

Electronic Supplementary Information

Implication of amino cross-reactions on the ignition characteristics of ammonia-blended typical small saturated and unsaturated fatty acid methyl esters

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Table S1. Reaction Energies (ΔE), Forward (V_f) and Reverse (V_r) Barrier Heights (in kcal mol⁻¹ without ZPE), and MUDs for the H-Abstraction Reaction R1a

MF:

Method/Basis set		ΔE_1	V_{f1}	V_{r1}	ΔE_2	V_{f1}	V_{r2}	MUDs
CCSD(T)/cc-pV(T,Q)Z		-8.7	9.4	18.1	-7.6	10.5	18.1	0.00
M062X	cc-pVTZ	-9.0	7.7	16.7	-8.0	8.6	16.6	1.20
	jul-cc- pVTZ	-9.2	8.3	17.5	-8.2	9.3	17.5	0.77
	maug-cc-pVTZ	-9.2	8.3	17.5	-8.3	9.2	17.5	0.80
	jun-cc- pVTZ	-9.1	8.4	17.5	-8.2	9.3	17.5	0.73
	MG3S	-9.2	8.0	17.2	-8.2	9.0	17.2	0.97
	ma-TZVP	-9.4	8.2	17.6	-8.4	9.1	17.5	0.87
M052X	cc-pVTZ	-8.6	8.6	17.2	-7.9	9.4	17.3	0.67
	jul-cc- pVTZ	-8.9	9.1	18	-8.3	9.9	18.2	0.33
	maug-cc-pVTZ	-8.7	9.2	17.9	-8.3	9.9	18.2	0.30
	jun-cc- pVTZ	-8.8	9.2	18	-8.1	10.0	18.1	0.23
	MG3S	-8.8	8.9	17.7	-8.3	9.7	18.0	0.43
	ma-TZVP	-9.1	8.8	17.9	-8.4	9.7	18.1	0.47
M08HX	cc-pVTZ	-9.6	8.3	17.9	-9.8	9.3	19.1	1.10
	jul-cc- pVTZ	-10.1	8.8	18.9	-10.3	9.9	20.2	1.37
	maug-cc-pVTZ	-10.0	8.9	18.9	-10.3	10.0	20.3	1.33
	jun-cc- pVTZ	-10.1	8.9	19	-10.2	10.0	20.2	1.33
	MG3S	-10.0	8.5	18.5	-10.4	9.5	19.9	1.37
	ma-TZVP	-10.2	8.7	18.9	-10.3	9.9	20.2	1.40
B3LYP	cc-pVTZ	-9.3	4.8	14.1	-8.2	7.5	15.7	2.53
	jul-cc- pVTZ	-9.5	5.8	15.3	-8.6	8.5	17.1	1.87
	maug-cc-pVTZ	-9.5	5.7	15.2	-8.6	8.4	17.0	1.93
	jun-cc- pVTZ	-9.5	5.8	15.3	-8.6	8.5	17.1	1.87
	MG3S	-9.5	5.6	15.1	-8.6	8.4	17.0	1.97
	ma-TZVP	-9.5	5.6	15.1	-8.5	8.3	16.8	2.00

MA:

Method/Basis set		V_{f1}	V_{r1}	ΔE_1	V_{f2}	V_{r2}	ΔE_2	MUDs
CCSD(T)/cc-Pv(T,Q)Z		10.4	19.9	-9.4	10.3	18.2	-8.0	0.00
M062X	cc-pVTZ	8.9	18.6	-9.8	8.2	16.4	-8.2	1.22
	jul-cc-pVTZ	9.5	19.7	-10.1	9.0	17.6	-8.6	0.73
	jun-cc-pVTZ	9.6	19.7	-10.1	9.0	17.5	-8.5	0.72
	maug-cc-pVTZ	9.5	19.7	-10.2	8.9	17.5	-8.6	0.77
	MG3S	9.3	19.5	-10.2	8.7	17.3	-8.6	0.90
	ma-TZVP	9.4	19.6	-10.2	8.8	17.6	-8.7	0.83
M052X	cc-pVTZ	9.1	19.3	-10.2	9.0	17.2	-8.2	0.89
	jul-cc-pVTZ	9.7	20.3	-10.6	9.7	18.3	-8.6	0.61
	jun-cc-pVTZ	9.7	20.3	-10.6	9.7	18.2	-8.6	0.59
	maug-cc-pVTZ	9.6	20.3	-10.7	9.6	18.2	-8.6	0.63
	MG3S	9.5	20.2	-10.7	9.4	18.1	-8.6	0.69
	ma-TZVP	9.4	20.1	-10.6	9.4	18.2	-8.7	0.68
M08HX	cc-pVTZ	9.9	20.4	-10.5	8.8	18.9	-10.1	1.06
	jul-cc-pVTZ	10.7	21.6	-10.9	9.6	20.2	-10.6	1.45
	jun-cc-pVTZ	10.7	21.7	-11.0	9.7	20.2	-10.6	1.47
	maug-cc-pVTZ	10.6	21.7	-11.1	9.7	20.2	-10.6	1.48
	MG3S	10.3	21.3	-11.0	9.3	19.9	-10.7	1.45
	ma-TZVP	10.6	21.4	-10.8	9.6	20.2	-10.5	1.36
B3LYP	cc-pVTZ	7.6	17.5	-9.9	7.3	15.8	-8.5	1.94
	jul-cc-pVTZ	8.6	18.9	-10.4	8.5	17.4	-8.9	1.22
	jun-cc-pVTZ	8.6	19.0	-10.4	8.5	17.4	-8.9	1.22
	maug-cc-pVTZ	8.4	18.9	-10.4	8.3	17.3	-9.0	1.31
	MG3S	8.4	18.9	-10.5	8.2	17.3	-9.0	1.35
	ma-TZVP	11.3	20.5	-9.2	11.2	19.0	-7.8	0.61

MP:

		V_{f1}	V_{r1}	ΔE_1	V_{f2}	V_{r2}	ΔE_2	V_{f3}	V_{r3}	ΔE_3	MUDs
CCSD(T)-F12/cc-pVTZ-F12		10.8	15.6	-4.8	6.5	27.7	-21.2	11.2	26.4	-15.1	0
M062X	cc-pVTZ	10.5	15.1	-4.5	6.0	27.6	-21.6	10.2	24.7	-14.6	0.60
	jul-cc-pVTZ	10.9	15.9	-5.0	6.9	28.4	-21.6	10.9	25.6	-14.8	0.39
	jun-cc-pVTZ	10.9	15.9	-5.0	6.7	28.4	-21.8	10.9	25.6	-14.7	0.38
	maug-cc-pVTZ	10.9	15.9	-5.1	6.6	28.6	-22.0	10.7	25.7	-14.9	0.41
	MG3S	10.7	15.7	-5.0	6.4	28.3	-21.9	10.5	25.4	-14.9	0.40
	ma-TZVP	10.7	15.8	-5.1	6.4	28.3	-21.9	10.7	25.6	-15.0	0.38
M052	cc-pVTZ	10.7	15.1	-4.4	6.2	28.8	-22.6	10.8	25.8	-15.0	0.54
	jul-cc-pVTZ	11.0	15.9	-4.9	6.9	29.7	-22.8	11.4	26.7	-15.3	0.56
	jun-cc-pVTZ	11.0	15.8	-4.9	6.9	29.6	-22.8	11.4	26.7	-15.2	0.55
	maug-cc-pVTZ	10.9	15.9	-4.9	6.8	29.8	-23.0	11.3	26.7	-15.4	0.58
	MG3S	10.8	15.7	-4.9	6.6	29.6	-23.0	11.1	26.5	-15.4	0.51
	ma-TZVP	10.7	15.6	-4.9	6.5	29.3	-22.8	11.1	26.6	-15.5	0.46

M08HX	cc-pVTZ	11.7	16.8	-5.0	7.2	29.3	-22.1	11.1	27.1	-16.1	0.82
	jul-cc-pVTZ	12.1	17.7	-5.6	7.9	30.2	-22.3	11.7	28.1	-16.4	1.40
	jun-cc-pVTZ	9.1	15.0	-5.8	4.9	27.4	-22.5	8.8	25.4	-16.5	1.25
	maug-cc-pVTZ	12.0	17.7	-5.7	7.9	30.4	-22.6	11.7	28.2	-16.5	1.49
	MG3S	11.7	17.5	-5.7	7.4	30.0	-22.6	11.3	28.0	-16.7	1.29
	ma-TZVP	12.0	17.5	-5.5	7.7	29.9	-22.2	11.6	28.0	-16.4	1.26
B3LYP	cc-pVTZ	9.0	13.0	-3.9	5.2	27.9	-22.7	8.7	23.9	-15.2	1.49
	jul-cc-pVTZ	9.6	14.1	-4.6	6.2	29.2	-23.0	9.7	25.2	-15.5	1.07
	jun-cc-pVTZ	9.6	14.2	-4.6	6.2	29.2	-23.0	9.7	25.2	-15.5	1.06
	maug-cc-pVTZ	9.5	14.1	-4.6	6.0	29.2	-23.2	9.5	25.1	-15.6	1.15
	MG3S	9.4	14.1	-4.7	5.9	29.2	-23.3	9.5	25.2	-15.7	1.18
	ma-TZVP	12.4	15.8	-3.4	8.9	30.8	-21.9	12.4	26.8	-14.4	1.28

MAe:

