

Supplementary Material

Hydrolysis of ketene catalysed by nitric acid and water in the atmosphere

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Table S1. Experimental and computational characteristic structure parameters of ketene

parameters	Previous GED Study ^C	M06-2X/6-311++G(d,p)	QCISD/cc-pVTZ
rC=O ^A	115.4	115.5	116.2
rC=C ^A	132.3	130.9	131.5
rC-H ^A	108.5	107.9	107.6
∠H-C-H ^B	121.3	121.4	121.8

^ABond lengths are given in picometers.

^Bbond angles (∠) indegrees.

^CAtkinson SJ, Noble-Eddy R, Masters SL(2016). Gas-Phase Structures of Ketene and Acetic Acid from Acetic Anhydride Using Very-High-Temperature Gas Electron Diffraction. *The Journal of Physical Chemistry A* **120**, 2041–2048.

doi:[10.1021/acs.jpca.6b00704](https://doi.org/10.1021/acs.jpca.6b00704)

Table S2. Zero-point energy corrected binding, activated, and reaction enthalpies (ΔH), free energies (ΔG), and energies barriers (ΔE) for all relevant complexes of various reactions at 298 K (in kcal/mol)

compounds	ΔH^A	ΔG^A	ΔE^A	ΔH^B	ΔG^B	ΔE^B
R1:CH ₂ =C=O + H ₂ O → CH ₃ COOH						
H ₂ C ₂ O+H ₂ O	0	0	0	0	0	0
H ₂ C ₂ O⋯H ₂ O	-2.74	3.83	-2.78	-1.42	5.15	-1.46
TS1	38.66	49.75	40.47	40.29	51.39	42.10
CH ₃ COOH	-35.04	-24.20	-33.27	-34.08	-23.23	-32.31
R2:CH ₂ =C=O + H ₂ O → H ₂ C ₂ (OH) ₂						
H ₂ C ₂ O+H ₂ O	0.00	0.00	0.00	0.00	0.00	0.00
TS2	35.78	47.16	37.73	36.51	47.88	38.46
H ₂ C ₂ (OH) ₂	-9.23	1.44	-7.64	-7.53	3.14	-5.94
R3:CH ₂ =C=O + H ₂ O + HNO ₃ → CH ₃ COOH + HNO ₃						
H ₂ C ₂ O+H ₂ O+HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00
H ₂ O⋯HNO ₃	-11.53	-2.86	-11.06	-8.59	0.08	-8.12
RC3	-12.45	4.73	-12.40	-8.03	9.14	-7.98
TS3	-2.54	18.72	-1.01	1.87	23.13	3.40
PC3	-42.55	-22.81	-41.17	-43.64	-23.90	-42.26
CH ₃ COOH+HNO ₃	-35.04	-24.20	-33.27	-34.08	-23.23	-32.31
R3':CH ₂ =C=O + H ₂ O + HNO ₃ → H ₂ C ₂ (OH) ₂ + HNO ₃						
H ₂ C ₂ O+H ₂ O+HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00
RC3'	-11.56	4.61	-11.69	-8.35	7.82	-8.48
TS3'	0.88	23.53	3.12	6.01	28.66	8.25
PC3'	-19.06	1.77	-17.53	-15.52	5.31	-13.99
H ₂ C ₂ (OH) ₂ +HNO ₃	-9.20	1.62	-7.55	-7.52	3.31	-5.87
R4:CH ₂ =C=O + 2H ₂ O + HNO ₃ → CH ₃ COOH + H ₂ O + HNO ₃						
H ₂ C ₂ O+2H ₂ O+HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00
H ₂ O⋯H ₂ O	-4.75	1.42	-4.25	-3.26	2.91	-2.76
H ₂ O⋯H ₂ O⋯H ₂ C ₂ O	-10.88	5.31	-10.09	-7.50	8.68	-6.71
RC4a	-24.88	1.26	-24.15	-18.45	7.68	-17.72
TS4a	-12.60	19.26	-9.90	-4.97	26.90	-2.26
PC4a	-54.34	-25.49	-52.41	-49.43	-20.58	-47.50
RC4b	-26.73	1.59	-25.53	-19.11	9.21	-17.91
TS4b	-8.22	22.97	-5.55	1.65	32.84	11.35
PC4b	-49.59	-20.78	-47.90	-43.47	-14.66	-41.79
CH ₃ COOH+HNO ₃ +H ₂ O	-35.04	-24.20	-33.27	-34.08	-23.23	-32.31
R4':CH ₂ =C=O + 2H ₂ O + HNO ₃ → H ₂ C ₂ (OH) ₂ + H ₂ O + HNO ₃						
H ₂ C ₂ O+2H ₂ O+HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00
RC4a'	-18.44	7.06	-17.99	-13.07	12.43	-12.63
TS4a'	-12.99	19.81	-9.70	-2.79	30.01	0.49
PC4a'	-29.61	1.20	-0.04	-22.06	8.76	-19.87
RC4b'	-26.38	-0.13	-25.46	-19.39	6.86	-18.47
TS4b'	-7.61	24.28	-4.58	1.22	33.11	4.24
PC4b'	-29.42	1.00	-27.15	-22.53	7.89	-20.26
H ₂ C ₂ (OH) ₂ +HNO ₃ +H ₂ O	-9.20	1.62	-7.55	-7.52	3.31	-5.87
R5:CH ₂ =C=O + 3H ₂ O + HNO ₃ → CH ₃ COOH + 2H ₂ O + HNO ₃						
H ₂ C ₂ O+3H ₂ O+HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00

H ₂ O··H ₂ O··H ₂ O	-16.30	0.21	-14.50	-11.92	4.59	-10.12
3H ₂ O··HNO ₃	32.57	-5.99	-30.78	-24.66	1.92	-22.87
3H ₂ O··H ₂ C ₂ O	19.45	5.33	-18.05	-14.50	10.29	-13.09
RC5a	-34.15	1.22	-32.73	-26.03	9.34	-24.61
TS5a	-22.42	16.33	-19.64	-14.22	24.53	-11.43
PC5a	-66.32	-27.77	-63.58	-59.32	-20.78	-56.59
RC5b	-28.72	5.68	-27.66	-20.90	13.50	-19.84
TS5b	-19.66	22.45	-15.82	-7.18	34.93	-3.34
PC5b	-60.11	-22.38	-57.98	-52.65	-14.93	-50.53
CH ₃ COOH+HNO ₃ +2H ₂ O	-35.04	-24.20	-33.27	-34.08	-87.34	-32.31
R6:CH ₂ =C=O + 3H ₂ O + HNO ₃ → H ₂ C ₂ (OH) ₂ + 2H ₂ O + HNO ₃						
H ₂ C ₂ O+3H ₂ O+HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00
RC6a	-36.63	0.70	-34.98	-26.42	10.91	-24.77
TS6a	-28.36	13.60	-24.56	-15.79	26.17	-11.99
PC6a	-39.53	0.30	-36.76	-29.80	10.03	-27.03
RC6b	-35.81	1.72	-34.16	-25.24	12.28	-23.60
TS6b	-23.15	19.28	-19.13	-11.40	31.02	-7.39
PC6b	-38.92	1.46	-36.14	-28.52	11.86	-25.73
H ₂ C ₂ (OH) ₂ +HNO ₃ +2H ₂ O	-9.20	1.62	-7.55	-7.52	3.31	-5.87
R7:H ₂ C ₂ (OH) ₂ → CH ₃ COOH						
H ₂ C ₂ (OH) ₂	0.00	0.00	0.00	0.00	0.00	0.00
TS7	44.65	45.41	45.07	44.50	45.26	44.92
CH ₃ COOH	-25.84	-25.82	-25.71	-26.56	-26.54	-26.44
R8:H ₂ C ₂ (OH) ₂ + HNO ₃ → CH ₃ COOH + HNO ₃						
H ₂ C ₂ (OH) ₂ +HNO ₃	0.00	0.00	0.00	0.00	0.00	0.00
RC8	-11.15	-0.26	-11.04	-8.76	2.12	-8.65
TS8	-9.36	3.54	-8.49	-5.38	7.52	-4.51
PC8	-37.32	-27.79	-37.45	-36.17	-26.63	-36.30
CH ₃ COOH+HNO ₃	-25.84	-25.82	-25.71	-26.56	-26.54	-26.44
R9:H ₂ C ₂ (OH) ₂ + H ₂ O → CH ₃ COOH + H ₂ O						
H ₂ C ₂ (OH) ₂ +H ₂ O	0.00	0.00	0.00	0.00	0.00	0.00
RC9	-7.98	0.90	-7.43	-5.69	3.19	-5.14
TS9	8.26	20.21	10.24	12.20	-85.41	14.18
PC9	-31.70	-24.42	-31.44	-31.44	-24.16	-31.18
CH ₃ COOH+H ₂ O	-25.84	-25.82	-25.71	-26.56	-26.54	-26.44

^AΔH, ΔG, and ΔE are computed at the M06-2X/6-311++G(d,p) level of theory.

^BΔH, ΔG, and ΔE are calculated at the CCSD(T)-F12a/cc-pVTZ-F12//M06-2X/6-311++G(d,p) level of theory.

Table S3. Cartesian coordinates (Å) for optimized structures of all species and complexes at the a M062X/6-311++G(d,p) level of theory.

