (GHZ): 0.0000000 51.7423275 51.7423275

Zero-point correction= 0.004736 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

1975.0513

CH2=C,

Geometry (Å):

C	0.82113300	-0.00012900	-0.00000300
C	-0.47973600	-0.00002500	0.00000200
H	-1.02339500	0.94840500	0.00000500
H	-1.02498600	-0.94748100	0.00000100

Rotational constants (GHZ): 279.0213509 39.4566701 34.5683302

Zero-point correction= 0.023778 (Hartree/Particle)

Harmonic Vibrational Frequencies scaled by 0.950 (cm^{-1}):

304.5775 738.0506 1141.9845

1651.6796 2994.4526 3084.6452

An intrinsic reaction coordinate (IRC) calculation was performed for each transition state (TS) at the M06-2X/aug-cc-pVDZ level of theory to identify whether the transition state belongs to the target reaction system.

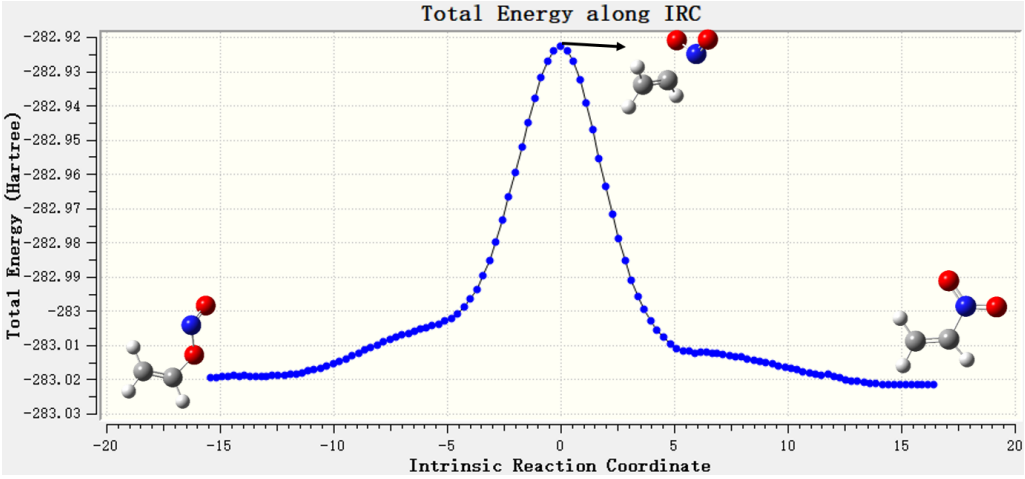

Fig. S1 Intrinsic reaction coordinate (IRC) calculation of the TS1 at the M06-2X/aug-cc-pVDZ level.

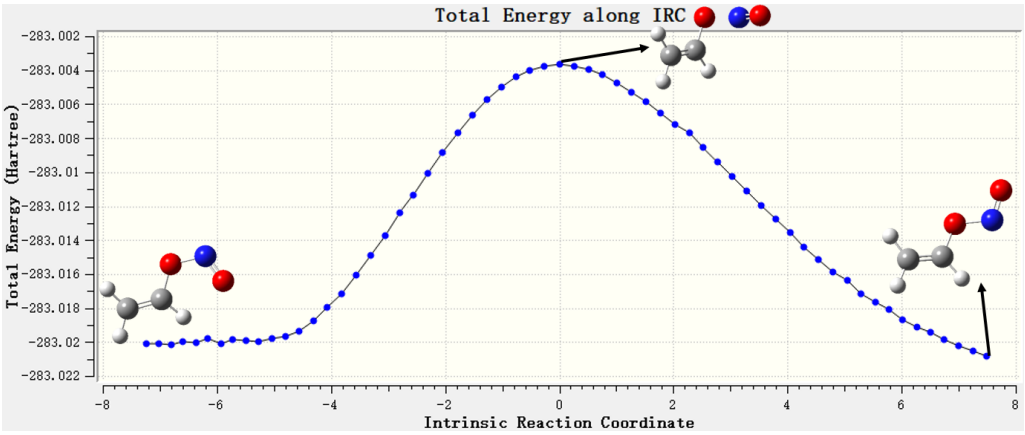

Fig. S2 Intrinsic reaction coordinate (IRC) calculation of the TS2 at the M06-2X/aug-cc-pVDZ level.

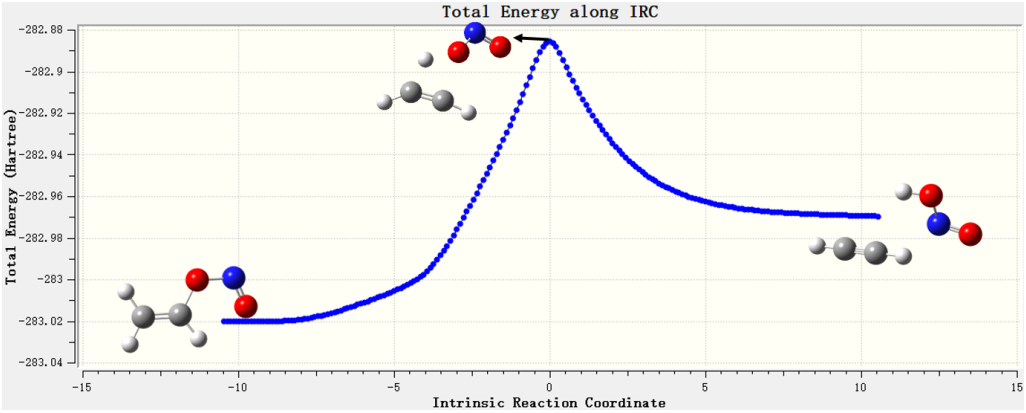

Fig. S3 Intrinsic reaction coordinate (IRC) calculation of the TS3 at the M06-2X/aug-cc-pVDZ level.

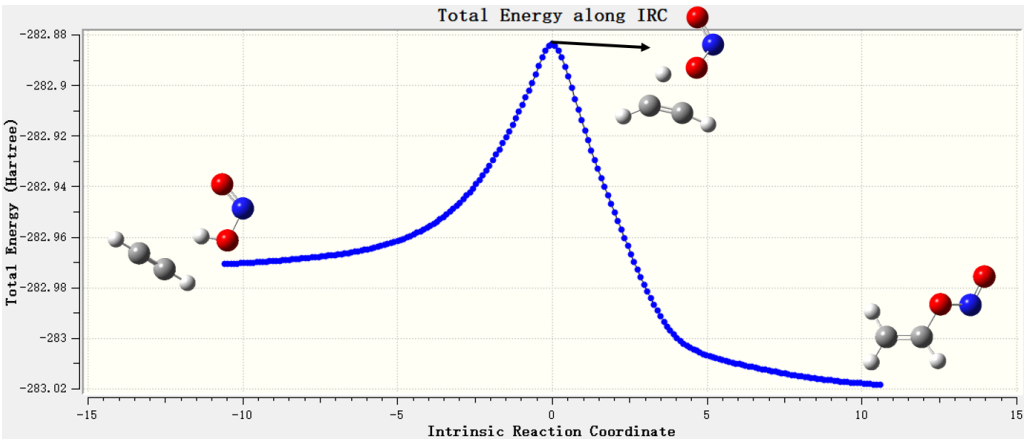

Fig. S4 Intrinsic reaction coordinate (IRC) calculation of the TS4 at the M06-2X/aug-cc-pVDZ level.

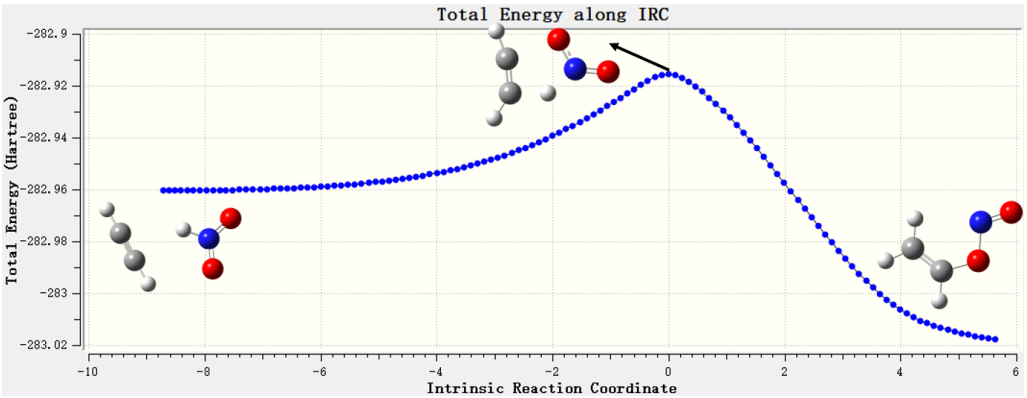

Fig. S5 Intrinsic reaction coordinate (IRC) calculation of the TS5 at the M06-2X/aug-cc-pVDZ level.

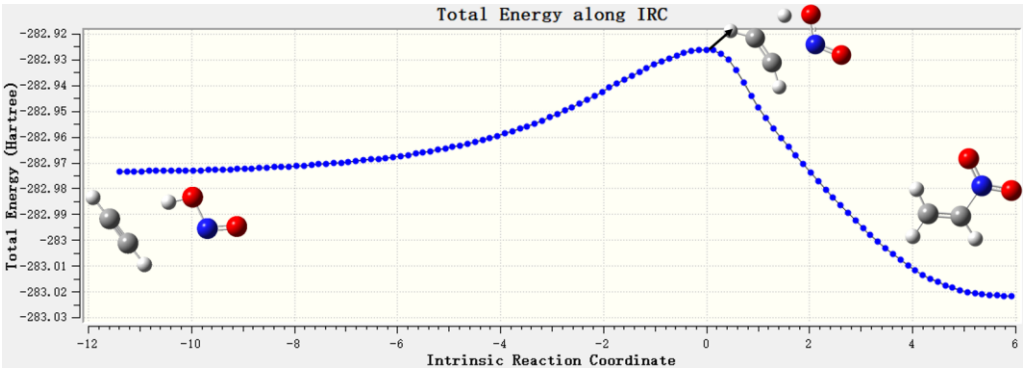

Fig. S6 Intrinsic reaction coordinate (IRC) calculation of the TS6 at the M06-2X/aug-cc-pVDZ level.

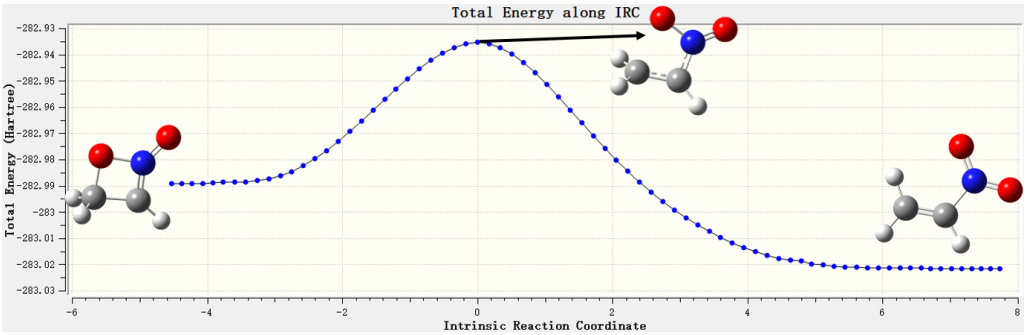

Fig. S7 Intrinsic reaction coordinate (IRC) calculation of the TS7 at the M06-2X/aug-cc-pVDZ level.

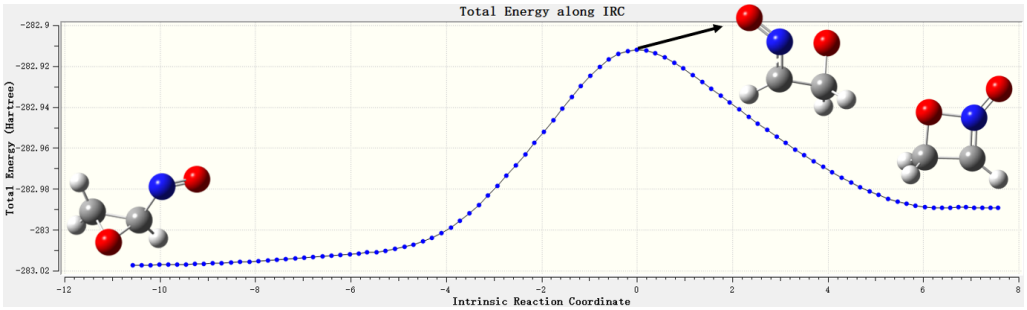

Fig. S8 Intrinsic reaction coordinate (IRC) calculation of the TS8 at the M06-2X/aug-cc-pVDZ level.

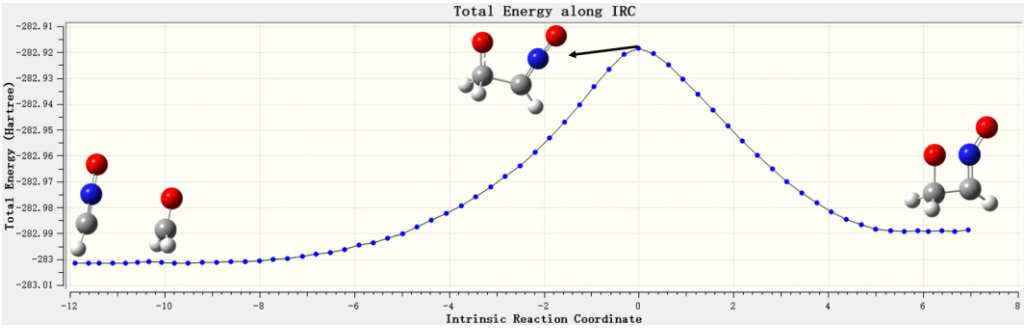

Fig. S9 Intrinsic reaction coordinate (IRC) calculation of the TS9 at the M06-2X/aug-cc-pVDZ level.

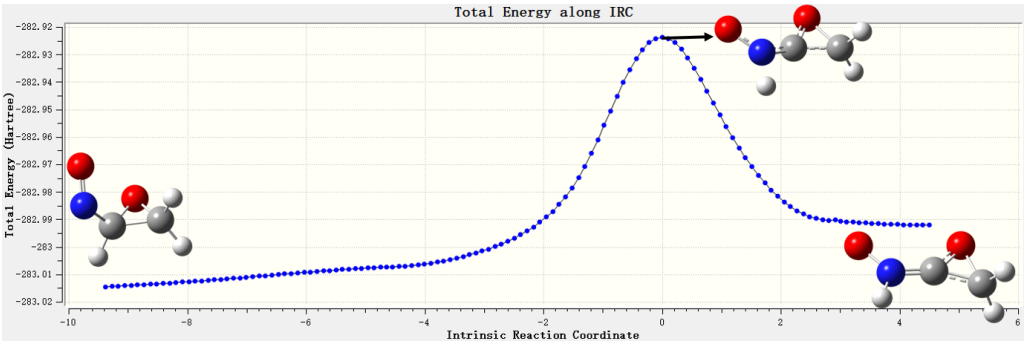

Fig. S10 Intrinsic reaction coordinate (IRC) calculation of the TS10 at the M06-2X/aug-cc-pVDZ level.

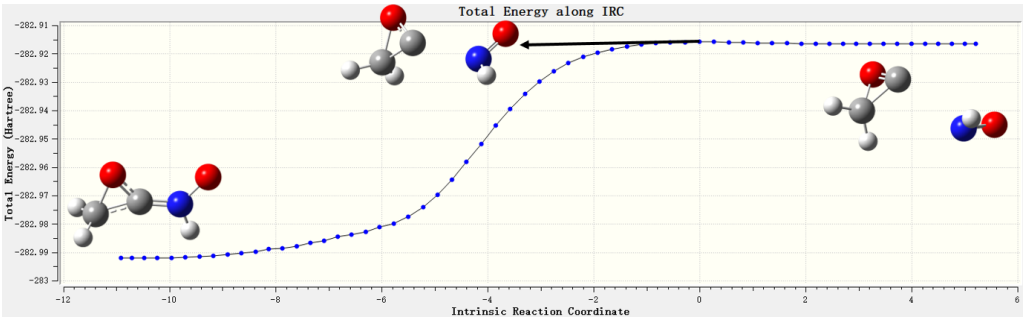

Fig. S11 Intrinsic reaction coordinate (IRC) calculation of the TS11 at the M06-2X/aug-cc-pVDZ level.

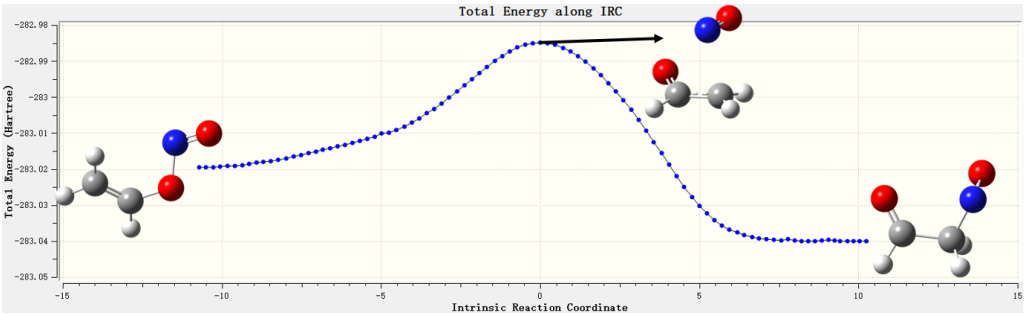

Fig. S12 Intrinsic reaction coordinate (IRC) calculation of the TS12 at the M06-2X/aug-cc-pVDZ level.

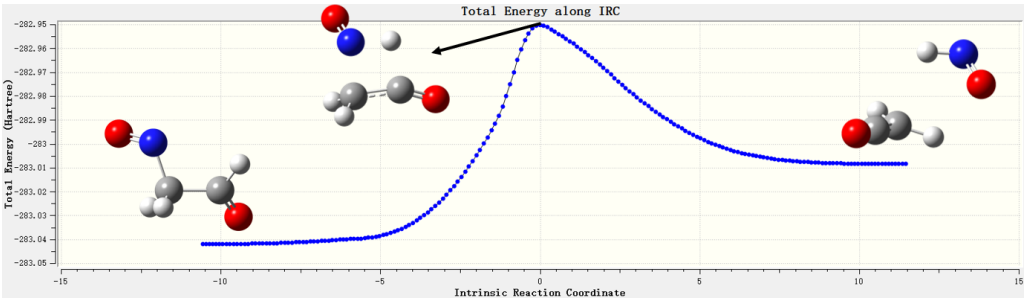

Fig. S13 Intrinsic reaction coordinate (IRC) calculation of the TS13 at the M06-2X/aug-cc-pVDZ level.

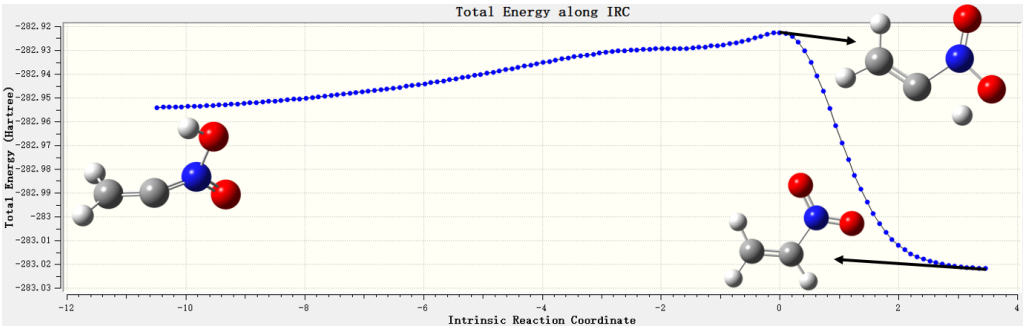

Fig. S14 Intrinsic reaction coordinate (IRC) calculation of the TS14 at the M06-2X/aug-cc-pVDZ level.

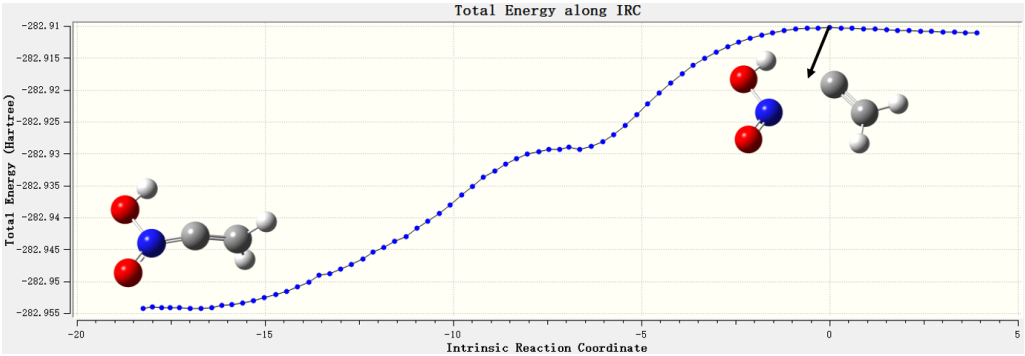

Fig. S15 Intrinsic reaction coordinate (IRC) calculation of the TS15 at the M06-2X/aug-cc-pVDZ level.

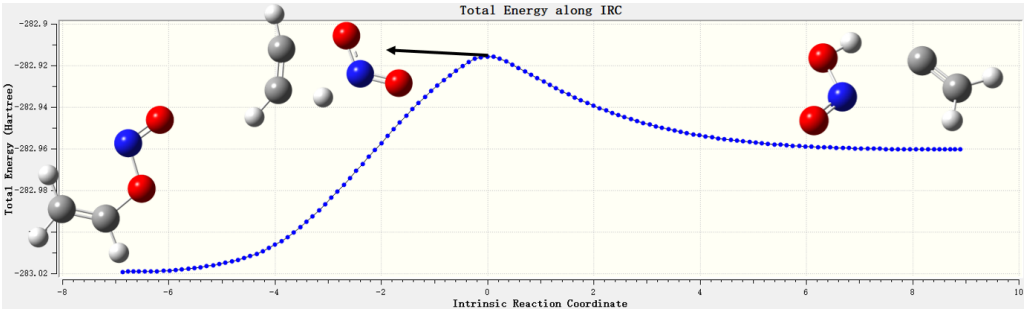

Fig. S16 Intrinsic reaction coordinate (IRC) calculation of the TS16 at the M06-2X/aug-cc-pVDZ level.