		V_{f1}	V_{r1}	ΔE_1	V_{f2}	V_{r2}	ΔE_2	V_{f3}	V_{r3}	ΔE_3	V_{f4}	V_{r4}	ΔE_4	MUDs
CCSD(T)/cc-pV(T,Q)Z		15.2	11.6	3.7	14.0	8.8	5.2	9.8	18.1	-8.3	15.3	10.8	4.5	0.00
M062X	cc-pVTZ	13.3	10.4	2.9	11.8	7.4	4.5	8.3	16.8	-8.4	13.2	9.8	3.5	1.57
	jul-cc-pVTZ	13.9	11.4	2.5	12.6	8.6	4.0	8.9	17.7	-8.8	13.9	10.9	3.0	0.71
	jun-cc-pVTZ	14.0	11.4	2.6	12.7	8.6	4.1	8.9	17.7	-8.8	14.0	10.9	3.1	0.92
	ma-TZVP	13.8	11.3	2.5	12.4	8.4	4.1	8.8	17.7	-8.9	13.7	10.7	3.1	0.85
	maug-cc-pVTZ	13.9	11.4	2.6	12.6	8.5	4.1	8.9	17.7	-8.8	13.9	12.7	1.2	0.98
	MG3S	13.7	11.1	2.6	12.3	8.2	4.1	8.6	17.4	-8.8	13.6	10.4	3.2	1.01
M052X	cc-pVTZ	14.3	10.1	4.2	12.9	6.7	6.2	9.1	17.5	-8.5	14.5	9.4	5.0	1.14
	jul-cc-pVTZ	14.8	11.1	3.7	13.5	7.8	5.7	9.6	18.4	-8.9	15.1	10.5	4.6	0.41
	jun-cc-pVTZ	14.9	11.1	3.8	13.6	7.8	5.8	9.6	18.4	-8.8	15.1	10.5	4.6	0.38
	ma-TZVP	14.6	10.8	3.8	13.3	7.5	5.8	9.3	18.3	-9.0	14.8	10.2	4.6	0.64
	maug-cc-pVTZ	14.8	11.0	3.8	13.5	7.7	5.8	9.6	18.4	-8.8	15.1	10.4	4.6	0.45
	MG3S	14.7	10.9	3.8	13.3	7.5	5.8	9.4	18.2	-8.9	14.8	10.2	4.6	0.59
M08HX	cc-pVTZ	14.6	10.1	4.4	13.2	8.1	5.1	9.0	19.3	-10.3	14.4	10.8	3.7	0.79
	jul-cc-pVTZ	15.2	11.4	3.8	14.0	9.4	4.5	9.5	20.4	-10.9	15.1	12.0	3.1	0.59
	jun-cc-pVTZ	15.3	11.5	3.8	14.1	9.5	4.6	9.6	20.4	-10.8	15.2	12.0	3.2	0.58
	ma-TZVP	15.1	11.2	4.0	13.9	9.2	4.6	9.5	20.3	-10.8	15.1	11.8	3.3	0.58
	maug-cc-pVTZ	15.2	11.4	3.8	14.0	9.4	4.6	9.6	20.4	-10.8	15.1	12.0	3.2	0.57
	MG3S	14.8	11.1	3.8	13.5	9.1	4.5	9.2	20.1	-11.0	14.6	11.6	3.1	0.71
B3LYP	cc-pVTZ	12.0	7.8	4.2	10.9	5.9	5.0	7.1	16.1	-9.0	12.6	7.7	4.9	2.93
	jul-cc-pVTZ	12.9	9.2	3.7	12.1	7.5	4.5	8.1	17.5	-9.5	13.6	9.2	4.4	1.67
	jun-cc-pVTZ	13.0	9.2	3.7	12.1	7.5	4.6	8.1	17.5	-9.4	13.7	9.2	4.4	1.66
	ma-TZVP	15.7	10.8	4.9	14.8	9.1	5.7	10.8	19.1	-8.3	16.3	10.7	5.6	0.67
	maug-cc-pVTZ	12.8	9.2	3.7	11.9	7.4	4.5	7.9	17.4	-9.5	13.5	9.1	4.4	1.78
	MG3S	12.8	9.2	3.6	11.8	7.4	4.4	7.9	17.4	-9.6	13.4	9.1	4.3	1.82

Table S2. The T1 diagnostics for all the reactants, TSs and products are determined at the CCSD (T)-F12/cc-pvtz-F12 level and CCSD(T)/cc-pVX(X = T, Q)Z.

	MF-TS1	MF-TS2	MA-TS1	MA-TS2	MP-TS1	MP-TS2	MP-TS3
T1	0.021	0.018	0.017	0.017	0.016	0.017	0.016
	MF	MF_1	MF_2	MA	MA_1	MA_2	MP

T1	0.015	0.019	0.019	0.014	0.017	0.017	0.014
	MP_1	MP_2	MP_3	MAe-TS1	MAe-TS2	MAe-TS3	MAe-TS4
T1	0.015	0.017	0.016	0.026	0.027	0.018	0.027
	MAe	MAe_1	MAe_2	MAe_3	MAe_4	NH ₂	NH ₃
T1	0.015	0.029	0.030	0.021	0.029	0.009	0.007

Table S3. Optimized geometries, rotational constants, and vibrational frequencies**NH₂:**

ZPE(Hartree): -55.889484

Cartesian Coordinates (Å)

N	0.00000000	0.00000000	0.14175400
H	0.00000000	0.80228800	-0.49614000
H	0.00000000	-0.80228800	-0.49614000

Frequencies (cm⁻¹):

1562.99 3395.39 3472.50

NH₃:

ZPE(Hartree): -56.571787

Cartesian Coordinates (Å)

N	0.00000000	0.00000000	0.11501700
H	0.00000000	0.93717000	-0.26837300
H	-0.81161300	-0.46858500	-0.26837300
H	0.81161300	-0.46858500	-0.26837300

Frequencies (cm⁻¹):

1085.27 1679.75 1679.80 3507.69 3619.93 3619.94

CH₃OC(=O)H + NH₂ → Products**CH₃OC(=O)H:**

ZPE(Hartree): -229.126340

Cartesian Coordinates (Å)

C	-0.82596700	0.43295000	0.00003500
O	-1.27721500	-0.67546400	0.00015100
O	0.47074100	0.73301700	-0.00009000
H	-1.42109900	1.34730500	0.00001700
C	1.35304700	-0.40117100	-0.00007900
H	2.35397900	0.00804000	-0.00019100
H	1.17828900	-1.00315500	0.88499300
H	1.17814400	-1.00328500	-0.88503500

Frequencies (cm⁻¹):158.95 318.69 344.11 789.93 967.05 1081.25 1201.68 1209.84 1268.22
1422.08 1496.93 1519.29 1529.03 1831.20 3130.12 3144.03 3201.68 3234.67**CH₃OC(=O):**

ZPE(Hartree): -228.458038

Cartesian Coordinates (Å)

C	0.81339800	0.51081000	-0.00003000
O	1.40922600	-0.50972900	-0.00001800
O	-0.47500200	0.73969300	-0.00000800
C	-1.30726200	-0.45579900	0.00003900
H	-2.32651400	-0.09712200	0.00005300
H	-1.09206200	-1.03635100	-0.88958700
H	-1.09202300	-1.03630800	0.88968500

Frequencies (cm⁻¹):136.44 289.47 381.75 772.36 932.87 1176.16 1180.33 1225.06
1483.48 1517.32 1523.30 1881.95 3134.84 3214.60 3247.78

CH₂OC(=O)H:

ZPE(Hartree): -228.457073

Cartesian Coordinates (Å)

C	-0.76488000	0.44717700	0.00002900
O	-1.29334100	-0.62150200	-0.00002100
O	0.57102800	0.64936900	0.00000100
H	-1.27280600	1.41015400	0.00010800
C	1.38068500	-0.44641000	-0.00017600
H	2.42598700	-0.21928300	0.00042600
H	0.93049400	-1.41841300	0.00050700

Frequencies (cm⁻¹):

120.21 261.89 346.29 371.48 767.44 1039.17 1047.71 1186.71
1268.90 1424.92 1470.53 1835.29 3169.09 3263.33 3422.20

MF-TS1:

ZPE(Hartree): -285.001211

Cartesian Coordinates (Å)

C	0.14753100	0.38096500	-0.09571400
O	-0.23821100	1.49980000	0.02210900
O	-0.58582300	-0.72198200	-0.08210500
H	1.37295600	0.04985000	-0.24412100
C	-2.00640300	-0.50408000	0.07218300
H	-2.45293400	-1.48856900	0.06314600
H	-2.19495300	0.00407000	1.01132900
H	-2.37160700	0.09918000	-0.75134400
N	2.59102000	-0.42492700	-0.07282400
H	2.88653900	0.15531200	0.71118100
H	2.36835700	-1.32921100	0.34073500F

Frequencies (cm⁻¹):

-1956.98 71.89 103.18 142.59 159.61 310.76 323.21 501.82 678.59 781.51 835.79 975.51 1157.18
1192.34 1229.35 1264.66 1488.12 1493.21 1518.31 1526.83 1548.85 1853.94 3132.47 3208.10
3239.87 3463.94 3554.95

MF-TS2:

ZPE(Hartree): -284.999969

Cartesian Coordinates (Å)

C	-1.30385200	-0.33518100	-0.27544200
O	-0.90291500	-1.19257700	0.45633400
O	-0.77533700	0.88743700	-0.38496900
H	-2.15476100	-0.43323400	-0.94914400
C	0.34205900	1.14787600	0.43305400
H	1.29507000	0.41000300	-0.02258900
H	0.64026600	2.17428000	0.27959400
H	0.17766100	0.85965900	1.46294900
N	2.11610700	-0.53266600	-0.37019200
H	1.57988100	-1.32676100	-0.02254800
H	2.84591000	-0.39032800	0.32648600F

Frequencies (cm⁻¹):

-1888.31	99.53	114.28	152.65	314.76	344.66	381.75	563.82	709.89	808.90	886.43	1004.21	1073.42
1184.85	1229.58	1273.44	1346.13	1422.38	1480.36	1499.48	1560.94	1823.82	3158.41	3169.50	3270.91	
3463.67	3551.72											

CH₃OC(=O)CH₃ + NH₂ → Products

CH₃OC(=O)CH₃:

ZPE(Hartree): -268.460183

Cartesian Coordinates (Å)

C	0.45814900	0.17077900	-0.00003700
O	0.27425200	1.35813800	-0.00000500
C	1.79484600	-0.50431500	0.00001100
H	1.87845100	-1.13892300	0.87799500
H	1.87787300	-1.14043800	-0.87691900
H	2.57442500	0.24599000	-0.00083200
O	-0.54264900	-0.72367600	-0.00004900
C	-1.85997300	-0.15818500	0.00003200
H	-2.53954500	-0.99998100	0.00001000
H	-2.00105000	0.45393900	0.88437200
H	-2.00111300	0.45403500	-0.88423100

Frequencies (cm⁻¹):

53.15	166.38	184.68	296.90	431.59	620.82	656.60	884.15	1005.02	1087.15	1103.35	1200.49	1233.42
1307.14	1421.02	1491.85	1499.05	1502.75	1518.18	1530.43	1840.19	3119.30	3127.54	3180.23		
3197.64	3227.17	3227.82										

CH₃OC(=O)CH₂:

ZPE(Hartree): -267.794798

Cartesian Coordinates (Å)

C	0.51895600	0.11983100	0.00003300
O	0.39000000	1.32480700	0.00018600
C	1.78513900	-0.56532600	-0.00000900
H	1.82478200	-1.63900700	-0.00013000
H	2.67926200	0.02932900	0.00008700
O	-0.52614000	-0.73123000	-0.00011500
C	-1.81074400	-0.09989400	-0.00007700
H	-2.53286900	-0.90552300	-0.00025600
H	-1.92113000	0.51930600	0.88417100
H	-1.92103400	0.51961500	-0.88412000

Frequencies (cm⁻¹):

160.62	180.68	299.59	340.80	431.06	647.53	667.37	806.84	882.20	1028.98	1108.79	1199.06	1236.02
1323.04	1474.34	1506.08	1515.29	1529.43	1746.50	3123.79	3192.14	3226.11	3245.62	3368.16		

CH₂OC(=O)CH₃:

ZPE(Hartree): -267.791524

Cartesian Coordinates (Å)

C	-0.41770200	0.18516000	-0.00065200
O	-0.27017100	1.37231300	0.00074500
C	-1.71746200	-0.55135300	-0.00173700
H	-1.76252300	-1.20659500	-0.86740700
H	-1.77957100	-1.17310600	0.88757600

H	-2.53074800	0.16188300	-0.02180300
O	0.62933100	-0.68874600	-0.00002200
C	1.88967400	-0.17255000	0.01698800
H	2.66386700	-0.90867600	-0.04674800
H	2.00863200	0.89042100	-0.04500200

Frequencies (cm⁻¹):

74.99 170.16 178.94 278.44 314.19 442.48 610.41 654.99 854.19 1018.26 1082.88 1194.16 1216.71
1285.15 1422.17 1466.54 1492.42 1498.89 1856.38 3118.33 3178.54 3229.48 3259.81 3415.92

MA-TS1:

ZPE(Hartree): -324.334504

Cartesian Coordinates (Å)

