atmosphere

MDPI

Supplementary Material

Experimental and Theoretical Studies of Trans-2-Pentenal Atmospheric Ozonolysis

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SPME-GC/MS (RASC-GSMA)

Sampling of the reaction gas mixture was done by exposing a polydimethylsiloxane / divinylbenzene (PDMS/DVB) fiber previously covered with O-(2,3,4,5,6-Pentafluorobenzyl) hydroxylamine hydrochloride (PFBHA) for 5 min in the simulation chamber. This method consists of exposing the PDMS/DVB fiber for one hour in the head space of a vial containing 4 mL of an aqueous solution of PFBHA (0.4 g/L) under a magnetic stir. These conditions ensure a maximum coating of the fiber by the PFBHA and a sufficient quantity of oxime for the detection. The aldehydes present in the simulation chamber adsorb on the PFBHA-doped fiber and form the corresponding oxime.

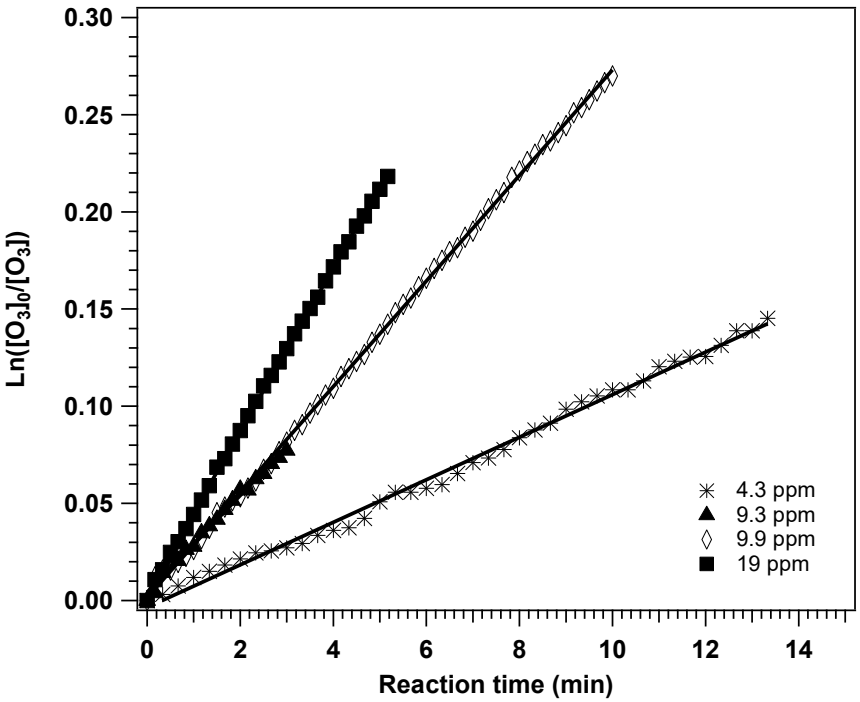

Figure S1. Ozone reaction profiles (Ln scale) as a function of reaction time for ($[T2P]_0 \approx 4.3$-19 ppm and $[O_3]_0 \approx 270$-440 ppb) at room temperature (T = 298 K) obtained in the ASC chamber.

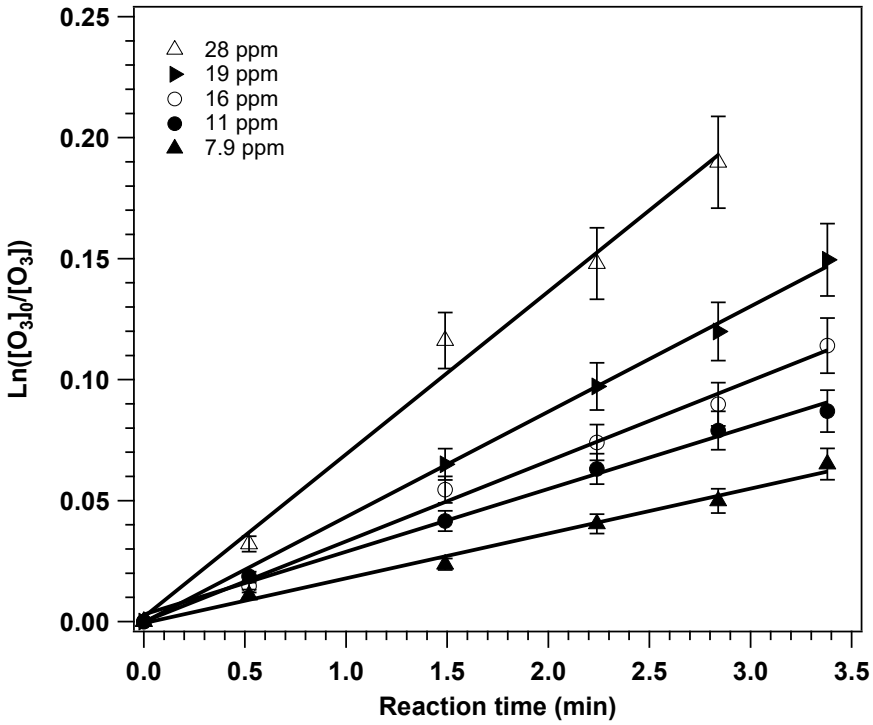

Figure S2. Ozone reaction profiles (Ln scale) as a function of reaction time for ($[T2P]_0 \approx 7.9$-28 ppm and $[O_3]_0 \approx 550$ ppb) without an OH scavenger at room temperature (T = 298 K) obtained in LFR. Error bars correspond to 1σ.