Species	Cartesian coordinates			
H ₂ C ₂ O	C	0.00043200	-1.20524500	0.00000000
	H	0.94128800	-1.73253300	0.00000000
	H	-0.94025400	-1.73288300	0.00000000
	C	0.00000000	0.10419900	0.00000000
	O	-0.00045300	1.25896100	0.00000000
HNO ₃	N	0.14209600	0.03406100	-0.00009100

	O	0.16009800	1.23581300	0.00001700
	O	1.04090100	-0.73992600	0.00004600
	O	-1.10989400	-0.55071800	-0.00001700
	H	-1.72350600	0.20021500	0.00027000
H ₂ O	O	0.00000000	0.00000000	0.11657000
	H	0.00000000	0.76160200	-0.46627900
	H	0.00000000	-0.76160200	-0.46627900
H ₂ C ₂ (OH) ₂	C	-1.39334200	-0.22136700	0.00005000
	H	-2.06982200	0.62016100	-0.00010800
	H	-1.78787800	-1.22459300	0.00020500
	C	-0.07644100	-0.03544400	-0.00002400
	O	0.81257200	-1.04348900	-0.00013000
	H	1.69853400	-0.66727000	0.00101900
	O	0.56882100	1.16060600	-0.00006900
	H	-0.07328200	1.87562900	0.00032500
CH ₃ COOH	C	0.09022800	0.12673200	0.00000500
	O	0.62694800	1.19865300	-0.00000200
	O	0.78650700	-1.02936500	-0.00000500
	H	1.72527900	-0.79894200	0.00002600
	C	-1.38966300	-0.12193600	-0.00000500
	H	-1.66017400	-0.70655400	-0.88038100
	H	-1.66024500	-0.70596100	0.88074700
	H	-1.91589900	0.82838300	-0.00032800
H ₂ O...H ₂ O	H	1.88210400	-0.00402700	0.76378400
	O	1.51034500	0.00059900	-0.11940800
	H	0.55288100	0.00005800	0.00811400
	O	-1.36471700	-0.00040300	0.09500100
	H	-1.79986200	0.76641600	-0.28528700
	H	-1.80015300	-0.76401500	-0.29135900
H ₂ O...H ₂ O...H ₂ O	O	-1.48416700	0.57167600	0.07166700
	H	-2.10144400	1.03385400	-0.49734200
	H	-0.65498600	1.07801000	0.05851900
	O	0.23967900	-1.57287500	-0.10167900
	H	0.17342400	-2.26707300	0.55627600
	H	-0.59922700	-1.08263000	-0.06989000
	O	1.24294800	0.99027500	0.08165800
	H	1.95783100	1.30473000	-0.47352100
	H	1.23671600	0.02050400	0.01279900
H ₂ C ₂ O ...H ₂ O	C	0.85537800	0.18468400	0.00376300
	C	1.16163200	-1.08712800	0.00054700
	O	0.60043800	1.31383400	0.00602600
	H	0.34938400	-1.79604100	-0.02905600
	H	2.19761400	-1.38579900	0.01936300
	O	-1.85154900	-0.25328900	-0.03501100

	H	-1.93450700	0.70378900	-0.02517200
	H	-2.70566700	-0.59165500	0.2408880
HNO ₃ ...H ₂ O	O	-2.33245600	-0.02591500	-0.06448300
	H	-2.08386200	0.90131700	0.02039100
	H	-3.11990000	-0.16628200	0.46603700
	O	0.22002100	1.11550300	-0.00395600
	O	0.11409000	-1.07264900	-0.00846800
	H	-0.83761500	-0.78844300	-0.02232300
	N	0.83908400	0.07300800	0.00193400
	O	2.01931900	-0.07414600	0.01720200
H ₂ O... H ₂ O...H ₂ C ₂ O	C	-1.21804300	-0.55079500	-0.06389500
	C	-2.15736800	0.24931100	0.36371900
	O	-0.40549100	-1.29254400	-0.43616600
	H	-3.12035200	-0.15977900	0.62694900
	H	-1.91486200	1.29728000	0.44935400
	O	0.47872400	1.65936600	-0.16058800
	H	0.71613400	2.16001200	-0.94315900
	H	1.24788300	1.10168800	0.03191500
	O	2.29086700	-0.45493500	0.22210900
	H	1.61749800	-1.12418300	0.05354700
	H	2.79336600	-0.76120900	0.97960400
	3H ₂ O... H ₂ C ₂ O	C	1.71932900	0.54427000
C		2.58286900	-0.25538800	-0.60240200
O		0.98271600	1.30056000	0.44916500
H		3.44092600	0.16958400	-1.10016900
H		2.38771300	-1.31531800	-0.55356000
O		0.27597600	-1.71182600	0.55883400
H		0.17383700	-2.06473600	1.44446900
H		-0.62951200	-1.61483400	0.21520700
O		-2.28860300	-1.10953600	-0.34032500
H		-2.64811200	-1.33694500	-1.19957500
H		-2.28404700	-0.13726100	-0.29157200
O		-1.85504500	1.61073300	-0.08293900
H		-0.90461300	1.65855500	0.08714100
H		-2.26974300	2.18821800	0.56117200
3H ₂ O ... HNO ₃	O	2.00749100	-1.96096500	-0.08590100
	H	2.21675600	-2.63118200	-0.73914500
	H	1.04500600	-1.94413600	0.00226100
	O	-0.37401700	-0.64423000	0.23445800
	O	-1.85732000	0.91242700	-0.07975600
	H	-0.96602200	1.43491000	-0.04729700
	O	2.54441600	0.73554100	0.03162000
	H	3.13781700	0.84308000	0.77813000
	H	2.42280300	-0.22773500	-0.07470300

	N	-1.55088500	-0.37635100	0.04963600
	O	-2.45415900	-1.15186400	-0.02479800
	O	0.30938300	2.19189700	-0.02582000
	H	0.47355100	2.86946800	-0.68538000
	H	1.11992600	1.62759600	0.02026000
HCOOH	C	0.00000000	0.42117800	0.00000000
	H	-0.37506500	1.45116900	0.00000000
	O	1.15248200	0.11068400	0.00000000
	O	-1.02342400	-0.44083800	0.00000000
	H	-0.65740200	-1.33700000	0.00000000
H ₂ O ... HCOOH	O	1.87395300	-0.02043500	-0.07079200
	H	1.39358600	0.81759600	-0.00933600
	H	2.68047200	0.06416400	0.44085500
	C	-1.19863300	0.05469500	0.00534800
	H	-2.28915800	-0.05736900	0.00596000
	O	-0.64321900	1.12386500	0.00414400
	O	-0.60142300	-1.12401100	0.00740000
	H	0.37240700	-0.98791500	0.00441100
TS1	C	0.34784500	0.17067900	0.09388900
	C	-0.58689500	1.21051900	-0.06540600
	O	1.44967900	-0.19268300	-0.00011500
	H	-1.32843500	1.25853100	0.72652500
	H	-0.18889800	2.15796100	-0.40501600
	O	-0.85908700	-1.04335100	0.06345000
	H	-0.56882400	-1.78815900	-0.47745600
	H	-1.20427400	-0.02724800	-0.52162800
TS2	C	0.21047700	0.18405500	-0.01339200
	C	1.47664400	-0.21006900	0.00465700
	O	-0.55659100	1.18493600	0.01876900
	H	1.74005200	-1.24974000	-0.09462000
	H	2.24350200	0.54581200	0.07567100
	O	-0.91318700	-0.90940600	-0.09665600
	H	-0.94136600	-1.46039200	0.69815700
	H	-1.40668500	0.11615700	-0.00369500
RC3	C	2.37252600	-0.42338900	0.02418200
	C	1.59406500	-1.02553200	0.90278200
	O	3.04308100	0.06039600	-0.77314300
	H	1.73462300	-2.08357100	1.06881400
	H	1.03177400	-0.41000800	1.59024000
	O	0.66991900	1.66834800	0.04993500
	H	-0.06836800	1.91670000	0.61459800
	H	0.94522000	2.46449000	-0.41041500
	O	-1.54589800	0.28657500	1.03389100
	O	-0.96155900	-0.83652400	-0.75356000