C	-0.19011800	0.55787600	-0.06733600
O	-0.51820400	1.12792200	0.94241700
C	1.06061000	0.79861400	-0.81040300
H	1.02892800	0.52331600	-1.85523900
H	1.49508300	1.76435200	-0.59711200
H	1.91116300	-0.02342900	-0.31915600
O	-0.91858500	-0.42943900	-0.61830700
C	-2.12498600	-0.75256300	0.08509200
H	-2.58793700	-1.55093100	-0.47954000
H	-1.89210500	-1.07531200	1.09453300
H	-2.77261500	0.11642800	0.12977600
N	2.52309500	-0.94658400	0.37939000
H	2.29364000	-0.61601400	1.31619200
H	1.88345000	-1.72374500	0.21782000

Frequencies (cm⁻¹):

-1799.69 32.44 76.68 125.50 164.36 186.47 301.41 387.30 436.32 516.69 656.46 729.35 815.45
835.77 893.70 1035.69 1049.73 1104.58 1201.10 1233.97 1307.42 1356.28 1413.83 1468.04 1502.99
1517.10 1530.27 1559.98 1811.43 3126.18 3183.75 3196.10 3227.08 3276.07 3459.75 3548.14

MA-TS2:

ZPE(Hartree): -324.334509

Cartesian Coordinates (Å)

C	0.90242000	-0.13897200	0.14964300
O	0.42121700	-0.95265000	0.89037800
C	2.24641400	-0.22668900	-0.49880600
H	2.11828500	-0.24632300	-1.57789000
H	2.82937100	0.65561000	-0.25013600
H	2.74832300	-1.12403700	-0.16210600
O	0.26225000	0.99495800	-0.20342300
C	-1.02492600	1.16653600	0.33431700
H	-1.76341800	0.27399900	-0.21846400
H	-1.05865200	0.99013500	1.40145000
H	-1.40087400	2.12650500	0.01165600
N	-2.37006800	-0.80578900	-0.62923500
H	-3.25332400	-0.70200800	-0.13194600
H	-1.84041800	-1.47706700	-0.07448300

Frequencies (cm⁻¹):

-1857.95	58.22	85.88	105.15	143.24	209.47	292.85	379.23	432.19	564.94	615.25	645.85	746.40
871.22	897.02	1017.18	1086.39	1130.85	1214.97	1239.46	1297.67	1353.88	1422.79	1478.85	1493.14	
1499.49	1502.66	1557.49	1838.05	3120.30	3166.21	3181.76	3229.84	3265.18	3462.92	3550.61		

CH₃OC(=O)CH₂CH₃ + NH₂ → Products

CH₃OC(=O)CH₂CH₃:

ZPE(Hartree): -307.783045

Cartesian Coordinates (Å)

C	-0.05122000	0.07962100	-0.00026800
O	-0.10342500	1.27858300	-0.00042700
O	-1.14315400	-0.70081600	-0.00005900
C	1.21181700	-0.74216100	-0.00043800
H	1.17173000	-1.40065200	0.87009600
H	1.17223900	-1.39921800	-0.87209200
C	2.46208400	0.11906200	0.00058300
H	2.48758400	0.76218300	0.87904100
H	3.35455800	-0.50538700	0.00024500
H	2.48795300	0.76369100	-0.87675400
C	-2.38881000	-0.00784000	0.00040900
H	-2.47332200	0.62004300	0.88629300
H	-2.47406500	0.61988800	-0.88550800
H	-3.15726100	-0.77477200	0.00084300

Frequencies (cm⁻¹):

58.39	150.88	169.87	216.77	228.24	347.84	454.67	591.38	671.15	826.44	884.04	1010.63	1053.89
1129.08	1131.29	1200.39	1225.13	1255.40	1298.23	1411.92	1440.73	1484.24	1500.71	1516.05	1516.32	
1525.52	1530.40	1834.92	3110.91	3113.21	3126.09	3138.89	3179.33	3184.56	3195.97	3225.94		

CH₃OC(=O)CH₂CH₂:

ZPE(Hartree): -307.110866

Cartesian Coordinates (Å)

C	0.00337200	0.09669300	-0.00010300
O	-0.06616300	1.29351600	-0.00022900
O	-1.07295400	-0.70262800	0.00009800
C	1.27697200	-0.71428800	-0.00024900
H	1.23205100	-1.38651700	0.86572500
H	1.23235600	-1.38556200	-0.86699000
C	2.50000100	0.11959500	0.00039200
H	3.47149700	-0.34851300	0.00010600
H	2.42043000	1.19475800	0.00061300
C	-2.33120000	-0.03156900	0.00014900
H	-2.42636000	0.59427600	0.88627100
H	-2.42645400	0.59419600	-0.88602300
H	-3.08544700	-0.81232600	0.00021800

Frequencies (cm⁻¹):

54.03	153.95	171.58	187.02	228.27	358.50	463.91	472.30	590.49	662.17	876.40	926.15	1024.07
1044.12	1146.90	1199.21	1207.05	1224.11	1255.07	1411.69	1454.03	1470.58	1501.88	1516.40		
1530.22	1839.95	3054.53	3064.79	3127.06	3197.58	3227.60	3235.59	3348.66				

CH₃OC(=O)CHCH₃:

ZPE(Hartree): -307.126608

Cartesian Coordinates (Å)

C	0.02728800	0.08325000	0.00021000
O	0.10709700	1.29173400	0.00017300
C	-1.20931100	-0.66836900	0.00029800
H	-1.14142400	-1.74699000	0.00020200
C	-2.51852500	0.01581200	-0.00026700
H	-2.38442400	1.09534100	-0.00012200
H	-3.10774400	-0.27124400	-0.87639500
H	-3.10846100	-0.27147300	0.87528700
O	1.11001100	-0.72226900	0.00007000
C	2.36226700	-0.04707300	-0.00023800
H	3.12078000	-0.82408500	-0.00058600
H	2.45677200	0.58063800	-0.88572000
H	2.45732500	0.58037400	0.88537400

Frequencies (cm⁻¹):

88.19 111.87 162.54 199.92 221.57 352.47 472.65 599.26 681.61 763.85 884.59 1006.07 1026.73
1092.55 1179.37 1199.22 1226.04 1245.98 1414.81 1452.41 1496.28 1496.47 1514.60 1527.06
1531.81 1747.00 3067.48 3101.97 3122.06 3189.75 3194.31 3222.73 3272.18

CH₂OC(=O)CH₂CH₃:

ZPE(Hartree): -307.114518

Cartesian Coordinates (Å)

C	-0.09649300	0.11067800	-0.00362300
O	-0.13157600	1.30550700	-0.00718200
C	1.13831000	-0.74653000	-0.00032800
H	1.07615300	-1.40602100	0.86841200
H	1.08254700	-1.40017500	-0.87402500
C	2.41174500	0.07998600	0.00670800
H	2.45253800	0.71963000	0.88709900
H	3.28575400	-0.56969800	0.00781500
H	2.45848700	0.72493700	-0.86946400
O	-1.21864900	-0.66104500	-0.00209000
C	-2.42667300	-0.03618600	-0.02920000
H	-2.45422200	1.03022700	0.11457800
H	-3.26078900	-0.70228000	0.09842300

Frequencies (cm⁻¹):

60.05 153.50 173.30 221.76 226.92 285.60 366.27 463.71 581.38 665.10 821.23 859.08 1022.35
1096.20 1125.31 1161.68 1201.99 1265.33 1295.76 1404.13 1441.46 1469.74 1482.26 1517.45 1525.45
1851.36 3108.24 3114.49 3135.97 3181.79 3184.93 3260.61 3416.44

MP-TS1:

ZPE(Hartree): -363.656316

Cartesian Coordinates (Å)

C	-0.49384200	-0.19437800	0.14186300
O	-0.28174500	0.74900500	0.85579700
O	-1.68686800	-0.43819400	-0.41209300
C	0.51601900	-1.24662300	-0.24275800
H	0.10712700	-2.21501500	0.06408900

H	0.56129300	-1.27260700	-1.33397400
C	1.87159400	-0.98815000	0.35598900
H	2.63145300	-1.70145800	0.04746200
H	2.23808300	0.12150700	-0.16788600
H	1.86158400	-0.82594000	1.43007100
C	-2.70744500	0.51271400	-0.11410100
H	-2.88312300	0.55545800	0.95975200
H	-2.41596200	1.50146700	-0.46515000
H	-3.59585900	0.16860800	-0.63429100
N	2.43153000	1.33701800	-0.59314700
H	1.76056400	1.80009300	0.02658300
H	3.34508000	1.52089100	-0.17022300

Frequencies (cm⁻¹):

-1774.17 35.98 92.50 135.09 155.19 162.12 183.51 214.34 345.73 382.29 454.90 546.83 599.27
672.26 737.28 837.42 896.08 910.52 1019.58 1052.75 1105.88 1144.88 1200.62 1224.70 1250.36
1271.83 1380.92 1414.79 1452.49 1468.49 1477.93 1503.42 1518.78 1529.72 1562.08 1828.72 3083.55
3127.78 3128.98 3155.92 3199.93 3230.77 3232.58 3465.37 3553.30

MP-TS2:

ZPE(Hartree): -363.660507

Cartesian Coordinates (Å)

C	-0.34337500	-0.39849900	-0.02094000
O	-0.55740900	-0.99807900	-1.04169900
O	-1.29643100	0.27914600	0.64278200
C	0.98620500	-0.26038500	0.63122500
H	1.38405100	0.86405200	0.27922000
H	0.89864800	-0.14077200	1.70917600
C	2.03047000	-1.24076300	0.16454300
H	2.08191600	-1.25450900	-0.92325700
H	3.00861900	-0.97557500	0.56301300
H	1.78691800	-2.25326700	0.49373600
C	-2.59257400	0.24273600	0.05099100
H	-2.56596700	0.67222400	-0.94982300
H	-2.94977200	-0.78376300	-0.01704300
H	-3.23461600	0.82843500	0.70175500
N	1.66061900	2.05965700	-0.32129400
H	0.79322500	2.54808700	-0.07654200
H	1.51901400	1.77041200	-1.29475500

Frequencies (cm⁻¹):

-1646.29 36.40 70.13 103.69 138.42 147.73 160.05 204.88 219.73 344.55 454.21 524.46 601.60
676.50 756.37 835.09 888.95 921.96 1026.84 1082.81 1098.24 1147.62 1201.05 1224.91 1248.94
1312.96 1402.26 1415.63 1436.84 1500.57 1506.66 1515.87 1516.93 1530.62 1551.44 1813.67 3096.94
3126.02 3158.51 3179.31 3193.57 3195.88 3226.28 3455.48 3543.78

MP-TS3:

ZPE(Hartree): -363.657430

Cartesian Coordinates (Å)

C	0.42566200	-0.20127100	0.15769700
O	0.14192700	0.69896600	0.89888400
O	-0.45879100	-1.14837600	-0.21353000
C	1.77162500	-0.43356600	-0.47216200
H	2.09109900	-1.44129700	-0.19714700
H	1.62097500	-0.45366800	-1.55387800
C	2.79029800	0.61487000	-0.06265200
H	2.92934900	0.61863700	1.01746700
H	3.75062000	0.41612400	-0.53627100
H	2.45842100	1.61016700	-0.35427700
C	-1.75485400	-1.02174300	0.30213300
H	-2.34238300	-1.86436500	-0.04620500
H	-1.76634700	-0.87249400	1.37901300
H	-2.25122900	0.02751300	-0.22786300
N	-2.57004600	1.24258500	-0.62024600
H	-3.46292100	1.35065100	-0.13062900
H	-1.89873800	1.75618300	-0.04142500