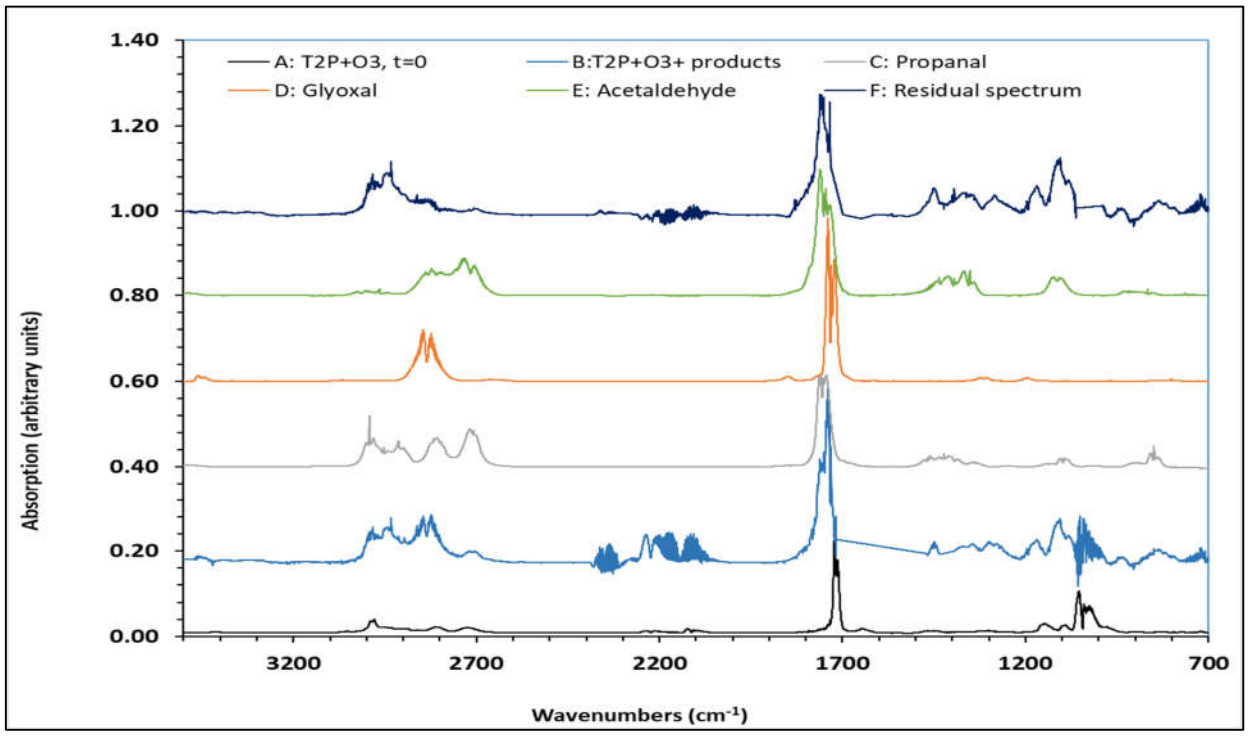

Figure S3. IR spectra from QUAREC. From bottom to top: Panel A shows the IR spectrum of a mixture air/T2P. Panel B shows the IR spectrum at the end of the reaction, including the product. Panels C, D and E show the reference spectra of propanal, glyoxal, and acetaldehyde. Panel F shows the resulting IR spectrum after removing the residual T2P and O_3.

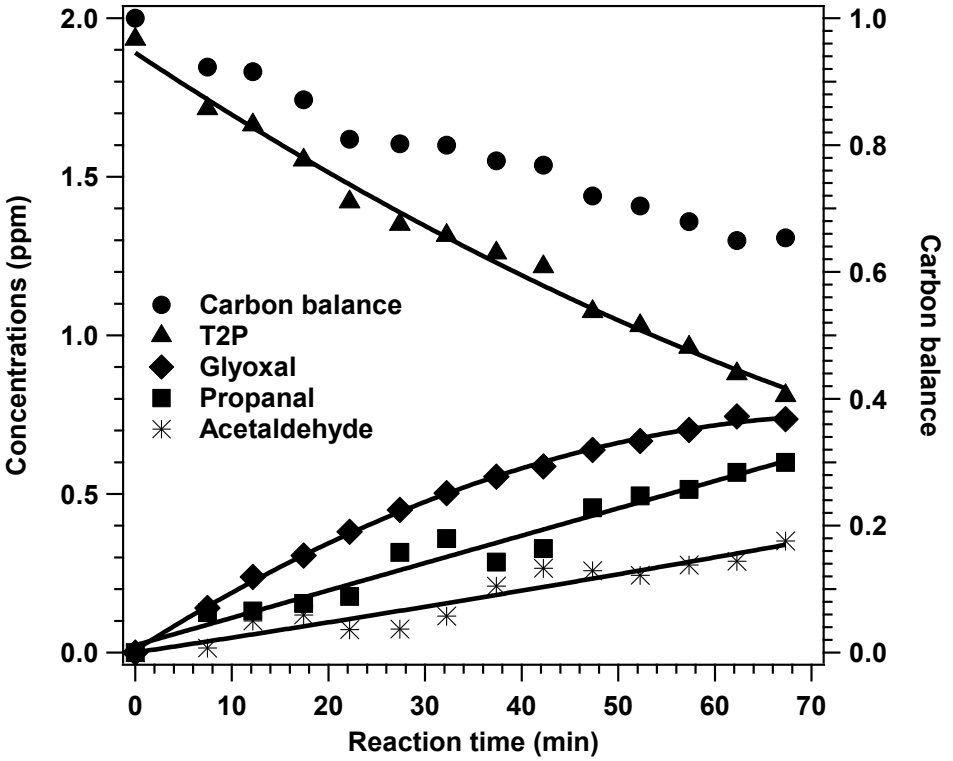

Figure S4. Temporal evolution of T2P and the products identified by FTIR during ozonolysis in QUAREC.