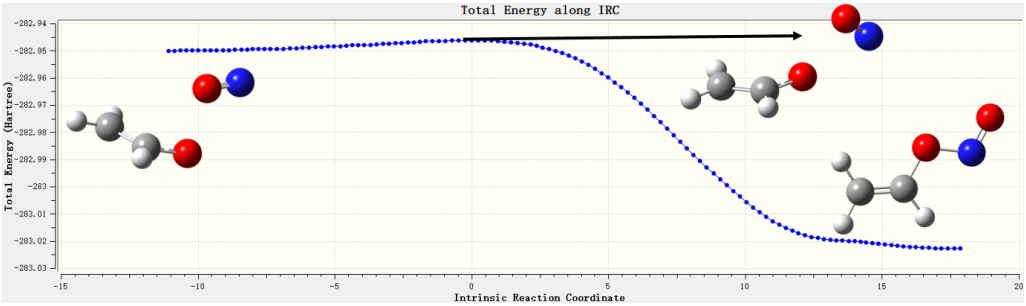

Fig. S17 Intrinsic reaction coordinate (IRC) calculation of the TS17 at the M06-2X/aug-cc-pVDZ level.

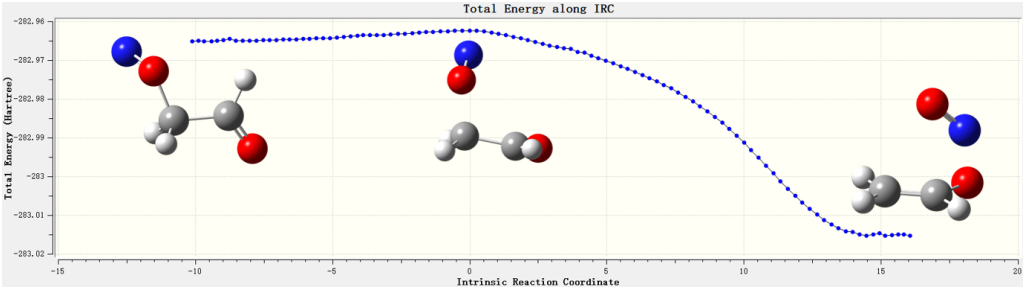

Fig. S18 Intrinsic reaction coordinate (IRC) calculation of the TS18 at the M06-2X/aug-cc-pVDZ level.

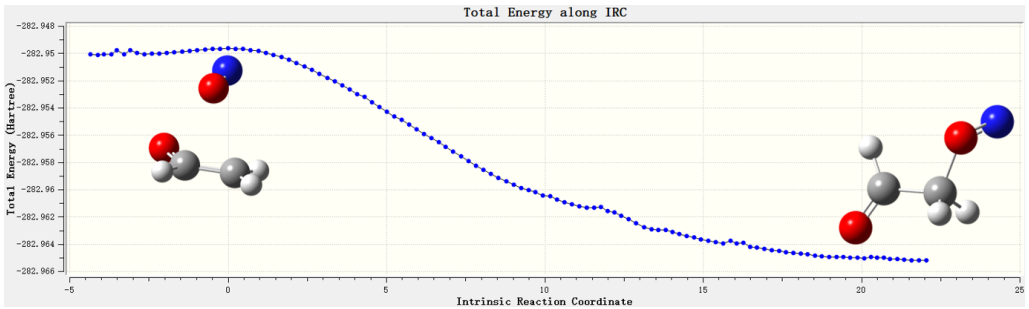

Fig. S19 Intrinsic reaction coordinate (IRC) calculation of the TS19 at the M06-2X/aug-cc-pVDZ level.

Table S2 T1 diagnostic values for all stationary points on the PES of C_2H_3 + NO_2 system

Species	*T1 diagnostics* *CCSD(T)-F12a/aVTZ-F12//M06-2X/aug-cc-pVDZ*
$C_2H_3NO_2$	*0.018*
C_2H_3	*0.017*
NO_2	*0.023*
$TS_{C2H3NO2→C2H3ONO}$	*0.021*
C_2H_3ONO	*0.019*
CH_2CHO	*0.0006*
NO	*0.020*
$TS_{C2H3ONO→ONCH2CHO}$	*0.023*
$ONCH_2CHO$	*0.015*
$TS_{ONCH2CHO→CH2CO+HNO}$	*0.023*

HNO	*0.015*
CH_2CO	*0.016*
$TS_{C2H3ONO→CH2CHO+NO}$	*0.041*
$TS_{C2H3NO2→CH2C+HNO2}$	*0.036*
CH_2C	*0.017*
HNO_2	*0.019*
$TS_{C2H3ONO→cis-C2H3ONO}$	*0.017*
cis-C_2H_3ONO	*0.019*
$TS_{cis-C2H3ONO→C2H2+HONO}$	*0.025*
C_2H_2	*0.013*
HONO	*0.020*
$TS_{C2H3ONO→C2H2+cis-HONO}$	*0.025*
Cis-HONO	*0.020*
$TS_{C2H3ONO→C2H2+HNO2}$	*0.025*
$TS_{C2H3NO2→C2H2+HONO}$	*0.023*
$TS_{C2H3NO2→CH2OCHNO}$	*0.025*
CH_2OCHNO	*0.017*
$TS_{CH2OCHNO→W}$	*0.052*

$TS_{W\rightarrow CH2OCNOH}$	*0.023*
CH_2OCNOH	*0.020*
$TS_{CH2OCNOH\rightarrow CH2(O)C+HNO}$	*0.018*
$CH_2(O)C$	*0.018*
$TS_{C2H3NO2\rightarrow CH2CNOOH}$	*0.019*
CH_2CNOOH	*0.012*
$TS_{CH2CNOOH\rightarrow CH2=C+HONO}$	*0.020*
$CH_2=C$	*0.017*
$TS_{cis\text{-}C2H3ONO\rightarrow NOCH2CH}$	*0.030*
$NOCH_2CHO$	*0.022*
$TS_{NOCH2CHO\rightarrow NO+CH2CHO}$	*0.036*

S1.2. Kinetics calculations

The calculated barrier-less processes of $\dot{C}_2H_3 + NO_2$ reaction is shown in Fig. S20 (N-attack), and the values in parentheses represent the imaginary frequency of the corresponding geometry in cm^{-1}. To simplify, all calculated points of this potential curve and their imaginary frequencies do not list here, but the existing data can also show the pattern of change. Note that the given potential energies in Fig. S20 have been scaled by the CCSD(T)-F12 values, since the $\dot{C}_2H_3 + NO_2$ reaction PES given in the manuscript is at the CCSD(T)-F12 level.

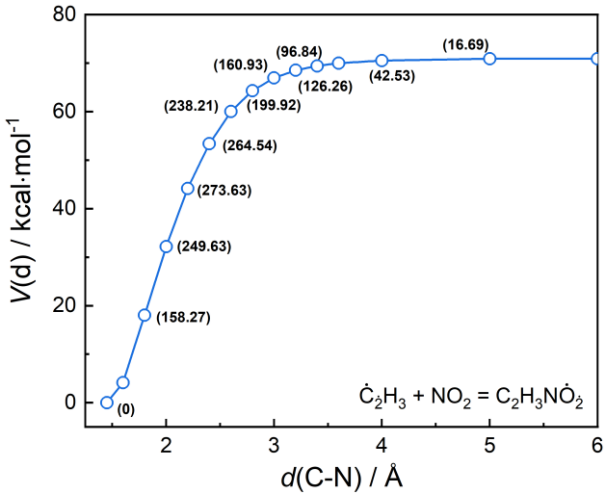

Fig. S20 Calculated points of potential curve of the association reaction, the CASPT2(12e,9o)/aug-cc-pVTZ energies are scaled by CCSD(T)-F12a energy.

In order to explore the possibility of an O-attack on the $\dot{C}_2H_3$ moiety, the barrier-less reaction process of $C_2H_3ONO \leftrightarrow C_2H_3 + NO_2$ reaction at different fixed C−O distances was calculated at the UB2PLYPD3/cc-pVTZ method, the UM06-2X/aug-cc-pVDZ method and the CASPT2/aVTZ method (shown in Fig. S **21**-S24).

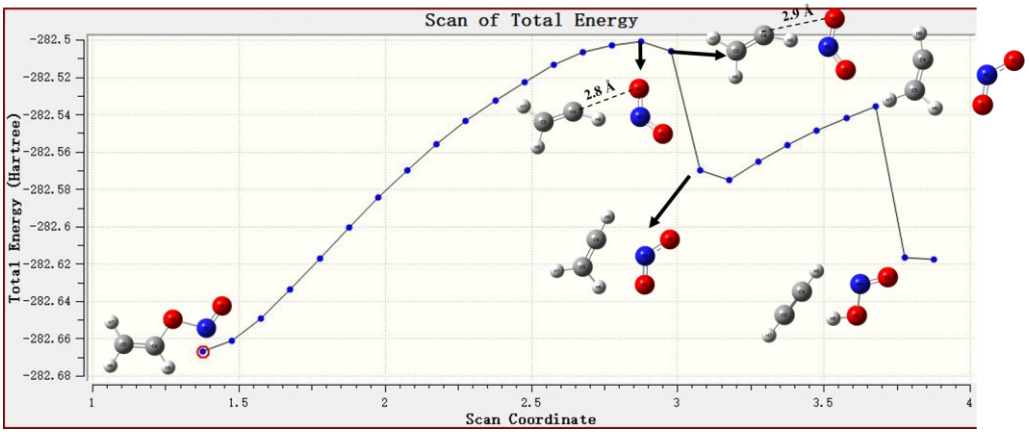

Fig. S 21 Relax scan for CH_2CH-ONO bond of C_2H_3ONO at the UB2PLYPD3/cc-pVTZ level of theory

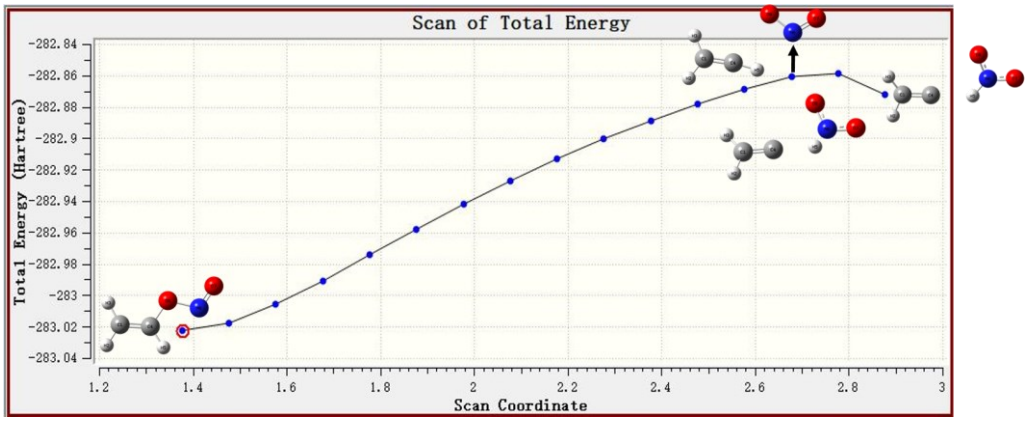

Fig. S 22 Relax scan for CH_2CH-ONO bond of C_2H_3ONO at the UM06-2X/aug-cc-pVDZ level of theory

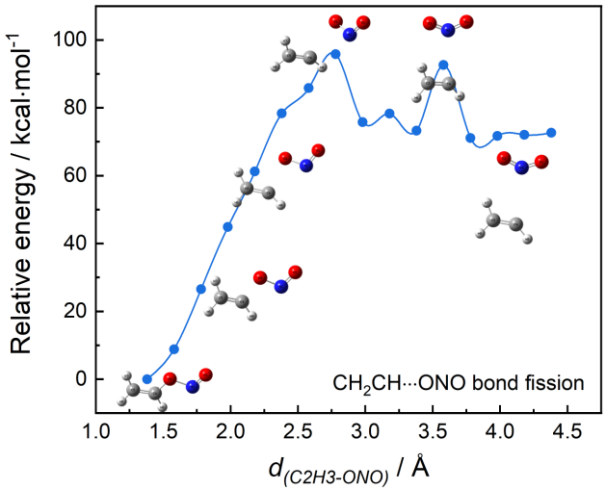

Fig. S 23 Relative Energy of the CH_2CH-ONO bond fission at the CASPT2(8e,7o)/aVTZ level of theory

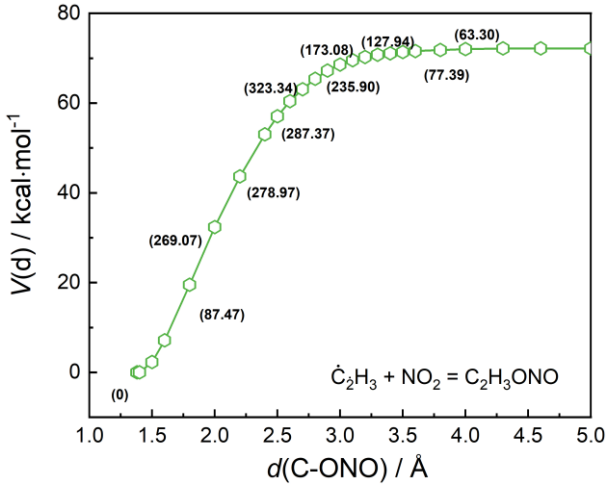

Fig. S 24 Relative Energy of the CH_2CH-ONO bond fission at the CASPT2(12e,9o)/aVTZ level of theory

In order to explore the possibility of the direct release of NO from C_2H_3ONO, a restricted scan (with frozen CON angle and CONO dihedral) of the C_2H_3O-NO bond was carried out (shown in Fig. S 25). It is clear that the C_2H_3ONO molecule cannot release NO directly via simple O-NO bond fission.

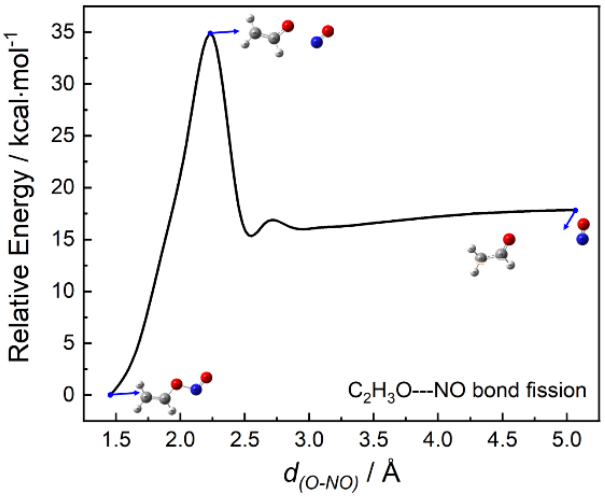

Fig. S 25 Relative Energy of the C_2H_3O-NO bond fission (a restricted scan with frozen CON angle and CONO dihedral) calculated at the CASPT2(8e,7o)/aVTZ method

The calculated barrier-less processes of the NO elimination reaction is shown in Fig. S26, and the values in parentheses represent the imaginary frequency of the corresponding geometry in cm^{-1}. To simplify, all calculated points of this potential curve and their imaginary frequencies do not list here, but the existing data can also show the pattern of change. Note that the given potential energies in Fig. S26 have been scaled by the CCSD(T)-F12 values, since the reaction PES given in the manuscript is at the CCSD(T)-F12 level.

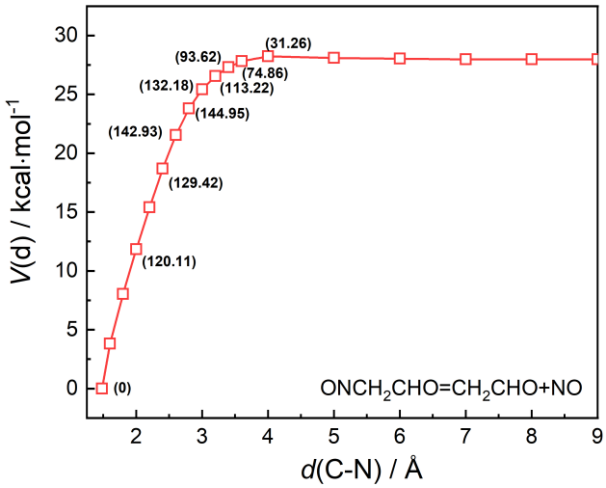

Fig. S26 Calculated points of potential curve of the NO elimination reaction, the CASPT2(6e,5o)/aug-cc-pVTZ energies are scaled by CCSD(T)-F12a energy. The active space of (6e,5o) is selected: five electrons in four orbitals for nitric oxide, and one electron in one orbital for the carbon-centered radical.

The variational effect plays an important effect for such system without reaction barrier (e. g. $\dot{C}_2H_3 + NO_2 \rightarrow C_2H_3NO_2$, $\dot{C}_2H_3 + NO_2 \rightarrow C_2H_3ONO$, $ONCH_2CHO \rightarrow CH_2CHO + NO$ and $CH_2OCNOH \rightarrow CH_2(O)C\cdots HNO$,). For the case shown in Fig. S27, the association reaction of $\dot{C}_2H_3 + NO_2$ is briefly illustrated here as an example. It is clear that the optimum transition state locates at different dividing surface with temperature change. "R=" means the separation of two fragments ($\dot{C}_2H_3$ radical and NO_2 molecule).

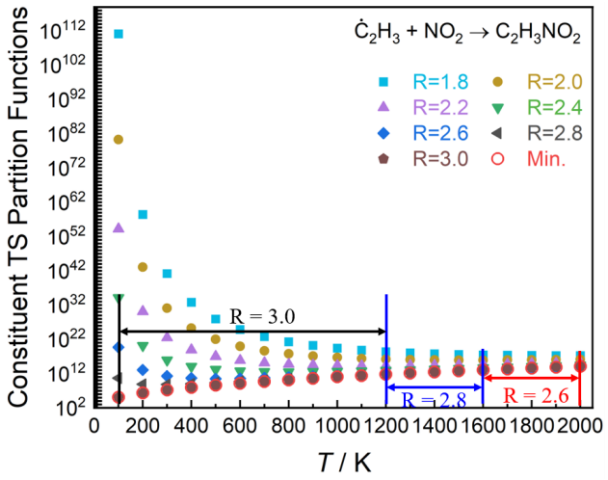

Fig. S27 Constituent transition state partition functions for one of the $\dot{C}_2H_3 + NO_2$ reaction process

In a microcanonical ensemble, the microcanonical energy-resolved classical rate coefficient (which is obtained by firstly integrating the E, J-resolved rate coefficient k^{GT}(E, J, s) over the angular momentum J distribution) is $k^{GT}(E,s) = N^{GT}(E,s)/\rho_R(E)h$, where N^{GT}(E,s) is the phase-space volume of the generalized transition state (it is, quantum mechanically, the number of states for the generalized transition state), and ρ_R(E) is the density of states for reactant. In microcanonical variational transition state theory, the variational rate coefficient is obtained by minimizing $k^{GT}(E,s) = N^{GT}(E,s)/\rho_R(E)h$ with respect to s: $k^{\mu VT}(E) = \min_s N^{GT}(E,s)/\rho_R(E)h$. That is, the optimum transition states for microcanonical ensembles correspond to a minimum sum of states. The density of states is the inverse Laplace transform of the partition function. As presented in Fig. S27, the optimum transition state located at different dividing surface with temperature changing, since the TS structure with the minimum partition function is not the same TS structure ("R" is changing, Fig. S27) as the temperature changes. For instance, at 500 K, the optimum transition state located at a structure where the distance between NO_2 and $\dot{C}_2H_3$ is 3.0 Å, whereas the optimum transition state located at a structure where the distance between NO_2 and $\dot{C}_2H_3$ is 2.8 Å at 1300 K. Similarly, for the case shown in Fig. S28, the optimum transition state located at a structure where the distance between NO and $\dot{C}H_2CHO$ is 3.0 Å at 500 K, whereas the optimum transition state located at a structure where the distance between NO and $\dot{C}H_2CHO$ is 2.8 Å at 1200 K.

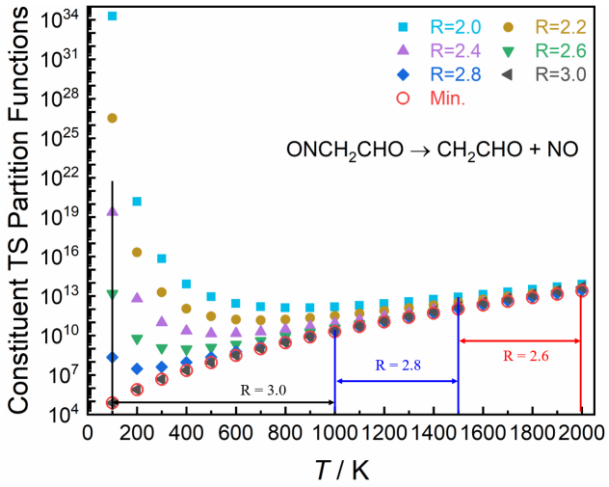

Fig. S28 Constituent transition state partition functions for the NO release process

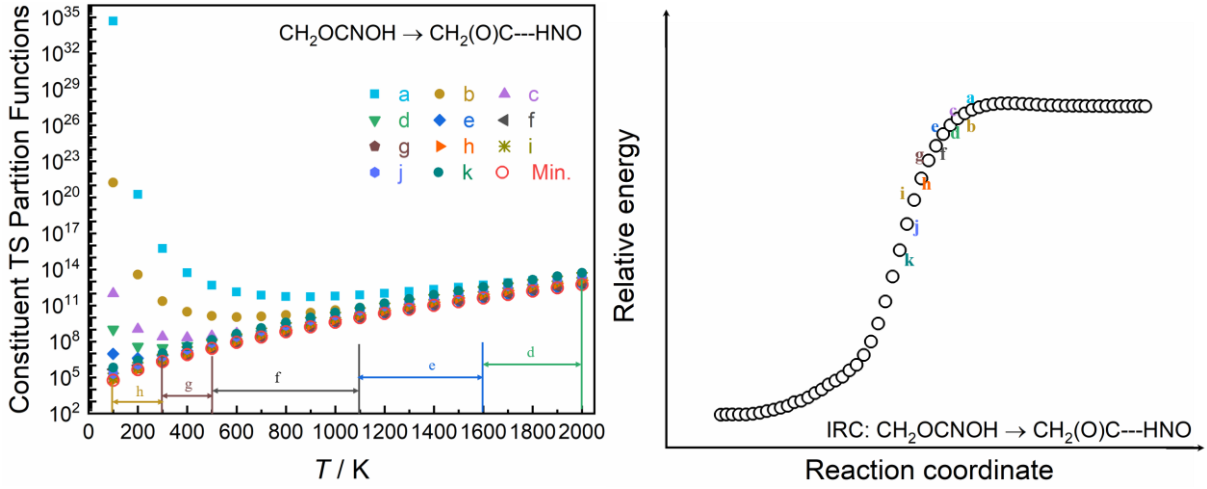

Fig. S29 Constituent transition state partition functions for the reaction via TS11

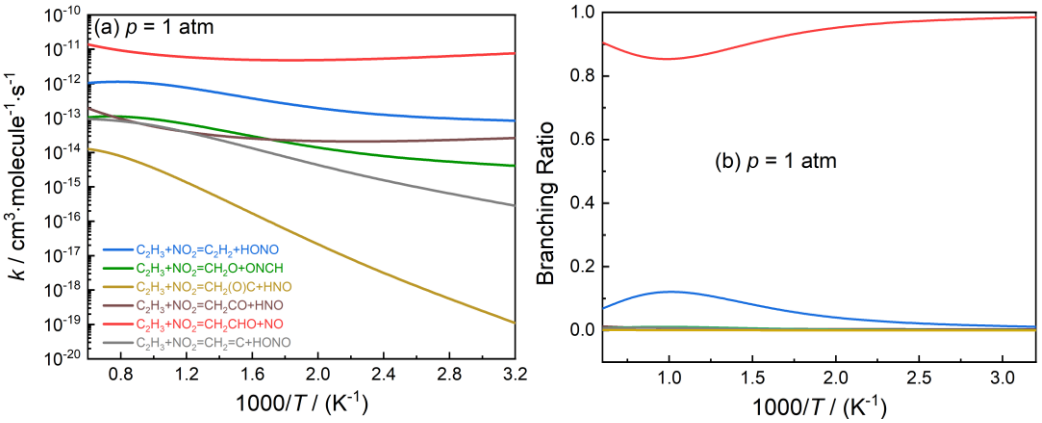

Fig. S30 Rate coefficients of $\dot{C}_2H_3$ + NO_2 various bimolecular products at 1 atm (a) and branching ratio (b) of various products.