	H	-0.11765400	-0.76890200	-0.24383200
	N	-1.89262000	-0.16255300	-0.03746200
	O	-2.96514300	-0.08970800	-0.54699200
TS3	C	2.15648400	-0.38349500	0.03252100
	C	1.22121400	-0.91233300	0.93104200
	O	2.98177000	-0.25112100	-0.72070400
	H	1.55682000	-1.89937400	1.25006100
	H	1.03330200	-0.21422400	1.74496700
	O	1.09844100	1.54231700	0.00560700
	H	0.12528200	1.39767500	0.14963400
	H	1.19772400	2.19853700	-0.68861100
	O	-1.39745200	0.91079100	0.50129900
	O	-1.04921700	-0.99963800	-0.46998700
	H	0.18985600	-0.96626800	0.29149900
	N	-1.86811300	-0.09198400	-0.09142500
	O	-3.04508900	-0.21453600	-0.30233300
PC3	C	-2.10398600	0.00450400	0.01349400
	C	-1.52476300	1.20889900	0.68644700
	O	-3.18823000	-0.10714000	-0.46993300
	H	-2.30881100	1.94570500	0.83597500
	H	-1.07665400	0.92769100	1.64065500
	O	-1.21333200	-1.03869500	-0.01091900
	H	0.51777500	-0.93548600	0.34069500
	H	-1.63090900	-1.77383700	-0.48187500
	O	1.45971100	-0.90887400	0.62392700
	O	1.32003300	0.65907600	-0.89598700
	H	-0.73862800	1.62059500	0.04996500
	N	2.04410200	0.06192000	-0.13586100
	O	3.20944500	0.20831600	0.04865700
RC3'	C	-2.24526400	-0.67906000	0.12004000
	C	-3.44344500	-0.36706400	-0.28291100
	O	-1.18712900	-0.99611500	0.48787900
	H	-3.64834800	0.67330200	-0.48084300
	H	-4.18238900	-1.14443400	-0.40130500
	O	-1.31041600	1.80759100	-0.14245000
	H	-1.31527800	2.72767000	-0.41295700
	H	-0.42008800	1.63616200	0.18530900
	O	1.37824100	0.82013600	0.51152600
	O	1.46948200	-1.20033200	-0.32796900
	H	0.53274400	-1.10625100	-0.05208200
	N	2.07373500	-0.02847600	-0.00235600
	O	3.23100400	0.02992300	-0.25953600
TS3'	C	1.88529700	-0.23562300	-0.07436900
	C	3.09802100	-0.23218200	0.46474000

	O	1.04454600	-1.01446100	-0.54593800
	H	3.62183300	0.68026900	0.69989400
	H	3.58085900	-1.18507900	0.61630000
	O	1.29848400	1.25514500	-0.20790500
	H	1.57983300	1.82663200	0.51850100
	H	0.27424400	1.16119700	-0.21248100
	O	-1.20521900	1.03321100	-0.15359200
	O	-1.27355100	-1.14216700	0.13233100
	H	-0.21708700	-1.05166900	-0.15799500
	N	-1.88399100	0.00926100	0.07023100
	O	-3.05821600	0.03210400	0.23784500
PC3'	C	2.05407900	-0.06007400	-0.01444500
	C	3.36685300	0.12862200	-0.06038300
	O	1.43636500	-1.19980400	-0.32334600
	H	3.79798600	1.10176500	0.12231900
	H	4.00891400	-0.70330500	-0.30172900
	O	1.14270400	0.91865700	0.32986600
	H	1.60396400	1.68521700	0.68495800
	H	-0.51260100	0.99896300	-0.18631000
	O	-1.47406900	1.08737400	-0.39142000
	O	-1.31706000	-0.92737500	0.45677500
	H	0.54405700	-1.21733300	0.05563700
	N	-2.05541200	-0.06551100	0.02358200
	O	-3.23544300	-0.10610300	-0.08324700
RC4a	C	-1.41500100	1.60402200	-0.09378300
	C	-0.32966500	2.10363800	0.43140100
	O	-2.38635000	1.18221800	-0.57013500
	H	-0.11534700	3.15241000	0.29177800
	H	0.32367600	1.45601200	0.99843000
	O	-0.70624900	-1.02284000	0.66770900
	H	-0.46451200	-1.25716600	1.56745100
	H	-1.60084800	-1.36610100	0.47800600
	H	0.53826300	-0.90079500	-0.33116500
	O	-3.28369000	-1.48824000	-0.04530700
	H	-3.47104500	-0.61293600	-0.40386200
	H	-3.68173600	-2.12449100	-0.64331600
	O	2.03723700	-0.20455100	1.08027000
	O	1.34234600	-0.75981700	-0.91502700
	N	2.31045200	-0.29556000	-0.09917200
	O	3.34250400	-0.02226600	-0.62861300
TS4a	C	-1.32670400	1.05945600	0.09694400
	C	-0.27359100	1.88765900	0.43811400
	O	-2.22953900	0.95855900	-0.66433500
	H	-0.34525000	2.88625100	0.02539000

	H	0.10869600	1.79379400	1.44701800
	O	-1.14176000	-0.30800500	0.98420000
	H	-0.18037700	-0.56794900	0.95849000
	H	-1.72127700	-1.00871500	0.57132800
	H	0.88428300	1.14572900	-0.31399300
	O	-2.77239800	-1.74221700	-0.43265700
	H	-3.08330300	-0.97120700	-0.92685100
	H	-3.52961100	-2.30084400	-0.24352700
	O	1.42810500	-0.79398700	0.78473800
	O	1.75655000	0.67281600	-0.80971000
	N	2.17238300	-0.35567000	-0.10304100
	O	3.24178200	-0.80842400	-0.36310100
PC4a	C	1.52524900	0.84940400	-0.11237700
	C	0.61044600	2.01904300	-0.30216000
	O	2.67140200	0.90699800	0.24972100
	H	1.18205100	2.94001900	-0.23054300
	H	0.11166000	1.95114300	-1.27030500
	O	0.92413000	-0.32947800	-0.38754300
	H	-0.77044700	-0.58693800	-0.63102900
	H	1.56463500	-1.06399500	-0.21998700
	H	-0.15700300	1.99039300	0.47425000
	O	3.00820700	-1.84028200	0.27835900
	H	3.50166500	-1.02059300	0.42120000
	H	3.60441300	-2.48284400	-0.11123100
	O	-1.71345900	-0.75768600	-0.86925400
	O	-1.84597000	0.29320500	1.04461600
	N	-2.45372700	-0.25635700	0.15709000
	O	-3.62869300	-0.41567800	0.05350500
RC4b	C	-2.81468800	-0.20197200	0.63798600
	C	-1.80146200	-0.22797700	1.47500800
	O	-3.71535400	-0.14668800	-0.07904700
	H	-1.98402600	0.01128100	2.51207300
	H	-0.86011700	-0.64294400	1.14171300
	O	-1.04363500	-0.58884000	-1.54058400
	H	-0.24624200	-1.10171500	-1.35826200
	H	-1.46625500	-0.96736800	-2.31490500
	H	1.26830500	1.30721700	-0.11995500
	O	1.27676200	-0.90622100	-0.04385900
	O	2.24692600	1.04824600	0.07627600
	N	2.31385000	-0.28306600	0.13761700
	O	3.38467300	-0.74748700	0.36979700
	O	-0.14531000	1.73850700	-0.39623800
	H	-0.55027900	1.07959400	-0.99029800
	H	-0.69393400	1.69495300	0.39759300

TS4b	C	2.37801500	-0.25246200	-0.00905400
	C	1.97821500	0.55125700	-1.06447200
	O	3.08385000	-0.46109000	0.88033100
	H	2.79084500	1.17564000	-1.42403400
	H	1.37928400	0.06003100	-1.82187900
	O	0.98887700	-1.46040300	0.07955900
	H	0.06984000	-1.14212200	-0.21583400
	H	0.93581600	-1.85656600	0.95666000
	H	-0.72356400	1.38624600	0.39960900
	O	-1.26113000	-0.66465800	-0.78582100
	O	-1.75543600	0.66213400	0.86009300
	N	-2.13340000	-0.21174700	0.00503100
	O	-3.27210000	-0.57649300	-0.02605100
	O	0.09100000	2.00440800	0.02329500
	H	0.36692700	2.65039300	0.68116900
	H	0.97677900	1.38465200	-0.42100600
PC4b	C	-2.12725800	-0.17887400	-0.22327300
	C	-2.09614100	-1.03178800	1.00545100
	O	-2.93136200	0.65257600	-0.51486600
	H	-2.97682400	-0.82587100	1.60743300
	H	-2.06609900	-2.08572100	0.72493200
	O	-1.08129500	-0.47614200	-1.05990000
	H	0.46614200	-0.83362900	-0.36274400
	H	-1.11238500	0.14114300	-1.80460700
	H	0.38855100	1.87069900	0.36633600
	O	1.30091600	-1.11764000	0.08340600
	O	1.81544800	0.80042200	-0.83107300
	N	2.18608300	-0.11609300	-0.12647900
	O	3.24250700	-0.25055100	0.40085200
	O	-0.20193300	1.44709700	0.99782900
	H	-0.62532400	2.15839800	1.48410300
	H	-1.19050500	-0.79448700	1.56683800
RC4a'	C	-2.03371600	-1.02538400	-0.39954400
	C	-3.25182400	-1.42432200	-0.17759600
	O	-0.93546700	-0.70867800	-0.63663800
	H	-3.85474300	-0.83694200	0.49656700
	H	-3.61342500	-2.31345600	-0.67144000
	O	-0.45613100	2.25933900	-0.60261500
	H	0.37167300	2.68101600	-0.35673200
	H	-0.17901400	1.44302700	-1.03417200
	O	1.88598800	0.58447400	-0.62752900
	O	1.55951200	-1.25484600	0.51242100
	H	0.67741700	-1.04871200	0.13565600
	O	-2.29344100	1.11565000	1.15214500