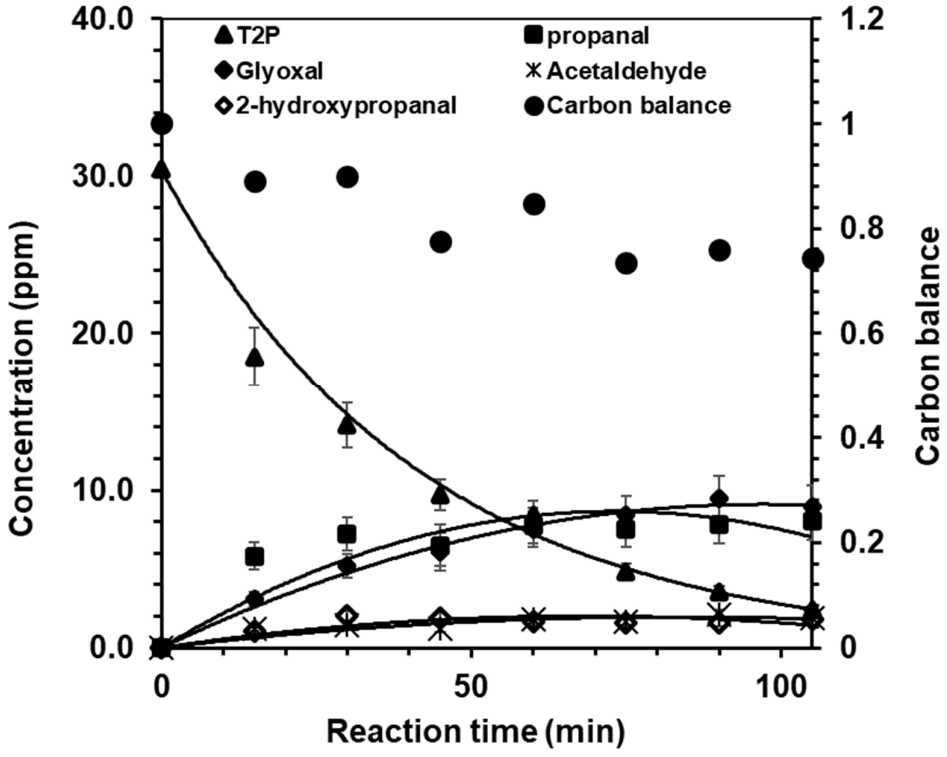

Figure S5. Temporal evolution of T2P and the products identified by SPME-GC / MS and FTIR during ozonolysis in RASC.

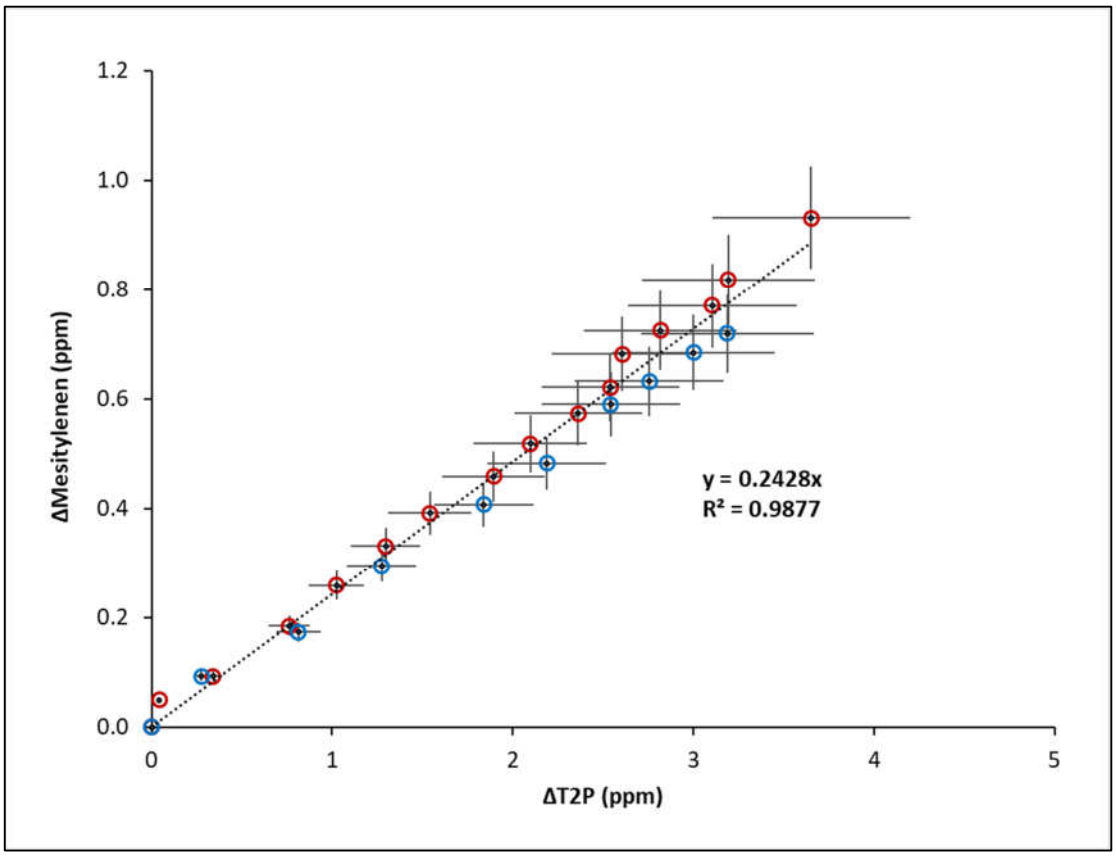

Figure S6. OH production in two T2P + O3/mesitylene experiments (BUW). The error bars represent the errors due to evaluation and calibration procedures, 15% and 10% for T2P and mesitylene, respectively.

Table S1. Data for Figure 1.

[T2P]-ASC (molecule/cm3)	k'-ASC (s-1)	[T2P]-LFR (molecule/cm3)	k'-LFR (s-1)
0	0.00003	0	0.000083
2.29E+14	0.000453	2.77E+14	0.000432
4.78E+14	0.0007	3.95E+14	0.0005533
1.05E+14	0.000183	1.96E+14	0.0003083
2.43E+14	0.000415	6.87E+14	0.00112
		4.64E+14	0.000725

Table S2. Data for Figure 2.