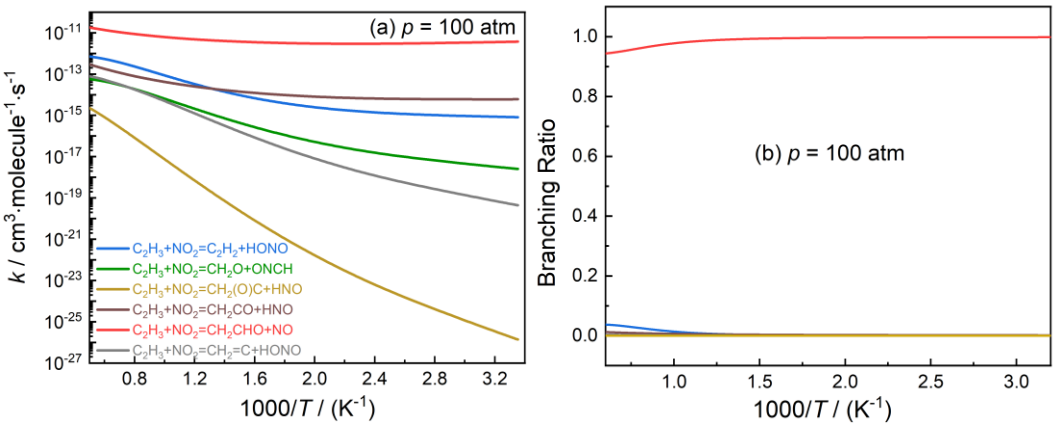

Fig. S 31 Rate coefficients of $\dot{C}_2H_3$ + NO_2 various bimolecular products at 100 atm (a) and branching ratio (b) of various products.

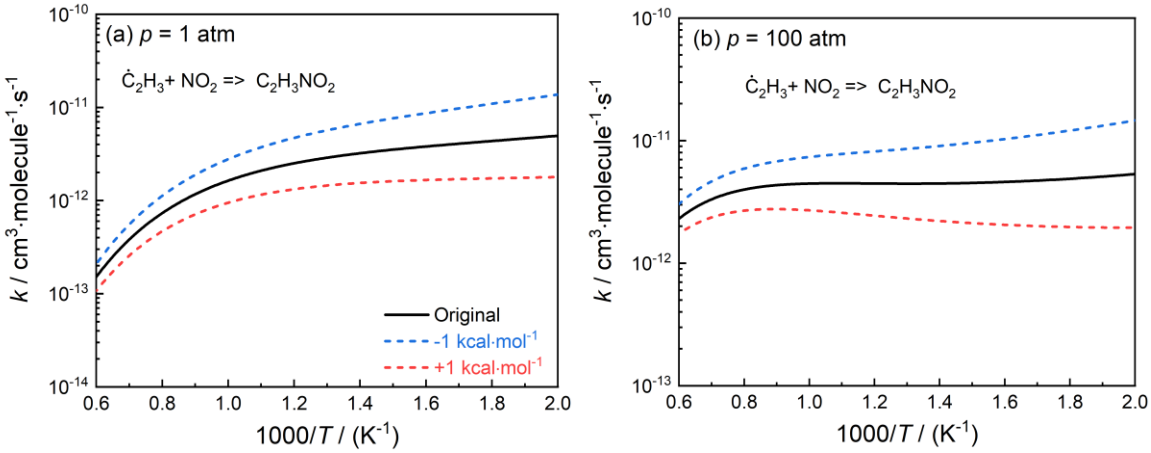

Fig. S 32 Effect of uncertainty introduced by the energy parameter on the calculated rate coefficients of $\dot{C}_2H_3$ + NO_2 = $C_2H_3NO_2$ reaction channel at p = 1 atm (a) and p = 100 atm (b).

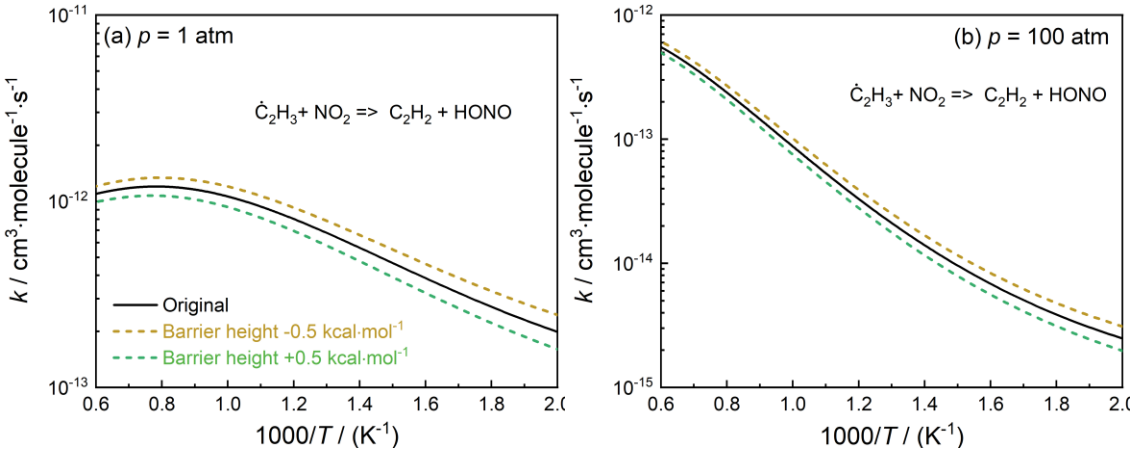

Fig. S33 Effect of uncertainty introduced by the energy parameter on the calculated rate coefficients of $\dot{C}_2H_3$ + NO_2 = C_2H_2 + HONO reaction channel at p = 1 atm (a) and p = 100 atm (b).

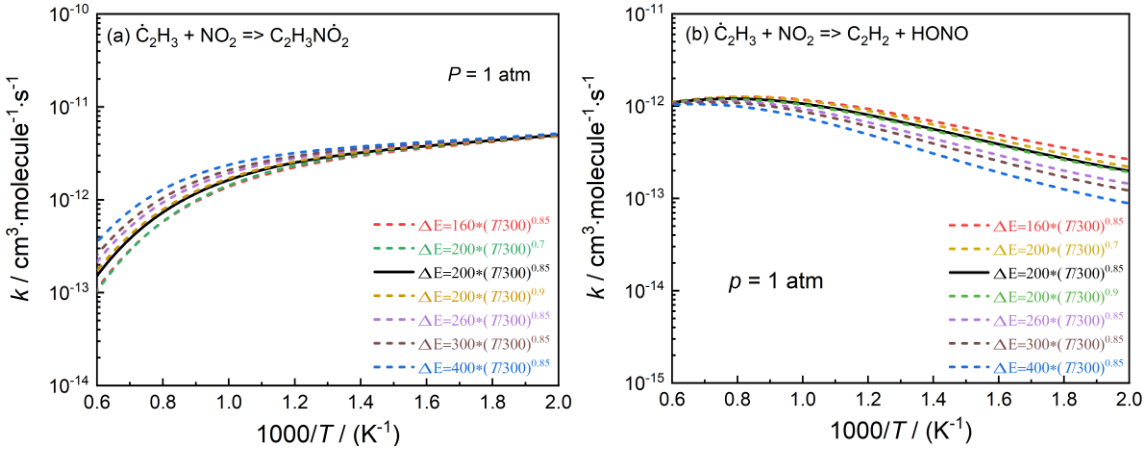

Fig. S34 Effect of collisional parameters on the rate coefficient of the association reaction and the chemically activated reaction of $\dot{C}_2H_3$ + NO_2 system (p = 1 atm)

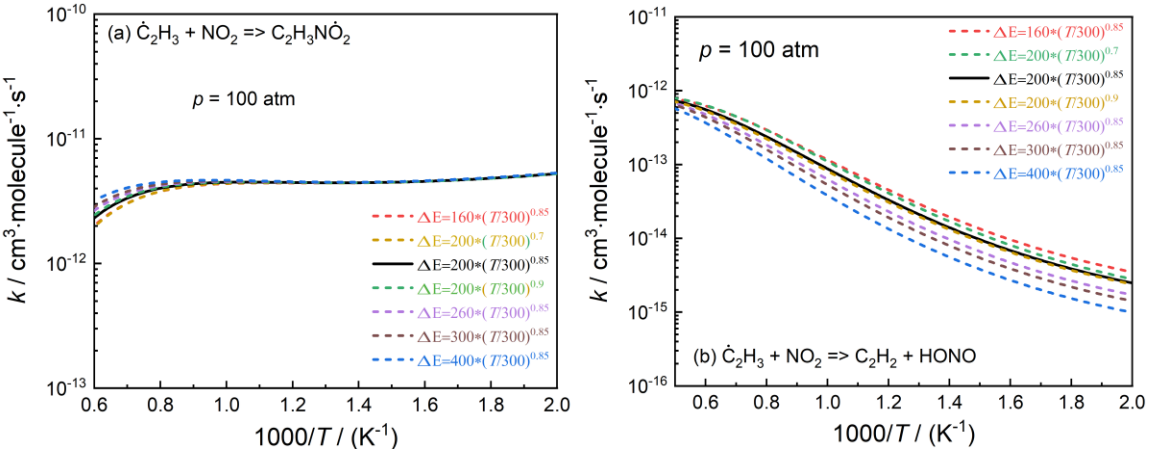

Fig. S35 Effect of collisional parameters on the rate coefficient of the association reaction and the chemically activated reaction of $\dot{C}_2H_3$ + NO_2 system (p = 100 atm)

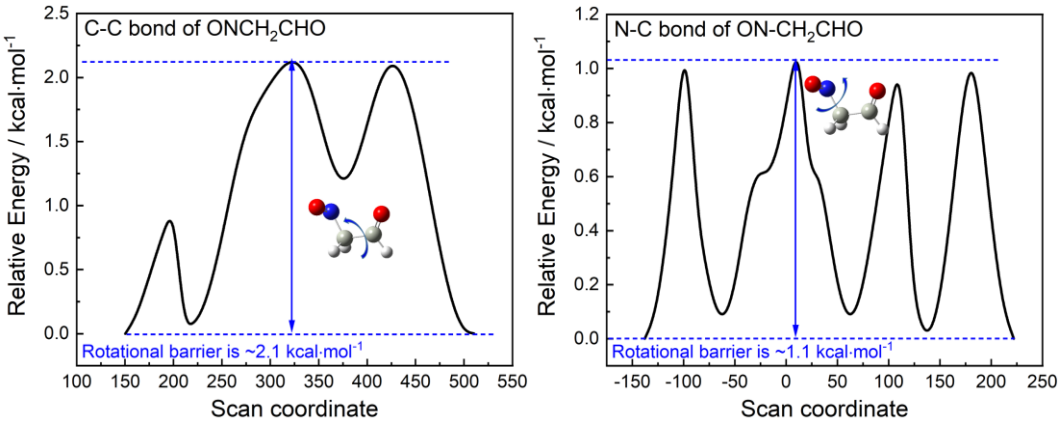

Fig. S36 Rotational potential energy surfaces of $ONCH_2CHO$ calculated at the M06-2X/aug-cc-pVDZ level.

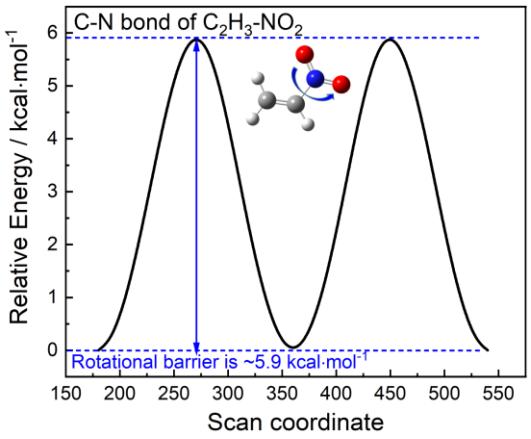

Fig. S37 Rotational potential energy surfaces of $C_2H_3NO_2$ calculated at the M06-2X/aug-cc-pVDZ level.

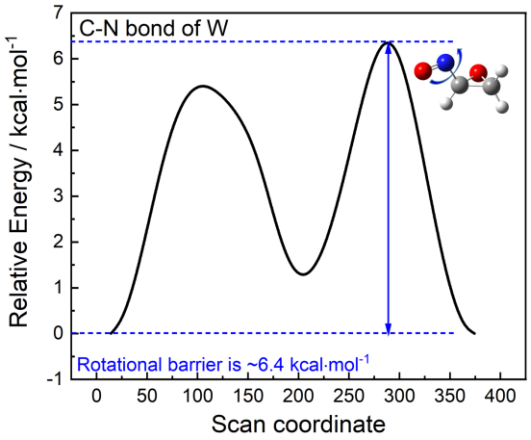

Fig. S38 Rotational potential energy surfaces of W calculated at the M06-2X/aug-cc-pVDZ level.

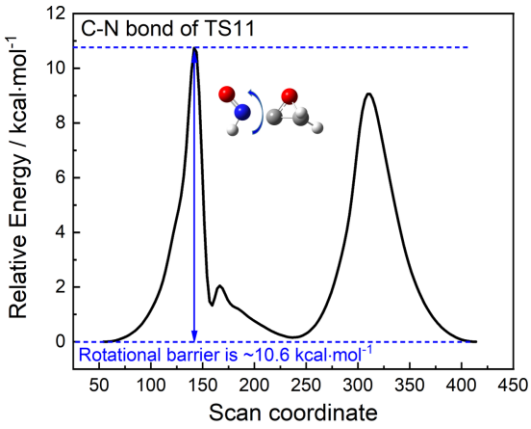

Fig. S39 Rotational potential energy surfaces of TS11 calculated at the M06-2X/aug-cc-pVDZ level.

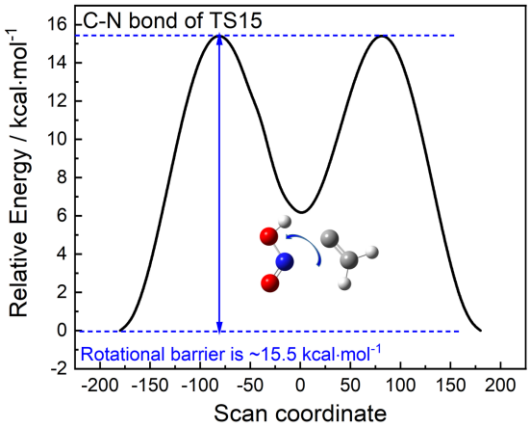

Fig. S40 Rotational potential energy surfaces of TS15 calculated at the M06-2X/aug-cc-pVDZ level.

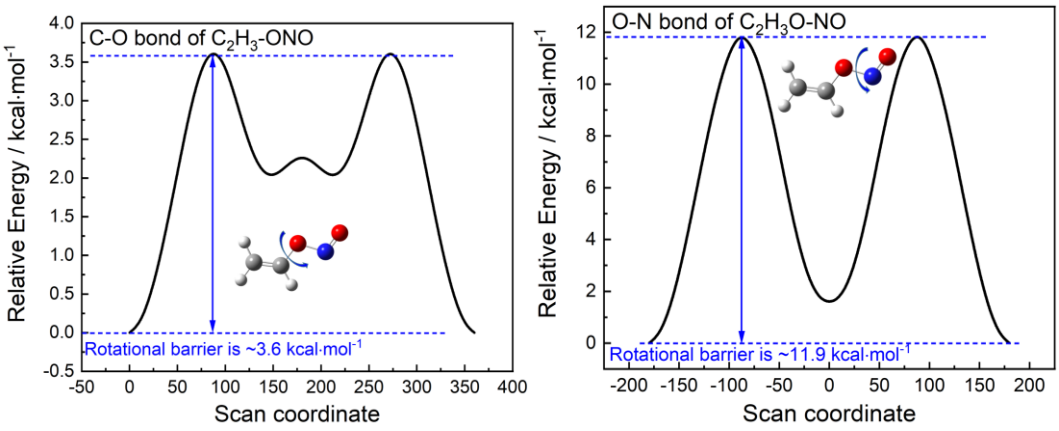

Fig. S41 Rotational potential energy surfaces of C_2H_3ONO calculated at the M06-2X/aug-cc-pVDZ level.

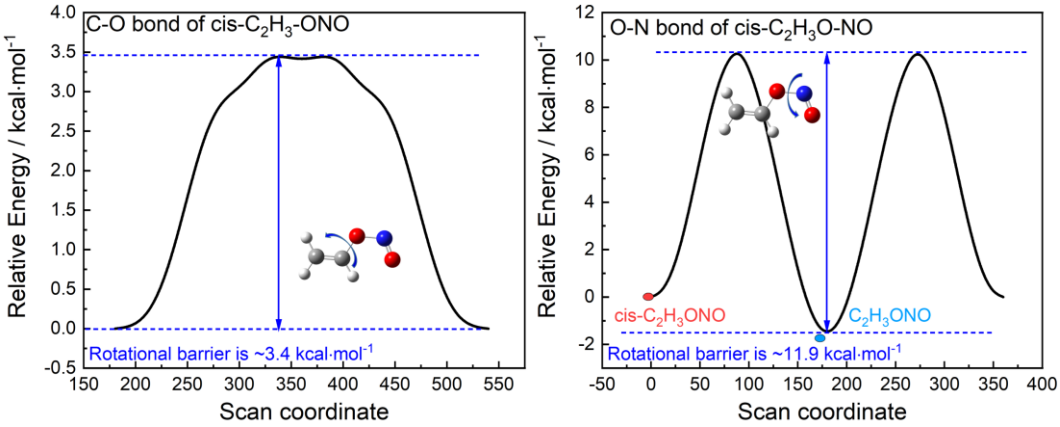

Fig. S42 Rotational potential energy surfaces of cis-C_2H_3ONO calculated at the M06-2X/aug-cc-pVDZ level.

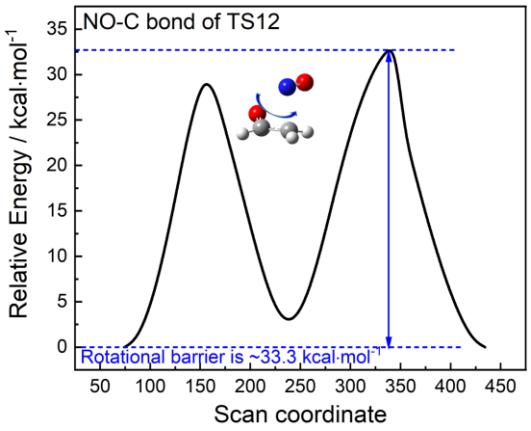

Fig. S43 Rotational potential energy surfaces of TS12 calculated at the M06-2X/aug-cc-pVDZ level.

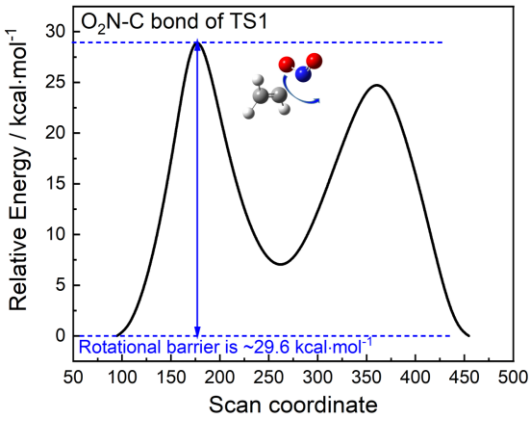

Fig. S44 Rotational potential energy surfaces of TS1 calculated at the M06-2X/aug-cc-pVDZ level.

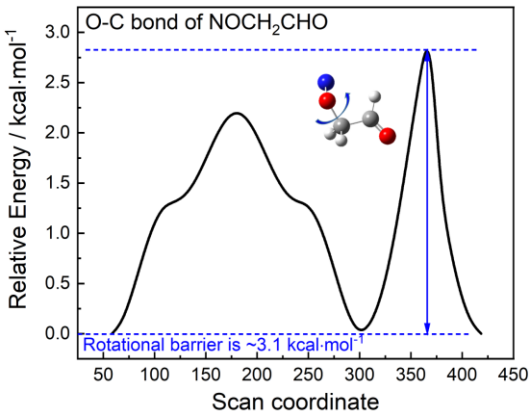

Fig. S45 Rotational potential energy surfaces of $NOCH_2CHO$ calculated at the M06-2X/aug-cc-pVDZ level.