	H	-2.81585500	1.71505800	1.68731700
	H	-1.69186000	1.67353000	0.63050900
	N	2.38255500	-0.26237100	0.08045400
	O	3.50718500	-0.34327500	0.45371000
TS4a'	C	1.59158600	-0.77600800	-0.03916200
	C	1.72582500	-1.55732600	1.02753300
	O	0.79078700	-0.67528900	-1.02338300
	H	2.52161300	-1.39167300	1.73534000
	H	1.02632800	-2.36823100	1.16763400
	O	0.97207500	2.09066600	0.06370100
	H	0.90655500	2.60840300	0.87284400
	H	0.10711800	1.61175100	-0.04570100
	O	-1.39928900	1.00671500	0.21596600
	O	-1.52040800	-1.04902800	-0.51541800
	H	-0.42316200	-0.85688300	-0.75612700
	O	2.59664900	0.33917900	-0.10819100
	H	2.95407400	0.32643800	-1.00919900
	H	1.91571200	1.24322500	-0.00992400
	N	-2.08235100	-0.01323600	0.03688900
	O	-3.23184500	-0.09729000	0.34941100
PC4a'	C	1.59786200	-0.66131500	0.29875600
	C	0.86898000	-0.69821000	1.40791800
	O	1.51144300	-1.47839000	-0.77063500
	H	1.03532800	0.02816600	2.18872100
	H	0.12246700	-1.46780500	1.54169200
	O	0.52531400	2.22372000	-0.35263800
	H	0.64660100	3.14554200	-0.11395500
	H	-0.85794500	1.43294100	0.00164800
	O	-1.71695800	1.05800300	0.35813200
	O	-1.09117300	-0.50554800	-1.02983300
	H	0.58178500	-1.68825300	-0.93405400
	O	2.55701600	0.29130000	0.10025200
	H	3.01932400	0.07049000	-0.71723400
	H	1.34868300	1.75805600	-0.13757700
	N	-1.86175800	-0.17498700	-0.15020500
	O	-2.74376400	-0.82621900	0.31749000
RC4b'	C	-2.94446200	0.02725400	-0.56805000
	C	-3.23928200	-1.21176900	-0.85917700
	O	-1.02785900	-0.85856400	1.36454100
	H	-3.94890500	-1.41512300	-1.64607600
	H	-2.75208600	-1.99497000	-0.30046100
	O	-0.02649800	1.62693200	0.65880600
	H	-0.69483000	2.06398800	0.12094100
	H	1.29153900	1.24318700	0.00339300

	O	2.17522400	1.01953300	-0.46382000
	O	1.64669900	-0.88792000	0.45808100
	H	-0.17394300	-1.22955200	1.10216900
	O	-2.69595200	1.13362600	-0.32626900
	H	-0.47807100	0.85321100	1.04436400
	N	2.43684800	-0.27052000	-0.23722200
	O	3.42868200	-0.70133400	-0.73558100
	H	-1.20153400	-1.17821100	2.25351500
TS4b'	C	-2.21090200	-0.18089600	0.07017100
	C	-2.91943400	-0.99999800	-0.69333100
	O	-1.06153500	-1.07569400	0.85013500
	H	-3.69682200	-0.56663400	-1.30484100
	H	-2.74456000	-2.06203200	-0.68984900
	O	-0.00392300	2.03551100	-0.34116000
	H	-0.00824600	2.19844400	-1.28889800
	H	0.92183100	1.40934100	0.01346100
	O	1.92339400	0.84139900	0.42473500
	O	1.05250100	-0.92184800	-0.51629000
	H	-0.18193100	-1.00645400	0.32672100
	O	-2.09601300	1.00323500	0.40835200
	H	-0.93671000	1.63911100	-0.03539600
	N	2.07722000	-0.33644900	-0.08473300
	O	3.16410600	-0.82048900	-0.12685100
	H	-0.94032500	-0.66817600	1.71952700
PC4b'	C	-1.72936300	-0.71349800	-0.04369600
	C	-1.72863000	-2.00178800	-0.35576000
	O	-1.02743600	-0.25637500	1.05453900
	H	-2.24012600	-2.32752000	-1.24724800
	H	-1.24298200	-2.71574400	0.29150600
	O	-0.84875500	2.36905200	0.23876900
	H	-0.97238500	3.31817300	0.31363000
	H	0.05818400	2.20893400	-0.05791900
	O	1.31049600	0.80078700	-0.55939600
	O	1.51197900	-0.91180300	0.78728400
	H	0.55764800	-0.63895100	0.91141000
	O	-2.40505900	0.23062400	-0.71926300
	H	-1.94661800	1.08381100	-0.66300200
	N	2.02969300	-0.09077700	-0.14363500
	O	3.14872900	-0.31871500	-0.46895400
	H	-1.19324700	0.68989900	1.18997500
RC5a	C	-0.57054500	1.78538200	0.08984700
	C	0.49392600	2.06752100	0.78953500
	O	-1.51900000	1.56945600	-0.54481200
	H	0.88408600	3.07385300	0.76064200

	H	0.96645800	1.28784600	1.36845500
	O	-0.28819300	-0.96513200	0.64823400
	H	0.08227600	-1.32551300	1.45913800
	H	-1.14645200	-1.41616200	0.47492500
	H	0.86594700	-0.79681700	-0.40052300
	O	-2.69504900	-2.02376600	0.16184700
	H	-2.85801200	-2.67813800	-0.52051300
	H	-3.31457400	-1.28817000	-0.00270100
	O	2.51576300	-0.53577500	0.99526400
	O	1.65214800	-0.61384400	-1.00962500
	N	2.70021700	-0.38742500	-0.19679400
	O	3.71324300	-0.06367000	-0.73596200
	O	-4.09530800	0.27167100	-0.35416300
	H	-3.39408000	0.92597500	-0.46547800
	H	-4.79629900	0.70015800	0.14104700
TS5a	C	-0.70978300	1.39356300	0.29446200
	C	0.40831800	2.09316000	0.59585600
	O	-1.65414600	1.25497800	-0.39623100
	H	0.49781500	3.05344200	0.10480600
	H	0.89841100	1.92735700	1.54202300
	O	-0.62123300	-0.01762900	1.42949600
	H	0.26273200	-0.41200200	1.34219300
	H	-1.29789300	-0.70009000	1.15850700
	H	1.57532600	1.07798600	-0.38262300
	O	-2.43599600	-1.75178600	0.66109200
	H	-2.25990700	-2.66949300	0.44434800
	H	-3.01311000	-1.39250100	-0.04291500
	O	1.98117100	-0.81606000	0.70758700
	O	2.29261600	0.60466800	-0.93262900
	N	2.61463000	-0.53166000	-0.29643700
	O	3.49808100	-1.16368200	-0.77855400
	O	-3.73285200	-0.40725900	-1.30195100
	H	-3.14773800	0.35953600	-1.23081900
	H	-4.63039800	-0.06879400	-1.31284200
PC5a	C	0.90061000	1.08457400	-0.19381200
	C	-0.13484200	2.16311500	-0.29846700
	O	2.05651500	1.27173400	0.10351900
	H	0.34521700	3.13599300	-0.24297600
	H	-0.68862800	2.06146800	-1.23319900
	O	0.41566500	-0.13239000	-0.45689800
	H	-1.24071700	-0.48941800	-0.67305300
	H	1.11840500	-0.85209500	-0.34233400
	H	-0.84185400	2.04567000	0.52582200
	O	2.19976100	-1.97211000	-0.18298600

	H	2.06430100	-2.68951300	0.44018500
	H	3.07218000	-1.57165200	0.02008700
	O	-2.18646100	-0.68999400	-0.88675100
	O	-2.28236100	0.12102100	1.14263800
	N	-2.90120500	-0.35488200	0.22025200
	O	-4.07056700	-0.56756900	0.14763600
	O	4.25992900	-0.38915700	0.44830300
	H	3.66783600	0.37842200	0.38777700
	H	5.07724700	-0.15311300	0.00591000
RC5b	C	-1.53461500	1.33716200	-0.49103500
	C	-1.24828700	2.27692800	0.38584100
	O	-1.75094100	0.55608800	-1.31172900
	H	-1.26765900	3.30424000	0.05059400
	H	-1.28289000	1.99148200	1.42737800
	O	-1.61745900	-0.41755000	1.56845900
	H	-0.79911300	-0.85594900	1.31324800
	H	-2.31749600	-0.97149700	1.19581100
	H	2.54906900	0.72191300	-0.16577000
	O	0.85329300	-0.60511600	0.11547900
	O	2.27043200	-2.22202200	-0.06578200
	N	1.96550700	-1.07086200	-0.05206900
	O	2.96380800	-0.19474600	-0.24703200
	O	1.85106200	2.12917100	-0.02639600
	H	2.16957100	2.81784100	0.56199300
	H	0.89163100	2.04649700	0.12385100
	O	-3.37685500	-1.67945000	-0.27199700
	H	-3.53836200	-2.57463100	-0.57665500
	H	-3.01260000	-1.19940100	-1.02281600
TS5b	C	-1.63826300	0.83837800	0.49845000
	C	-0.61060900	1.62622800	0.99696900
	O	-2.68986300	0.98746000	-0.05295100
	H	-0.90526400	2.65404900	1.17570300
	H	0.02977100	1.16985600	1.74260800
	O	-1.26089600	-0.67403400	0.65430500
	H	-0.31984600	-0.86286100	0.32734200
	H	-1.94419000	-1.21202600	0.14897800
	H	2.03315100	1.11318900	-0.68806600
	O	0.99803000	-0.85880900	-0.42115400
	O	2.68864200	-1.69969900	0.62492700
	N	2.17941600	-0.81530400	0.00222500
	O	2.84456800	0.24415300	-0.27985300
	O	1.23413000	1.90496700	-0.94401800
	H	1.57752400	2.80239600	-0.87997900
	H	0.42611500	1.78560200	-0.22956800