ΔT2P	[C2H5CHO] (ppmv)	[GLY] (ppmv)	[CH3CHO] (ppmv)
0	0	0	0
0.21827606	0.06308	0.070434	0.007336
0.26962521	0.0655975	0.1191645	0.049911
0.38007949	0.0774725	0.1530165	0.059212
0.51241539	0.0883975	0.190281	0.036025
0.58281146	0.158175	0.224952	0.037073
0.61835822	0.1797875	0.251433	0.0577055
0.67311333	0.1427375	0.2772315	0.1048655
0.71662658	0.1640175	0.293475	0.1330305
0.85836084	0.2282375	0.31941	0.1288385
0.90281759	0.2468575	0.3334695	0.121699
0.97029179	0.2572125	0.3509415	0.138074
1.05443111	0.284145	0.3722355	0.143838
0.08749025	0.0232275	0.023751	0.0287545
0.22335142	0.0475475	0.0819	0.0405445
0.33486937	0.0703	0.1259895	0.0294095
0.45971218	0.10963	0.164073	0.049911
0.55207084	0.12787	0.203931	0.06157
0.63013329	0.14269	0.2340975	0.061439
0.7125139	0.1656325	0.2597595	0.064714
0.83427001	0.1911875	0.276549	0.090914
0.85888942	0.192755	0.301938	0.0727705
0.91497896	0.203775	0.3220035	0.0853465
1.01065373	0.2354575	0.319956	0.1005425
0.98976373	0.22211	0.3544905	0.0715915
0.19169996	0.094335	0.112749	0.067334
0.23896544	0.106875	0.145782	0.022139
0.31656875	0.10545	0.18291	0.028034
0.42209166	0.144495	0.209937	0.052138
0.4524295	0.16017	0.25116	0.048732
0.5271749	0.19741	0.265083	0.102311
0.6069766	0.18392	0.276549	0.059736
0.64742705	0.205865	0.300027	0.074015
0.71227968	0.222775	0.316134	0.073229
0.79581865	0.27284	0.331149	0.139515
0.78614572	0.265905	0.357084	0.123009
1.06204417	0.289655	0.337974	0.160475

1.10007639	0.29127	0.376194	0.136633
0.06225927	0.011875	0.034944	0.015982
0.13681075	0.036385	0.063882	0.016637
0.19475977	0.05187	0.092274	0.012707
0.25462445	0.06935	0.114387	0.034191
0.33604042	0.0969	0.13923	0.035239
0.39191412	0.108965	0.157521	0.043885
0.38441108	0.100985	0.176631	0.046243
0.50621576	0.149055	0.188643	0.047029
0.51323988	0.147155	0.211575	0.056068
0.52345679	0.143925	0.22659	0.063404
0.6270626	0.18221	0.238329	0.056723
0.58922812	0.167485	0.256347	0.070609
0.03836758	0.007505	0.018564	ND
0.07466632	0.014535	0.036582	ND
0.105887	0.023085	0.053508	ND
0.1472638	0.032965	0.066339	ND
0.16889258	0.035435	0.071253	ND
0.17998908	0.02964	0.085995	ND
0.20876477	0.05092	0.095004	ND
0.21910897	0.05871	0.104832	ND
0.26556383	0.059565	0.107835	ND
0.28455955	0.062795	0.116298	ND
0.30750486	0.06783	0.126399	ND
0.32781711	0.07163	0.140049	ND
0.37784542	0.090345	0.140049	ND
0.38894193	0.09994	0.151515	ND
0.41658916	0.09937	0.151788	ND
0.39627691	0.08987	0.15561	ND

Table S3: Data for Figure 3

Δ[T2P] (ppmv)	[Glyoxal] (ppmv)	Δ[T2P] (ppmv)	[Propanal] (ppmv)	Δ[T2P] (ppmv)	[Acetaldehyde] (ppmv)	Δ[T2P] (ppmv)	[2-hydroxypropanal] (ppmv)
0.00	0.00	0.00	0.00	0	0	0	0
0.59	0.65	0.59	1.13	0.5915126	0.24165066	0.82559705	0.1065092
3.27	1.16	3.27	1.62	3.27352626	0.41127136	2.02444772	0.19294595
3.49	3.49	8.87	4.42	6.58272074	0.79964005	2.82613571	0.17630492
6.58	3.38	8.89	2.35	7.77121359	0.71796972	2.95212866	0.33448791
7.16	4.80	9.23	4.38	8.87268902	1.242788	3.53612581	0.06393475
7.77	4.00	10.71	5.31	8.88649146	1.08042131	3.9112879	0.2879868
8.87	2.96	11.51	5.92	9.22539218	1.26270447	4.44787208	0.40386952
8.89	5.41	12.22	5.62	10.1487658	1.17313787	4.633426	0.09329255
10.15	5.82	12.36	5.42	10.7054296	1.43011124	5.17793301	0.37469957
10.71	4.97	12.55	5.60	10.767593	1.19385073	5.68682234	0.37124779
10.77	6.70	12.75	4.39	11.0864905	1.26830169	6.67345708	0.49305613
11.09	6.32	12.79	4.72	11.5092039	1.37705484	6.91345407	0.25501247
11.51	4.94	12.81	3.92	12.2159011	0.75123044	8.1386609	0.45713347
12.22	6.90	13.05	5.67	12.357504	1.02977656	8.25329325	0.47714268
12.35	7.56	13.05	5.06	12.5549642	1.2412959	8.63995313	0.4761807
12.36	7.44	13.05	6.50	12.752001	1.02152259	9.18169391	0.52261816
12.55	7.23	13.11	5.74	12.7851224	1.02761572	9.35940651	0.57775184
12.75	6.49	13.11	5.60	12.80121	1.16054584	9.58064983	0.40591133
12.79	6.18	13.37	4.75	12.808695	0.98954475	9.65219772	0.42876877
12.80	8.39	13.52	5.27	13.0489067	1.15084523	9.83001863	0.58470561
12.81	6.49	13.53	5.21	13.0522112	1.2214693	9.86535001	0.65169855
13.05	8.64	13.64	6.04	13.1084405	1.12980388	10.5188544	0.49752043
13.05	7.41	13.66	5.78	13.518354	1.2868676	11.0133847	0.42227872
13.05	5.82	13.68	4.97	13.5307908	1.49676899	11.0801839	0.34616803
13.11	6.01	13.97	5.99	13.6371714	0.96166811	11.1090268	0.72231047
13.11	7.39	14.17	5.97	13.6838555	1.18482057	11.2422438	0.63167535
13.37	5.94	14.18	6.26	13.9742261	1.28355873	11.4190147	0.46752287
13.52	8.33	14.22	5.77	14.0132507	1.07097707	11.692467	0.28638301