Frequencies (cm⁻¹):

-1852.56 45.03 61.66 103.60 161.79 190.10 216.84 236.11 343.07 376.52 453.61 564.77 586.82
662.40 741.61 822.95 871.86 897.32 1020.82 1078.03 1128.99 1140.02 1199.04 1232.80 1258.18
1297.87 1353.25 1411.98 1441.52 1476.88 1483.19 1500.28 1517.74 1526.34 1560.11 1833.50
3111.10 3114.26 3139.65 3165.18 3181.04 3185.27 3264.10 3463.02 3550.79

CH₃OC(=O)CH=HCH + NH₂ → Products

CH₃OC(=O)CH=HCH:

ZPE(Hartree): -306.550288

Cartesian Coordinates (Å)

C	-0.04305900	0.10543500	0.00006000
O	0.06067100	1.30439300	0.00012000
O	1.01017500	-0.72431700	-0.00002200
C	2.28836100	-0.07597400	-0.00008000
H	3.02046500	-0.87240900	-0.00031500
H	2.38859400	0.54423300	-0.88445800
H	2.38882800	0.54392800	0.88448500
C	-1.31658500	-0.64828400	0.00008400
C	-2.46745400	0.00309200	-0.00013100
H	-1.24929000	-1.72411500	0.00035000
H	-3.40992100	-0.52029100	0.00003400
H	-2.47302700	1.08243300	-0.00048200

Frequencies (cm⁻¹):

90.67 162.55 198.66 232.62 358.35 481.42 539.11 680.72 853.82 891.20 1042.83 1048.21 1055.97
1095.98 1200.05 1227.15 1261.17 1354.14 1458.27 1501.44 1515.75 1529.15 1739.64 1823.15
3126.72 3196.83 3214.73 3228.10 3265.39 3309.39

CH₃OC(=O)CH=HC:

ZPE(Hartree): -305.861016

Cartesian Coordinates (Å)

C	-0.09316700	0.46123200	-0.00001000
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O	0.45820400	1.52887600	-0.00001000
O	0.55457400	-0.70933300	0.00002600
C	1.98523700	-0.60387500	0.00006600
H	2.35164200	-1.62161900	0.00009000
H	2.31718500	-0.07186300	-0.88488900
H	2.31713400	-0.07183800	0.88502500
C	-1.57449600	0.30681600	-0.00005000
C	-2.16617900	-0.85466200	-0.00004700
H	-2.11465400	1.24277900	-0.00008200
H	-1.88190200	-1.89087600	-0.00002100

Frequencies (cm⁻¹):

96.96 167.49 182.72 225.08 345.44 510.73 601.63 639.80 833.59 879.85 897.69 926.24 1086.59
 1201.32 1232.40 1235.74 1313.90 1501.61 1518.28 1530.77 1689.83 1821.03 3129.33 3200.83
 3225.36 3230.86 3319.55

CH₃OC(=O)C=HCH:

ZPE(Hartree): -305.860872

Cartesian Coordinates (Å)

C	-0.01665000	0.29116100	-0.06707900
O	0.34406600	1.44175000	0.02193400
O	0.81903200	-0.75933700	-0.05464700
C	2.20509400	-0.41298800	0.07541000
H	2.74010300	-1.35285600	0.05635000
H	2.50682400	0.22356500	-0.74970600
H	2.37173800	0.10972000	1.01128600
C	-1.37942900	-0.10722300	-0.24468700
C	-2.59003500	-0.35603900	0.12849600
H	-3.36515200	-0.60284200	-0.58559200
H	-2.87217900	-0.32635500	1.17652100

Frequencies (cm⁻¹):

89.05 121.43 164.23 191.30 271.83 344.48 553.67 609.58 737.12 879.50 939.77 950.04 1051.05
 1198.28 1228.16 1262.40 1437.45 1496.20 1515.62 1528.93 1738.04 1888.75 3126.07 3137.29
 3196.38 3218.75 3229.93

CH₂OC(=O)CH=HCH:

ZPE(Hartree): -305.882306

Cartesian Coordinates (Å)

C	-0.00125400	0.13595200	-0.00031400
O	-0.09087300	1.33175500	-0.00003900
O	-1.08797600	-0.68737600	-0.00009700
C	-2.31714900	-0.11264700	0.00097300
H	-3.12884400	-0.80983000	-0.00153800
H	-2.38544500	0.95641100	-0.00180800
C	1.24125300	-0.65484200	-0.00024500
C	2.41277100	-0.03871000	0.00022200
H	1.14001700	-1.72780600	-0.00016400
H	3.33772300	-0.59206700	0.00044400

H	2.45362200	1.03974100	0.00033900
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Frequencies (cm⁻¹):

96.16	177.87	200.79	239.74	306.01	378.39	490.78	538.11	675.93	835.08	867.18	1039.14	1046.03
1097.56	1155.73	1202.62	1255.20	1349.15	1455.71	1476.49	1733.06	1832.07	3216.55	3262.43	3268.53	
3311.65	3419.50											

CH₃OC(=O)CH=CH:

ZPE(Hartree): -305.859678

Cartesian Coordinates (Å)

C	-0.06087500	0.44374000	-0.00000900
O	0.49459400	1.51081900	-0.00000600
O	0.58066700	-0.72773000	0.00002800
C	2.01090400	-0.62939000	0.00007300
H	2.37162000	-1.64915300	0.00009400
H	2.34617900	-0.09903400	-0.88479800
H	2.34612200	-0.09901800	0.88495600
C	-1.53767600	0.29814200	-0.00005200
C	-2.15122200	-0.85157500	-0.00005700
H	-2.07373600	1.24127500	-0.00007900
H	-3.15905600	-1.22427900	-0.00008500

Frequencies (cm⁻¹):

98.97	170.24	186.08	212.27	344.64	535.93	564.57	622.76	827.25	829.04	896.23	909.69	1094.11
1200.95	1231.43	1242.96	1329.02	1502.06	1518.38	1530.18	1698.37	1819.38	3128.09	3170.52		
3198.67	3230.51	3315.67										

MAe-TS1:

ZPE(Hartree): -362.415499

Cartesian Coordinates (Å)

C	-0.77517700	0.19836900	0.00770000
O	-1.08988600	1.35740600	-0.05372200
O	-1.65809100	-0.80854400	0.02496000
C	-3.03319800	-0.40533800	-0.03302400
H	-3.60729700	-1.32179300	-0.00936500
H	-3.26941700	0.22395000	0.81833000
H	-3.21800000	0.14623100	-0.94858600
C	0.61729000	-0.31539000	0.07399900
C	1.62833600	0.52431500	0.08106400
H	0.74695200	-1.38608600	0.12195800
H	2.82768300	-0.04857300	0.15249100
H	1.56669500	1.60030800	0.03329200
N	3.96639000	-0.48776300	0.00354300
H	4.02783700	-0.52524800	-1.01166700
H	4.52112800	0.32291600	0.27040800

Frequencies (cm⁻¹):

-1906.73	48.93	74.90	84.05	98.35	164.57	208.25	226.32	325.93	413.68	520.98	569.73	683.75
720.13	815.97	875.31	928.87	988.85	1054.14	1102.38	1200.85	1223.63	1240.65	1257.77	1340.59	

1428.36 1499.72 1517.00 1528.90 1569.35 1706.24 1819.25 3127.85 3198.67 3230.06 3245.74
3266.60 3479.74 3568.54

MAe-TS2:

ZPE(Hartree): -362.417305

Cartesian Coordinates (Å)

C	-0.41267600	-0.50007800	-0.00572700
O	-1.05843700	-1.51249000	0.06938800
O	-0.95691100	0.72241600	-0.04537500
C	-2.39114000	0.74281500	0.00153400
H	-2.67005000	1.78696100	-0.04283700
H	-2.79518400	0.19631300	-0.84369100
H	-2.73682100	0.28640500	0.92272900
C	1.06008300	-0.45124500	-0.06821200
C	1.84083900	-1.50797700	-0.01793300
H	1.63592400	0.75050200	-0.20260400
H	2.91560100	-1.41851700	-0.06648000
H	1.40722800	-2.49668000	0.06726900
N	2.04237600	1.89338100	-0.05164300
H	2.33410200	1.87296800	0.92314800
H	1.15271300	2.38789100	-0.04610900

Frequencies (cm⁻¹):

-1884.26 45.31 91.63 116.89 131.16 165.49 220.42 236.38 330.42 399.10 494.92 560.08 664.37
680.28 790.48 833.12 891.30 1022.62 1049.77 1108.49 1201.06 1231.81 1271.76 1301.87 1427.70
1463.20 1501.25 1517.04 1529.02 1576.86 1735.22 1809.57 3129.28 3178.98 3201.10 3231.38
3274.40 3483.44 3569.23

MAe-TS3:

ZPE(Hartree): -362.424606

Cartesian Coordinates (Å)

C	-0.51869500	0.14505900	-0.18426700
O	-0.22122900	-0.72120900	-0.96398000
O	0.34639200	1.09387800	0.22496300
C	1.63591400	1.03130300	-0.33131200
H	1.61994000	0.89780400	-1.40575100
H	2.19654100	1.88553600	0.01893100
H	2.25231800	-0.00663600	0.10108400
C	-1.83933400	0.32296500	0.45228800
C	-2.82365200	-0.51461500	0.17001000
H	-1.94684300	1.14932200	1.13583100
H	-3.79773000	-0.40807600	0.61917200
H	-2.65851900	-1.32453100	-0.52400300
N	2.63006300	-1.17331200	0.54772500
H	1.97439100	-1.74042800	0.01157800
H	2.22275600	-1.12943200	1.48090100

Frequencies (cm⁻¹):

-1852.53 59.99 86.77 118.50 163.93 215.14 235.39 357.17 370.44 481.84 534.15 595.26 681.21

776.41 840.48 854.81 895.57 1040.59 1051.12 1091.74 1097.69 1153.75 1233.00 1262.89 1352.42
1409.87 1459.21 1464.98 1489.43 1564.34 1738.63 1819.51 3163.32 3215.68 3265.40 3265.80
3310.50 3463.45 3550.21

MAe-TS4:

ZPE(Hartree): -362.417425

Cartesian Coordinates (Å)

C	-0.47267900	0.12756900	0.00945800
O	-0.15253800	-1.03223400	0.06739100
O	-1.74899700	0.52953900	-0.03971100
C	-2.71883100	-0.52627700	-0.01253000
H	-3.68281100	-0.03758300	-0.05563000
H	-2.57639600	-1.18103800	-0.86553900
H	-2.61437900	-1.10025300	0.90189100
C	0.43979800	1.29397100	-0.02047800
C	1.74907600	1.18451600	0.05690500
H	-0.04205300	2.25964800	-0.10252400
H	2.44848100	2.00688000	0.03462200
H	2.38346500	-0.00749300	0.21127700
N	2.86484600	-1.10403200	0.05517300
H	3.25344000	-1.03090200	-0.88254600
H	2.00442600	-1.63815300	-0.04932800

Frequencies (cm⁻¹):