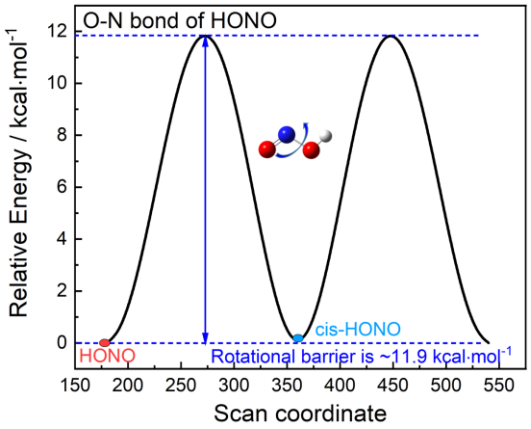

Fig. S46 Rotational potential energy surfaces of HONO calculated at the M06-2X/aug-cc-pVDZ level.

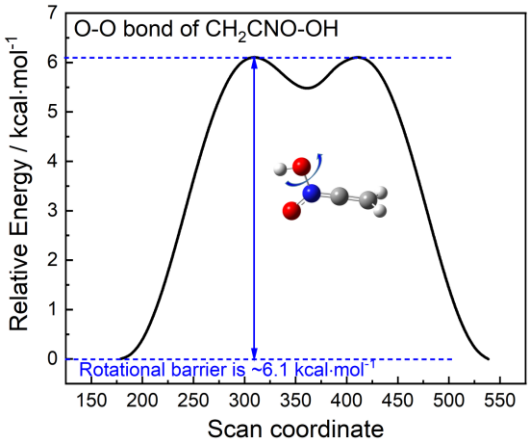

Fig. S47 Rotational potential energy surfaces of CH_2CNOOH calculated at the M06-2X/aug-cc-pVDZ level.

S2. Results and discussion

S2.1. Theoretically calculated rate coefficients

S2.1.1. High-pressure limit rate coefficients

Table S3 High-pressure limit rate coefficient for vinyl + NO_2 reaction. Units are cm^3, mol, s, cal.

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)
$C_2H_3NO_2 = \dot{C}_2H_3+NO_2$	2.44E+26	-3.15	73180.0	298-2000
$C_2H_3NO_2 = C_2H_2+HONO$	1.47E+14	-0.12	56900.0	298-2000
$C_2H_3NO_2 = CH_2O+ONCH$	3.37E+17	-1.14	65850.0	298-2000
$C_2H_3NO_2 = CH2(O)C+HNO$	4.43E+06	1.99	77850.0	298-2000
$C_2H_3NO_2 = CH2CO+HNO$	1.43E+09	0.79	61350.0	298-2000
$C_2H_3NO_2 = CH_2CHO+NO$	4.55E+15	-0.60	60810.0	298-2000
$C_2H_3NO_2 = CH_2=C+HONO$	3.25E+23	-2.66	74920.0	298-2000
$\dot{C}_2H_3+NO_2 = C_2H_3NO_2$	3.15E+15	-1.04	71.1	298-2000
$\dot{C}_2H_3+NO_2 = C_2H_2+HONO$	1.08E-03	4.47	-642.7	298-2000
$\dot{C}_2H_3+NO_2 = CH_2O+ONCH$	3.61E+00	3.20	3346.0	298-2000
$\dot{C}_2H_3+NO_2 = CH_2(O)C+HNO$	6.35E-09	5.70	11180.0	298-2000
$\dot{C}_2H_3+NO_2 = CH_2CO+HNO$	1.42E-02	3.90	-2358.0	298-2000
$\dot{C}_2H_3+NO_2 = CH_2CHO+NO$	7.96E-16	2.40	-2025.0	298-2000
$\dot{C}_2H_3+NO_2 = CH_2=C+HONO$	6.90E+02	2.67	7095.0	298-2000

S2.1.2. Pressure-dependent rate coefficients

Table S4 Pressure-dependent rate coefficient for vinyl + NO_2 reaction. Units are cm^3, mol, s, cal. Mean and maximum deviations of the Arrhenius fits are reported for each channel.

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)	Average, Max [%] ($k_{calcfit}/k_{calc}$)
$C_2H_3NO_2 = \dot{C}_2H_3+NO_2$	-	-	-	-	-
0.01 atm	3.81E+60	-14.35	85440.0	298-2000	1.8; 3.5
	1.82E+45	-10.15	75500.0		
0.1 atm	7.71E+60	-13.97	87220.0	298-2000	2.3; 5.6
	6.33E+45	-10.04	76310.0		

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)	Average, Max [%] ($k_{calcfit}/k_{calc}$)
1 atm	2.35E+60	-13.42	89540.0	298-2000	3.9; 10.6
	4.08E+40	-8.17	75520.0		
10 atm	1.00E+57	-12.11	90560.0	298-2000	5.0; 14.6
	1.92E+34	-6.00	74220.0		
100 atm	3.34E+49	-9.73	88680.0	298-2000	4.7; 13.2
	3.75E+28	-4.08	72890.0		
$C_2H_3NO_2$ = C_2H_2+HONO	-	-	-	-	-
0.01 atm	1.60E+57	-13.32	75370.0	298-2000	3.2; 8.5
	8.55E+35	-7.63	61160.0		
0.1 atm	5.31E+55	-12.60	77020.0	298-2000	4.8; 14.6
	1.74E+31	-5.99	60300.0		
1 atm	2.28E+52	-11.37	77610.0	298-2000	6.0; 15.4
	1.91E+26	-4.30	59260.0		
10 atm	5.92E+45	-9.27	76070.0	298-2000	6.0; 14.6
	2.29E+21	-2.65	58120.0		
100 atm	5.55E+34	-5.96	71210.0	298-2000	4.9; 12.9
	5.75E+16	-1.13	56960.0		
$C_2H_3NO_2$ = CH_2O+ONCH	-	-	-	-	-
0.01 atm	5.87E+56	-13.44	77920.0	298-2000	2.7; 7.2
	1.11E+39	-8.79	65760.0		
0.1 atm	1.21E+56	-12.93	79930.0	298-2000	3.8; 10.5
	6.50E+35	-7.54	65760.0		
1 atm	3.11E+53	-11.92	80960.0	298-2000	4.8;13.4
	1.32E+33	-6.48	66350.0		
10 atm	3.51E+47	-9.97	80260.0	298-2000	5.4; 13.5
	3.13E+27	-4.66	65990.0		
100 atm	2.51E+41	-7.96	80770.0	298-2000	5.4; 13.8
	1.27E+17	-1.42	64100.0		
$C_2H_3NO_2$ = $CH_2(O)C$+HNO	-	-	-	-	-
0.01 atm	2.56E+62	-15.11	87710.0	298-2000	2.7; 6.4
	1.01E+48	-11.38	77060.0		

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)	Average, Max [%] ($k_{calcfit}/k_{calc}$)
0.1 atm	9.45E+60	-14.32	91260.0	298-2000	4.9; 11.3
	3.77E+42	-9.51	78170.0		
1 atm	7.17E+54	-12.25	93070.0	298-2000	7.4;16.0
	1.27E+32	-6.24	77540.0		
10 atm	2.07E+46	-9.55	94450.0	298-2000	8.2; 13.5
	2.31E+19	-2.34	76480.0		
100 atm	1.50E+35	-6.18	95230.0	298-2000	8.9; 13.8
	8.06E+03	2.29	74830.0		
$C_2H_3NO_2$ = CH_2CO+HNO					
0.01 atm	7.08E+54	-13.46	77490.0	298-2000	2.8; 7.5
	1.11E+35	-8.18	64230.0		
0.1 atm	1.24E+54	-12.89	79700.0	298-2000	4.4; 13.1
	8.97E+29	-6.39	63340.0		
1 atm	2.93E+51	-11.82	81080.0	298-2000	5.8; 17.2
	1.81E+24	-4.43	62220.0		
10 atm	2.58E+45	-9.81	80570.0	298-2000	6.3; 17.6
	7.59E+18	-2.60	61540.0		
100 atm	9.93E+25	-4.00	72010.0	298-2000	8.3; 18.8
	2.16E+17	-2.31	61850.0		
$C_2H_3NO_2$ = CH_2CHO+NO	-	-	-	-	-
0.01 atm	8.11E+57	-13.67	76910.0	298-2000	2.7; 7.0
	4.64E+38	-8.54	63900.0		
0.1 atm	6.07E+56	-13.04	78760.0	298-2000	4.1; 12.4
	1.22E+34	-6.93	63080.0		
1 atm	6.79E+53	-11.92	79660.0	298-2000	5.3; 13.2
	9.92E+28	-5.19	62020.0		
10 atm	5.21E+47	-9.94	78560.0	298-2000	5.4; 13.6
	3.30E+24	-3.66	61350.0		
100 atm	1.12E+38	-6.96	75750.0	298-2000	5.3; 13.7
	8.64E+17	-1.57	60510.0		
$C_2H_3NO_2$ =CH_2=C+HONO	-	-	-	-	

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)	Average, Max [%] ($k_{calcfit}/k_{calc}$)
0.01 atm	4.73E+63	-15.55	86110.0	298-2000	1.7; 2.9
	5.73E+47	-11.12	76000.0		
0.1 atm	2.96E+62	-14.78	87240.0	298-2000	2.3; 4.8
	3.44E+48	-11.15	76890.0		
1 atm	4.00E+60	-13.89	88990.0	298-2000	4.2; 9.2
	4.38E+44	-9.75	77110.0		
10 atm	3.23E+55	-12.10	89850.0	298-2000	6.5; 14.2
	1.95E+36	-7.08	75960.0		
100 atm	1.34E+45	-8.85	88330.0	298-2000	5.5; 17.3
	9.16E+22	-2.94	73040.0		
$\dot{C}_2H_3+NO_2 = C_2H_3NO_2$	-	-	-	-	-
0.01 atm	1.10E+49	-12.04	12120.0	298-2000	0.1; 0.3
	1.90E+38	-9.30	3523.0		
0.1 atm	2.09E+50	-11.96	14390.0	298-2000	0.1; 0.3
	1.99E+36	-8.34	3781.0		
1 atm	2.79E+49	-11.30	16520.0	298-2000	0.3; 0.8
	3.59E+30	-6.29	2808.0		
10 atm	1.28E+46	-10.00	17650.0	298-2000	0.3; 0.6
	7.92E+23	-4.02	1400.0		
100 atm	1.31E+39	-7.75	16210.0	298-2000	0.3; 0.4
	8.77E+17	-2.02	7.5		
$\dot{C}_2H_3+NO_2 = C_2H_2+HONO$	-	-	-	-	-
0.01 atm	3.42E+19	-2.36	2772.0	298-2000	0.7; 1.5
	2.52E+09	0.56	-2085.0		;
0.1 atm	9.69E+27	-4.80	8418.0	298-2000	0.; 0.8
	6.00E+10	0.24	-339.4		;
1 atm	6.88E+27	-4.58	11100.0	298-2000	0.; 2.2
	5.65E+07	1.09	-314.9		;
10 atm	1.44E+25	-3.65	13190.0	298-2000	2.; 6.0
	5.04E+05	1.54	-226.6		;
100 atm	1.66E+20	-2.14	14310.0	298-2000	3.8;11.0
	1.67E-02	3.77	-1533.0		

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)	Average, Max [%] ($k_{calcfit}/k_{calc}$)
$\dot{C}_2H_3+NO_2$ = $CH_2O+ONCH$					
0.01 atm	2.77E+23	-3.75	6512.0	298-2000	0.3; 0.7
	8.29E+11	-0.43	-370.1		;
0.1 atm	1.45E+24	-3.87	7880.0	298-2000	0.4; 0.9
	9.92E+10	-0.17	289.6		;
1 atm	7.84E+24	-3.97	10590.0	298-2000	0.6; 1.9
	1.92E+09	0.26	785.8		;
10 atm	7.37E+24	-3.85	13950.0	298-2000	1.9; 5.7
	4.83E+07	0.67	1847.0		;
100 atm	3.43E+20	-2.51	15740.0	298-2000	4.2; 10.5
	1.99E+00	2.84	1573.0		
$\dot{C}_2H_3+NO_2$ = $CH_2(O)C+HNO$					
0.01 atm	1.17E+26	-4.71	9529.0	298-2000	0.2; 0.6
	7.17E+13	-1.14	2829.0		
0.1 atm	1.63E+28	-5.14	13750.0	298-2000	0.5; 1.4
	5.99E+14	-1.39	5781.0		
1 atm	4.19E+26	-4.48	17730.0	298-2000	1.8; 4.9
	7.27E+14	-1.57	8758.0		
10 atm	2.33E+21	-2.84	20970.0	298-2000	3.5; 8.1
	2.93E+04	1.47	9027.0		
100 atm	-1.48E-03	0.15	-6264.0	298-2000	7.5;9.1
	3.95E-14	7.20	8198.0		
$\dot{C}_2H_3+NO_2$ = $CH_2CO+HNO$					
0.01 atm	7.67E-01	3.33	-2947.0	298-2000	0.1; 0.4
	3.08E+11	0.00	9379.0		
0.1 atm	1.03E+04	2.13	2504.0	298-2000	0.2; 0.6
	1.51E+00	3.21	-2881.0		
1 atm	2.14E+04	2.09	2665.0	298-2000	0.1; 0.4
	4.24E+00	3.05	-2810.0		
10 atm	1.88E+06	1.53	4473.0	298-2000	0.1; 0.4
	1.67E+00	3.19	-2788.0		

Reaction	A	n	E_a (cal·mol^{-1})	Fitting T (K)	Average, Max [%] ($k_{calcfit}/k_{calc}$)
100 atm	6.79E+04	2.00	3145.0	298-2000	0.4; 0.8
	1.44E+00	3.14	-2230.0		
$\dot{C}_2H_3+NO_2$ = $CH_2CHO+NO$					
0.01 atm	2.40E+05	2.22	-2400.0	298-2000	0.2; 0.6
	3.98E+04	2.19	-2798.0		
0.1 atm	1.89E+06	1.93	-1501.0	298-2000	0.1; 0.4
	3.67E+04	2.36	-2957.0		
1 atm	2.95E+08	1.27	1552.0	298-2000	0.1; 0.2
	3.98E+05	2.13	-2496.0		
10 atm	4.64E+09	0.95	3267.0	298-2000	0.1; 0.3
	5.08E+05	2.10	-2430.0		
100 atm	5.45E+08	1.27	1485.0	298-2000	0.1; 0.2
	4.47E+05	2.06	-2170.0		
$\dot{C}_2H_3+NO_2$ = $CH_2=C+HONO$					
0.01 atm	4.83E+25	-4.52	8662.0	298-2000	0.3; 0.8
	8.58E+09	0.26	564.5		
0.1 atm	7.19E+26	-4.76	9986.0	298-2000	0.3; 0.8
	1.66E+10	0.20	1834.0		
1 atm	1.35E+28	-4.95	13240.0	298-2000	0.5; 1.3
	2.99E+09	0.44	3381.0		
10 atm	2.85E+24	-3.66	15180.0	298-2000	1.1; 3.5
	2.91E+09	0.26	5096.0		
100 atm	1.34E+21	-2.57	18190.0	298-2000	3.2; 8.8
	1.39E+01	2.68	4564.0		

S2.1.3. Calculated Uncertainty

Table S4 The calculated uncertainties of the high-pressure limit rate coefficient for vinyl + NO_2 reaction. Units are cm^3, mol, s, cal.

Reaction	*Lower limit*			*Upper limit*		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
$C_2H_3NO_2 = \dot{C}_2H_3+NO_2$	8.30E+25	-3.04	73760.0	3.19E+25	-2.87	72410.0
$C_2H_3NO_2 = C_2H_2+HONO$	2.66E+14	-0.20	57530.0	3.03E+13	0.09	56180.0
$C_2H_3NO_2 = CH_2O+ONCH$	3.84E+18	-1.45	66640.0	1.10E+16	-0.69	64970.0
$C_2H_3NO_2$ = CH2(O)C+HNO	1.27E+09	1.33	78870.0	5.79E+04	2.54	76730.0
$C_2H_3NO_2$ = CH2CO+HNO	1.59E+10	0.47	61880.0	2.48E+07	1.33	60510.0
$C_2H_3NO_2 = CH_2CHO+NO$	4.03E+16	-0.88	61410.0	1.59E+14	-0.15	59990.0
$C_2H_3NO_2 = CH_2$=C+HONO	1.01E+26	-3.40	76190.0	3.80E+21	-2.08	73890.0
$\dot{C}_2H_3+NO_2 = C_2H_3NO_2$	1.50E+15	-0.98	652.6	4.12E+14	-0.77	-698.5
$\dot{C}_2H_3+NO_2 = C_2H_2+HONO$	8.74E-04	4.51	13.4	5.37E-05	4.84	-1512.0
$\dot{C}_2H_3+NO_2 = CH_2O+ONCH$	3.52E+00	3.21	3880.0	1.19E-01	3.63	2569.0
$\dot{C}_2H_3+NO_2 = CH_2$(O)C+HNO	1.58E-06	5.06	12240.0	5.64E-11	6.29	10170.0
$\dot{C}_2H_3+NO_2 = CH_2CO+HNO$	2.35E-03	4.16	-1976.0	4.08E-03	4.07	-2841.0
$\dot{C}_2H_3+NO_2 = CH_2CHO+NO$	6.58E+03	2.75	-1679.0	3.47E+04	2.52	-2513.0
$\dot{C}_2H_3+NO_2 = CH_2$=C+HONO	3.35E+03	2.47	7680.0	1.00E+01	3.21	6184.0

Table S5 The calculated uncertainties of the pressure-dependent rate coefficient for vinyl + NO_2 reaction. Units are cm^3, mol, s, cal.