13.53	7.61	14.54	5.93	14.1676215	1.66356358	11.9656879	0.4728967
13.64	9.34	14.61	6.31	14.2230394	0.99837997	12.7713631	0.42678669
13.66	7.52	14.64	6.51	14.6100658	1.4614295	12.9030585	0.67531081
13.68	8.02	14.66	6.90	14.638213	1.62603407	13.2114809	0.78497667
13.75	8.74	14.68	7.03	14.6456038	1.46782418	13.6817164	0.48119313
13.97	8.37	14.70	6.02	14.6568688	1.50821352	14.4925876	0.57758004
14.01	7.59	14.87	7.38	14.6766686	1.40021563	15.2591751	0.73292474
14.17	9.44	14.89	5.16	14.7048446	1.29988189	17.3215003	0.67849124
14.22	7.41	15.01	6.52	14.761668	1.17592621		
14.61	8.56	15.03	5.46	14.8876184	1.41948012		
14.64	8.05	15.26	6.79	15.0062079	1.66985677		
14.66	9.11	15.76	7.34	15.033342	1.11837111		
14.68	8.41			15.4219414	1.46392453		
14.70	7.91						
14.76	8.09						
14.87	9.29						
14.89	9.79						
15.01	8.70						
15.03	8.87						
15.76	10.36						

Table S4. The Z-matrices, energies (in Hartree), imaginary frequencies of TS structures and multiplicity of all the optimized structures at M06-2X/6-311++G(d,p) level of theory.

Structures	Z-matrix	Key points
R	C C 1 R12 H 1 R13 2 A213 H 1 R14 3 A314 2 D2314 H 1 R15 4 A415 2 D2415 C 2 R26 1 A126 3 -D3126 H 2 R27 1 A127 3 D3127 H 2 R28 1 A128 3 -D3128 C 6 R69 2 A269 1 -D1269 H 6 R6_10 2 A26_10 1 D126_10 C 9 R9_11 6 A69_11 2 D269_11 H 9 R9_12 6 A69_12 2 -D269_12 O 11 R11_13 9 A9_11_13 6 D69_11_13 H 11 R11_14 9 A9_11_14 6 -D69_11_14 Variables: R12 = 1.53329851 R13 = 1.09100133 A213 = 110.79049116 R14 = 1.09155099 A314 = 108.34429345 D2314 = 121.52167087 R15 = 1.09247876 A415 = 107.98525521 D2415 = 121.61915346 R26 = 1.49514670 A126 = 111.41346710 D3126 = 178.72971541 R27 = 1.09248167 A127 = 110.44901336 D3127 = 59.09035241 R28 = 1.09542421 A128 = 109.12279315 D3128 = 58.59810536 R69 = 1.33443448 A269 = 125.68839356 D1269 = 118.68204083 R6_10 = 1.09146448 A26_10 = 116.16803820 D126_10 = 59.95469022 R9_11 = 1.47210442 A69_11 = 120.58567807 D269_11 = 178.86431177 R9_12 = 1.08609152 A69_12 = 122.40110792 D269_12 = 1.13906439 R11_13 = 1.20462230 A9_11_13 = 124.32429797	Multiplicity = 1 **Energies (Hartree)** ZPE = -270.375146 ZPE corr = 0.119069 H = -270.367184 S = 82.03cal/mol-K

	D69_11_13 = 179.89535836		
	R11_14 = 1.10954504		
	A9_11_14 = 114.91431372		
	D69_11_14 = 0.14577053		
	O		Multiplicity = 1
	O 1 R12		
	O 1 R13 2 A213		**Energies (Hartree)**
	Variables:		ZPE = -225.332374
O3	R12 = 1.39893400		ZPE corr = 0.007302
	R13 = 1.39886092		H = -225.328496
	A213 = 59.99929582		S = 58.27cal/mol-K
	C		
	C 1 R12		
	H 1 R13 2 A213		
	H 1 R14 3 A314 2 D2314		
	H 1 R15 4 A415 2 D2415		
	C 2 R26 1 A126 3 -D3126		
	H 2 R27 1 A127 3 D3127		
	H 2 R28 1 A128 3 -D3128		
	C 6 R69 2 A269 1 -D1269		
	H 6 R6_10 2 A26_10 1 D126_10		
	C 9 R9_11 6 A69_11 2 -D269_11		
	H 9 R9_12 6 A69_12 2 -D269_12		
	O 11 R11_13 9 A9_11_13 6 D69_11_13		
	H 11 R11_14 9 A9_11_14 6 -D69_11_14		
	O 1 R1_15 2 A21_15 6 -D621_15		
	O 15 R15_16 1 A1_15_16 2 -D21_15_16		
	O 15 R15_17 16 A16_15_17 1 D1_16_15_17		Multiplicity = 1
	Variables:		
	R12 = 1.53300727		**Energies (Hartree)**
	R13 = 1.09105306		
	A213 = 110.79686923		ZPE = -495.711709
RC1	R14 = 1.09144497		ZPE corr = 0.127444
	A314 = 108.34594789		H = -495.699070
	D2314 = 121.57720515		S = 110.82cal/mol-K
	R15 = 1.09253055		
	A415 = 107.98385519		
	D2415 = 121.57664373		
	R26 = 1.49467126		
	A126 = 111.64292836		
	D3126 = 178.39210505		
	R27 = 1.09267196		
	A127 = 110.58521565		
	D3127 = 59.25131542		
	R28 = 1.09607411		
	A128 = 109.06529365		
	D3128 = 58.47269615		
	R69 = 1.33416106		
	A269 = 125.54972180		
	D1269 = 119.35125805		
	R6_10 = 1.09131908		