	O	-3.20977500	-1.60599500	-0.74038700
	H	-3.92389100	-2.20486800	-0.51042300
	H	-3.57474700	-0.71019100	-0.80164300
PC5b	C	-1.69753200	0.82397100	0.22932700
	C	-0.58053200	1.75659500	0.56764700
	O	-2.87215400	1.08876000	0.25471400
	H	-0.98007200	2.75863100	0.69725400
	H	-0.11123500	1.41530700	1.49297700
	O	-1.26370700	-0.41383600	-0.11198900
	H	0.35204400	-0.88883900	-0.37886100
	H	-2.04495700	-0.98898500	-0.29922700
	H	2.45557400	0.80855700	-1.74816100
	O	1.27130500	-1.11510900	-0.67070900
	O	1.55483400	-0.51338300	1.41237000
	N	2.08438900	-0.82321700	0.37773600
	O	3.25230300	-0.91288500	0.14033500
	O	2.29470900	1.57241000	-1.18582300
	H	3.15485400	1.79619100	-0.82141500
	H	0.18986100	1.74271700	-0.20705200
	O	-3.69353700	-1.42063000	-0.55336300
	H	-4.26751100	-2.09153600	-0.17828900
	H	-4.02092400	-0.55553800	-0.26750800
RC6a	C	-1.76063600	-0.69847900	1.08538500
	C	-2.98847300	-1.13992100	1.00278600
	O	-0.67529400	-0.30459600	1.17905100
	H	-3.42211600	-1.25137100	0.02206100
	H	-3.52495600	-1.38536900	1.90577100
	O	-1.48588700	-0.52346100	-1.71558700
	H	-1.80029500	-0.92695800	-2.52726300
	H	-0.53116200	-0.69518900	-1.66743300
	O	1.13792800	-0.14834900	-1.07517400
	O	2.29018400	0.00843400	0.75950900
	H	1.78288300	0.91633600	0.72773300
	O	-1.21634500	2.08134100	-0.75959600
	H	-1.34680600	2.73420700	-1.45049500
	H	-1.42919700	1.21806400	-1.15613400
	N	1.81541600	-0.72648900	-0.23434500
	O	2.09807800	-1.88595900	-0.23479700
	O	1.00284200	2.16205200	0.77917700
	H	0.60149200	2.28573200	1.64401100
	H	0.24485300	2.10467800	0.15246100
TS6a	C	-1.13421700	0.67779700	0.67807200
	C	-0.89958300	1.31507700	1.81674300
	O	-0.63392400	0.76221900	-0.51641300

	H	-1.43484800	1.04582800	2.71334200
	H	-0.16585100	2.10764000	1.83208900
	O	-0.53190500	-2.18836100	0.32365900
	H	-0.26251400	-2.80417500	1.01170900
	H	0.28074600	-1.69179900	0.05442500
	O	1.80139900	-1.01873600	-0.06697000
	O	1.72752400	1.11305200	-0.52357400
	H	0.54880100	0.91880700	-0.52444000
	O	-2.12169700	-0.40401700	0.73084500
	H	-2.68996400	-0.29224000	-0.09263900
	H	-1.50602400	-1.28559100	0.59534500
	N	2.41227600	0.04454200	-0.26375000
	O	3.60619700	0.12818400	-0.22310000
	O	-3.07461200	0.26739500	-1.55097400
	H	-3.44612500	-0.15202300	-2.32980500
	H	-2.19120600	0.60663200	-1.77044600
PC6a	C	1.03223800	-0.35550000	0.88542100
	C	0.06839400	-0.41119400	1.79867800
	O	1.27495100	-1.29784200	-0.06756000
	H	-0.04606100	0.39505200	2.50696700
	H	-0.59030200	-1.26650300	1.84822300
	O	-0.11557700	2.25580900	-0.42915000
	H	-0.15229500	3.18673200	-0.19737600
	H	-1.44288800	1.36852800	-0.27689500
	O	-2.32962600	0.93476600	-0.07183800
	O	-1.25797000	-0.70035500	-1.03986000
	H	0.42667800	-1.64797800	-0.37193700
	O	1.86867800	0.70395800	0.77420600
	H	2.62661100	0.46874000	0.19720200
	H	0.67328000	1.88441300	0.00433700
	N	-2.24014900	-0.35756000	-0.40953400
	O	-3.14479300	-1.05020200	-0.05753200
	O	3.74191400	-0.36030400	-0.87879800
	H	4.15041000	-0.09240000	-1.70445500
	H	3.13119800	-1.08014800	-1.07966200
RC6b	C	2.91985600	-0.08037000	0.45913100
	C	3.83841700	-0.44637300	-0.39018000
	O	2.10616900	0.24851300	1.22296800
	H	4.84647400	-0.61764700	-0.04574700
	H	3.54092800	-0.57005000	-1.42064900
	O	0.94588200	-0.07835200	-1.52281700
	H	0.46665500	-0.08376400	-2.35639100
	H	0.49561500	-0.74019100	-0.96689100
	H	-1.28893900	1.35386100	0.52903300

	O	-1.95030300	0.15787200	-1.20017200
	O	-2.06893700	0.78963000	0.88238400
	N	-2.37156800	-0.07798200	-0.09217900
	O	-3.03419400	-1.02239900	0.24167900
	O	0.01919500	1.98339100	0.06521900
	H	0.69437200	2.02354200	0.75035500
	H	0.38556900	1.37951000	-0.61421600
	O	-0.07839200	-1.56063500	0.57912200
	H	-0.89135900	-2.01167100	0.82900500
	H	0.28666000	-1.17143200	1.37999700
TS6b	C	1.83621800	0.33980400	-0.26644500
	C	2.69564200	0.96630300	-1.06393700
	O	1.36263200	0.51060700	0.89648500
	H	3.17349600	1.86470400	-0.70258100
	H	2.92159400	0.58139600	-2.04476800
	O	1.25231100	-0.91948000	-0.92349000
	H	0.28853000	-0.67813000	-1.12250800
	H	1.24307900	-1.61298200	-0.19259700
	H	-1.46690000	1.38178200	0.73756100
	O	-1.03775400	0.13011800	-1.10664100
	O	-2.35994800	0.58391200	0.54598700
	N	-2.00982400	-0.22156800	-0.39501000
	O	-2.61071800	-1.24089800	-0.55863600
	O	-0.54028100	2.08325900	0.99223100
	H	0.30889500	1.46217000	0.98587100
	H	-0.42305200	2.74637300	0.30443100
	O	1.16832800	-2.14293300	1.31059700
	H	1.66844700	-2.79649400	1.80382500
	H	1.28696700	-1.27117400	1.72585800
PC6b	C	-1.53169800	0.56136100	0.14490800
	C	-2.04076500	1.73685500	0.50042100
	O	-0.89705300	0.28896000	-1.02520900
	H	-2.01058800	2.57307400	-0.18312400
	H	-2.51569000	1.84048800	1.46369300
	O	-1.51028000	-0.51104900	0.98112000
	H	0.20599000	-0.25446900	1.47765600
	H	-1.53205600	-1.33637800	0.43823000
	H	1.68650400	2.02498600	-0.92847900
	O	1.07144900	0.19725300	1.30670800
	O	2.54513500	0.04600800	-0.25498700
	N	1.66792800	-0.52663700	0.32516500
	O	1.27316700	-1.64830700	0.15096200
	O	0.79713800	2.39739600	-0.92559200
	H	-0.43220600	1.09705800	-1.31974300

	H	0.60475200	2.55974600	0.00499300
	O	-1.35391700	-2.49088800	-0.84642600
	H	-1.08959500	-1.82363300	-1.49293500
	H	-0.56293300	-3.01868900	-0.70102900
TS7	C	1.24174400	-0.59766000	-0.04992000
	H	1.85107400	-0.35440700	0.81723300
	H	1.37392300	-1.59930100	-0.43784100
	C	-0.04957600	-0.02757800	0.03432300
	O	-1.20724100	-0.64768600	0.03318800
	H	-1.90838900	0.00288800	-0.11065400
	O	0.00513200	1.25186100	-0.00939500
	H	1.14725900	0.86884600	-0.36549700
RC8	C	-1.81338700	0.03022600	0.11627700
	C	-1.34490600	-0.78462200	1.07830500
	O	-2.76039600	-0.35409300	-0.74252000
	H	-0.71221600	-0.38588900	1.85859400
	H	-1.77864100	-1.76720100	1.18421200
	O	-1.40637600	1.28336900	-0.12948500
	H	-0.56517200	1.45251200	0.32051500
	H	-2.84862800	0.32087500	-1.42563900
	O	1.31273300	0.88283500	0.55224300
	O	1.21133200	-1.10316000	-0.37474300
	H	0.31040600	-1.01239600	0.05001600
	N	1.90773100	0.01053700	-0.05360800
	O	3.04144300	0.02163900	-0.40298600
TS8	C	-1.73935300	0.03169500	0.12459200
	C	-1.11380100	-0.96370300	0.86868800
	O	-2.84334000	-0.21602900	-0.54331500
	H	-0.58983900	-0.61332300	1.75286900
	H	-1.65369400	-1.89635400	0.95743300
	O	-1.25129800	1.21963700	-0.05982400
	H	-0.27304600	1.22413000	0.20513400
	H	-3.03057600	0.52604600	-1.13556700
	O	1.23374000	0.94918900	0.47420000
	O	1.09436300	-0.98083800	-0.54330600
	H	0.03262600	-1.04231400	0.06446500
	N	1.81979000	-0.00190500	-0.08936700
	O	3.00340100	-0.04606000	-0.22506100
PC8	C	1.84084300	-0.10213800	0.07290300
	C	1.52823300	1.22767100	0.67962800
	O	3.03980600	-0.14159100	-0.50504100
	H	0.73478700	1.12211400	1.41530100
	H	2.42346600	1.65846700	1.12483700
	O	1.11267500	-1.07186900	0.06885900