-1864.76 46.00 135.34 140.85 168.71 173.78 219.26 249.13 354.05 476.70 479.02 601.40 633.09
746.51 777.01 851.62 917.11 981.84 1048.59 1078.04 1200.62 1201.66 1236.06 1288.22 1378.25
1467.63 1501.45 1517.87 1529.18 1578.02 1713.60 1814.91 3128.40 3199.26 3203.00 3231.04
3251.06 3480.50 3567.81

CH₃OC(=O)CH₂CH=CH₂ + NH₂ → Products

CH₃OC(=O)CH₂CH=CH₂:

ZPE(Hartree): -345.871359

Cartesian Coordinates (Å)

C	0.48480500	0.13477900	0.13012400
O	0.60919300	1.32351000	0.01164700
O	1.50311100	-0.72685800	0.00382800
C	2.77529700	-0.12404400	-0.27318900
H	3.47739100	-0.94395200	-0.34433800
H	2.72758100	0.42832200	-1.20537300
H	3.04787300	0.55194300	0.53018300
C	-0.79692600	-0.57935600	0.47206000
H	-0.83116900	-1.52768500	-0.05664700
H	-0.72847800	-0.81270300	1.53751700
C	-2.00506800	0.25577800	0.19667300
C	-3.05868200	-0.18561300	-0.46825200
H	-1.97812100	1.26819900	0.57224000
H	-3.91705000	0.44446400	-0.63887500
H	-3.09301100	-1.19106900	-0.86299900

Frequencies (cm⁻¹):

36.47 79.81 160.11 176.87 200.92 330.72 391.04 447.71 571.99 635.60 744.44 925.01 952.73
972.68 989.24 1050.43 1058.60 1162.14 1200.97 1217.82 1242.57 1262.25 1337.93 1388.10 1466.35
1486.01 1501.92 1518.07 1530.02 1755.12 1835.94 3080.08 3128.17 3161.33 3198.95 3199.05
3229.13 3237.40 3287.48

CH₂OC(=O)CH₂CH=CH₂:

ZPE(Hartree): -345.202507

Cartesian Coordinates (Å)

C	0.53156000	0.16033600	0.10258000
O	0.63376500	1.34571100	-0.01757200
O	1.58935600	-0.69051600	-0.00431700
C	2.82013800	-0.15124400	-0.23217100
H	3.59206900	-0.87714600	-0.38282300
H	2.89177100	0.90383700	-0.40457600
C	-0.72431800	-0.60154800	0.41915400
H	-0.75069600	-1.50710500	-0.18129200
H	-0.62636900	-0.91852100	1.46059900
C	-1.95439000	0.22591200	0.23231000
C	-3.01137300	-0.18728000	-0.44476300
H	-1.94296800	1.20614900	0.68593500
H	-3.88702800	0.43333200	-0.54856500
H	-3.03145900	-1.15916900	-0.91682800

Frequencies (cm⁻¹):

39.51 81.51 159.90 196.90 228.67 274.81 350.07 394.02 457.66 566.37 626.13 728.37 908.99
948.89 976.43 992.09 1054.32 1119.71 1169.84 1202.30 1245.42 1268.74 1338.76 1379.39 1463.64
1470.95 1486.41 1756.62 1852.27 3079.27 3155.80 3199.73 3236.91 3259.28 3288.42 3415.35

CH₃OC(=O)CHCH=CH₂:

ZPE(Hartree): -345.235557

Cartesian Coordinates (Å)

C	-0.48652100	0.14604200	0.00001000
O	-0.68441700	1.33869200	0.00006500
O	-1.48015900	-0.76153800	-0.00001000
C	-2.79958800	-0.20630800	0.00003600
H	-3.47342100	-1.05279200	0.00004100
H	-2.94575400	0.40533000	0.88419600
H	-2.94580300	0.40535800	-0.88409600
C	0.82338600	-0.49076200	-0.00004200
H	0.86158400	-1.56740500	-0.00010500
C	1.97639400	0.27689400	-0.00001100
C	3.23396500	-0.25889500	-0.00005600
H	1.84645200	1.34952500	0.00005400
H	4.10846300	0.36823800	-0.00002700
H	3.37926900	-1.32731500	-0.00012200

Frequencies (cm⁻¹):

90.39 160.42 162.69 182.12 220.01 329.00 397.78 456.45 583.09 713.06 741.05 852.87 914.54

942.12	1012.90	1044.68	1086.57	1199.30	1200.20	1232.24	1252.10	1309.68	1385.36	1495.97	1517.37
1527.41	1531.96	1554.57	1780.77	3125.28	3194.02	3217.47	3226.40	3240.04	3270.19	3317.41	

CH₃OC(=O)CH₂C=CH₂:

ZPE(Hartree): -345.187905

Cartesian Coordinates (Å)

C	0.35217800	0.02250400	-0.00018600
O	0.20611800	-1.16724000	-0.00028100
O	1.55162400	0.62007200	0.00011000
C	2.67459400	-0.27448900	0.00024500
H	3.55125700	0.35907000	0.00055400
H	2.64760000	-0.90102600	0.88512300
H	2.64804600	-0.90075000	-0.88484400
C	-0.74745800	1.06747200	-0.00032500
H	-0.58115800	1.70543400	0.86777700
H	-0.58183000	1.70464300	-0.86918100
C	-2.11083800	0.53086700	0.00040400
C	-2.77475400	-0.58778200	0.00016100
H	-3.85634000	-0.60237200	0.00092000
H	-2.25185000	-1.53909400	-0.00076800

Frequencies (cm⁻¹):

25.00	142.84	160.75	172.76	181.30	285.37	369.80	451.45	475.53	603.41	712.05	906.33	940.94
946.48	971.70	1027.38	1051.13	1201.38	1220.04	1246.85	1247.12	1371.39	1427.37	1459.15	1500.51	
1518.64	1530.27	1797.22	1840.55	3100.93	3127.46	3129.64	3141.58	3201.36	3228.98	3231.31		

CH₃OC(=O)CH₂CH=CH:

ZPE(Hartree): -345.182874

Cartesian Coordinates (Å)

C	-0.41790000	0.14497800	0.13769300
O	-0.56384900	1.32926700	0.00270800
O	-1.41590400	-0.73924500	0.01836300
C	-2.70025100	-0.16683300	-0.27088600
H	-3.38422800	-1.00248100	-0.33336900
H	-2.98920700	0.51357300	0.52286100
H	-2.66000100	0.37385500	-1.21014500
C	0.87728400	-0.53552800	0.49825700
H	0.85675500	-0.66729500	1.58207900
H	0.90577100	-1.52431900	0.05298300
C	2.07203100	0.29805800	0.10789800
C	3.10960500	-0.18042700	-0.51401000
H	2.01794400	1.34646400	0.37470400
H	3.44637300	-1.12146400	-0.91139100

Frequencies (cm⁻¹):

33.34	83.61	156.59	173.95	210.66	331.16	363.07	440.39	591.11	674.37	736.40	845.68	872.16
938.76	980.37	1031.53	1094.07	1199.20	1202.22	1228.52	1252.61	1281.14	1389.97	1473.38	1501.21	
1517.74	1529.47	1714.74	1835.88	3089.30	3128.96	3176.92	3197.39	3200.48	3230.41	3298.88		

MB-TS1:

ZPE(Hartree): -401.745557

Cartesian Coordinates (Å)

C	-0.01265400	0.13205500	-0.08905300
O	0.25559100	-0.78860100	-0.81121900
O	0.84870200	1.13427300	0.17269200
C	2.11508300	1.02766600	-0.42946100
H	2.69177200	0.03067700	0.13741200
H	2.05652400	0.80304600	-1.48630500
H	2.68581100	1.90839900	-0.17380000
C	-1.30149200	0.31621800	0.66328900
H	-1.07612600	0.04632000	1.69812100
H	-1.56640300	1.36996900	0.66450600
C	-2.40455800	-0.53542400	0.12418400
C	-3.60909100	-0.07087200	-0.15858700
H	-2.16902000	-1.57811300	-0.03085600
H	-4.38444500	-0.71870800	-0.53530200
H	-3.85526900	0.97243000	-0.02164100
N	3.09358600	-1.12827200	0.58069300
H	2.43467000	-1.70800500	0.06249500
H	3.96930500	-1.21135300	0.06650200

Frequencies (cm⁻¹):

-1860.30 29.78 50.00 83.66 102.58 155.29 191.32 211.40 328.53 377.75 390.32 449.14 563.37
570.88 628.82 710.31 767.44 882.89 926.03 953.19 975.79 991.17 1053.69 1087.68 1163.98 1193.33
1230.79 1248.98 1261.21 1337.89 1350.95 1387.95 1464.74 1479.04 1485.78 1501.52 1557.58
1755.39 1833.65 3080.90 3159.97 3167.37 3199.68 3237.35 3266.49 3288.56 3462.90 3550.99

MB-TS2:

ZPE(Hartree): -401.752880

Cartesian Coordinates (Å)

C	-0.56594800	-0.37193500	0.12258500
O	-0.75776900	-0.83165000	1.21848100
O	-1.55702900	-0.10346900	-0.74272300
C	-2.87473300	-0.40909900	-0.26584600
H	-3.54575800	-0.14443700	-1.07210300
H	-2.94817300	-1.46542900	-0.03133800
H	-3.09113500	0.17040300	0.62559800
C	0.75737400	0.03257700	-0.42174600
H	0.78079300	0.02383000	-1.50545000
H	0.79453700	1.23452300	-0.17475700
C	1.92196900	-0.58079100	0.23379900
C	3.07684900	-0.79816900	-0.38355200
H	1.79745200	-0.83862800	1.27553900
H	3.91396600	-1.23420400	0.13715700
H	3.21286000	-0.54731100	-1.42539200
N	0.53479700	2.56935800	0.22956400
H	-0.39678400	2.67446400	-0.17246900
H	0.36398400	2.38674500	1.21876100

Frequencies (cm⁻¹):

-1514.56 38.10 67.95 85.57 118.56 155.13 161.96 174.65 204.02 327.15 385.60 444.82 518.25
564.76 676.73 732.81 785.04 813.32 933.66 968.71 979.68 1010.49 1054.86 1065.77 1193.30
1200.68 1212.52 1240.51 1294.29 1330.06 1390.34 1400.94 1484.49 1503.84 1517.85 1530.02
1550.94 1723.24 1817.21 3127.09 3187.39 3197.78 3203.22 3228.67 3237.20 3293.40 3450.25
3538.83

MB-TS3:

ZPE(Hartree): -401.742193

Cartesian Coordinates (Å)

C	0.79168000	-0.08547700	-0.00889500
O	0.63113300	0.91849100	-0.64908600
O	1.99741700	-0.56587000	0.31376500
C	3.10839900	0.21559300	-0.15080800
H	3.99302300	-0.30589500	0.18888300
H	3.08734000	0.28080900	-1.23317400
H	3.05994500	1.21361700	0.27103400
C	-0.29986000	-0.96324200	0.55134900
H	-0.08123200	-1.99599100	0.27694100
H	-0.21899600	-0.90325500	1.63766700
C	-1.65693100	-0.56683800	0.10168200
C	-2.56462000	-1.28873800	-0.51348800
H	-1.95939200	0.68301600	0.41963900
H	-3.52846100	-0.88272300	-0.78101400
H	-2.37508000	-2.32544900	-0.76860100
N	-2.14203600	1.91042900	0.44256200
H	-2.94197400	1.98883200	-0.18201400
H	-1.34133300	2.18527200	-0.12376600