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
$C_2H_3NO_2 = \dot{C}_2H_3+NO_2$	-	-	-			
0.01 atm	1.55E+69	-17.04	90420.0	4.31E+59	-13.99	84710.0
	2.19E+42	-9.25	75470.0	5.56E+44	-9.93	74970.0
0.1 atm	1.51E+61	-14.13	88000.0	1.53E+60	-13.70	86720.0
	5.54E+45	-10.11	76870.0	7.34E+44	-9.71	75650.0
1 atm	7.54E+60	-13.62	90440.0	2.90E+59	-13.10	88970.0
	3.53E+40	-8.21	76110.0	3.29E+39	-7.79	74790.0
10 atm	3.11E+57	-12.30	91500.0	5.15E+55	-11.70	89740.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
	1.12E+34	-5.98	74780.0	1.84E+33	-5.66	73480.0
100 atm	4.04E+49	-9.78	89510.0	4.60E+47	-9.17	87340.0
	1.07E+28	-3.96	73390.0	6.04E+27	-3.82	72190.0
$C_2H_3NO_2$ = C_2H_2+HONO	-	-	-			
0.01 atm	9.50E+57	-13.58	76090.0	3.36E+56	-13.08	74850.0
	2.73E+34	-7.14	61310.0	1.51E+35	-7.37	60510.0
0.1 atm	2.75E+56	-12.83	77750.0	7.70E+54	-12.32	76420.0
	5.14E+31	-6.15	60920.0	2.55E+30	-5.71	59610.0
1 atm	1.56E+53	-11.62	78490.0	1.46E+51	-11.00	76770.0
	3.92E+26	-4.40	59850.0	2.90E+25	-4.02	58560.0
10 atm	8.36E+46	-9.61	77230.0	1.04E+44	-8.74	74830.0
	3.72E+21	-2.72	58700.0	3.71E+20	-2.39	57420.0
100 atm	4.83E+36	-6.52	72910.0	6.20E+26	-3.68	65340.0
	9.86E+16	-1.20	57560.0	1.44E+19	-1.99	56830.0
$C_2H_3NO_2$ = CH_2O+ONCH	-	-	-			
0.01 atm	2.03E+62	-15.13	81070.0	1.54E+56	-13.23	77440.0
	3.45E+33	-6.92	65060.0	2.34E+38	-8.55	65150.0
0.1 atm	7.09E+56	-13.17	80730.0	2.90E+55	-12.71	79440.0
	1.18E+36	-7.63	66270.0	1.58E+35	-7.31	65210.0
1 atm	1.78E+54	-12.14	81850.0	2.61E+52	-11.57	80200.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
	1.74E+33	-6.52	66810.0	2.54E+32	-6.24	65780.0
10 atm	1.48E+48	-10.15	80980.0	1.48E+46	-9.54	79420.0
	1.09E+28	-4.82	66610.0	1.64E+26	-4.26	65220.0
100 atm	3.86E+42	-8.31	81630.0	2.72E+33	-5.66	75650.0
	1.63E+18	-1.76	64880.0	7.76E+23	-3.83	64850.0
$C_2H_3NO_2$ = $CH_2(O)C+HNO$	-	-	-			
0.01 atm	1.53E+79	-20.22	95610.0	6.35E+61	-14.86	87210.0
	3.96E+41	-9.19	75850.0	8.86E+46	-11.01	76270.0
0.1 atm	2.14E+62	-14.75	91550.0	9.74E+59	-13.97	90560.0
	3.00E+44	-10.09	78830.0	1.78E+41	-9.07	77240.0
1 atm	4.66E+57	-13.06	94210.0	4.11E+53	-11.85	92240.0
	2.34E+34	-6.89	78430.0	3.81E+30	-5.75	76540.0
10 atm	8.70E+49	-10.56	96170.0	7.71E+44	-9.11	93580.0
	3.51E+21	-2.94	77360.0	7.04E+17	-1.87	75530.0
100 atm	5.04E+38	-7.14	96930.0	1.66E+34	-5.89	94720.0
	2.30E+06	1.63	75840.0	1.21E+02	2.83	73750.0
$C_2H_3NO_2$ = $CH_2CO+HNO$						
0.01 atm	5.02E+56	-14.04	78750.0	1.41E+54	-13.20	76990.0
	1.96E+32	-7.26	64110.0	1.63E+34	-7.89	63570.0
0.1 atm	5.29E+54	-13.10	80350.0	1.89E+53	-12.60	79150.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
	3.18E+30	-6.58	63970.0	9.58E+28	-6.06	62630.0
1 atm	1.69E+52	-12.05	81880.0	2.05E+50	-11.44	80350.0
	4.05E+24	-4.55	62800.0	2.03E+23	-4.11	61530.0
10 atm	5.11E+46	-10.19	81730.0	3.67E+43	-9.24	79430.0
	1.21E+19	-2.67	61970.0	7.60E+17	-2.27	60900.0
100 atm	1.09E+27	-4.32	72560.0	1.49E+33	-6.00	77360.0
	3.34E+18	-2.67	62450.0	1.64E+09	0.46	59890.0
$C_2H_3NO_2$ = CH_2CHO+NO	-	-	-			
0.01 atm	3.44E+59	-14.18	78090.0	1.72E+57	-13.43	76390.0
	2.41E+36	-7.78	63880.0	9.14E+37	-8.29	63280.0
0.1 atm	2.69E+57	-13.25	79440.0	9.54E+55	-12.76	78180.0
	3.76E+34	-7.10	63700.0	1.71E+33	-6.64	62400.0
1 atm	4.26E+54	-12.16	80510.0	5.11E+52	-11.56	78880.0
	2.07E+29	-5.30	62610.0	1.45E+28	-4.91	61330.0
10 atm	1.01E+49	-10.31	79790.0	7.35E+45	-9.38	77290.0
	3.71E+24	-3.68	61770.0	5.40E+23	-3.40	60740.0
100 atm	1.95E+39	-7.33	76570.0	2.58E+36	-6.47	74870.0
	8.37E+18	-1.87	61130.0	3.40E+16	-1.13	59740.0
$C_2H_3NO_2$ =CH_2=C+HONO	-	-	-			
0.01 atm	4.52E+70	-17.69	90090.0	2.17E+62	-15.08	85140.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
	1.49E+46	-10.59	76200.0	7.44E+47	-11.13	75570.0
0.1 atm	7.22E+62	-14.92	87790.0	9.83E+61	-14.59	86860.0
	5.54E+48	-11.24	77330.0	7.88E+47	-10.91	76340.0
1 atm	1.82E+61	-14.11	89600.0	4.13E+59	-13.56	88410.0
	1.23E+45	-9.89	77580.0	3.79E+43	-9.40	76450.0
10 atm	2.43E+56	-12.38	90350.0	1.03E+54	-11.63	89080.0
	3.20E+37	-7.44	76680.0	7.03E+34	-6.62	75170.0
100 atm	1.45E+48	-9.73	90040.0	4.06E+42	-8.09	86980.0
	4.73E+26	-4.05	74710.0	2.31E+21	-2.44	72170.0
$\dot{C}_2H_3+NO_2 = C_2H_3NO_2$	-	-	-			
0.01 atm	4.53E+53	-13.56	14980.0	1.91E+48	-11.74	11480.0
	4.11E+33	-7.83	2998.0	5.10E+37	-9.06	2982.0
0.1 atm	2.61E+50	-12.07	14940.0	3.51E+49	-11.66	13840.0
	2.31E+36	-8.45	4321.0	1.93E+35	-7.98	3085.0
1 atm	5.08E+49	-11.44	17160.0	3.28E+48	-10.97	15950.0
	4.81E+30	-6.40	3419.0	2.61E+29	-5.90	2060.0
10 atm	1.75E+46	-10.09	18250.0	7.39E+44	-9.60	16870.0
	7.60E+23	-4.07	1997.0	7.08E+22	-3.67	657.0
100 atm	4.64E+38	-7.66	16580.0	2.12E+37	-7.21	14940.0
	3.91E+17	-1.97	524.8	1.32E+17	-1.75	-699.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
$\dot{C}_2H_3+NO_2 = C_2H_2+HONO$						
0.01 atm	1.32E+26	-4.40	7442.0	1.20E+20	-2.52	2632.0
	9.82E+10	0.18	-616.5	2.93E+09	0.55	-2448.0
0.1 atm	2.93E+26	-4.37	8384.0	1.06E+28	-4.79	8227.0
	6.96E+09	0.52	-23.5	2.72E+10	0.34	-829.4
1 atm	7.78E+26	-4.31	11180.0	2.17E+27	-4.41	10760.0
	1.03E+07	1.31	86.3	2.74E+07	1.16	-832.2
10 atm	1.84E+24	-3.39	13270.0	5.02E+24	-3.50	12920.0
	3.89E+05	1.57	348.0	7.20E+04	1.79	-871.6
100 atm	3.92E+20	-2.23	15250.0	5.11E+18	-1.71	13410.0
	1.20E-02	3.82	-906.2	1.56E-03	4.07	-2259.0
$\dot{C}_2H_3+NO_2 = CH_2O+ONCH$						
0.01 atm	6.55E+21	-3.27	6546.0	4.43E+23	-3.81	6163.0/
	6.87E+10	-0.12	-96.0	8.15E+11	-0.42	-771.3/
0.1 atm	5.29E+23	-3.75	8365.0	1.92E+21	-2.99	6042.0/
	1.28E+10	0.10	652.3	1.06E+13	-0.98	-0.0
1 atm	9.33E+23	-3.70	10760.0	5.75E+24	-3.91	10390.0
	1.15E+09	0.31	1283.0	2.72E+09	0.18	425.2
10 atm	1.11E+24	-3.60	14110.0	3.56E+24	-3.74	13760.0
	3.46E+07	0.71	2340.0	9.42E+06	0.88	1340.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
100 atm	3.10E+20	-2.49	16310.0	2.08E+19	-2.16	15130.0
	3.84E+00	2.78	2263.0	7.63E-02	3.25	815.8
$\dot{C}_2H_3$+NO_2 = CH_2(O)C+HNO						
0.01 atm	5.65E+23	-4.05	8886.0	5.63E+26	-4.86	9468.0
	8.72E+12	-0.88	2852.0	1.43E+14	-1.22	2498.0
0.1 atm	2.06E+28	-5.23	13570.0	6.13E+27	-4.97	13330.0
	1.25E+14	-1.16	5847.0	2.10E+15	-1.59	5463.0
1 atm	2.78E+27	-4.74	17830.0	2.63E+26	-4.40	17520.0
	2.97E+15	-1.73	9155.0	8.79E+13	-1.30	8099.0
10 atm	3.33E+24	-3.74	22430.0	3.29E+20	-2.59	20530.0
	6.35E+06	0.82	10030.0	8.36E+02	1.93	8190.0
100 atm	4.16E-03	4.11	14620.0	-1.05E-05	0.65	-8062.0
	7.01E-10	3.15	972.8	3.46E-16	7.78	
$\dot{C}_2H_3$+NO_2 = CH_2CO+HNO						
0.01 atm	6.23E+11	-0.00	10200.0	6.14E-01	3.36	-3459.0
	1.04E-01	3.59	-2426.0	8.72E+12	-0.43	9890.0
0.1 atm	7.00E+05	1.69	5132.0	5.46E+03	2.22	1725.0
	2.98E-01	3.43	-2287.0	1.93E+00	3.17	-3367.0
1 atm	4.26E+05	1.77	4803.0	4.71E+04	1.99	2481.0
	4.28E-01	3.36	-2287.0	3.58E+00	3.07	-3320.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
10 atm	6.73E+07	1.15	6713.0	1.72E+06	1.54	3947.0
	1.76E-01	3.49	-2302.0	1.57E+00	3.20	-3252.0
100 atm	1.13E+05	1.97	4462.0	1.76E+05	1.89	3230.0
	4.36E-01	3.33	-1705.0	5.49E-01	3.25	-2712.0
$\dot{C}_2H_3+NO_2 = CH_2CHO+NO$						
0.01 atm	1.33E+10	0.87	5329.0	5.60E+06	1.76	-2289.0
	7.40E+04	2.38	-1905.0	1.29E+03	2.81	-3786.0
0.1 atm	4.57E+06	1.87	1527.0	2.91E+06	1.85	-1632.0
	1.30E+05	2.27	-1874.0	8.98E+04	2.28	-3291.0
1 atm	1.63E+08	1.45	2838.0	1.47E+08	1.38	975.7
	1.43E+05	2.25	-1871.0	6.62E+05	2.05	-2948.0
10 atm	2.33E+10	0.84	4977.0	4.51E+09	0.95	2815.0
	7.20E+04	2.36	-1905.0	4.99E+05	2.11	-2913.0
100 atm	6.69E+07	1.59	2340.0	2.00E+09	1.14	1653.0
	2.70E+05	2.14	-1534.0	5.99E+05	2.01	-2562.0
$\dot{C}_2H_3+NO_2 = CH_2=C+HONO$						
0.01 atm	9.41E+22	-3.69	8306.0	4.93E+25	-4.52	8180.0
	4.54E+08	0.63	784.4	1.00E+10	0.24	181.7
0.1 atm	5.20E+24	-4.13	9669.0	8.86E+26	-4.77	9777.0
	1.05E+09	0.55	1988.0	1.13E+10	0.25	1432.0

Reaction	Lower limit			Upper limit		
	A	n	E_a (cal·mol^{-1})	A	n	E_a (cal·mol^{-1})
1 atm	5.49E+26	-4.55	13080.0	5.36E+27	-4.80	12970.0
	3.92E+08	0.70	3535.0	1.37E+09	0.54	2959.0
10 atm	2.38E+23	-3.36	15040.0	9.47E+23	-3.51	14950.0
	3.69E+09	0.23	5548.0	2.39E+09	0.24	4707.0
100 atm	1.01E+21	-2.54	18370.0	5.79E+19	-2.16	17580.0
	4.68E+02	2.24	5531.0	2.78E-01	3.17	3713.0

S2.2. Additional model validation

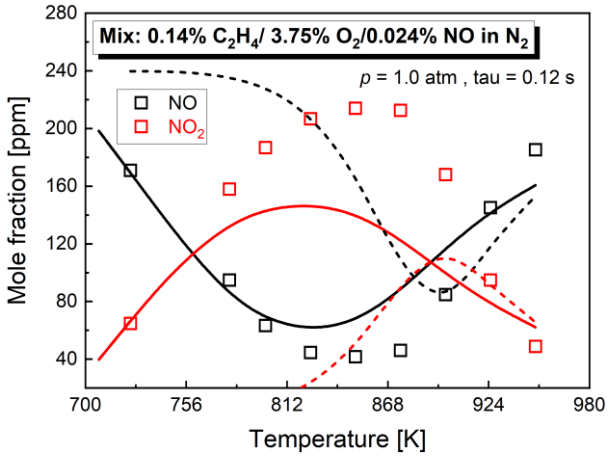

Fig. S48 Effect of newly $\dot{C}_2H_3$ + NO_2 kinetics on the temperature-dependent mole fractions of NO, NO_2 at a pressure of 1 atm with a residence time of 0.12 s . Solid lines means the updated Deng model[1] with the present $\dot{C}_2H_3$ + NO_2 kinetics, dash lines represent the original Deng model [1], and symbols represent the experimental measurement taken from Dagaut et al.[2].

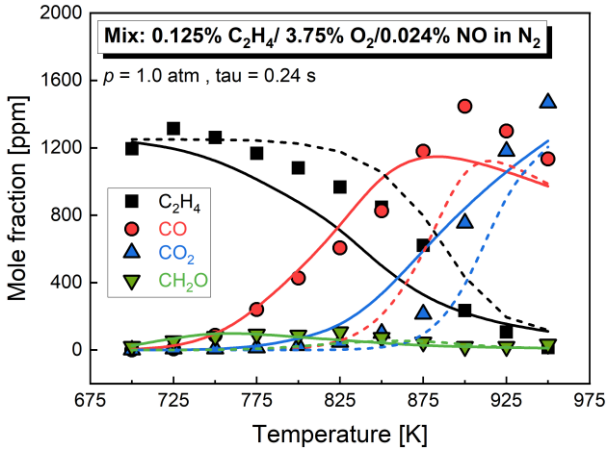

Fig. S49 Effect of newly $\dot{C}_2H_3 + NO_2$ kinetics on the temperature-dependent mole fractions of C_2H_4, CO, CO_2 and CH_2O at a pressure of 1 atm with a residence time of 0.24 s . Solid lines means the updated Deng model[1] with the present $\dot{C}_2H_3 + NO_2$ kinetics, dash lines represent the original Deng model [1], and symbols represent the experimental measurement taken from Dagaut et al.[2].

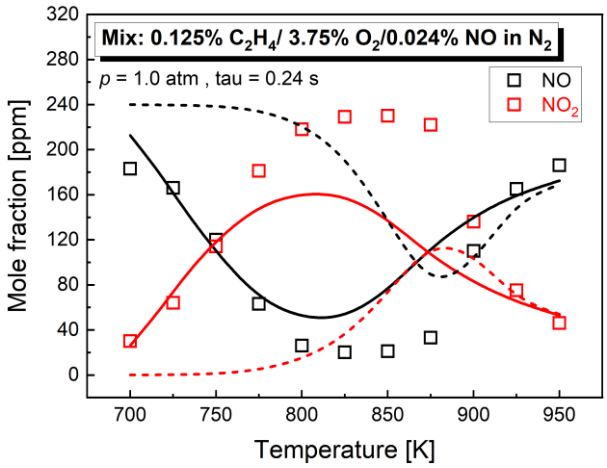

Fig. S50 Effect of newly $\dot{C}_2H_3 + NO_2$ kinetics on the temperature-dependent mole fractions of NO, NO_2 at a pressure of 1 atm with a residence time of 0.24 s . Solid lines means the updated Deng model[1] with the present $\dot{C}_2H_3 + NO_2$ kinetics, dash lines represent the original Deng model [1], and symbols represent the experimental measurement taken from Dagaut et al.[2].

References

[1] Deng Fuquan; Zhang Yingjia; Sun Wuchuan; Huang Wenlin; Zhao Qian; Qin Xiaokang; Yang Feiyu; H. Zuohua, Proc. Combust. Inst. 37 (1) (2019) 719-726
[2] Philippe Dagaut, Olivier Mathieu, André Nicolle, Guillaume Dayma, Combustion Science and Technology 177 (2005) 1767-1791

```
TemperatureList[K]                298.15  300  400  500  600  700  800  900 1000 1100 1200 1300 1400 1500
1600 1700 1800 1900 2000
PressureList[atm]                 0.01 0.1 1. 10  100  1000
EnergyStepOverTemperature         0.2
ExcessEnergyOverTemperature       30
ModelEnergyLimit[kcal/mol]        400
!WellCutoff                       10
ChemicalEigenvalueMax             0.2
ChemicalEigenvalueMin             1.e-6
CalculationMethod                 direct
MicroRateOutput                   C2H3+NO2_AES_N2-ke.out
MicroEnerMin[kcal/mol]            -10.
MicroEnerMax[kcal/mol]            10.
MicroEnerStep[kcal/mol]           1.0
Model
 EnergyRelaxation
  Exponential
   Factor[1/cm]             200
   Power                    0.85
   ExponentCutoff           10
  End
 CollisionFrequency
  LennardJones
    Epsilons[1/cm]          57    227
    Sigmas[angstrom]          3.74   5.85
    Masses[amu]             28    73
  End
!**************************************WELL**************************************!
 Well      C2H3NO2
 Species
  RRHO
```

Geometry[angstrom] 8

N	0.00000000	-0.56087700	0.00000000
O	0.78019400	-1.49423700	0.00000000
O	-1.21031700	-0.65536600	0.00000000
C	0.60816600	0.77629900	0.00000000
H	1.69209800	0.72667000	0.00000000
C	-0.15888400	1.85585700	0.00000000
H	-1.24266700	1.75973300	0.00000000
H	0.29585600	2.84362900	0.00000000

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #CH2CH-NO2 Bond

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.163227771

0.632030706

1.361078773

2.280727204

3.290125808

4.278779575

5.123396067

5.711667398

5.940010575

5.754594068

5.170365153

4.293358503

3.266712173

2.235952518

1.319511289

0.606949779

0.156295674

End

Frequencies[1/cm] 17

324.8630 519.4505

532.3126 637.3883 808.9326

877.7017 932.9365 977.9366

1028.7780 1216.7599 1323.2844

1412.1195 1607.1252 1663.7521

3036.7577 3118.1623 3140.9974

ZeroEnergy[kcal/mol] 0

ElectronicLevels[1/cm] 1

0 1

End

End

Well C2H3ONO

Species

RRHO

Geometry[angstrom] 8

C	2.27230800	-0.18783700	-0.00000100
H	3.16004700	0.43732700	-0.00000100
H	2.38288800	-1.26950700	-0.00000700
C	1.07532200	0.38501500	0.00000400
H	0.89384500	1.45936800	0.00000100
N	-1.21721900	0.43175900	-0.00000500
O	-2.18100900	-0.22254600	0.00000200
O	-0.06924500	-0.38152500	0.00000100

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #CH2CH-ONO

Group 6 7

Axis 4 8

Symmetry 1

Potential[kcal/mol] 36

0

0.104418208

0.406767973

0.869829823

1.446059247

2.078844847

2.700108745

3.229119334

3.568782068

3.640535897

3.444329992

3.062120858

2.627849771

2.268118027

2.061448401

2.023941531

2.110287465

2.22407188

2.277765986

2.224860032

2.111539347

2.023078705

2.059543282

2.267452867

2.626971258

3.062769075

3.44588245

3.640641946

3.56556169

3.228849504

2.70410598

2.079823762

1.446132038

0.868596767

0.407440036

0.104763338

End

Frequencies[1/cm] 17

204.0962 244.4417

462.1626 617.9026 681.3238

845.3884 877.5298 933.9089

940.9483 1168.5193 1255.6881

1343.1392 1652.1332 1767.6118

3041.4279 3063.9089 3143.9509

ZeroEnergy[kcal/mol] -1.48

ElectronicLevels[1/cm] 1

0 1

End

End

Well cis-C2H3ONO

Species

RRHO

Geometry[angstrom] 8

C -2.14995600 0.10898100 -0.00003500

H -2.83595400 0.95118500 -0.00000100

H -2.55074300 -0.90201800 -0.00012800

C -0.84040400 0.33591100 0.00004200

H -0.38157400 1.32042000 0.00013900

N 1.40790400 -0.48047400 -0.00000300

O 1.70520400 0.65187100 -0.00003600

O 0.02668400 -0.73632400 0.00003100

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #CH2CH-ONO

Group 6 7

Axis 4 8

Symmetry 1

Potential[kcal/mol] 36

0

0.010340102

0.046841074

0.130379532

0.30381249

0.600858544

1.025866964

1.533033947

2.049649968

2.487689877

2.786556964

2.940146817

3.04305461

3.16259768

3.30710998

3.415196609

3.448814175

3.428611507

3.411506225

3.427756211

3.448529286

3.417914352

3.307965275

3.163583497

3.042097658

2.943102387

2.786513666

2.490313494

2.05058684

1.539336652

1.028698914

0.599985051

0.303054458

0.128538419

0.047480507

0.009525594

End

Frequencies[1/cm] 17

274.3551 276.1906

402.5880 682.8323 735.2088

818.9777 894.4738 938.3378

940.6655 1117.2967 1254.6574

1344.5188 1646.7399 1709.0215

3037.9452 3102.3691 3139.6901

ZeroEnergy[kcal/mol] 0.29

ElectronicLevels[1/cm] 1

0 1

End

End

Well ONCH2CHO

Species

RRHO

Geometry[angstrom] 8

N	1.05718100	0.01656700	-0.52623100
C	0.05502100	0.94673500	0.05716600
O	-1.47383000	-0.90481500	-0.05081500
C	-1.30787600	0.27608300	0.08818000
H	0.33587900	1.22309300	1.08435800
H	0.00522100	1.83658300	-0.58316800
O	1.71599000	-0.52979500	0.30559600
H	-2.16152200	0.96432600	0.27210000

Core RigidRotor

SymmetryFactor 0.5

End

Rotor Hindered #CH2CH-ONO

Group 7

Axis 1 2

Symmetry 1

Potential[kcal/mol] 36

0

0.081852967

0.32827783

0.7132091

1.180223632

0.497005722

0.2531731

0.090601704

0.079208014

0.233586019

0.496787348

0.623699262

0.604556457

0.696822944

0.902776582

1.134955725

0.602048302

0.625842835

0.387318316

0.156306969

0.063192716

0.14023394

0.343604749

0.599367581

0.854247507

1.062354758

0.212157824

0.02795241

0.019098879

0.192752093

0.51588309

0.882782247

1.061175668

0.741366706

0.375194832

0.103918711

End

Frequencies[1/cm] 17

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521.9691 604.7614 750.3945

811.1858 923.0794 1053.2849

1147.7675 1209.6598 1330.1225

1354.2642 1680.6541 1773.0524

2829.7425 2913.3352 2987.0897

ZeroEnergy[kcal/mol] -11.59

ElectronicLevels[1/cm] 1

0 1

End

End

Well CH2OCHNO

Species

RRHO

Geometry[angstrom] 8

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H 0.18730700 2.09773500 -0.00036500

C 1.43206400 -0.00122600 0.00008300

H 2.03850400 -0.08281600 0.90790100

H 2.03955000 -0.08227400 -0.90711800

N -0.55856600 0.08490900 -0.00002800

O 0.37284500 -1.00555800 -0.00016400

O -1.75233800 -0.08110400 0.00006700

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 18

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664.6377 729.1171 876.6685

926.4279 966.5398 1015.9699

1057.5041 1149.9219 1261.9914

1298.3422 1419.2964 1720.8243

```
2954.5597    3016.9797    3158.4593
     ZeroEnergy[kcal/mol]             21.29
     ElectronicLevels[1/cm]        1
          0   1
  End
  End

  Well    W
  Species
    RRHO
     Geometry[angstrom]    8
 C                 0.18109400   -0.12056700    0.41687800
 H                -0.04808700   -0.36946000    1.45536200
 C                 1.36353100    0.66205500    0.00540000
 H                 2.05539900    0.98735200    0.78175400
 H                 1.29636900    1.26199500   -0.90216900
 N                -0.96905200    0.01914500   -0.47293600
 O                 1.28035000   -0.73779800   -0.19756800
 O                -2.00385700    0.07994500    0.12780900
     Core   RigidRotor
      SymmetryFactor     0.5
     End
           Rotor Hindered         #CH2OCH-NO
      Group       8
      Axis        1 6
      Symmetry    1
     Potential[kcal/mol]     36
0
0.25084253
0.858658272
1.721393473
```