	H	-0.51867000	-1.02715100	0.35909600
	H	3.15272100	-1.01734000	-0.90156300
	O	-1.50108300	-1.01374900	0.52413100
	O	-1.16207500	0.77388700	-0.68866800
	H	1.17678500	1.88729200	-0.11651500
	N	-1.97665900	0.07149000	-0.13293900
	O	-3.15769000	0.21869600	-0.08250000
RC9	C	-0.75136400	0.08766900	-0.09963100
	C	-0.30042100	1.33894900	-0.23246400
	O	-1.96915900	-0.18834800	0.40318100
	H	0.61899300	1.53296900	-0.76454800
	H	-0.91854200	2.15986400	0.09506000
	O	-0.10037000	-1.04231800	-0.43841400
	H	0.85540600	-0.86294100	-0.46729100
	H	-2.02904300	-1.14248000	0.51903300
	H	2.00607900	0.61032100	0.74145100
	O	2.40305400	-0.06770100	0.18234200
	H	3.10961500	-0.47051300	0.69199000
TS9	C	0.63718100	0.02979100	0.13974800
	C	0.03271600	1.29896200	0.17645200
	O	1.86722800	-0.09903400	-0.35733700
	H	-0.50616600	1.50391800	1.09829300
	H	0.61945400	2.12138000	-0.20888800
	O	0.02264100	-1.04756200	0.43347700
	H	-1.16428500	-0.76938600	0.18411400
	H	2.04200300	-1.04445800	-0.45601400
	H	-1.27289800	0.74037700	-0.33673200
	O	-2.05761000	-0.11504000	-0.21601000
	H	-2.39556300	-0.43125900	-1.05901600
PC9	C	-0.74759800	-0.09411700	-0.00289300
	C	-0.32606500	1.34303600	-0.00520100
	O	-2.08262200	-0.23407000	0.00218600
	H	0.75821300	1.41218600	-0.04991900
	H	-0.78201600	1.84804100	-0.85776900
	O	-0.01439300	-1.05229600	-0.00216000
	H	1.86772500	-0.60492900	0.00981600
	H	-2.27658700	-1.18140300	0.00866200
	H	-0.70179100	1.82162300	0.90069600
	O	2.61888000	0.00451400	0.01787000
	H	3.40152200	-0.53420700	-0.10608000
RCS1	C	1.81861000	-0.55947000	-0.09988900
	C	1.24430000	-0.91258200	1.03697800
	O	2.29520900	-0.31987100	-1.11674200
	H	1.35619400	-1.93881000	1.35730300

	H	0.96853300	-0.11936600	1.71627600
	O	0.73409900	1.86467900	0.41070500
	H	-0.19661500	1.72030800	0.18543500
	H	0.97137400	2.71600800	0.03930700
	C	-2.29624600	-0.20800800	-0.25754600
	H	-3.32378900	-0.44579100	-0.55627800
	O	-1.87212700	0.91650000	-0.19070000
	O	-1.61717300	-1.30689200	0.00950900
	H	-0.69575500	-1.08731600	0.27852000
TSS1	C	1.51337800	-0.20356400	0.00246900
	C	0.83699900	-1.15049600	0.76140400
	O	2.27408500	-0.06994100	-0.88526900
	H	1.25935900	-2.14550900	0.68491500
	H	0.53606200	-0.82688000	1.75063000
	O	0.85057200	1.25242900	0.44817000
	H	-0.21197000	1.19721800	0.30933600
	H	1.23263600	1.91709600	-0.14033800
	C	-2.12996000	0.02142000	-0.24587200
	H	-3.19007400	0.05982600	-0.51842300
	O	-1.56269700	1.07673600	0.06869000
	O	-1.61114300	-1.14005300	-0.29149800
	H	-0.55505400	-1.15927100	0.08512600
PCS1	C	-1.71607300	-0.02728500	-0.00053300
	C	-1.18529800	1.21470400	0.64096400
	O	-2.78038900	-0.17941500	-0.52051400
	H	-1.96354600	1.97245800	0.64954300
	H	-0.85834900	0.99201200	1.65809800
	O	-0.81161400	-1.05393700	0.05853100
	H	1.02117100	-0.96775700	0.31318200
	H	-1.21115500	-1.81697600	-0.38235200
	C	2.50214500	0.12032200	-0.12198400
	H	3.59597300	0.12047700	-0.04118000
	O	1.99333900	-0.98221600	0.41431400
	O	1.86438600	1.00233600	-0.62567000
	H	-0.31452800	1.55920300	0.07874300

Table S4 Calculated frequencies optimized at the M062X/6-311++G(d,p) level and total electronic energies at the CCSD(T)-F12a /VTZ-F12 level for all structures.

Species	Frequencies (cm ⁻¹)						E (hartree)
H ₂ C ₂ O	449.03	578.23	619.33	993.59	1184.93	1416.63	-152.42772
	2269.65	3206.72	3311.47				
HNO ₃	464.85	624.78	710.06	815.29	980.84	1361.84	-280.65539
	1428.85	1831.95	3797.21				

H₂O	1594.97	3896.30	4002.18				-76.37409552
H₂C₂(OH)₂	206.90	372.77	460.66	545.11	660.31	691.52	-228.8192013
	756.70	955.57	982.68	1199.20	1243.77	1424.16	
	1443.38	1783.40	3205.78	3306.41	3891.84	3917.00	
CH₃COOH	126.53	432.53	548.30	601.23	663.80	887.80	-228.862368
	1016.42	1079.21	1234.13	1351.36	1429.13	1479.95	
	1482.59	1885.35	3087.63	3164.29	3192.42	3840.01	
HCOOH	647.01	678.44	1074.98	1170.43	1315.14	1417.71	-189.5932677
	1878.14	3107.25	3814.92				
H₂O...H₂O	136.55	150.71	153.88	208.18	354.94	657.26	-152.756125
	1606.72	1620.69	3809.68	3884.52	3967.72	3985.45	
H₂O...H₂O...H₂O	47.85	173.55	209.51	214.09	232.70	256.46	-229.147292
	338.82	351.02	443.56	559.25	693.64	847.95	
	1616.17	1621.70	1645.91	3668.03	3725.13	3734.39	
	3961.17	3966.32	3967.41				
H₂C₂O...H₂O	55.37	113.34	145.30	155.84	231.07	238.78	-228.80623100
	439.55	580.23	624.37	987.26	1178.27	1405.14	
	1607.72	2258.52	3217.99	3327.93	3880.47	3988.04	
HNO₃...H₂O	69.80	140.11	183.41	227.02	302.11	447.51	-357.0456104
	671.63	727.29	809.41	832.75	1024.87	1416.18	
	1519.01	1596.40	1817.67	3291.46	3856.85	3973.61	
H₂O... HCOOH	153.69	193.09	212.13	229.30	366.71	538.67	-265.98363244
	704.51	889.11	1088.28	1250.00	1396.18	1454.94	
	1590.63	1836.17	3103.46	3508.34	3789.72	3968.72	
H₂C₂O...H₂O... H₂O	27.05	107.15	139.87	154.51	169.21	207.29	-305.19299209
	223.40	233.34	275.44	334.34	431.51	456.06	
	580.01	651.30	707.41	985.33	1177.57	1401.99	
	1608.25	1637.62	2245.17	3212.08	3324.65	3749.38	
3H₂O... H₂C₂O	28.99	33.56	40.87	113.86	156.02	161.18	-381.58120740
	168.00	199.05	231.38	239.73	252.93	293.94	
	307.80	359.84	422.82	434.52	515.11	581.66	
	662.61	704.62	861.56	983.73	1177.44	1400.20	
	1621.99	1637.07	1656.44	2241.06	3210.74	3324.28	
3642.78	3693.77	3813.33	3954.18	3958.06	3960.55		
3H₂O... HNO₃	30.46	36.78	67.99	76.31	140.28	162.33	-509.82413307
	183.37	193.75	233.31	263.86	298.73	320.82	
	348.53	402.07	512.66	540.15	705.22	734.78	
	791.74	830.68	949.86	1066.68	1069.99	1418.39	
	1575.73	1612.15	1644.67	1674.21	1809.63	2573.46	
	3344.95	3609.23	3813.89	3943.26	3946.23	3967.49	