Frequencies (cm⁻¹):

-1879.09 26.61 67.79 112.92 135.97 155.96 171.00 176.66 245.39 305.83 344.52 426.65 510.70
582.90 632.92 672.99 744.05 796.59 928.89 948.98 962.32 973.31 1052.44 1151.84 1200.32 1205.75
1227.38 1250.61 1286.30 1383.38 1446.78 1457.77 1477.18 1502.66 1518.52 1530.31 1566.89
1762.98 1832.58 3089.14 3124.61 3130.11 3162.14 3202.32 3232.10 3257.86 3477.30 3562.87

MB-TS4:

ZPE(Hartree): -401.737866

Cartesian Coordinates (Å)

C	-1.19419400	0.07386300	0.16435900
O	-1.09701700	1.26823000	0.24686800
O	-2.33437300	-0.55300800	-0.14897000
C	-3.45977900	0.31011200	-0.37092400
H	-4.28725100	-0.34526700	-0.60709200
H	-3.66491100	0.88813200	0.52365800
H	-3.25091700	0.98450400	-1.19418200
C	-0.08431100	-0.91023400	0.43074700
H	-0.25345200	-1.28592800	1.44243000
H	-0.18189300	-1.75587800	-0.24303600

C	1.26854400	-0.26868000	0.33683300
C	2.27142800	-0.79007800	-0.33096200
H	1.38032100	0.67390900	0.85511300
H	3.43900600	-0.16476500	-0.36232700
H	2.28298600	-1.70911300	-0.89990100
N	4.39702600	0.61423400	-0.25940500
H	4.42549900	0.73421200	0.75080500
H	3.97241800	1.46888100	-0.61313600

Frequencies (cm⁻¹):

-1877.53 25.99 55.03 62.19 91.97 117.23 159.72 178.55 217.35 319.54 338.96 442.97 543.62
600.59 613.61 719.82 746.98 773.44 928.85 941.37 994.12 1011.51 1051.85 1131.32 1201.54
1212.71 1233.87 1255.06 1312.64 1352.93 1367.78 1400.12 1470.01 1502.33 1519.03 1530.27
1568.22 1733.93 1834.69 3085.67 3129.47 3167.99 3200.99 3220.39 3230.11 3231.32 3479.54
3568.53

CH₃OC(=O)CH=CHCH₃ + NH₂ → Products

CH₃OC(=O)CH=CHCH₃:

ZPE(Hartree): -345.879172

Cartesian Coordinates (Å)

C	-0.56203600	0.16116600	0.00008300
O	-0.78351500	1.34558700	0.00014400
O	-1.53617400	-0.76384700	-0.00003000
C	0.77048800	-0.46933700	0.00011900
C	1.86208500	0.28352600	-0.00018000
H	0.80798700	-1.54762700	0.00040800
H	1.72539300	1.35718300	-0.00057500
C	3.25410400	-0.24242300	0.00000200
H	3.79387000	0.11915100	0.87421100
H	3.27002700	-1.32810000	0.00066000
H	3.79365100	0.11803300	-0.87480700
C	-2.86760900	-0.23628300	-0.00010100
H	-3.52362300	-1.09670400	-0.00012400
H	-3.02603100	0.37213800	0.88406500
H	-3.02594800	0.37211400	-0.88429800

Frequencies (cm⁻¹):

78.06 150.08 159.32 180.25 211.46 244.93 328.08 393.40 456.52 722.74 745.06 886.07 932.59
974.11 1022.17 1074.60 1100.91 1146.58 1201.07 1225.50 1248.93 1342.37 1369.46 1428.70 1500.30
1501.30 1508.09 1518.07 1529.99 1761.19 1815.98 3090.03 3126.19 3137.16 3176.07 3195.48
3223.57 3226.45 3253.87

CH₂OC(=O)CH=CHCH₃:

ZPE(Hartree): -345.211441

Cartesian Coordinates (Å)

C	0.61258000	0.19361100	0.00006900
O	0.83692600	1.37297000	0.00009600
O	1.60638900	-0.74368600	-0.00000500
C	-0.70246200	-0.45706200	0.00012600
C	-1.80666900	0.27977200	-0.00009700

H	-0.72228500	-1.53554800	0.00034200
H	-1.68775800	1.35544800	-0.00035600
C	-3.18928900	-0.26850000	-0.00004000
H	-3.73450400	0.08476300	0.87420100
H	-3.73430100	0.08411700	-0.87467300
H	-3.18811100	-1.35419200	0.00034600
C	2.88999000	-0.30390700	-0.00005800
H	3.62256400	-1.08388600	-0.00031000
H	3.07297700	0.75153500	-0.00027200

Frequencies (cm⁻¹):

82.36 150.19 160.88 162.61 210.86 237.99 312.42 350.96 394.29 466.89 714.48 729.05 875.11
924.91 974.72 1019.65 1099.58 1130.60 1178.90 1202.89 1254.49 1340.14 1361.09 1429.30 1470.79
1500.81 1506.74 1754.09 1826.28 3090.29 3137.36 3177.48 3224.84 3257.65 3262.75 3419.05

CH₃OC(=O)C=CHCH₃:

ZPE(Hartree): -345.188471

Cartesian Coordinates (Å)

C	-0.58078600	0.17950800	-0.00003900
O	-0.85137700	1.35416800	-0.00001500
O	-1.49212100	-0.79362800	-0.00003000
C	-2.85430100	-0.34286300	0.00005100
H	-3.45673000	-1.24109800	0.00010400
H	-3.04638200	0.25423700	0.88505100
H	-3.04649600	0.25420700	-0.88494300
C	0.78895100	-0.33117200	-0.00006000
C	1.94409400	0.28404000	0.00001700
H	1.91895200	1.37241400	0.00010800
C	3.28361800	-0.37745200	0.00002300
H	3.85096100	-0.06959700	0.87659600
H	3.18716700	-1.45744100	-0.00009300
H	3.85106200	-0.06940400	-0.87641700

Frequencies (cm⁻¹):

42.37 119.74 124.89 173.10 188.24 244.25 312.68 363.92 446.12 729.01 745.40 838.81 897.67
977.59 1078.35 1081.90 1130.21 1200.71 1234.53 1269.00 1337.80 1423.46 1500.15 1505.49 1506.07
1518.76 1529.12 1766.39 1793.14 3095.69 3128.27 3134.22 3145.30 3193.98 3198.82 3231.82

CH₃OC(=O)CH=CCH₃:

ZPE(Hartree): -345.194577

Cartesian Coordinates (Å)

C	-0.63427900	0.53098200	-0.00000500
O	-1.43071200	1.43465400	-0.00000800
O	-0.98785700	-0.76082500	0.00000100
C	0.82845900	0.73546600	-0.00000800
C	1.70179300	-0.23792200	0.00000300
H	1.13119500	1.77797300	-0.00001800
C	3.14770900	-0.44635500	0.00000900
H	3.45225800	-1.01022000	-0.87917500

H	3.67422400	0.51166300	-0.00000900
H	3.45225400	-1.01018600	0.87921600
C	-2.40068800	-0.99485500	0.00000600
H	-2.51724300	-2.07052300	0.00000600
H	-2.85104400	-0.55662100	0.88440200
H	-2.85105100	-0.55662000	-0.88438700

Frequencies (cm⁻¹):

83.49 123.78 125.00 171.22 200.40 244.49 290.13 357.40 490.94 691.58 703.13 876.76 878.33
 971.91 1056.13 1078.43 1100.79 1200.87 1233.07 1267.68 1327.44 1411.83 1475.15 1488.34 1501.63
 1517.88 1530.96 1782.28 1812.17 3053.76 3126.79 3132.35 3155.29 3161.67 3196.48 3227.43

CH₃OC(=O)CH=CHCH₂:

ZPE(Hartree): -345.235557

Cartesian Coordinates (Å)

C	-0.48664000	0.14592200	0.00015300
O	-0.68442700	1.33857300	0.00013300
O	-1.48032300	-0.76157200	-0.00009200
C	0.82349800	-0.49065000	0.00074500
C	1.97660400	0.27691800	0.00005100
H	0.86161300	-1.56734400	0.00069500
H	1.84681500	1.34961600	-0.00006000
C	-2.79979200	-0.20619700	-0.00030500
H	-3.47372300	-1.05265600	-0.00023800
H	-2.94602700	0.40564400	0.88376500
H	-2.94585400	0.40534500	-0.88461100
C	3.23416300	-0.25890300	-0.00041900
H	4.10872900	0.36821600	-0.00098000
H	3.37945900	-1.32737400	-0.00024400

Frequencies (cm⁻¹):

90.77 161.14 162.78 182.83 220.19 329.06 397.75 456.41 583.39 713.10 741.10 853.01 914.75
 942.15 1012.83 1044.84 1086.45 1199.32 1200.25 1232.24 1252.07 1309.65 1385.36 1496.00 1517.41
 1527.40 1531.96 1554.62 1780.84 3124.86 3193.57 3217.03 3226.01 3239.58 3269.71 3316.94

MC-TS1:

ZPE(Hartree): -401.753809

Cartesian Coordinates (Å)

C	-0.06763600	0.21090800	0.27175400
O	-0.39299500	-0.62680800	1.07354700
O	-0.94387300	1.09110800	-0.25887100
C	-2.26875900	0.98847600	0.19625000
H	-2.79666700	-0.09930200	-0.22524700
H	-2.33522000	0.90997900	1.27424400
H	-2.84036500	1.79321500	-0.24274000
C	1.28507300	0.42551800	-0.26425400
C	2.28907900	-0.34089300	0.14204100
H	1.41272200	1.21897500	-0.98386600
H	2.06493400	-1.11128500	0.86842300

C	3.69458000	-0.21465000	-0.32801100
H	4.35669200	-0.02003800	0.51461900
H	4.02585900	-1.14888800	-0.77937200
H	3.80276500	0.58561200	-1.05361100
N	-3.07892700	-1.30897500	-0.63495100
H	-2.59898300	-1.28886800	-1.53379600
H	-2.43832300	-1.80713500	-0.01809200

Frequencies (cm⁻¹):

-1840.60 46.98 76.73 106.22 126.35 161.08 174.10 212.45 250.32 326.67 364.80 394.93 456.91
592.10 721.53 737.82 778.54 851.47 884.19 933.80 979.80 1021.46 1100.39 1101.08 1144.19
1163.05 1228.42 1256.39 1339.37 1367.27 1412.05 1429.31 1465.22 1487.29 1500.71 1507.32
1562.19 1756.94 1811.57 3091.07 3138.79 3161.86 3177.33 3222.84 3255.54 3262.68 3462.62
3548.77

MC-TS2:

ZPE(Hartree): -401.746748

Cartesian Coordinates (Å)

C	-0.75161300	-0.51859600	-0.00656100
O	-1.13208400	-1.65898200	-0.08421400
O	-1.58510100	0.53055100	0.05363600
C	0.65728800	-0.10645200	0.03760500
C	1.68405400	-0.93319400	-0.00311900
H	0.92712300	1.20125500	0.14408300
H	1.46140600	-1.99424400	-0.06949500
C	3.11581200	-0.52092700	0.04217200
H	3.61422900	-1.00038100	0.88315500
H	3.62823700	-0.85030100	-0.86063600
H	3.21256400	0.55554200	0.13848100
C	-2.97835800	0.19181800	0.02406300
H	-3.50925800	1.13253000	0.08405300
H	-3.21350900	-0.32857300	-0.89816200
H	-3.22206200	-0.44572700	0.86707500
N	1.03784400	2.41464500	0.02411400
H	0.07289600	2.68198600	0.20785100
H	1.13784600	2.49695300	-0.98553900