2.702305028

3.653729285

4.449006587

5.010023298

5.327130831

5.428917892

5.361468151

5.189317195

4.943882542

4.616792587

4.150778305

3.488228674

2.673664867

1.909833321

1.403873666

1.236439699

1.386836156

1.81825584

2.49350438

3.340496623

4.278369811

5.20338282

5.964970393

6.389255921

6.333691837

5.781847433

4.852220974

3.72654486

2.56764651

1.512353744

0.671504819

```
0.144997365
  End
    Frequencies[1/cm]      17
        332.8639    396.5927
522.4933    804.2698    876.8006
903.2681    1019.3220    1083.0665
1088.0613    1096.3354    1184.2263
1330.2865    1435.7825    1662.5180
2986.0702    3018.7224    3090.5960
    ZeroEnergy[kcal/mol]            7.08
    ElectronicLevels[1/cm]       1
        0   1
  End
  End

Well  CH2OCNOH
  Species
    RRHO
    Geometry[angstrom]    8
 C              0.25613100   -0.20044900    0.00002500
 H             -1.19942600   -1.49978600    0.00000300
 C              1.67455900   -0.40992500   -0.00001200
 H              2.18949600   -0.63733800   -0.93239500
 H              2.18954400   -0.63734500    0.93234300
 N             -0.98807700   -0.49549800    0.00000500
 O              0.99135700    0.90798100    0.00000300
 O             -1.97225900    0.33016900   -0.00001100
    Core   RigidRotor
      SymmetryFactor    1
    End
    Frequencies[1/cm]      18
```

```
167.9079    216.6871    439.1394
547.1558    781.4693    796.8752
943.5390    1002.8839    1027.8306
1060.3010    1154.0392    1228.3908
1400.5429    1443.2067    1861.8736
2997.1160    3100.4858    3245.6123
    ZeroEnergy[kcal/mol]             21.09
    ElectronicLevels[1/cm]       1
        0   1
 End
 End

  Well  CH2CNOOH
 Species
  RRHO
    Geometry[angstrom]    8
N              0.42899900    0.11153000   -0.00003200
O              1.10617800   -1.11072400   -0.00002700
O              1.15675000    1.13511800    0.00001200
C             -0.82932500    0.02137300   -0.00013900
H              2.02723500   -0.79795000    0.00045800
C             -2.13010100   -0.03257400    0.00006400
H             -2.68838000   -0.05529900    0.93686000
H             -2.68871700   -0.05540000   -0.93652500
    Core   RigidRotor
     SymmetryFactor      1
    End
          Rotor Hindered         #CH2CN(O)-OH Bond
     Group       5
     Axis        1 2
     Symmetry    1
```

Potential[kcal/mol] 36

0

0.07527855

0.31884448

0.743713592

1.317185739

2.004486227

2.759972524

3.53116664

4.264558955

4.913382443

5.441033846

5.823595013

6.049459527

6.125011043

6.073348814

5.931182771

5.739678167

5.560957187

5.464090428

5.520853682

5.683130149

5.87889115

6.03957437

6.120264561

6.084872398

5.904889496

5.568388154

5.081256294

4.465161192

3.752273377

2.986519142

2.220502607

1.508084169

0.897426437

0.426286029

0.122223163

End

Frequencies[1/cm] 17

108.1144 179.7811

501.1876 557.8711 595.9901

630.8638 794.3376 903.2524

946.4607 1088.7641 1207.0396

1360.5615 1517.1112 2058.4590

2989.7425 3077.9428 3576.4906

!1D-Hindered 282.4664

ZeroEnergy[kcal/mol] 38.40

ElectronicLevels[1/cm] 1

0 1

End

End

Well IRCP

Species

RRHO

Geometry[angstrom] 8

N	0.94913400	-0.28240600	0.00000100
O	1.08904900	1.06994500	-0.00000200
O	1.98648700	-0.83614200	0.00000000
C	-1.71537900	0.53596500	0.00000300
H	0.15379500	1.36862300	0.00000000

```
 C              -2.55161100   -0.45561500   -0.00000100
 H              -2.17240700   -1.48077100   -0.00000500
 H              -3.62768100   -0.26354200   -0.00000100
    Core   RigidRotor
     SymmetryFactor   1
    End
    Frequencies[1/cm]      18
38.0337    83.0044    149.7903
160.3893    182.7790    225.3599
389.9987    703.3371    755.8704
767.8138    944.4367    1145.9774
1378.8233    1664.9576    1737.6963
2993.3947    3084.1291    3372.8135
!1D-Hindered 282.4664
    ZeroEnergy[kcal/mol]            64.77
    ElectronicLevels[1/cm]       1
         0   1
 End
 End

 Well    IRCP3
 Species
  RRHO
    Geometry[angstrom]    8
 N               1.10599300   -0.10935600    0.00005100
 O               2.26148200   -0.45864100   -0.00012600
 O               0.68883500    1.03414300    0.00006500
 C              -1.72378900   -0.75442800    0.00013100
 H               0.35321100   -0.84601700    0.00020600
 C              -2.69309800    0.05142400   -0.00010000
 H              -3.60014500    0.63446800   -0.00039700
```

```
 H              -1.59622300    0.59105200    0.00014000
    Core   RigidRotor
     SymmetryFactor    1
    End
    Frequencies[1/cm]       18
60.1075    83.4196    146.4814
209.1819    210.2161    286.6321
592.3181    595.2070    766.8077
1072.3514    1108.8790    1383.9058
1450.0892    1653.1442    1813.3277
2317.3180    2949.0181    3229.0158
!1D-Hindered 282.4664
    ZeroEnergy[kcal/mol]             71.44
    ElectronicLevels[1/cm]        1
         0   1
 End
 End

Well  NOCH2CHO
 Species
  RRHO
    Geometry[angstrom]    8
 C              -0.02730500    0.75954200    0.15839200
 H               0.23262800    1.66512900   -0.39797300
 H              -0.13019500    0.95964800    1.22864300
 C               0.97530600   -0.35098400   -0.08233300
 H               0.54174500   -1.33999900   -0.34394500
 N              -1.80713900   -0.70773100    0.21347500
 O              -1.36837200    0.31687000   -0.31572800
 O               2.15809600   -0.16462100    0.01105200
    Core   RigidRotor
```

```
      SymmetryFactor    0.5
    End
    Frequencies[1/cm]      18
53.4902    176.0650    281.1468
425.8245    583.6975    716.4890
772.4984    994.9559    1047.2097
1146.0184    1189.8226    1319.4692
1347.4307    1419.2616    1775.8169
2847.1075    2966.6297    3041.9561
!1D-Hindered 282.4664
    ZeroEnergy[kcal/mol]            33.272
    ElectronicLevels[1/cm]       1
         0   1
  End
  End


!****************************************Tight Transition
States*************************************!
   Barrier          TS1   C2H3NO2   C2H3NO2
    RRHO
     Geometry[angstrom]    8
 C              1.70283300   -0.52634100   -0.22969700
 H              2.73673000   -0.58172700    0.10029600
 H              1.35814600   -1.15910200   -1.04202200
 C              0.88356400    0.28915500    0.43000500
 H              1.07637100    0.94611900    1.26762300
 N             -0.72890600    0.04432800    0.31221500
 O             -1.53713100   -0.77755500    0.01006700
 O             -0.41128000    1.01599600   -0.47422300
     Core    RigidRotor
```

```
      SymmetryFactor    0.5
    End
    Tunneling      Eckart
      ImaginaryFrequency[1/cm]  812.8284
      WellDepth[kcal/mol]       58.19
      WellDepth[kcal/mol]       59.67
    End
    Frequencies[1/cm]     17
162.2771    299.6946
469.1226    532.0735    559.7191
759.5644    792.2235    918.6585
934.0316    1169.2289    1236.6017
1297.0618    1547.1372    1594.9398
3043.3407    3143.8398    3155.2074
    ZeroEnergy[kcal/mol]       58.19
    ElectronicLevels[1/cm]         1
        0   1
  End

  Barrier            TS2   C2H3ONO  cis-C2H3ONO
    RRHO
    Geometry[angstrom]     8
C              2.13492300   -0.19871200   -0.20946700
H              2.90468500   -0.81415000    0.24675900
H              2.36390200    0.35955300   -1.11394900
C              0.93852900   -0.12249400    0.36470800
H              0.67565600   -0.66908200    1.27290800
N             -1.37552300    0.26644600    0.34424600
O             -1.80140600   -0.55585900   -0.34401000
O             -0.04313100    0.70408200   -0.12435100
    Core     RigidRotor
```

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 238.1417

WellDepth[kcal/mol] 10.826

WellDepth[kcal/mol] 9.054

End

Frequencies[1/cm] 17

36.8138 271.2450

404.2994 601.0988 676.3487

773.8219 860.1579 910.0382

925.2349 1113.1787 1271.7992

1342.4859 1641.8263 1793.0100

3027.9224 3045.7262 3142.9648

ZeroEnergy[kcal/mol] 9.35

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS3 cis-C2H3ONO P1

RRHO

Geometry[angstrom] 8

C	2.05965900	-0.18544200	-0.28681900
H	3.04570800	-0.39067000	-0.67387100
H	0.94112200	-0.93620700	-0.06048300
C	1.31789900	0.72309500	0.16259400
H	0.82693500	1.61662000	0.51262500
N	-1.30882300	-0.51565500	-0.20177400
O	-1.83185000	0.55267000	-0.18452100
O	-0.15782000	-0.54093000	0.48195900

```
      Core     RigidRotor
        SymmetryFactor     0.5
      End
      Tunneling      Eckart
        ImaginaryFrequency[1/cm]    1603.2886
        WellDepth[kcal/mol]         77.812
        WellDepth[kcal/mol]         52.484
      End
      Frequencies[1/cm]     17
89.3196    181.2495
236.3158    342.4559    473.2681
663.9491    668.7792    694.1137
811.3370    849.0677    970.4715
1060.8513    1549.2940    1630.0366
1752.2682    3178.1046    3244.5825
      ZeroEnergy[kcal/mol]        78.1
      ElectronicLevels[1/cm]          1
          0   1
  End


 Barrier TS4   C2H3ONO   P2
             RRHO
      Geometry[angstrom]     8
 C                -1.87248500   -0.67522800    0.02247700
 H                -2.66580100   -1.40014100    0.11939900
 H                -0.60608300   -0.66129800   -0.51663400
 C                -1.57075000    0.52242600    0.25984500
 H                -1.52101400    1.56253100    0.53903400
 N                 1.25572600    0.42116200    0.22005900
 O                 1.91779000   -0.56113000    0.15326700
```

```
O                0.16498900    0.36957900   -0.57528500
    Core     RigidRotor
     SymmetryFactor    0.5
    End
    Tunneling      Eckart
     ImaginaryFrequency[1/cm]    1600.6207
     WellDepth[kcal/mol]         80.764
     WellDepth[kcal/mol]         53.374
    End
    Frequencies[1/cm]     17
74.4583    201.9947
223.9757    337.5646    512.4357
644.3386    668.7961    701.2254
752.1680    885.5151    974.6240
1077.3902    1545.8201    1651.4847
1743.8460    3176.3858    3239.0497
    ZeroEnergy[kcal/mol]        79.28
    ElectronicLevels[1/cm]          1
        0   1
  End


    Barrier         TS5  C2H3ONO  P3
          RRHO
    Geometry[angstrom]     8
C              -1.62360600   -0.44439100    0.00025500
H              -1.90830600   -1.48159400    0.00031900
H              -0.26731100    0.94773900   -0.00038100
C              -1.63568500    0.80637800   -0.00007100
H              -2.29997000    1.65643600   -0.00008500
N               0.80637000    0.17358000   -0.00016300
```

O 1.98783900 0.39057400 0.00022000

O 0.31050300 -0.95426900 -0.00019700

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 977.8993

WellDepth[kcal/mol] 62.717

WellDepth[kcal/mol] 27.004

End

Frequencies[1/cm] 17

213.4192 345.8000

411.2837 495.2214 571.9494

675.3724 701.1856 714.9063

809.8039 954.3334 1131.6961

1378.5446 1603.8579 1642.0759

1786.4409 3182.2228 3259.8556

ZeroEnergy[kcal/mol] 61.24

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS6 C2H3NO2 P1

RRHO

Geometry[angstrom] 8

N -0.80646800 -0.17378600 -0.00003600

O -0.31040800 0.95402500 0.00071400

O -1.98800800 -0.39037100 -0.00038300

C 1.62338100 0.44450000 -0.00069300

H 1.90805500 1.48183600 -0.00135900

```
C               1.63589400   -0.80625800    0.00040900
H               0.26772800   -0.94842000    0.00036200
H               2.30117100   -1.65559500    0.00030600
    Core     RigidRotor
     SymmetryFactor     0.5
    End
    Tunneling      Eckart
     ImaginaryFrequency[1/cm]    979.7493
     WellDepth[kcal/mol]         56.37
     WellDepth[kcal/mol]         30.749
    End
    Frequencies[1/cm]    17
213.5103    345.7829
411.2170    494.5769    571.7984
675.6634    701.9057    715.1695
809.7594    955.0151    1131.7854
1378.2562    1603.5436    1641.9933
1786.4244    3181.6599    3258.8135
    ZeroEnergy[kcal/mol]        56.37
    ElectronicLevels[1/cm]          1
        0   1
  End

   Barrier           TS7   C2H3NO2  CH2OCHNO
          RRHO
    Geometry[angstrom]     8
C               0.50804100   -0.92341600   -0.04578300
H               0.41807200   -1.96565600   -0.31686600
C               1.58664300   -0.02571800    0.11023600
H               2.49697300   -0.11586800   -0.49340000
H               1.68348000    0.58103500    1.00982800
```

N -0.52471200 -0.04681800 -0.01790200

O 0.03403400 1.13731000 -0.14990400

O -1.72074000 -0.19693200 0.09228300

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 884.6389

WellDepth[kcal/mol] 51.47

WellDepth[kcal/mol] 30.178

End

Frequencies[1/cm] 17

252.4228 527.5502

565.8445 703.6988 732.2315

843.2253 960.1377 997.0402

1033.3435 1122.7912 1250.5810

1320.6733 1466.5234 1598.1308

2973.1128 3068.2228 3154.1976

ZeroEnergy[kcal/mol] 51.47

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS8 CH2OCHNO P4

RRHO

Geometry[angstrom] 8

C 0.08391600 1.03930800 -0.06746600

H -0.19174900 2.09785900 -0.14579700

C 1.39828700 0.17732300 0.05668100

H 1.74580500 0.52135500 1.06484800

H 2.13924900 0.55885600 -0.68435100

N -0.86500800 0.22262900 0.02465700

O 0.99561600 -1.07637000 -0.05948100

O -1.81204900 -0.42816300 0.01665800

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1097.3339

WellDepth[kcal/mol] 39.652

WellDepth[kcal/mol] 56.447

End

Frequencies[1/cm] 17

155.8968 224.1952

360.5366 559.9455 585.1468

668.3500 871.8546 1021.0629

1055.6662 1120.2407 1193.6826

1272.3155 1381.7350 2037.2085

2690.4896 2757.1320 2994.2604

ZeroEnergy[kcal/mol] 60.95

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS9 CH2OCHNO W

RRHO

Geometry[angstrom] 8

C -0.12827900 0.84312600 -0.12269000

H 0.17857100 1.69234300 -0.74989300

C -1.45165700 0.25370700 0.14197500

H -2.17317700 0.63583100 -0.60118100

H -1.84954100 0.33741600 1.16278200

N 0.78247900 -0.03260100 0.35227100

O -0.91622400 -0.97080800 -0.21020500

O 1.89702500 -0.15648900 -0.08895900

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 792.6315

WellDepth[kcal/mol] 35.078

WellDepth[kcal/mol] 49.296

End

Frequencies[1/cm] 17

228.8495 283.4952

443.1246 594.0265 831.5378

874.1567 995.9889 1052.8242

1096.2024 1139.0429 1203.6956

1352.3471 1377.5288 1614.5839

2872.6598 2942.9832 2967.5976

ZeroEnergy[kcal/mol] 56.37

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS10 W CH2OCNOH

RRHO

Geometry[angstrom] 8

C 0.24404300 -0.18642300 -0.17056300

H -0.59023900 -1.00640000 -1.02101000

C 1.63280600 -0.40981500 0.14854300

H 2.32822800 -0.70451400 -0.63437200

H 1.92393900 -0.57726700 1.18422100

```
 N              -1.04055200   -0.55111000    0.06930700
 O               0.98945000    0.90906700   -0.07989000
 O              -1.94434400    0.30635600    0.09465600
     Core     RigidRotor
      SymmetryFactor    0.5
     End
     Tunneling      Eckart
      ImaginaryFrequency[1/cm]    1466.6165
      WellDepth[kcal/mol]         55.633
      WellDepth[kcal/mol]         41.614
     End
     Frequencies[1/cm]    17
194.8562    220.3810
479.2635    556.1282    782.5188
885.7012    965.7769    1010.4000
1046.3845    1059.4475    1176.9977
1350.3750    1404.9049    1594.0933
1897.9223    3006.4509    3114.3252
     ZeroEnergy[kcal/mol]        62.71
     ElectronicLevels[1/cm]         1
         0   1
  End

    Barrier           TS12   C2H3ONO   ONCH2CHO
           RRHO
     Geometry[angstrom]     8
 N               0.94123900    0.00076600   -0.50008200
 C              -0.90401000    1.11266700    0.12281500
 O              -0.50195800   -1.15991200    0.21905800
 C              -1.29569100   -0.21368800   -0.06984100
 H              -0.24843400    1.37055200    0.94960300
```

H -1.46903900 1.92197600 -0.33630600

O 1.81969000 0.12939300 0.18121900

H -2.21484900 -0.44760300 -0.63278300

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 373.6542

WellDepth[kcal/mol] 17.513

WellDepth[kcal/mol] 27.627

End

Frequencies[1/cm] 17

234.2742 330.8774

382.5389 426.0745 545.5508

730.5521 807.6917 926.1721

982.6005 1180.4049 1282.6757

1406.2090 1475.2986 1942.9571

2909.1394 3031.6007 3126.9886

ZeroEnergy[kcal/mol] 16.03

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS13 ONCH2CHO P6

RRHO

Geometry[angstrom] 8

N -1.09154100 -0.02568600 -0.50622700

C 0.02859600 1.02757900 0.11986800

O 2.02964500 -0.51251200 0.10017000

C 0.99811800 0.01023500 -0.06903700

H 0.09513100 1.89661600 -0.53669700

H -0.24684700 1.24653500 1.15262900

O -1.80001400 -0.54637400 0.34423300

H -0.20482200 -0.71914400 -0.93255200

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1074.1003

WellDepth[kcal/mol] 49.528

WellDepth[kcal/mol] 37.936

End

Frequencies[1/cm] 17

106.1025 290.5119

378.7398 441.8750 534.0235

606.0915 833.0339 896.5188

949.0634 1066.4710 1209.7908

1318.9062 1404.8655 1810.0464

1974.1515 2981.6756 3073.8694

ZeroEnergy[kcal/mol] 37.93

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS14 C2H3NO2 CH2CNOOH

RRHO

Geometry[angstrom] 8

N 0.47038500 0.11924200 -0.00008200

O 1.40589300 -0.77559200 0.00014300

O 0.69491100 1.28136500 -0.00003200

C -0.77306100 -0.70930000 -0.00024000

H 0.54679600 -1.53610500 0.00001900

C -1.88330000 0.03721400 0.00009500

H -1.84767200 1.13050700 0.00032500

H -2.86008600 -0.44276400 0.00021100

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1196.1523

WellDepth[kcal/mol] 60.803

WellDepth[kcal/mol] 22.406

End

Frequencies[1/cm] 17

93.5998 305.5067

480.6182 554.4877 715.7015

811.5781 812.5128 956.8125

1020.5001 1056.3076 1266.7120

1327.5208 1567.8623 1660.1317

2171.8292 2990.3196 3101.5676

ZeroEnergy[kcal/mol] 60.80

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS15 CH2CNOOH IRCP

RRHO

Geometry[angstrom] 8

N -0.65604100 -0.04127500 0.37492800

O -1.41553400 0.95349100 -0.12613000

O -1.26883800 -0.84977800 0.96517800

C 1.30850000 0.79240100 -0.43129500

H -0.73407900 1.50342800 -0.56660500

```
C               2.22238600   -0.06059000   -0.04607300
H               2.06927400   -0.96760500    0.53388000
H               3.23385300    0.21350200   -0.36690200
    Core     RigidRotor
     SymmetryFactor      0.5
    End
    Tunneling      Eckart
     ImaginaryFrequency[1/cm]    103.9823
     WellDepth[kcal/mol]         28.036
     WellDepth[kcal/mol]         1.665
    End
    Frequencies[1/cm]    17
90.1681    165.4710
191.0672    269.9362    466.8129
581.9353    699.4366    725.2737
798.0926    980.1606    1187.7593
1356.6856    1629.1036    1748.9509
2989.6559    3111.7554    3434.1949
    ZeroEnergy[kcal/mol]        66.43
    ElectronicLevels[1/cm]          1
        0   1
  End


     Barrier        TSPST    IRCP  P8
   RRHO
    Stoichiometry  C2H3O2N1
    Core      PhaseSpaceTheory
     FragmentGeometry[angstrom]      4   #CH2=C
C               0.82113300   -0.00012900   -0.00000300
C              -0.47973600   -0.00002500    0.00000200
H              -1.02339500    0.94840500    0.00000500
```

H -1.02498600 -0.94748100 0.00000100

FragmentGeometry[angstrom] 4 #HONO

H 1.71227700 0.41688300 0.00000100

O 1.01652600 -0.25681800 -0.00000100

N -0.15884000 0.48433800 0.00000200

O -1.09157600 -0.21908800 -0.00000100

SymmetryFactor 2

PotentialPrefactor[au] 143.

PotentialPowerExponent 6.