TS1	-1803.09	308.82	450.12	482.34	567.90	614.09	-228.735912
	731.78	817.36	881.75	1062.74	1119.53	1323.97	
	1452.10	1885.37	2066.32	3160.83	3259.76	3861.52	
TS2	-1487.24	403.82	439.48	567.93	634.20	639.67	-228.743127
	736.40	801.79	989.42	1018.08	1201.91	1333.88	
	1443.04	1871.05	2206.76	3220.83	3326.0	3829.88	
RC3	22.28	28.20	70.60	81.71	110.77	141.08	-509.474271
	165.58	191.10	212.97	242.05	354.86	364.40	
	447.07	589.63	592.94	658.67	717.24	725.04	
	828.33	998.18	1025.78	1173.51	1405.86	1416.42	
	1436.26	1596.12	1797.45	2276.81	3199.02	3307.38	
	3427.90	3865.71	3975.96				
TS3	-360.41	46.51	68.82	89.04	114.08	184.55	-509.454702
	248.46	289.19	337.92	411.77	486.21	517.20	
	585.90	734.35	743.75	851.75	898.21	957.08	
	966.95	1059.96	1098.83	1167.60	1392.19	1409.85	
	1443.49	1601.45	1646.82	1663.92	2344.77	3117.24	
	3202.35	3204.71	3932.81				
PC3	25.05	27.34	69.13	69.13	98.09	118.47	-509.534963
	159.34	170.62	435.91	519.41	600.45	635.31	
	650.04	721.28	770.69	824.57	869.37	1006.76	
	1017.17	1078.21	1233.15	1325.94	1415.26	1421.16	
	1445.77	1480.35	1484.46	1810.24	1914.87	3085.32	
	3157.50	3205.10	3508.22	3822.87			
RC3'	13.93	29.14	59.97	63.89	86.39	118.63	-509.474976
	163.14	166.80	181.01	261.69	290.86	409.07	
	433.55	571.63	647.14	650.77	657.36	724.14	
	820.14	975.67	1023.92	1180.46	1402.25	1414.02	
	1440.34	1622.70	1811.14	2243.91	3213.83	3324.78	
	3585.51	3851.02	3969.44				
TS3'	-302.84	42.40	52.14	90.51	189.05	298.81	-509.449409
	394.28	458.15	480.28	558.24	626.92	656.28	
	699.25	754.24	770.30	822.83	901.89	1013.42	
	1081.60	1107.26	1160.59	1205.57	1313.50	1458.92	
	1524.48	1657.34	1734.58	1773.18	1997.49	2667.57	
	3219.82	3321.45	3856.32				
PC3'	33.33	48.78	68.58	134.14	145.95	175.88	-509.489511
	310.91	469.25	490.97	551.51	650.41	654.42	
	700.78	727.88	743.77	792.48	819.10	934.59	
	992.47	1026.89	1221.30	1266.77	1388.39	1423.42	
	1448.34	1480.60	1795.43	1817.56	3212.54	3315.22	

	3435.93	3758.15	3894.45				
RC4a	13.38	29.28	39.66	59.64	87.22	96.43	-585.867724
	127.27	142.71	152.87	200.24	206.18	227.25	
	276.72	299.36	335.14	395.29	444.74	538.66	
	570.85	653.89	677.76	728.54	812.74	824.97	
	887.14	980.33	1037.57	1183.68	1408.11	1417.43	
	1539.80	1604.28	1627.37	1807.73	2248.51	3076.82	
	3200.95	3307.80	3596.37	3851.31	3938.63	3969.00	
TS4a	-317.53	37.89	52.41	84.35	98.84	157.16	-585.843174
	174.31	186.98	241.55	267.55	353.85	365.61	
	452.00	495.61	529.85	608.85	655.23	702.25	
	709.50	742.17	754.62	830.78	1035.87	1060.93	
	1076.72	1097.31	1183.46	1215.51	1274.05	1456.87	
	1493.55	1591.88	1634.72	1680.53	1761.06	2009.55	
	3161.27	3173.85	3206.51	3271.24	3812.55	3962.59	
PC4a	21.05	25.57	56.40	81.13	96.52	106.49	-585.920845
	134.56	160.46	183.81	194.64	245.78	359.08	
	454.93	521.21	592.01	643.98	655.65	723.20	
	801.35	828.67	887.01	903.97	1015.84	1030.32	
	1080.74	1298.02	1408.61	1424.53	1454.58	1463.86	
	1481.75	1485.04	1590.61	1806.11	1870.03	3083.85	
	3155.48	3203.72	3360.43	3444.29	3804.58	3966.89	
RC4b	36.35	45.44	60.76	75.09	99.38	110.94	-585.868858
	139.59	154.46	154.46	236.50	238.14	280.56	
	307.29	321.30	388.44	446.25	474.22	552.90	
	585.26	661.35	676.50	734.63	817.01	831.15	
	996.43	1061.98	1180.65	1192.42	1404.48	1413.36	
	1533.36	1589.61	1687.03	1792.26	2267.43	2611.80	
	3194.47	3302.59	3664.44	3833.03	3848.18	3964.34	
TS4b	-883.89	27.16	41.02	75.32	85.75	96.38	-585.828827
	124.24	149.56	336.04	338.24	364.99	420.04	
	459.72	500.36	548.40	584.78	638.63	714.41	
	758.00	780.74	797.15	869.02	927.70	981.66	
	1071.50	1103.68	1122.47	1160.23	1305.20	1333.31	
	1448.01	1588.38	1643.55	1665.54	1772.38	1980.37	
	2149.03	2803.93	3155.13	3253.40	3888.52	3902.57	
PC4b	20.25	35.36	71.03	79.89	87.18	114.07	-585.911104
	133.65	169.71	178.92	192.69	217.56	287.46	
	357.05	437.04	536.55	599.32	645.85	666.57	
	725.87	793.08	832.65	869.41	1011.42	1029.96	
	1075.08	1225.58	1318.28	1409.85	1417.40	1470.11	

	1481.56	1492.95	1606.02	1809.90	1913.18	3085.07	
	3159.34	3203.01	3418.95	3824.12	3859.28	3968.14	
RC4a'	18.69	26.43	37.63	57.68	77.02	94.02	-585.85951
	119.42	135.33	159.66	166.40	173.72	188.17	
	241.74	289.69	295.44	389.91	431.94	549.50	
	575.11	649.81	654.23	664.74	686.97	724.01	
	819.65	972.18	1020.44	1177.45	1399.29	1418.36	
	1444.61	1632.63	1653.35	1813.72	2232.13	3213.99	
	3326.47	3583.21	3691.23	3864.69	3951.69	3959.76	
TS4a'	-304.84	36.11	48.98	59.43	105.72	137.44	-585.838692
	171.18	277.54	330.90	411.46	449.46	513.87	
	565.17	602.99	645.92	695.43	717.67	747.13	
	770.01	809.20	831.67	867.66	924.78	1016.39	
	1118.87	1144.96	1252.53	1331.31	1412.00	1444.12	
	1470.63	1588.41	1600.94	1616.98	1729.56	1767.74	
	1884.54	3215.18	3280.85	3322.37	3798.92	3904.94	
PC4a'	41.43	44.34	89.09	93.73	115.10	149.24	-585.876523
	179.54	187.22	202.20	249.21	340.24	374.63	
	457.69	469.44	545.74	628.48	665.22	682.11	
	728.50	733.31	810.38	831.21	909.09	961.37	
	977.56	1051.61	1213.82	1263.69	1401.22	1432.89	
	1438.67	1488.20	1631.56	1785.96	1789.73	3123.84	
	3206.11	3307.64	3743.32	3826.44	3861.47	3950.05	
RC4b'	8.68	24.98	38.29	72.41	91.85	106.03	-585.86926
	117.42	142.18	174.47	184.23	221.92	262.60	
	298.90	317.44	369.11	433.98	474.71	563.39	
	580.17	641.06	685.16	735.22	821.23	828.81	
	982.61	1040.40	1063.34	1180.24	1404.44	1418.76	
	1563.95	1615.06	1663.36	1806.72	2253.83	2723.48	
	3215.94	3325.04	3645.58	3816.68	3908.20	3949.29	
TS4b'	-596.10	30.39	45.34	57.61	76.68	89.49	-585.831357
	135.44	318.42	349.29	378.05	430.36	459.11	
	524.12	566.75	600.63	637.59	694.04	709.70	
	736.20	786.05	798.54	858.20	934.99	1024.27	
	1116.43	1118.89	1150.37	1208.52	1391.12	1446.12	
	1526.14	1604.58	1674.95	1679.37	1735.72	1865.29	
	2283.18	2681.01	3220.97	3333.98	3828.82	3918.47	
PC4b'	24.71	43.67	52.21	84.67	123.94	149.80	-585.877697
	175.02	210.15	225.23	270.34	345.85	432.96	
	455.36	580.02	603.69	621.71	661.21	667.13	
	724.87	730.77	812.10	825.13	905.85	972.76	