	A26_10 = 116.23548859		
	D126_10 = 60.06886200		
	R9_11 = 1.47087570		
	A69_11 = 120.54602441		
	D269_11 = 179.20589676		
	R9_12 = 1.08633016		
	A69_12 = 122.31593378		
	D269_12 = 0.86879217		
	R11_13 = 1.20483445		
	A9_11_13 = 124.42572465		
	D69_11_13 = 178.20803228		
	R11_14 = 1.10970255		
	A9_11_14 = 114.83473614		
	D69_11_14 = 1.46225875		
	R1_15 = 5.45050734		
	A21_15 = 13.65761921		
	D621_15 = 40.84382744		
	R15_16 = 1.39863791		
	A1_15_16 = 55.36755875		
	D21_15_16 = 26.23765920		
	R15_17 = 1.39901676		
	A16_15_17 = 60.01732312		
	D1_16_15_17 = 61.67824231		
	C		
	C 1 R12		
	H 1 R13 2 A213		
	H 1 R14 3 A314 2 D2314		
	H 1 R15 4 A415 2 D2415		
	C 2 R26 1 A126 3 -D3126		
	H 2 R27 1 A127 3 D3127		
	H 2 R28 1 A128 3 -D3128		
	C 6 R69 2 A269 1 -D1269	Multiplicity = 1	
	H 6 R6_10 2 A26_10 1 D126_10		
	C 9 R9_11 6 A69_11 2 D269_11	**Energies (Hartree)**	
	H 9 R9_12 6 A69_12 2 -D269_12		
	O 11 R11_13 9 A9_11_13 6 -D69_11_13	ZPE = -495.740511	
	H 11 R11_14 9 A9_11_14 6 D69_11_14	ZPE corr = 0.129201	
	O 1 R1_15 2 A21_15 6 D621_15	H = -495.729749	
TS1	O 15 R15_16 1 A1_15_16 2 -D21_15_16	S = 98.12cal/mol-K	
	O 15 R15_17 16 A16_15_17 1 -D1_16_15_17		
	Variables:		
	R12 = 1.53470824	Imaginary frequency =	
	R13 = 1.09101315	326 *i*	
	A213 = 110.46039038		
	R14 = 1.09166599		
	A314 = 108.42576591		
	D2314 = 121.64050249		
	R15 = 1.09215241		
	A415 = 107.99256652		
	D2415 = 121.67230548		
	R26 = 1.49950055		

	A126	=	110.96954756
	D3126	=	178.47409969
	R27	=	1.09457447
	A127	=	109.81041122
	D3127	=	60.88795365
	R28	=	1.09131834
	A128	=	109.96464542
	D3128	=	57.11350788
	R69	=	1.37076731
	A269	=	122.49386278
	D1269	=	85.14953772
	R6_10	=	1.08771745
	A26_10	=	117.78705587
	D126_10	=	79.95760853
	R9_11	=	1.47940728
	A69_11	=	120.22336851
	D269_11	=	167.56627583
	R9_12	=	1.08598621
	A69_12	=	121.67823346
	D269_12	=	0.53109539
	R11_13	=	1.20130115
	A9_11_13	=	123.77306992
	D69_11_13	=	165.27692704
	R11_14	=	1.10794801
	A9_11_14	=	114.73022039
	D69_11_14	=	15.10008798
	R1_15	=	4.64025626
	A21_15	=	13.29579099
	D621_15	=	48.05298767
	R15_16	=	1.25848455
	A1_15_16	=	98.76529492
	D21_15_16	=	168.12072174
	R15_17	=	1.26477213
	A16_15_17	=	112.93562669
	D1_16_15_17	=	68.82346597

					C				
				C	1	R12			
			H	1	R13		2	A213	
	H	1	R14		3	A314		2	D2314
	H	1	R15		4	A415		2	D2415
	C	2	R26		1	A126		3	D3126
	H	2	R27		1	A127		3	D3127
	H	2	R28		1	A128		3	-D3128
	C	6	R69		2	A269		1	-D1269
I1	H	6	R6_10		2	A26_10		1	D126_10
	O	6	R6_11		2	A26_11		1	D126_11
	C	9	R9_12		6	A69_12		2	D269_12
	H	9	R9_13		6	A69_13		2	D269_13
	O	9	R9_14		6	A69_14		2	-D269_14
	O	12	R12_15		9	A9_12_15		6	-D69_12_15
	H	12	R12_16		9	A9_12_16		6	D69_12_16

Multiplicity = 1

Energies (Hartree)