Frequencies (cm⁻¹):

-1871.89 46.54 85.86 96.61 115.10 142.56 170.49 176.62 216.29 247.80 312.78 388.17 402.71
491.74 631.77 698.06 768.88 804.00 892.77 935.85 978.96 1088.83 1091.22 1146.57 1201.16
1232.10 1253.11 1307.09 1323.87 1425.91 1442.53 1500.06 1504.78 1509.01 1517.49 1529.90
1577.94 1752.60 1800.47 3092.54 3128.18 3140.68 3167.41 3192.07 3199.28 3228.42 3480.86
3565.81

MC-TS3:

ZPE(Hartree): -401.749559

Cartesian Coordinates (Å)

C	0.85507900	-0.05229900	0.01395800
O	0.85185100	1.15157300	0.08331600

O	1.98691900	-0.77047900	-0.04526600
C	-0.32252100	-0.93979800	-0.01919900
C	-1.56456400	-0.49747900	0.03710800
H	-0.11278500	-2.00024200	-0.08695600
H	-1.81255300	0.80679600	0.15849900
C	-2.82877000	-1.26383500	0.01484000
H	-3.43824200	-0.95936700	-0.83469000
H	-2.64023200	-2.33442300	-0.05012800
H	-3.40709600	-1.05551700	0.91315900
C	3.19485600	-0.00052600	-0.01598500
H	4.00089200	-0.72019200	-0.06818900
H	3.22389100	0.67654300	-0.86307900
H	3.24637600	0.57373300	0.90289400
N	-2.04708400	2.01301800	0.04792200
H	-1.08072200	2.33371400	0.02259200
H	-2.36457700	2.06269600	-0.91829200

Frequencies (cm⁻¹):

-1923.17 48.11 103.81 133.43 145.08 154.13 167.79 176.87 233.50 253.63 297.82 359.62 425.12
529.79 645.97 729.28 752.88 782.63 892.21 952.99 987.47 1059.89 1076.00 1129.08 1201.65
1203.76 1237.24 1270.31 1364.80 1417.41 1451.31 1484.86 1495.39 1502.21 1517.49 1530.04
1572.88 1751.88 1810.35 3081.79 3127.21 3144.39 3152.35 3196.77 3197.38 3228.35 3474.63
3560.33

MC-TS4:

ZPE(Hartree): -401.756175

Cartesian Coordinates (Å)

C	-1.16975400	-0.01020500	-0.17816800
O	-1.34989200	0.60151500	-1.20153900
O	-2.14302200	-0.23783200	0.71847900
C	-3.42317000	0.30121800	0.36848300
H	-4.08491000	0.03580700	1.18221400
H	-3.35513100	1.37846000	0.25933700
H	-3.76479600	-0.13099300	-0.56609600
C	0.10643500	-0.59837300	0.25936900
C	1.18596100	-0.49964300	-0.51694700
H	0.12036200	-1.10753500	1.21028100
H	1.07182400	0.02477200	-1.45680200
C	2.50892100	-1.00724900	-0.16292400
H	3.18753000	-0.05780900	0.26227700
H	2.52019300	-1.69308400	0.67650000
H	3.09297300	-1.36732800	-1.00198500
N	3.82014900	1.11912200	0.61075300
H	4.18585200	1.37418200	-0.30606900
H	2.97801000	1.68571700	0.71068400

Frequencies (cm⁻¹):

-1700.38 40.59 60.00 77.19 101.14 159.41 166.13 207.42 244.78 326.81 387.24 395.59 457.77
593.36 707.19 751.49 768.28 835.77 907.01 949.29 1000.78 1026.04 1076.10 1092.69 1157.65

1200.63	1227.44	1251.01	1335.09	1349.78	1381.94	1415.57	1490.46	1501.75	1517.00	1529.80
1548.75	1721.02	1809.10	3126.92	3146.50	3196.98	3213.37	3227.42	3228.99	3255.10	3456.00
3544.25										

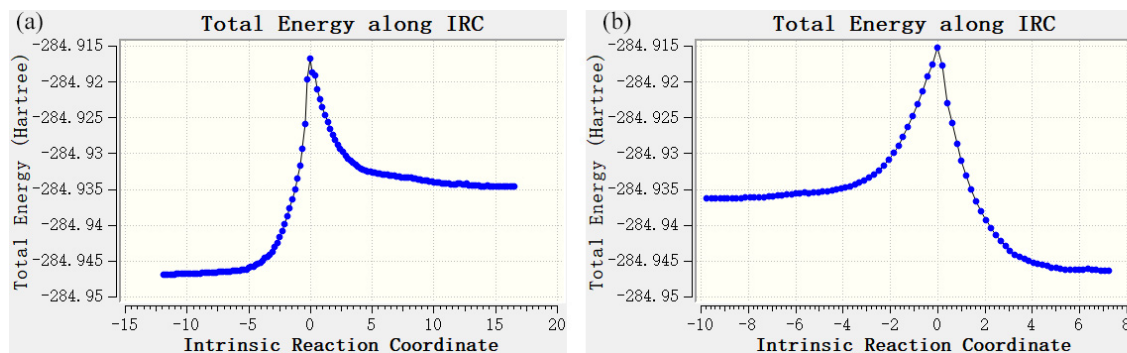


Figure S1. IRC diagrams of MF. (a) TS1; (b) TS2.

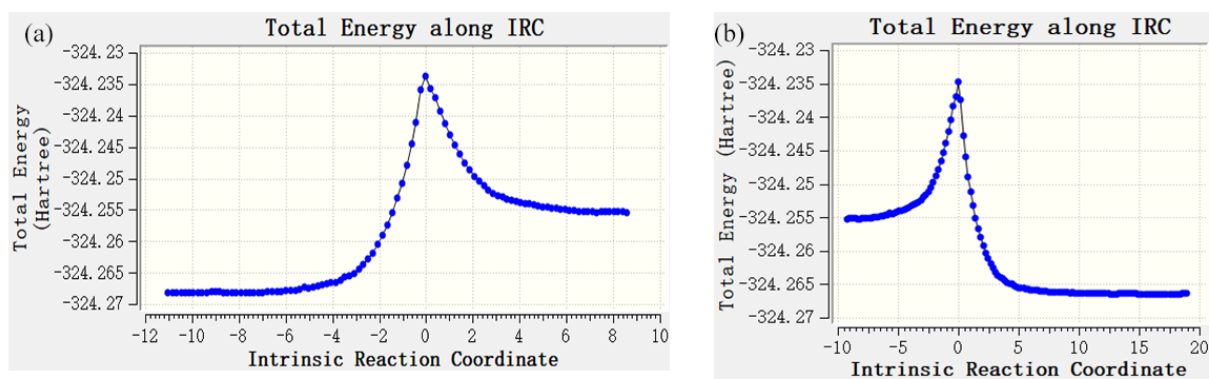


Figure S2. IRC diagrams of MA. (a) TS1; (b) TS2.

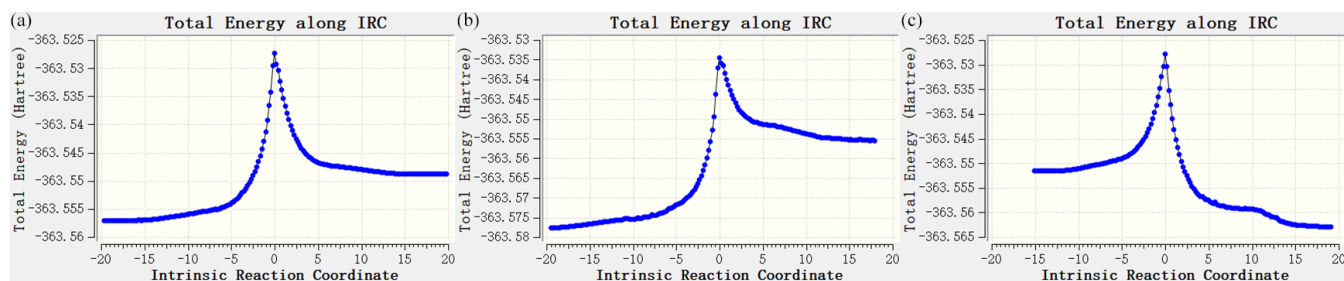


Figure S3. IRC diagrams of MP. (a) TS1; (b) TS2; (c) TS3.

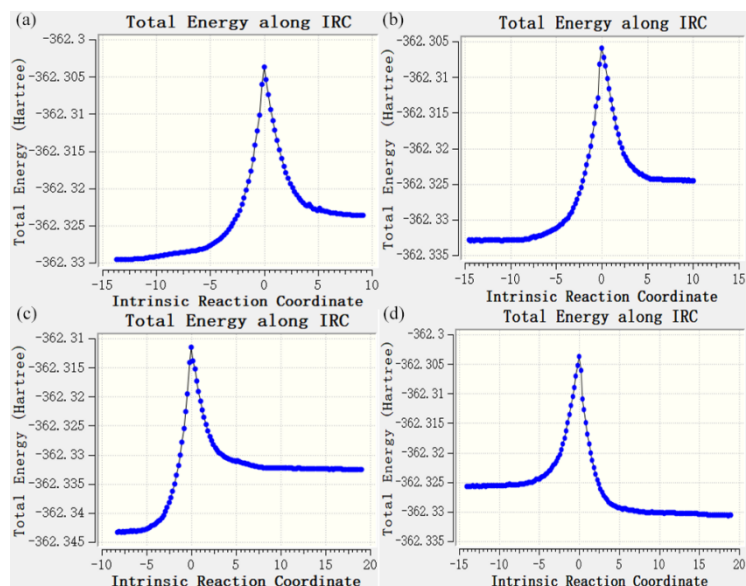


Figure S4. IRC diagrams of MAe. (a) TS1; (b) TS2; (c) TS3; (d) TS4.

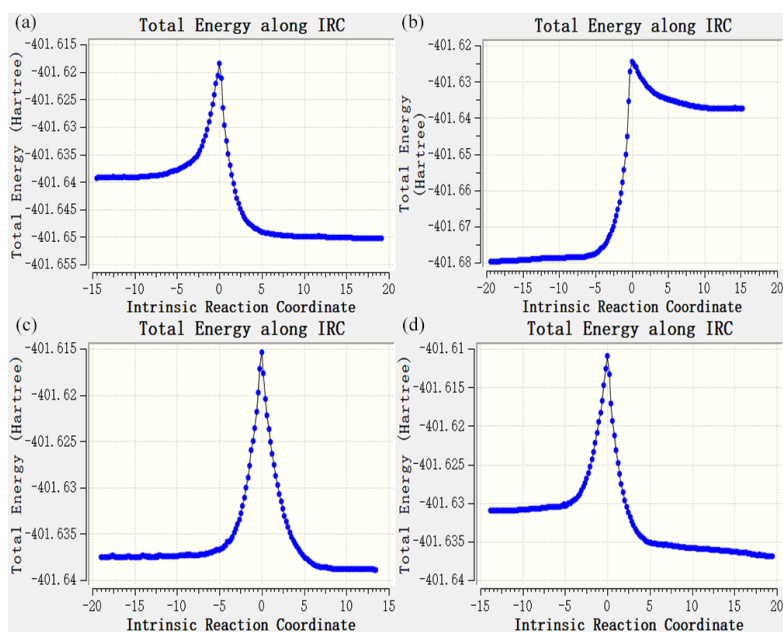


Figure S5. IRC diagrams of MB. (a) TS1; (b) TS2; (c) TS3; (d) TS4.