End

Frequencies[1/cm] 12

304.5775 555.1843 668.0000

738.0506 871.0246 1141.9845

1282.6071 1651.6796 1757.3695

2994.4526 3084.6452 3636.2941

ZeroEnergy[kcal/mol] 69.72

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS16 C2H3NO2 IRCP3

RRHO

Geometry[angstrom] 8

N 0.83316600 -0.02995600 -0.00023000

O 1.88490600 -0.61732000 0.00043500

O 0.65542200 1.16183400 -0.00023500

C -1.40280400 -0.90398000 -0.00041000

H -0.19183500 -0.99866200 -0.00093700

C -2.13142800 0.16390400 0.00036000

H -3.21971000 0.19304400 0.00065400

H -1.53784600 1.09964500 0.00058900

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 1069.0895

WellDepth[kcal/mol] 77.08

WellDepth[kcal/mol] 5.65

End

Frequencies[1/cm] 17

85.7299 198.3267

263.7914 351.3943 379.5041

466.7874 680.2104 794.2808

834.5603 910.5525 1173.3099

1356.6762 1624.7064 1632.9683

2095.7336 2858.0470 3091.1594

ZeroEnergy[kcal/mol] 77.08

ElectronicLevels[1/cm] 1

0 1

End

Barrier TS17 C2H3ONO P7

RRHO

Geometry[angstrom] 8

C	1.35505200	-0.48608500	-0.06334300
O	0.10712500	-0.34952400	0.25087600
N	-2.25400000	0.09495800	0.41848700
O	-1.73769100	0.20387100	-0.54178200
H	1.68620300	-1.47792100	-0.41633200
C	2.28199600	0.51126800	0.01460300
H	1.99513100	1.50257600	0.36295300
H	3.31890100	0.32477300	-0.25634000

```
      Core     RigidRotor
       SymmetryFactor    0.5
      End
      Tunneling      Eckart
       ImaginaryFrequency[1/cm]    119.9312
       WellDepth[kcal/mol]         34.206
       WellDepth[kcal/mol]         16.353
      End
      Frequencies[1/cm]    17
          69.6664    98.0200
289.3212    395.2902    497.5292
685.4065    837.2506    950.1301
965.5454    1222.9969    1251.2117
1363.6840    1515.1871    2094.9134
2900.1221    3023.8782    3126.0938
      ZeroEnergy[kcal/mol]        32.73
      ElectronicLevels[1/cm]          1
          0   1
  End

       Barrier        TS18   NOCH2CHO   NOCH2CHO
            RRHO
      Geometry[angstrom]     8
 C              -1.20108900    0.20572000   -0.40113200
 H              -1.87919700    1.00361900   -0.71108200
 H              -1.40171000   -0.77756500   -0.82768500
 C              -0.89523000    0.15963900    1.05676700
 H              -0.86746800    1.13180200    1.59266900
 N               1.02387700   -0.23442500   -1.23928800
 O               0.21353400    0.63187200   -1.08881800
 O              -0.61155600   -0.87111200    1.61857800
```

```
    Core     RigidRotor
     SymmetryFactor     0.5
    End
    Tunneling      Eckart
     ImaginaryFrequency[1/cm]    165.4072
     WellDepth[kcal/mol]         35.086
     WellDepth[kcal/mol]         2.106
    End
    Frequencies[1/cm]    17
        102.0042    148.8659
303.2083    465.6921    530.8790
871.7849    957.1457    1033.2827
1082.5106    1116.6476    1333.2386
1369.7168    1475.6513    1740.5501
2841.1393    2984.5311    3087.5646
    ZeroEnergy[kcal/mol]        35.378
    ElectronicLevels[1/cm]          1
        0   1
  End


   Barrier          TS19  NOCH2CHO  P7
          RRHO
    Geometry[angstrom]     8
 C              1.29093800    1.02508100   -0.14909300
 H              0.65105800    1.40819200   -0.94301300
 H              1.99691000    1.70512400    0.32203800
 C              1.29497700   -0.32217200    0.16250200
 H              2.02875400   -0.67827900    0.90829500
 N             -2.08704300    0.23024800   -0.15755900
 O             -1.12985700    0.11593200    0.36807600
```

```
O               0.43199300   -1.14896000   -0.27618300
    Core     RigidRotor
     SymmetryFactor     0.5
    End
    Tunneling      Eckart
     ImaginaryFrequency[1/cm]    93.8207
     WellDepth[kcal/mol]         9.964
     WellDepth[kcal/mol]         36.863
    End
    Frequencies[1/cm]    17
        146.5590    253.1503
283.0293    383.6523    509.1154
650.6460    784.1629    943.4155
966.1227    1199.0547    1274.8278
1391.0199    1469.7415    2076.2791
2883.0281    3019.4621    3121.2753
    ZeroEnergy[kcal/mol]       43.236
    ElectronicLevels[1/cm]         1
        0   1
  End
!***************************************Full C2H3+NO2
PES***************************************!
!***************************************Finish barrierless channel
1***************************************!
  BarrierTSdecomp   ONCH2CHO   P7
            Variational

  RRHO  #d=2.0 angstrom
       Geometry[angstrom]                          8
O        0.0000000000       0.0000000000       0.0000000000
N        0.0000000000       0.0000000000       1.1484290194
```

```
C         0.0000000000       1.9522902151       1.8848634667
C         0.7483687028       2.5041347155       0.7920802502
O         0.2657667347       2.6246168815      -0.3353215909
H        -1.0782958180       2.0279721547       1.8417779071
H         0.4584595509       1.8475814566       2.8578381385
H         1.8197431816       2.7007797481       0.9614042734
   Core RigidRotor
      SymmetryFactor     0.5
    End
     Frequencies[1/cm]     17
163.45
178.30
281.51
484.26
525.27
779.23
888.45
981.03
1014.00
1184.27
1405.64
1482.99
1642.34
1828.17
2984.86
3174.96
3287.71
     ZeroEnergy[kcal/mol]             11.84
     ElectronicLevels[1/cm]           1
          0   1
  End
```

RRHO #d=2.2 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.1431978602
C	0.0000000000	2.1671959351	1.8723497005
C	0.7399710045	2.5354329950	0.7119422084
O	0.2409737109	2.5324440776	-0.4198411584
H	-1.0794508112	2.1822283309	1.8236556525
H	0.4776620345	2.1190193466	2.8398403186
H	1.8194947917	2.7156897613	0.8391861560

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 17

156.35

182.05

274.13

448.31

511.60

706.04

842.48

974.74

1012.09

1191.85

1401.72

1485.09

1610.29

1861.57

2990.17

3184.13

3301.60

ZeroEnergy[kcal/mol] 15.39

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.4 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.1421955482
C	0.0000000000	2.3869969808	1.8388115750
C	0.7386598638	2.5829592380	0.6424639314
O	0.2282397504	2.4856982119	-0.4832244527
H	-1.0787528200	2.3636844040	1.7908071400
H	0.4877256460	2.4065323936	2.8019151878
H	1.8242832606	2.7384550017	0.7426658335

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 17

144.11

174.56

251.09

400.01

508.66

644.06

821.91

974.37

1008.05

1191.83

1399.72

1487.01

1579.14

1875.89

2996.53

3189.30

3309.69

ZeroEnergy[kcal/mol] 18.68

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.6 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.1437509596
C	0.0000000000	2.6068525218	1.7933479520
C	0.7436086789	2.6521491497	0.5862163775
O	0.2273136220	2.4888900451	-0.5300142217
H	-1.0779945772	2.5673911724	1.7458923706
H	0.4902465705	2.6920099365	2.7513439785
H	1.8336907458	2.7775599281	0.6740431892

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 17

131.12

156.59

216.95

348.59

506.41

589.52

812.99

975.46

1001.25

1185.47

1399.60

1487.88

1558.94

1882.92

3002.34

3192.42

3314.80

ZeroEnergy[kcal/mol] 21.54

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.8 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.1463731912
C	0.0000000000	2.8239316855	1.7444484430
C	0.7536788791	2.7409631861	0.5436678715
O	0.2375838095	2.5345185675	-0.5644395243
H	-1.0776970926	2.7878903519	1.6924773112
H	0.4871412379	2.9644447404	2.6972913127
H	1.8468735357	2.8307146894	0.6325168589

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 17

118.85

131.91

178.67

295.75

503.92

541.29

805.52

976.43

993.24

1177.34

1401.31

1487.52

1554.06

1888.48

3006.46

3194.50

3318.31

ZeroEnergy[kcal/mol] 23.79

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=3.0 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.1489059684
C	0.0000000000	3.0388512665	1.6895491031
C	0.7660513570	2.8450515004	0.5065211372
O	0.2553424462	2.6045927509	-0.5954727323
H	-1.0773872955	3.0192383006	1.6268267017
H	0.4804153417	3.2256929228	2.6376727760

```
H         1.8605440733        2.8977600474        0.6061363919
    Core RigidRotor
        SymmetryFactor    0.5
    End
     Frequencies[1/cm]     17
104.00
108.31
142.42
244.67
499.45
505.18
797.19
976.32
986.81
1171.06
1403.56
1486.78
1558.30
1893.17
3009.16
3195.93
3320.69
    ZeroEnergy[kcal/mol]             25.43
    ElectronicLevels[1/cm]            1
         0   1
  End
  End

Barrier TSaddition   C2H3NO2  R
            Variational
                    RRHO  #d=1.80000 angstrom
```

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.2120730697
O	0.0000000000	0.9383131577	-0.7643862239
C	-0.0000000243	-1.6901223064	-0.7978551434
H	-0.0000000748	-2.4343349583	-0.0203019897
C	-0.0000000041	-1.6467538175	-2.1082784108
H	-0.0000001781	-0.6855390849	-2.6058259406
H	0.0000003303	-2.5564257941	-2.6928151980

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 17

138.87

214.67

454.56

461.45

712.62

776.53

899.25

900.00

963.90

1136.12

1317.73

1381.01

1639.10

1682.25

3175.31

3277.04

3308.11

ZeroEnergy[kcal/mol] 18.04

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.00000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.2061809658
O	0.0000000000	0.9186970364	-0.7812175165
C	-0.0000006799	-1.8544193525	-0.9175004662
H	-0.0000014591	-2.6170950800	-0.1589543178
C	0.0000004294	-1.7041710773	-2.2163414280
H	-0.0000029158	-0.7031789610	-2.6329107964
H	0.0000050710	-2.5585663306	-2.8817718792

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.177124596

0.677840154

1.430986469

2.313260433

3.199215368

3.990264512

4.634225428

5.062835752

5.208439291

5.042668224

4.578217695

3.884523513

3.038781269

2.133448213

1.279976308

0.597170043

0.155626121

End

Frequencies[1/cm] 16

187.66

400.17

422.98

636.62

760.55

823.47

863.53

951.72

1072.90

1305.12

1377.82

1649.22

1676.22

3154.47

3252.56

3315.49

ZeroEnergy[kcal/mol] 32.18

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.20000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.2017630257
O	0.0000000000	0.9019005423	-0.7958791911
C	-0.0000011465	-2.0072532002	-1.0579247755
H	0.0000014698	-2.8121193672	-0.3453103733
C	-0.0000043878	-1.7463972497	-2.3374884704
H	-0.0000044264	-0.7141261343	-2.6725501583
H	-0.0000060000	-2.5388296872	-3.0778682759

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.193739166

0.737119722

1.529918362

2.39926061

3.2006235

3.881025148

4.41929966

4.766115375

4.87973099

4.743388864

4.35973081

3.770478682

3.023402894

2.165593643

1.312674573

0.615650825

0.159115701

End

Frequencies[1/cm] 16

156.39

346.43

380.45

556.53

731.20

774.41

834.99

944.83

1037.41

1312.70

1381.81

1652.99

1684.35

3138.71

3232.05

3321.80

ZeroEnergy[kcal/mol] 44.16

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.40000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.1985504549
O	0.0000000000	0.8841836868	-0.8117445784
C	0.0000053741	-2.1572971002	-1.2008045062
H	0.0000061230	-3.0129619794	-0.5503216232
C	0.0000065139	-1.8067122690	-2.4587924164
H	0.0000029066	-0.7559690358	-2.7306515004
H	0.0000114070	-2.5459435619	-3.2540052799

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.223053272

0.847231952

1.721119252

2.591867122

3.293718299

3.859624564

4.29697484

4.571948876

4.659653369

4.550622338

4.242516429

3.756110597

3.110685073

2.282063799

1.394963659

0.654369417

0.167392552

End

Frequencies[1/cm] 16

129.85

292.45

330.22

469.65

702.96

758.86

819.75

939.99

1028.23

1328.12

1387.35

1651.72

1695.00

3129.99

3219.56

3321.11

ZeroEnergy[kcal/mol] 53.37

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.60000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.1966082435
O	0.0000000000	0.8706777683	-0.8236866768
C	0.0000003398	-2.3027808187	-1.3493163979
H	0.0000000451	-3.2102792888	-0.7727844347
C	0.0000009411	-1.8724698548	-2.5834909078
H	0.0000011229	-0.8090925401	-2.7980460624
H	0.0000011396	-2.5619803916	-3.4232365400

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.306186986

1.115567564

2.197948033

3.14097935

3.743377175

4.209114725

4.559009003

4.775566296

4.843720103

4.756791212

4.511252392

4.11594337

3.566181669

2.643176063

1.608683982

0.752599754

0.195234521

End

Frequencies[1/cm] 16

107.03

237.14

273.70

380.07

697.98

755.75

813.77

936.57

1032.52

1347.81

1391.86

1647.84

1700.61

3126.04

3216.07

3314.76

ZeroEnergy[kcal/mol] 60.01

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.80000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.1959701298
O	0.0000000000	0.8623443134	-0.8315721246
C	0.0000038630	-2.4358487702	-1.5158123265
H	0.0000547198	-3.3935324305	-1.0261798482
C	-0.0000648572	-1.9171669440	-2.7167574989
H	-0.0000991143	-0.8426688166	-2.8615408822
H	-0.0000911349	-2.5466743937	-3.6029204958

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.038340861

0.143260533

0.291290142

0.4580823

0.621987912

0.76869975

0.884475345

0.958145019

0.983747427

0.95820777

0.884224341

0.769013505

0.621987912

0.45745479

0.291290142

0.143260533

0.038340861

End

Frequencies[1/cm] 16

89.82

187.11

217.71

296.49

700.83

756.51

812.75

934.29

1040.87

1360.29

1394.93

1644.75

1699.49

3124.15

3217.19

3307.40

ZeroEnergy[kcal/mol] 64.30

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=3.00000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.1959288012
O	0.0000000000	0.8582107402	-0.8358501896
C	-0.0000079702	-2.5449028285	-1.7152573667
H	-0.0000215356	-3.5509045457	-1.3335120225
C	0.0000126482	-1.9163258411	-2.8635183719
H	0.0000218947	-0.8337103600	-2.9127663807
H	0.0000202298	-2.4626024250	-3.8035251490

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.025037649

0.094252002

0.191892558

0.302208816

0.411583809

0.509161614

0.585906087

0.634851867

0.651606384

0.634600863

0.585780585

0.50891061

0.411772062

0.302208816

0.192080811

0.094377504

0.025037649

End

Frequencies[1/cm] 16

79.74

146.37

167.76

227.44

704.64

758.30

813.56

933.17

1048.95

1366.28

1397.34

1642.66

1696.00

3123.41

3219.68

3301.19

ZeroEnergy[kcal/mol] 66.95

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=3.20000 angstrom

Geometry[angstrom] 8

N	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	1.1960625725
O	0.0000000000	0.8564387673	-0.8379479990
C	0.0000372195	-2.6210498340	-1.9535424251
H	0.0000666828	-3.6674697500	-1.7016253918
C	0.0000177562	-1.8656605373	-3.0234366616
H	-0.0000129110	-0.7846007345	-2.9527717918
H	0.0000321614	-2.3031483978	-4.0188528420

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-NO2

Group 2 3

Axis 1 4

Symmetry 2

Potential[kcal/mol] 18

0

0.024974898

0.094063749

0.191704305

0.302146065

0.411458307

0.509036112

0.585780585

0.634726365

0.651480882

0.634475361

0.585655083

0.508785108

0.41164656

0.302083314

0.191955309

0.094252002

0.024912147

End

Frequencies[1/cm] 16

75.48

116.38

125.77

176.04

708.68

759.82

815.33

932.83

1055.71

1368.68

1399.36

1641.39

1692.52

3123.32

3222.45

3296.48

ZeroEnergy[kcal/mol] 68.54

ElectronicLevels[1/cm] 1

0 1

End

End

Barrier TSadd2 C2H3ONO R

Variational

RRHO #d=2.00000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2026075291
O	0.0000000000	1.2985909285	1.6910160048
C	0.0000109382	0.9576784290	3.6617464957
C	0.0000205283	2.0655564817	4.3817358448
H	0.0000237979	1.9738243992	5.4729944335
H	0.0000250571	3.0532415724	3.9203893333
H	0.0000061138	-0.1267359390	3.7384093754

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 17

60.63

181.05

220.07

356.89

564.70

638.40

826.70

850.69

876.68

924.35

1082.35

1363.43

1618.40

1667.97

3182.02

3305.06

3339.34

ZeroEnergy[kcal/mol] 32.37

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.20000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2086537486
O	0.0000000000	1.2842882912	1.6884880842
C	0.0000549756	0.8372359817	3.8425874852
C	0.0001136363	1.9252907348	4.5852220902
H	0.0001495085	1.8098855180	5.6760481250
H	0.0001233985	2.9245772318	4.1480268410
H	0.0000222706	-0.2491626323	3.8128193201

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 17

54.55

153.84

210.77

313.59

511.99

639.76

770.74

789.24

863.46

919.47

1024.55

1355.86

1589.26

1661.14

3164.92

3292.25

3345.96

ZeroEnergy[kcal/mol] 43.65

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.40000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2128026974
O	0.0000000000	1.2781642868	1.6792831426
C	0.0000178718	0.7424139721	4.0187214512
C	0.0000231292	1.8079445508	4.7898954271
H	0.0000325345	1.6675211935	5.8792234186
H	0.0000176711	2.8200995999	4.3814774638
H	0.0000177178	-0.3389755184	3.9139153128

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 17

49.36

127.45

199.44

278.47

459.89

603.03

689.30

762.97

855.24

919.42

979.49

1353.14

1564.09

1657.24

3149.67

3279.31

3350.30

ZeroEnergy[kcal/mol] 53.02

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.50000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2141537688
O	0.0000000000	1.2802701541	1.6657422762
C	0.0000099658	0.7376005886	4.1061335855

```
C         0.0000127913       1.7987669040       4.8843724210
H         0.0000060168       1.6568613592       5.9740348770
H         0.0000214828       2.8140380278       4.4828197465
H         0.0000109115      -0.3444825414       4.0088584662
      Core RigidRotor
        SymmetryFactor    1
      End

     Frequencies[1/cm]     17
  45.99
 114.89
 191.10
 260.88
 428.31
 551.83
 675.34
 759.59
 847.69
 922.03
 969.10
1357.13
1551.07
1654.40
3143.31
3272.81
3348.40
     ZeroEnergy[kcal/mol]                    57.04
     ElectronicLevels[1/cm]          1
          0   1
  End
```

RRHO #d=2.60000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2162063583
O	0.0000000000	1.2825666748	1.6463253599
C	-0.0000479443	0.7666737507	4.1946295978
C	-0.0000198057	1.8307383032	4.9720506062
H	-0.0000471743	1.6979493114	6.0631965487
H	0.0000307190	2.8456555479	4.5686468643
H	-0.0000945708	-0.3187251318	4.1394723812

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 17

37.92

102.02

178.19

236.33

385.96

471.65

680.78

762.40

821.42

925.16

976.48

1364.91

1530.05

1650.16

3138.53

3265.90

3340.49

ZeroEnergy[kcal/mol] 60.44

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.70000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2203423750
O	0.0000000000	1.2835972059	1.6190166299
C	0.0000194654	0.8223013901	4.2793185244
C	0.0000959154	1.8964581851	5.0467584665
H	0.0001332681	1.7822223473	6.1401493151
H	0.0001258069	2.9071881191	4.6321357821
H	-0.0000303421	-0.2651278511	4.2834890806

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 17

34.42

89.99

163.74

203.69

318.78

343.10

693.99

770.86

811.03

927.85

996.71

1372.47

1494.31

1645.79

3135.48

3261.18

3329.23

ZeroEnergy[kcal/mol] 63.10

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.80000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2380894298
O	0.0000000000	1.2777683530	1.5464927575
C	0.0000024928	0.9588895529	4.3282756949
C	0.0001041441	2.0693891230	5.0481222578
H	0.0001114624	2.0123891114	6.1459836244
H	0.0001817624	3.0602147738	4.5872272822
H	-0.0000851006	-0.1234919937	4.4429706614

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-ONO

Group 1 2

Axis 3 4

Symmetry 1

Potential[kcal/mol] 36

0

0.004204317

0.016629015

0.036207327

0.061872486

0.09287148

0.128200293

0.167858925

0.209274585

0.244854402

0.266817252

0.274974882

0.267695766

0.247427193

0.210717858

0.166164648

0.116026599

0.080446782

0.067645578

0.079442766

0.116905113

0.164031114

0.210968862

0.246109422

0.267821268

0.274974882

0.267131007

0.243599382

0.209462838

0.167482419

0.128765052

0.092620476

0.061684233

0.036019074

0.016629015

0.004141566

End

Frequencies[1/cm] 16

76.13

139.24

153.83

283.87

473.67

716.20

785.25

923.70

930.34

1027.88

1380.79

1444.28

1640.07

3133.78

3256.61

3312.78

ZeroEnergy[kcal/mol] 65.41

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=2.90000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2458824165
O	0.0000000000	1.2699923537	1.5338106498
C	0.0000091365	0.9080430654	4.4111345302
C	0.0000397526	2.0006016595	5.1606269761
H	0.0000461988	1.9197787491	6.2569656454
H	0.0000588253	3.0028237949	4.7244157319
H	-0.0000152020	-0.1750402673	4.5254603502

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-ONO

Group 1 2

Axis 3 4

Symmetry 1

Potential[kcal/mol] 36

0

0.004580823

0.019013553

0.040725399

0.069151602

0.101342865

0.132906618

0.166854909

0.198230409

0.228476391

0.246925185

0.259538136

0.258785124

0.246862434

0.222640548

0.188504004

0.151606416

0.122113446

0.110755515

0.122113446

0.151606416

0.188692257

0.228476391

0.246925185

0.259538136

0.258785124

0.246862434

0.228476391

0.198230409

0.166854909

0.132906618

0.101342865

0.069151602

0.040725399

0.019013553

0.004580823

End

Frequencies[1/cm] 16

75.35

123.79

136.23

240.77

711.97

783.70

791.51

931.37

949.66

1040.46

1384.46

1495.11

1637.62

3132.86

3253.18

3302.71

ZeroEnergy[kcal/mol] 67.24

ElectronicLevels[1/cm] 1

0 1

End

RRHO #d=3.00000 angstrom

Geometry[angstrom] 8

O	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.2470902673
O	0.0000000000	1.2686617954	1.5304285185
C	-0.0000149484	0.8211257174	4.4968592793
C	0.0000001212	1.8820808891	5.2918690812
H	-0.0000044772	1.7584041187	6.3841672083