ZPE = -495.847525
ZPE corr = 0.133385
H = -495.837626
S = 93.89cal/mol-K

		O	14	R14_17	9	A9_14_17	6	D69_14_17	
					Variables:				
				R12	=	1.52761653			
				R13	=	1.09030721			
				A213	=	110.63010406			
				R14	=	1.09292735			
				A314	=	107.78868031			
				D2314	=	122.77915460			
				R15	=	1.09284958			
				A415	=	107.46038807			
				D2415	=	122.00287443			
				R26	=	1.51867336			
				A126	=	111.36232712			
				D3126	=	179.06575767			
				R27	=	1.09387056			
				A127	=	111.22241733			
				D3127	=	57.89184394			
				R28	=	1.09259550			
				A128	=	110.32118025			
				D3128	=	61.21365252			
				R69	=	1.56619127			
				A269	=	112.67424181			
				D1269	=	69.76124073			
				R6_10	=	1.09416999			
				A26_10	=	111.18108310			
				D126_10	=	56.82726859			
				R6_11	=	1.42197792			
				A26_11	=	113.35159692			
				D126_11	=	175.21523860			
				R9_12	=	1.51354113			
				A69_12	=	111.19261469			
				D269_12	=	125.98483268			
				R9_13	=	1.09297461			
				A69_13	=	110.94791584			
				D269_13	=	2.16610569			
				R9_14	=	1.41383311			
				A69_14	=	103.56028750			
				D269_14	=	117.72377661			
				R12_15	=	1.19735153			
				A9_12_15	=	122.43122666			
				D69_12_15	=	95.94976457			
				R12_16	=	1.10657347			
				A9_12_16	=	114.78602529			
				D69_12_16	=	81.48242796			
				R14_17	=	1.41832329			
				A9_14_17	=	103.36463933			
				D69_14_17	=	26.06310686			
					C				Multiplicity = 1
				C	1	R12			
			H	1	R13		2	A213	**Energies (Hartree)**
TS2		H	1	R14		3	A314	2	D2314

H	1	R15	4	A415	2	D2415
C	2	R26	1	A126	3	-D3126
H	2	R27	1	A127	3	D3127
H	2	R28	1	A128	3	-D3128
H	6	R69	2	A269	1	D1269
O	6	R6_10	2	A26_10	1	D126_10
O	10	R10_11	6	A6_10_11	2	D26_10_11
C	1	R1_12	2	A21_12	6	D621_12
C	12	R12_13	1	A1_12_13	2	-D21_12_13
H	12	R12_14	13	A13_12_14	1	D1_13_12_14
O	12	R12_15	13	A13_12_15	1	-D1_13_12_15
O	13	R13_16	12	A12_13_16	14	D14_12_13_16
H	13	R13_17	12	A12_13_17	14	-D14_12_13_17

ZPE = -495.815948
ZPE corr = 0.130528
H = -495.805937
S = 93.28cal/mol-K
Imaginary frequency = 512*i*

Variables:

R12	=	1.52483417
R13	=	1.08995740
A213	=	110.16624096
R14	=	1.09232486
A314	=	107.66808366
D2314	=	121.91028876
R15	=	1.09206957
A415	=	107.94983529
D2415	=	122.64189802
R26	=	1.50703219
A126	=	111.66032710
D3126	=	179.15152525
R27	=	1.09026541
A127	=	112.09588265
D3127	=	57.32091349
R28	=	1.09723677
A128	=	110.84499489
D3128	=	61.46798964
R69	=	1.08922685
A269	=	118.42841142
D1269	=	30.51960160
R6_10	=	1.33037903
A26_10	=	118.55678459
D126_10	=	167.98938130
R10_11	=	1.30337102
A6_10_11	=	110.48729056
D26_10_11	=	44.57200355
R1_12	=	3.42512321
A21_12	=	48.99714532
D621_12	=	45.49609541
R12_13	=	1.51386425
A1_12_13	=	121.83387031
D21_12_13	=	121.73741927
R12_14	=	1.10066429
A13_12_14	=	114.36205141
D1_13_12_14	=	55.90978617
R12_15	=	1.27098434

	A13_12_15	=	117.77036061
	D1_13_12_15	=	156.62239028
	R13_16	=	1.19936218
	A12_13_16	=	122.56747042
	D14_12_13_16	=	16.50736742
	R13_17	=	1.10688304
	A12_13_17	=	114.31892762
	D14_12_13_17	=	163.81597677

C
C 1 R12
H 1 R13 2 A213
H 1 R14 3 A314 2 D2314
H 1 R15 3 A315 2 -D2315
C 2 R26 1 A126 3 -D3126
H 2 R27 1 A127 3 D3127
H 2 R28 1 A128 3 -D3128
H 6 R69 2 A269 1 D1269
O 6 R6_10 2 A26_10 1 -D126_10
O 10 R10_11 6 A6_10_11 2 D26_10_11
C 1 R1_12 2 A21_12 6 D621_12
C 12 R12_13 1 A1_12_13 2 -D21_12_13
H 12 R12_14 13 A13_12_14 1 D1_13_12_14
O 12 R12_15 13 A13_12_15 1 -D1_13_12_15
O 13 R13_16 12 A12_13_16 14 -D14_12_13_16
H 13 R13_17 12 A12_13_17 14 D14_12_13_17

Variables:

	R12	=	1.52658611
	R13	=	1.08952502
	A213	=	110.10122775
	R14	=	1.09063981
I2	A314	=	108.35205421
	D2314	=	120.22708792
	R15	=	1.09244151
	A315	=	107.87406943
	D2315	=	122.06586882
	R26	=	1.47503332
	A126	=	111.70765166
	D3126	=	176.31420126
	R27	=	1.08819918
	A127	=	112.87512370
	D3127	=	61.07839917
	R28	=	1.10052369
	A128	=	111.62614334
	D3128	=	58.34309966
	R69	=	1.08956291
	A269	=	122.16211409
	D1269	=	28.13140207
	R6_10	=	1.24683435
	A26_10	=	125.25488009
	D126_10	=	155.57690708
	R10_11	=	1.37227235

Multiplicity = 1

Energies (Hartree)