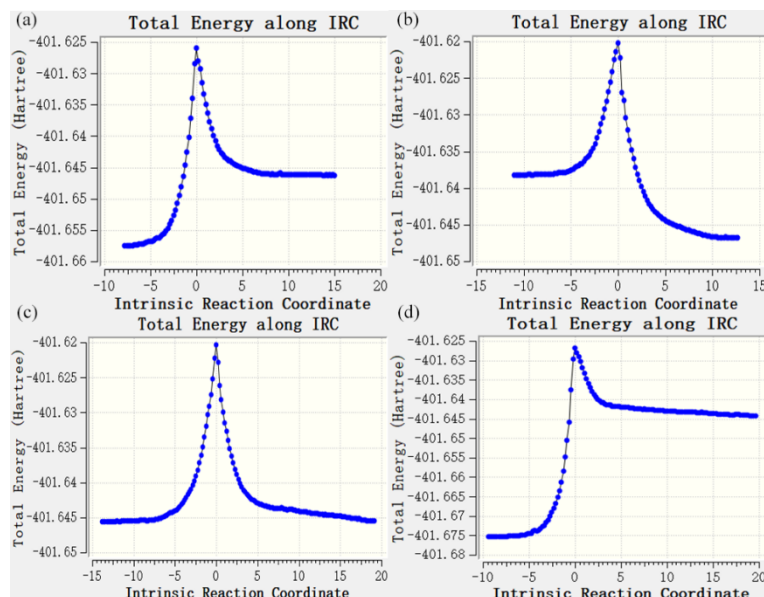


Figure S6. IRC diagrams of MC. (a) TS1; (b) TS2; (c) TS3; (d) TS4.

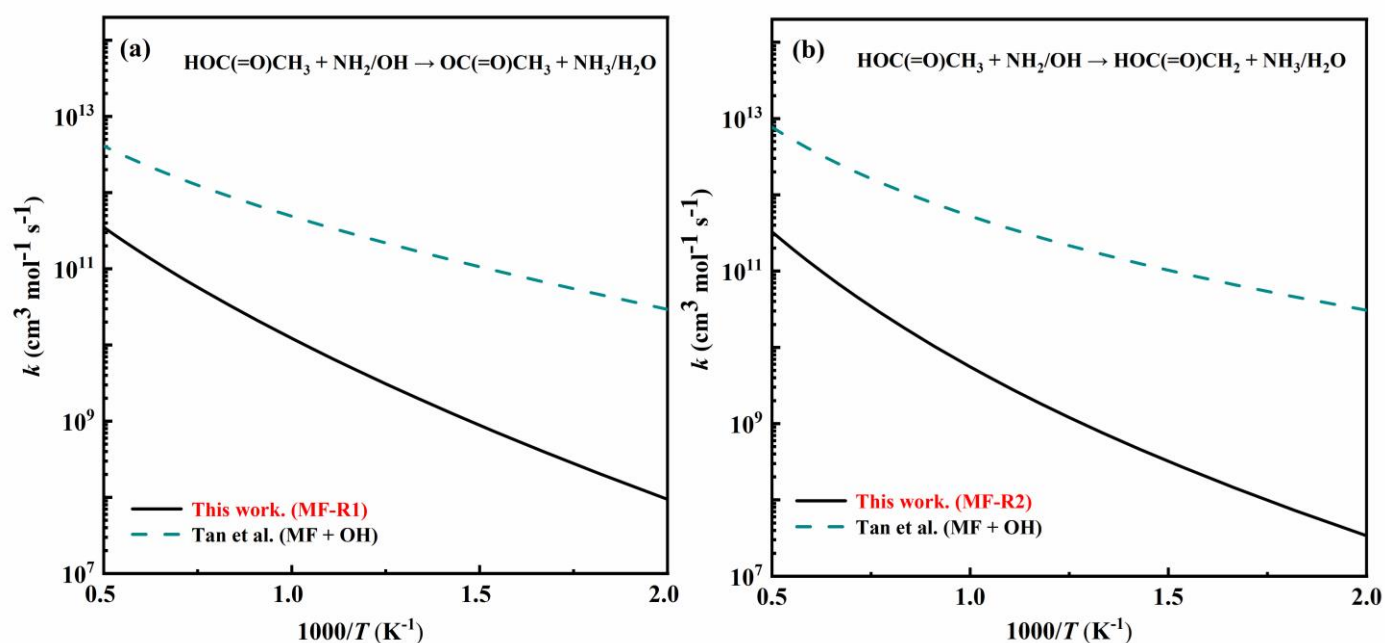


Figure S7. Calculated rate constants for H-abstraction from MF by the NH_2 radical (R1–R2) at 500–2000 K using the MS-CVT/SCT method. The theoretical results for R1 and R2 by Tan et al. are also included (dashed lines).

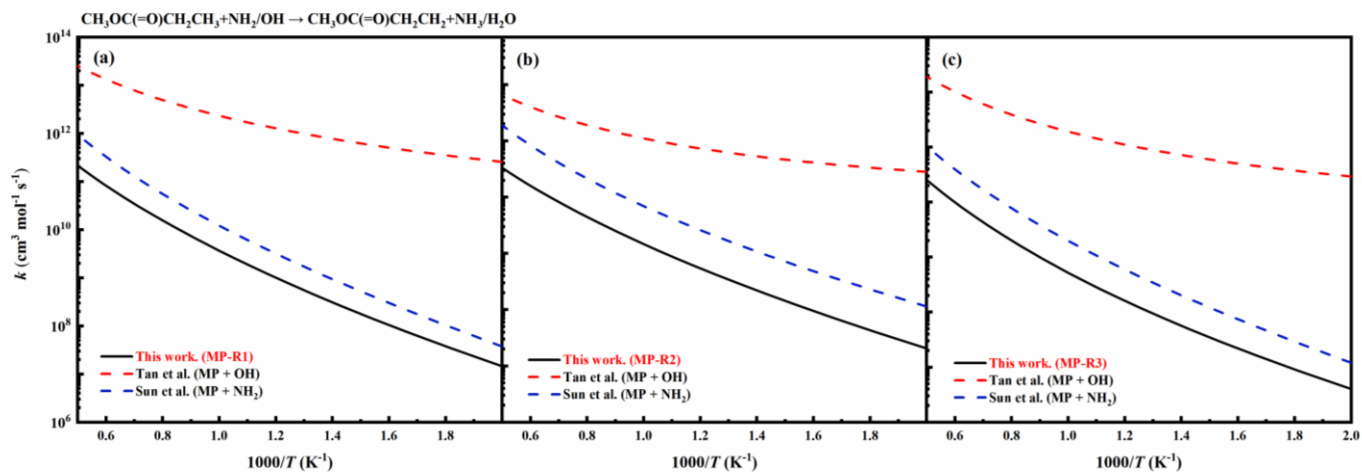


Figure S8. Calculated rate constants for H-abstraction from MP by the NH_2 radical (R1–R3) at 500–2000 K using the MS-CVT/SCT method. The theoretical results for R1, R2 and R3 by Tan et al. and Sun et al. are also included (dashed lines).

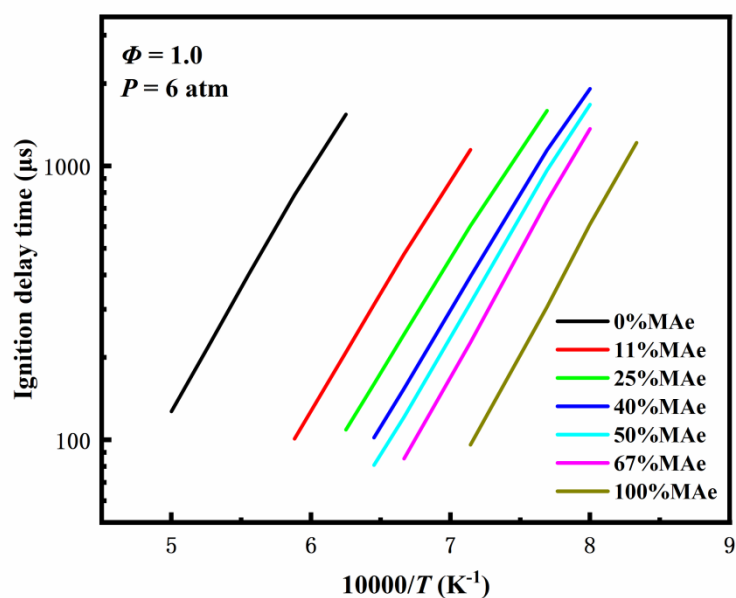


Figure S9. The comparisons between the predictions of current model ignition delay time of MAe/ NH_3 mixtures at 6 atm and $\Phi = 1.0$.

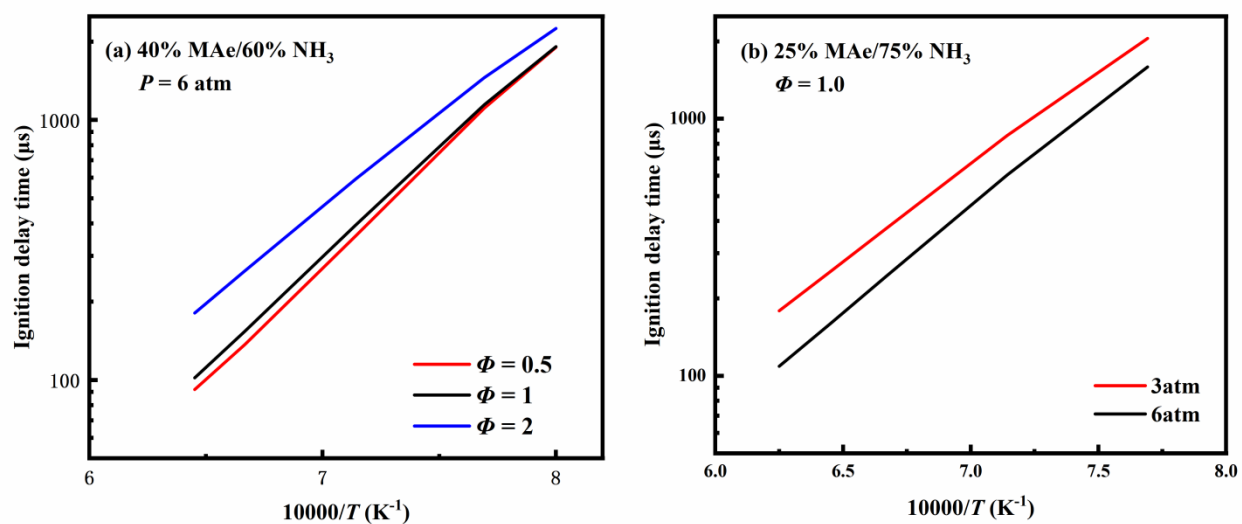


Figure S10. Ignition delay times of (a) 75%NH₃/25%MAe mixture at $\Phi = 1$ and different pressures; (b) 60%NH₃/40%MAe mixture at 6 atm and various equivalence ratios.