H 0.0000172402 2.9015012696 4.8970459520

H -0.0000310162 -0.2651045610 4.5811998285

Core RigidRotor

SymmetryFactor 1

End

Rotor Hindered #C2H3-ONO

Group 1 2

Axis 3 4

Symmetry 1

Potential[kcal/mol] 36

0

0.004580823

0.019013553

0.040725399

0.069151602

0.101342865

0.132906618

0.166854909

0.198230409

0.228476391

0.246925185

0.259538136

0.258785124

0.246862434

0.222640548

0.188504004

0.151606416

0.122113446

0.110755515

0.122113446

0.151606416

0.188692257

0.228476391

0.246925185

0.259538136

0.258785124

0.246862434

0.228476391

0.198230409

0.166854909

0.132906618

0.101342865

0.069151602

0.040725399

0.019013553

0.004580823

End

Frequencies[1/cm] 16

79.31

112.29

134.86

208.54

716.89

766.88

794.80

931.88

1047.72

1120.69

```
 1386.46
 1583.19
 1636.49
 3132.49
 3251.04
 3296.78
     ZeroEnergy[kcal/mol]                 68.58
     ElectronicLevels[1/cm]          1
          0   1
  End

End


 BarrierTS11   CH2OCNOH  P5
    Variational
                  RRHO  #left10
        Geometry[angstrom]                        8
C              -0.47289400   -0.05687400    0.56390500
H               1.33176700   -1.20376800    0.74694800
C              -1.61055400   -0.61390400   -0.24259400
H              -2.53767500   -0.90662800    0.24518100
H              -1.40749200   -1.01090200   -1.23645700
N               1.08514500   -0.42056900    0.09143800
O              -1.26720900    0.78659500   -0.10831200
O               2.04494800    0.28151500   -0.19740500
      Core RigidRotor
        SymmetryFactor    0.5
      End
     Frequencies[1/cm]     17
         184.7217    239.3819
```

405.1952 569.6697 793.1199

886.2870 909.7374 957.6142

1061.6491 1097.0679 1294.0511

1424.9460 1438.3831 1453.2967

2981.9507 2997.9355 3105.8920

ZeroEnergy[kcal/mol] 51.89

ElectronicLevels[1/cm] 1

0 1

End

RRHO #left9

Geometry[angstrom] 8

C	-0.51876200	-0.04427000	0.59078300
H	1.37620200	-1.16941300	0.78632100
C	-1.62454200	-0.61445500	-0.25013100
H	-2.56592600	-0.90027500	0.21372800
H	-1.39238000	-1.01471000	-1.23546400
N	1.12562100	-0.43438700	0.07738200
O	-1.27989600	0.78667300	-0.10692100
O	2.06513300	0.28216600	-0.20156200

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 17

161.4933 214.0720

366.1739 510.8935 781.3655

873.6627 897.6681 939.9518

1063.1758 1089.1339 1306.6063

1429.5395 1438.4606 1500.9525

2962.5055 3002.0714 3110.7351

ZeroEnergy[kcal/mol] 58.06

```
    ElectronicLevels[1/cm]          1
        0   1
  End

                RRHO  #left8
      Geometry[angstrom]                        8
C            -0.56465600   -0.03286700    0.61568900
H             1.41987200   -1.13636100    0.82047000
C            -1.63977700   -0.61465900   -0.25715900
H            -2.59532600   -0.89319400    0.18126600
H            -1.37745900   -1.01894600   -1.23262100
N             1.16676700   -0.44834400    0.06559300
O            -1.29424100    0.78723500   -0.10530700
O             2.08747800    0.28315800   -0.20655200
      Core RigidRotor
        SymmetryFactor    0.5
      End
      Frequencies[1/cm]     17
         134.9286    190.9671
327.4001    449.8271    753.2721
863.8549    885.0274    924.3747
1063.8637    1083.0988    1319.9917
1436.5504    1441.1070    1547.3752
2943.6612    3004.4559    3114.4220
    ZeroEnergy[kcal/mol]                    62.31
    ElectronicLevels[1/cm]          1
        0   1
  End

                RRHO  #left7
      Geometry[angstrom]                        8
```

```
C              -0.58736100   -0.02781400    0.62746400
H               1.44042600   -1.11903900    0.83654400
C              -1.64783000   -0.61455500   -0.26053700
H              -2.61037900   -0.88949000    0.16458000
H              -1.37022400   -1.02099700   -1.23062300
N               1.18753100   -0.45538900    0.06055500
O              -1.30207100    0.78772900   -0.10442400
O               2.09940400    0.28376800   -0.20941200
      Core RigidRotor
        SymmetryFactor    0.5
      End
     Frequencies[1/cm]     17
          120.9088    180.5788
309.4074    420.2062    731.6197
860.5693    878.6691    917.1499
1064.0677    1080.4560    1326.4023
1440.1103    1443.6553    1567.0763
2943.0831    3005.1987    3115.8717
    ZeroEnergy[kcal/mol]                  63.69
    ElectronicLevels[1/cm]          1
         0   1
  End


                RRHO  #left6
       Geometry[angstrom]                          8
C              -0.61000900   -0.02307200    0.63883000
H               1.46438800   -1.10606400    0.84989500
C              -1.65624500   -0.61436600   -0.26379300
H              -2.62592400   -0.88548100    0.14702700
H              -1.36301700   -1.02314700   -1.22803500
N               1.20825500   -0.46200900    0.05644700
```

```
O               -1.31033000    0.78833700   -0.10360800
O                2.11184000    0.28432200   -0.21261400
      Core RigidRotor
        SymmetryFactor    0.5
      End
     Frequencies[1/cm]     17
         108.9950    171.0551
293.5547    392.5155    710.8945
857.7204    872.8898    910.6177
1064.1033    1077.9072    1332.0976
1444.3182    1447.1405    1583.6405
2922.3085    3006.3734    3117.7090
    ZeroEnergy[kcal/mol]                    64.64
    ElectronicLevels[1/cm]          1
         0   1
  End

                  RRHO  #left5
       Geometry[angstrom]                          8
C               -0.63251700   -0.01877000    0.64993700
H                1.48600700   -1.09094000    0.86352300
C               -1.66474300   -0.61402800   -0.26698600
H               -2.64130800   -0.88147400    0.12948400
H               -1.35607900   -1.02513600   -1.22520800
N                1.22909300   -0.46880700    0.05260700
O               -1.31879700    0.78907500   -0.10276400
O                2.12449500    0.28497400   -0.21596500
      Core RigidRotor
        SymmetryFactor    0.5
      End
     Frequencies[1/cm]     17
```

```
          96.4646    162.2495
277.0000    365.7195    685.3595
854.9634    868.7097    903.9487
1064.1690    1076.0349    1337.0481
1447.2645    1451.1045    1598.2458
2919.6496    3007.0024    3118.9516
     ZeroEnergy[kcal/mol]                    65.25
     ElectronicLevels[1/cm]          1
          0   1
  End

                    RRHO  #left4
        Geometry[angstrom]                          8
 C              -0.65509700   -0.01471700    0.66089600
 H               1.50864200   -1.07759900    0.87563500
 C              -1.67328500   -0.61360400   -0.27007200
 H              -2.65663400   -0.87733500    0.11160800
 H              -1.34922200   -1.02713400   -1.22198200
 N               1.24994400   -0.47552600    0.04920500
 O              -1.32737100    0.78992000   -0.10201000
 O               2.13727100    0.28567700   -0.21948800
       Core RigidRotor
         SymmetryFactor    0.5
       End
      Frequencies[1/cm]     17
          85.0503    153.8078
260.1379    339.9423    657.6869
851.5756    866.7754    897.5961
1064.1662    1074.9497    1341.4855
1450.5201    1455.3268    1610.9207
2912.5517    3007.6351    3120.1002
```

ZeroEnergy[kcal/mol] 65.59

ElectronicLevels[1/cm] 1

0 1

End

RRHO #left3

Geometry[angstrom] 8

C	-0.67771000	-0.01092800	0.67179100
H	1.52981000	-1.06333300	0.88778300
C	-1.68175000	-0.61306800	-0.27309200
H	-2.67165900	-0.87320200	0.09359600
H	-1.34238600	-1.02905600	-1.21842300
N	1.27085500	-0.48239100	0.04589000
O	-1.33596800	0.79085400	-0.10127900
O	2.15006000	0.28647000	-0.22308000

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 17

73.8958 145.8953

242.8939 315.1004 626.8034

848.1094 866.1902 891.6814

1064.1785 1074.3704 1345.6075

1453.8996 1459.4435 1622.2390

2906.6700 3008.4546 3121.4473

ZeroEnergy[kcal/mol] 65.71

ElectronicLevels[1/cm] 1

0 1

End

RRHO #left2

```
        Geometry[angstrom]                      8
C              -0.70039800   -0.00745400    0.68263700
H               1.55083900   -1.04941400    0.89913800
C              -1.69023600   -0.61241100   -0.27609100
H              -2.68657000   -0.86892700    0.07531700
H              -1.33562200   -1.03102100   -1.21454500
N               1.29169900   -0.48919500    0.04278400
O              -1.34455700    0.79185000   -0.10057300
O               2.16297500    0.28730900   -0.22676100
      Core RigidRotor
        SymmetryFactor    0.5
      End
     Frequencies[1/cm]     17
         63.5027    138.7466
225.7010    291.6509    591.6305
844.7644    865.7122    886.3538
1064.1834    1073.8197    1349.4037
1457.5570    1463.5382    1631.7665
2897.3177    3009.2484    3122.8011
    ZeroEnergy[kcal/mol]                  65.66
    ElectronicLevels[1/cm]          1
          0   1
  End


                 RRHO  #left1
        Geometry[angstrom]                      8
C              -0.72316700   -0.00381700    0.69361800
H               1.57070500   -1.03624000    0.90952000
C              -1.69807800   -0.61161900   -0.27892800
H              -2.70049500   -0.86497700    0.05654800
H              -1.32792300   -1.03285700   -1.20991700
```

```
N                1.31281600   -0.49708000    0.03917900
O               -1.35312800    0.79311500   -0.09997300
O                2.17516600    0.28866000   -0.23007800
      Core RigidRotor
        SymmetryFactor   0.5
      End
     Frequencies[1/cm]     17
          54.1047    131.4810
208.2322    268.5820    555.0612
841.6438    864.2238    881.1459
1063.6236    1072.8887    1352.7791
1461.3829    1467.4061    1639.7845
2892.3126    3011.5348    3125.6795
    ZeroEnergy[kcal/mol]                    65.51
    ElectronicLevels[1/cm]           1
          0   1
  End


                  RRHO  #TS11
       Geometry[angstrom]                          8
C               -0.71430800    0.03747800    0.70794300
H                1.61997000   -0.98285000    0.92408000
C               -1.67396800   -0.57284500   -0.27847200
H               -2.68224300   -0.82304400    0.04085900
H               -1.28837900   -0.99686300   -1.20165400
N                1.36572600   -0.46629900    0.03913900
O               -1.32967700    0.83224200   -0.09614300
O                2.21970500    0.32763900   -0.23061800
      Core RigidRotor
        SymmetryFactor  0.5
      End
```

```
      Frequencies[1/cm]     17
          45.9901    124.0757
192.0064    246.7792    520.0842
838.6974    862.4160    876.9659
1062.9820    1071.8910    1355.8571
1465.5610    1471.7276    1647.4406
2892.1508    3013.5860    3128.3158
     ZeroEnergy[kcal/mol]                    65.32
     ElectronicLevels[1/cm]          1
          0   1
  End
End

!**************************************Reactant &
Products**************************************!
   Bimolecular      R    # C2H3 + NO2
   Fragment    C2H3
     RRHO
      Geometry[angstrom]     5
 C              0.05027400   -0.58843500    0.00000000
 H              0.97945600   -1.16207700    0.00000000
 H             -0.88410400   -1.16169200    0.00000000
 C              0.05027400    0.72383000    0.00000000
 H             -0.69864400    1.51139800    0.00000000
       Core     RigidRotor
       SymmetryFactor   1
       End
       Frequencies[1/cm]      9
680.8507    801.7926    902.1903
1003.4532    1312.4594    1594.9018
2948.4748    3041.4441    3100.3317
```

```
      ZeroEnergy[1/cm]           0
      ElectronicLevels[1/cm]     1
        0   2
   End
   Fragment      NO2
    RRHO
     Geometry[angstrom]    3
N              0.00000000    0.00000000    0.31821200
O              0.00000000    1.09413100   -0.13921800
O              0.00000000   -1.09413100   -0.13921800
      Core     RigidRotor
      SymmetryFactor    2
      End
      Frequencies[1/cm]     3
735.0660    1402.6203    1708.0344
      ZeroEnergy[1/cm]           0
      ElectronicLevels[1/cm]     1
        0   2
   End
    GroundEnergy[kcal/mol]      70.7
  End

 Bimolecular     P1    # C2H2 + HONO
   Fragment     C2H2
    RRHO
     Geometry[angstrom]    4
C             -0.60312200   -0.00027500    0.00000100
H             -1.67430300    0.00180900    0.00000400
C              0.60312200   -0.00035800   -0.00000100
H              1.67429900    0.00198700   -0.00000400
      Core     RigidRotor
```

```
        SymmetryFactor    2
        End
        Frequencies[1/cm]      6    !
584.4096    585.2118    714.6745
1993.9341    3260.1722    3363.0038
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]       1
          0   1
    End
    Fragment        HONO
     RRHO
       Geometry[angstrom]     4
 H              1.71227700    0.41688300    0.00000100
 O              1.01652600   -0.25681800   -0.00000100
 N             -0.15884000    0.48433800    0.00000200
 O             -1.09157600   -0.21908800   -0.00000100
        Core     RigidRotor
        SymmetryFactor     1
        End
        Frequencies[1/cm]      6    !
555.1843    668.0000    871.0246
1282.6071    1757.3695    3636.2941
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]       1
          0   1
    End
    GroundEnergy[kcal/mol]       25.62
  End

  Bimolecular      P2    # C2H2 + cis-HONO
    Fragment     C2H2
```

```
    RRHO
      Geometry[angstrom]   4
C              -0.60312200   -0.00027500    0.00000100
H              -1.67430300    0.00180900    0.00000400
C               0.60312200   -0.00035800   -0.00000100
H               1.67429900    0.00198700   -0.00000400
      Core    RigidRotor
      SymmetryFactor    2
      End
      Frequencies[1/cm]    6   !
584.4096    585.2118    714.6745
1993.9341    3260.1722    3363.0038
      ZeroEnergy[1/cm]          0
      ElectronicLevels[1/cm]       1
        0   1
  End
   Fragment       cis-HONO
    RRHO
      Geometry[angstrom]   4
H               0.91321000    1.03682800   -0.00010900
N              -0.15665800   -0.51905300   -0.00002100
O              -1.04741000    0.25352500    0.00001200
O               1.07033400    0.07104300    0.00002000
      Core    RigidRotor
      SymmetryFactor   1
      End
      Frequencies[1/cm]    6   !
658.8506    671.3542    936.7171
1311.9489    1703.5772    3470.8668
      ZeroEnergy[1/cm]          0
      ElectronicLevels[1/cm]       1
```

```
        0   1
   End
    GroundEnergy[kcal/mol]       25.91
  End

  Bimolecular      P3    # C2H2 + HNO2
    Fragment     C2H2
      RRHO
        Geometry[angstrom]     4
 C              -0.60312200   -0.00027500    0.00000100
 H              -1.67430300    0.00180900    0.00000400
 C               0.60312200   -0.00035800   -0.00000100
 H               1.67429900    0.00198700   -0.00000400
        Core     RigidRotor
        SymmetryFactor    2
        End
        Frequencies[1/cm]      6    !
584.4096    585.2118    714.6745
1993.9341    3260.1722    3363.0038
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]        1
          0   1
    End
     Fragment        HNO2
      RRHO
        Geometry[angstrom]     4
 H               0.00017800    1.35203600    0.00001800
 N              -0.00002600    0.30909200   -0.00000800
 O               1.08658600   -0.21974000    0.00000200
 O              -1.08658500   -0.21971900    0.00000200
        Core     RigidRotor
```

```
        SymmetryFactor     2
        End
        Frequencies[1/cm]      6    !
768.3296    1033.2560    1413.0784
1438.3168    1667.8811    3081.7040
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]       1
          0   1
    End
     GroundEnergy[kcal/mol]       34.23
   End

  Bimolecular      P4    # CH2O + ONCH
    Fragment     CH2O
      RRHO
       Geometry[angstrom]    4
 C              0.52835500    0.00000000    0.00000100
 H              1.10993900   -0.94567600   -0.00000100
 H              1.10994900    0.94567200   -0.00000100
 O             -0.67375200    0.00000100    0.00000000
        Core     RigidRotor
        SymmetryFactor       2
        End
        Frequencies[1/cm]      6
1150.7705    1193.4630    1446.2771
1768.7477    2801.3901    2876.9467
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]       1
          0   1
    End
     Fragment        ONCH
```

```
    RRHO
      Geometry[angstrom]    4
C              -1.17759800   -0.00042100   -0.02499600
H              -2.24514100   -0.00140600   -0.04764400
N              -0.01984500   -0.00012600   -0.00041800
O               1.18120600    0.00060200    0.02506900
      Core     RigidRotor
      SymmetryFactor      1
      End
      Frequencies[1/cm]     6
325.5452    488.8221    543.5700
1254.7799    2254.5936    3348.0337
      ZeroEnergy[1/cm]            0
      ElectronicLevels[1/cm]        1
        0   1
   End
    GroundEnergy[kcal/mol]      4.5
  End

  Bimolecular      P5    # CH2(O)C + HNO
   Fragment     CH2(O)C
    RRHO
      Geometry[angstrom]     5
C               0.55301000    0.72075500   -0.00001400
C              -0.80330900    0.05033600   -0.00000400
H              -1.34153400   -0.07278700   -0.93618500
H              -1.34146600   -0.07268400    0.93623600
O               0.52309900   -0.56013400    0.00000700
      Core     RigidRotor
      SymmetryFactor   1
      End
```

```
        Frequencies[1/cm]     9
811.9485    842.0727    872.9607
1058.5485    1066.2696    1366.6120
1479.0126    3009.6981    3123.6788
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]        1
          0   1
    End
     Fragment        HNO
      RRHO
       Geometry[angstrom]     3
 H              -0.94388800    0.90874400    0.00000000
 N               0.06292600    0.57700300    0.00000000
 O               0.06292600   -0.61847100    0.00000000
        Core     RigidRotor
        SymmetryFactor     1
        End
        Frequencies[1/cm]    3
1500.1005    1682.4430    2838.4261
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]        1
          0   1
    End
     GroundEnergy[kcal/mol]      65.54
   End

  Bimolecular      P6    # CH2CO + HNO
    Fragment     CH2CO
     RRHO
      Geometry[angstrom]     5
 C              -1.21233500    0.00002800   -0.00002000
```

```
 O                1.26533200    0.00004500   -0.00004300
 C                0.10471100   -0.00015000    0.00009800
 H               -1.73819500    0.94782200   -0.00006400
 H               -1.73871900   -0.94744700   -0.00006400
       Core     RigidRotor
       SymmetryFactor   2
       End
       Frequencies[1/cm]      9
419.4754    534.7753    586.5015
931.2574    1122.3523    1335.8301
2143.7886    3067.6794    3174.3680
       ZeroEnergy[1/cm]           0
       ElectronicLevels[1/cm]        1
          0   1
   End
    Fragment        HNO
     RRHO
      Geometry[angstrom]     3
 H               -0.94388800    0.90874400    0.00000000
 N                0.06292600    0.57700300    0.00000000
 O                0.06292600   -0.61847100    0.00000000
       Core     RigidRotor
       SymmetryFactor      1
       End
       Frequencies[1/cm]    3
1500.1005    1682.4430    2838.4261
       ZeroEnergy[1/cm]           0
       ElectronicLevels[1/cm]        1
          0   1
   End
    GroundEnergy[kcal/mol]      -0.0013
```

```
 End

 Bimolecular      P7    # CH2CHO + NO
  Fragment     CH2CHO
   RRHO
    Geometry[angstrom]     6
C              -1.16989000   -0.17091700    0.00000200
H              -2.06044400    0.45368400    0.00000100
H              -1.26510500   -1.25476300    0.00000500
C               0.13868600    0.40939800   -0.00000100
H               0.20135300    1.51672600   -0.00000300
O               1.16392800   -0.26831600   -0.00000100
      Core     RigidRotor
      SymmetryFactor   1
      End
      Frequencies[1/cm]      12
421.8496    477.4042    735.1005
928.3551    933.3477    1111.5095
1320.2524    1395.0820    1544.0939
2857.1528    3023.8982    3141.5198
      ZeroEnergy[1/cm]           0
      ElectronicLevels[1/cm]       1
        0   2
  End
   Fragment       NO
    RRHO
     Geometry[angstrom]     2
O               0.00000000    0.00000000    0.53374700
N               0.00000000    0.00000000   -0.60999700
      Core     RigidRotor
      SymmetryFactor      1
```

```
        End
        Frequencies[1/cm]    1
1975.0513
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]       1
          0   2
    End
    GroundEnergy[kcal/mol]      16.37
  End

    Bimolecular      P8    # CH2=C + HONO
   Fragment     CH2=C
     RRHO
       Geometry[angstrom]     4
 C                 0.82113300   -0.00012900   -0.00000300
 C                -0.47973600   -0.00002500    0.00000200
 H                -1.02339500    0.94840500    0.00000500
 H                -1.02498600   -0.94748100    0.00000100
        Core     RigidRotor
        SymmetryFactor       2
        End
        Frequencies[1/cm]      6
304.5775    738.0506    1141.9845
1651.6796    2994.4526    3084.6452
        ZeroEnergy[1/cm]           0
        ElectronicLevels[1/cm]       1
          0   1
    End
    Fragment        HONO
     RRHO
       Geometry[angstrom]     4
```

```
 H                1.71227700    0.41688300    0.00000100
 O                1.01652600   -0.25681800   -0.00000100
 N               -0.15884000    0.48433800    0.00000200
 O               -1.09157600   -0.21908800   -0.00000100
       Core     RigidRotor
       SymmetryFactor     1
       End
       Frequencies[1/cm]    6
555.1843    668.0000    871.0246
1282.6071    1757.3695    3636.2941
       ZeroEnergy[1/cm]            0
       ElectronicLevels[1/cm]        1
          0   1
   End
    GroundEnergy[kcal/mol]      69.72
  End

End
```