ZPE = -495.867187
ZPE corr = 0.129263
H = -495.855340
S = 103.34cal/mol-K

	A6_10_11	=	117.93621939
	D26_10_11	=	5.90386358
	R1_12	=	4.78251092
	A21_12	=	45.76263413
	D621_12	=	93.38498195
	R12_13	=	1.51922926
	A1_12_13	=	62.05599662
	D21_12_13	=	96.90663846
	R12_14	=	1.10674033
	A13_12_14	=	114.80762071
	D1_13_12_14	=	12.61724440
	R12_15	=	1.19591236
	A13_12_15	=	121.81331385
	D1_13_12_15	=	169.91842269
	R13_16	=	1.20762167
	A12_13_16	=	121.35892266
	D14_12_13_16	=	16.36399647
	R13_17	=	1.10209055
	A12_13_17	=	115.03722448
	D14_12_13_17	=	167.93492835

				C			
				C 1 R12			
				H 1 R13	2 A213		
			H 1 R14	3 A314	2 D2314		
			H 1 R15	4 A415	2 D2415		
			C 2 R26	1 A126	3 -D3126		
			H 2 R27	1 A127	3 D3127		
			H 2 R28	1 A128	3 -D3128		
			H 6 R69	2 A269	1 D1269		
			O 6 R6_10	2 A26_10	1 -D126_10		
			C 1 R1_11	4 A41_11	2 D241_11		Multiplicity = 1
			C 11 R11_12	1 A1_11_12	2 -D21_11_12		
			H 11 R11_13	12 A12_11_13	1 D1_12_11_13		**Energies (Hartree)**
			O 11 R11_14	12 A12_11_14	1 -D1_12_11_14		
			O 12 R12_15	11 A11_12_15	13 D13_11_12_15		ZPE = -495.806516
			H 12 R12_16	11 A11_12_16	13 -D13_11_12_16		ZPE corr = 0.130271
TS3			O 14 R14_17	11 A11_14_17	12 D12_11_14_17		H = -495.796445
				Variables:			S = 93.51cal/mol-K
				R12	=	1.52476948	
				R13	=	1.09057073	Imaginary frequency =
				A213	=	110.45735745	576*i*
				R14	=	1.09150119	
				A314	=	107.86565441	
				D2314	=	123.42942189	
				R15	=	1.09341828	
				A415	=	107.28714441	
				D2415	=	122.22950686	
				R26	=	1.52119312	
				A126	=	114.04005955	
				D3126	=	172.23883488	
				R27	=	1.09400636	

	A127	=	112.15727306
	D3127	=	64.24675841
	R28	=	1.09434074
	A128	=	109.99038638
	D3128	=	53.71655876
	R69	=	1.10302315
	A269	=	115.99561432
	D1269	=	38.86027410
	R6_10	=	1.27299837
	A26_10	=	118.80012680
	D126_10	=	176.14771574
	R1_11	=	3.18800186
	A41_11	=	59.33901109
	D241_11	=	29.00062161
	R11_12	=	1.49009536
	A1_11_12	=	90.82672926
	D21_11_12	=	151.91102763
	R11_13	=	1.08710239
	A12_11_13	=	119.94050590
	D1_12_11_13	=	61.19142000
	R11_14	=	1.32504186
	A12_11_14	=	111.43670131
	D1_12_11_14	=	157.33146488
	R12_15	=	1.19918339
	A11_12_15	=	122.87644691
	D13_11_12_15	=	22.17121771
	R12_16	=	1.10530030
	A11_12_16	=	114.40660843
	D13_11_12_16	=	159.38370017
	R14_17	=	1.29645169
	A11_14_17	=	111.23740237
	D12_11_14_17	=	171.70188454

				C				
			C	1	R12			
		H	1	R13	2	A213		
	H	1	R14	3	A314	2	D2314	
	H	1	R15	3	A315	2	-D2315	
	C	2	R26	1	A126	3	-D3126	Multiplicity = 1
	H	2	R27	1	A127	3	D3127	
	H	2	R28	1	A128	3	-D3128	**Energies (Hartree)**
	H	6	R69	2	A269	1	D1269	
	O	6	R6_10	2	A26_10	1	-D126_10	ZPE = -495.859266
I3	C	1	R1_11	2	A21_11	6	D621_11	ZPE corr = 0.128847
	C	11	R11_12	1	A1_11_12	2	D21_11_12	H = -495.847197
	H	11	R11_13	12	A12_11_13	1	D1_12_11_13	S =105.02cal/mol-K
	O	11	R11_14	12	A12_11_14	1	-D1_12_11_14	
	O	12	R12_15	11	A11_12_15	13	-D13_11_12_15	
	H	12	R12_16	11	A11_12_16	13	D13_11_12_16	
	O	14	R14_17	11	A11_14_17	12	D12_11_14_17	

Variables:

R12	=	1.52430633

R13	=	1.09050676
A213	=	110.82701428
R14	=	1.09050359
A314	=	108.67562624
D2314	=	121.19867888
R15	=	1.09306535
A315	=	107.64434036
D2315	=	121.53482369
R26	=	1.50549879
A126	=	113.08582113
D3126	=	175.98334121
R27	=	1.09264796
A127	=	112.27248574
D3127	=	61.65101872
R28	=	1.09770500
A128	=	110.66637470
D3128	=	57.38137130
R69	=	1.10630599
A269	=	116.07049277
D1269	=	23.53063837
R6_10	=	1.21175421
A26_10	=	123.79990819
D126_10	=	160.07778967
R1_11	=	4.84714915
A21_11	=	48.81902317
D621_11	=	48.73094602
R11_12	=	1.48791079
A1_11_12	=	131.46737190
D21_11_12	=	40.28964752
R11_13	=	1.08563147
A12_11_13	=	123.87001470
D1_12_11_13	=	132.59927858
R11_14	=	1.24738223
A12_11_14	=	115.77418859
D1_12_11_14	=	48.29755256
R12_15	=	1.19725448
A11_12_15	=	120.82050706
D13_11_12_15	=	4.09868407
R12_16	=	1.10248918
A11_12_16	=	115.32365792
D13_11_12_16	=	175.88964708
R14_17	=	1.34277776
A11_14_17	=	118.10957515
D12_11_14_17	=	176.05105782