	985.76	1045.86	1243.50	1348.96	1390.62	1419.98	
	1445.46	1492.78	1600.71	1802.40	1812.17	3140.59	
	3218.35	3323.93	3725.80	3759.79	3814.65	3956.66	
RC5a	10.75	26.71	41.27	43.13	54.67	75.63	
	98.11	109.20	138.19	142.67	160.75	178.00	
	206.41	242.83	247.23	260.28	291.47	327.74	
	394.46	399.51	444.39	495.11	547.71	574.33	
	662.25	682.42	729.88	789.69	826.56	920.17	-662.256607
	968.24	981.80	1041.45	1183.78	1406.05	1415.71	
	1561.77	1615.25	1627.72	1660.79	1810.45	2248.46	
	2922.26	3204.35	3309.96	3412.75	3626.55	3832.73	
	3920.15	3950.51	3965.68				
TS5a	-142.72	13.71	21.83	42.05	58.55	84.65	
	88.35	137.24	170.85	187.16	192.59	209.75	
	243.43	259.27	274.66	306.29	420.08	439.38	
	511.68	544.94	590.43	614.39	654.15	665.96	
	682.43	734.77	820.61	821.57	860.70	931.05	-662.237116
	1033.43	1046.42	1065.59	1167.60	1403.90	1448.10	
	1483.02	1610.84	1653.41	1691.41	1785.27	2029.11	
	2773.20	3151.68	3193.60	3305.92	3558.13	3739.82	
	3813.75	3951.14	3962.21				
PC5a	18.05	27.48	41.02	58.17	78.07	89.14	
	104.27	133.00	155.65	166.30	187.08	223.27	
	236.38	285.68	297.63	358.20	463.59	490.58	
	600.38	627.86	648.25	659.02	724.35	821.99	
	860.60	875.98	922.45	1018.08	1032.88	1061.25	-662.313082
	1081.12	1327.59	1413.67	1425.78	1462.36	1479.70	
	1486.47	1512.33	1611.11	1653.42	1803.86	1844.82	
	2877.91	3081.87	3152.70	3203.96	3377.94	3506.88	
	3734.55	3942.41	3962.11				
RC5b	12.77	19.60	27.01	46.72	55.52	66.50	
	104.45	121.99	123.25	146.64	154.52	163.28	
	182.42	205.49	221.85	229.97	266.35	309.40	
	349.85	373.65	428.79	449.17	480.85	599.10	
	625.26	664.43	688.65	699.58	731.26	828.20	-662.248283
	956.80	999.43	1048.99	1168.42	1396.08	1418.49	
	1543.80	1604.84	1628.48	1653.32	1808.50	2255.07	
	2976.92	3193.41	3308.82	3650.04	3793.01	3865.22	
	3906.02	3941.80	3977.04				
TS5b	-654.40	28.51	43.83	62.41	77.98	91.42	
	124.09	171.54	180.14	200.48	251.45	291.55	-662.220658

	362.08	418.06	426.63	447.59	482.20	539.48	
	555.38	597.47	645.00	699.59	710.01	753.62	
	811.65	824.21	870.13	874.76	1075.12	1092.18	
	1114.22	1138.34	1170.77	1269.86	1335.32	1459.35	
	1470.16	1590.43	1648.24	1660.95	1679.04	1814.76	
	1841.61	2044.79	2860.79	3030.84	3162.67	3256.00	
	3780.76	3895.41	3955.16				
PC5b	22.31	37.28	47.27	69.01	83.65	90.16	
	101.92	110.31	147.13	153.45	160.20	185.21	
	195.34	225.68	241.50	248.69	345.83	365.24	
	464.31	550.39	594.51	648.60	660.57	724.26	
	810.67	829.93	889.53	900.39	1022.11	1034.26	-662.302331
	1075.47	1292.27	1413.10	1434.97	1456.29	1474.42	
	1476.98	1490.51	1594.37	1617.80	1804.33	1865.85	
	3077.17	3145.78	3201.70	3344.22	3415.45	3790.59	
	3867.59	3963.36	3967.18				
RC6a	23.67	45.36	61.21	65.92	80.96	87.95	
	96.97	116.13	125.93	151.05	180.20	195.17	
	203.11	216.02	256.98	267.77	325.81	340.33	
	364.91	430.35	446.54	528.03	537.27	580.44	
	624.52	703.42	734.49	755.96	843.42	932.26	-662.256836
	982.21	1078.49	1101.25	1180.17	1405.41	1411.64	
	1584.81	1618.68	1641.84	1677.88	1805.42	2256.57	
	2481.17	3219.42	3328.54	3445.10	3672.65	3735.18	
	3923.34	3949.46	3953.62				
TS6a	-408.71	27.61	42.94	55.74	65.23	105.38	
	127.96	145.25	190.90	214.76	244.29	252.14	
	319.18	384.60	432.64	453.16	499.06	523.13	
	597.51	653.56	667.93	721.68	724.84	819.25	
	829.44	833.38	841.33	851.51	916.10	1013.89	-662.236245
	1129.41	1243.48	1354.83	1384.25	1435.81	1472.83	
	1514.31	1559.31	1598.33	1644.03	1669.72	1706.82	
	1824.42	2025.73	3033.58	3213.36	3319.58	3375.17	
	3742.52	3917.04	3960.04				
PC6a	28.52	38.16	45.26	86.75	91.40	116.03	
	126.75	166.68	179.70	189.21	204.18	219.00	
	231.06	276.65	307.39	394.10	443.16	465.66	
	488.82	588.69	624.45	672.59	692.94	700.75	-662.265533
	731.83	804.45	824.86	831.92	936.18	959.19	
	982.55	1056.01	1240.33	1341.23	1415.50	1441.16	
	1460.42	1501.66	1601.78	1640.53	1784.33	1786.35	

	3016.66	3205.14	3306.92	3506.54	3671.25	3833.62	
	3839.01	3943.81	3970.90				
RC6b	30.79	37.84	57.87	77.20	84.43	96.32	
	109.09	113.34	137.57	145.10	155.11	222.08	
	231.56	235.63	251.49	272.63	299.61	316.04	
	353.15	418.96	439.81	484.10	571.53	580.04	
	635.41	666.53	695.51	731.25	834.85	901.72	-662.255248
	979.45	1026.07	1054.19	1178.78	1400.80	1429.26	
	1578.89	1606.72	1652.36	1667.31	1805.12	2242.25	
	2699.37	3209.58	3320.32	3547.79	3682.42	3850.11	
	3904.80	3925.35	3949.99				
TS6b	-559.87	25.51	40.04	61.55	71.17	97.15	
	123.46	156.80	198.66	223.29	268.72	295.67	
	392.04	442.43	473.17	495.49	523.26	539.94	
	630.16	656.90	675.91	695.41	726.37	731.44	
	798.34	813.98	817.90	862.20	1027.07	1104.79	-662.229095
	1119.52	1191.27	1197.46	1311.12	1436.33	1446.35	
	1559.00	1580.68	1618.47	1681.81	1704.03	1749.73	
	1808.00	2356.01	2889.53	3026.16	3217.08	3324.63	
	3711.52	3905.23	3957.91				
PC6b	34.61	60.60	75.09	88.75	100.99	113.72	
	118.80	134.71	146.39	172.82	180.68	194.83	
	235.60	254.37	410.36	418.64	435.95	471.38	
	517.22	580.80	644.58	656.44	692.25	718.89	
	734.17	797.48	822.08	825.02	881.11	959.21	-662.263811
	980.94	1021.85	1282.25	1368.63	1434.92	1453.47	
	1461.06	1477.18	1627.17	1630.74	1779.74	1802.16	
	3206.82	3311.31	3336.52	3404.00	3585.40	3830.16	
	3838.30	3920.56	3935.08				
TS7	-2125.30	413.76	497.40	564.46	625.84	754.99	
	802.08	1016.97	1071.49	1151.75	1232.28	1422.41	-228.742878
	1547.07	1620.39	2022.10	3151.92	3249.22	3824.61	
RC8	47.59	67.07	86.36	148.98	156.54	195.80	
	396.82	468.31	525.91	571.09	655.33	687.30	
	720.06	731.25	751.54	815.72	841.26	982.94	
	998.83	1029.31	1239.46	1255.31	1403.53	1436.64	-509.490522
	1463.06	1478.57	1741.85	1802.76	3139.66	3202.37	
	3308.69	3789.10	3863.35				
TS8	-1138.39	68.74	99.54	126.16	190.11	259.29	
	418.72	490.53	584.17	591.32	694.30	729.57	-509.479690
	749.37	766.46	843.61	925.71	979.92	1003.91	

	1054.37	1099.06	1248.64	1278.90	1376.44	1410.90	
	1458.73	1557.59	1580.27	1706.28	1720.05	2885.28	
	3162.12	3268.46	3818.73				
PC8	27.08	36.99	75.62	107.20	150.43	157.89	-509.534963
	181.93	442.39	545.30	616.20	662.98	683.60	
	725.91	814.91	845.59	904.61	1025.94	1030.16	
	1075.64	1253.83	1373.27	1420.91	1434.33	1474.08	
	1484.31	1488.64	1802.71	1821.51	3091.19	3168.16	
	3201.60	3228.25	3820.75				
RC9	70.67	138.10	196.07	213.13	268.41	356.10	-305.205163
	373.13	469.66	563.33	642.39	681.67	734.33	
	773.07	974.71	986.00	1240.82	1309.31	1432.17	
	1467.64	1594.79	1766.69	3211.22	3313.78	3686.33	
	3841.60	3881.86	3966.56				
TS9	-1707.87	132.49	412.45	482.28	507.38	565.55	-305.169577
	582.12	596.74	696.39	746.65	771.70	867.15	
	979.89	1054.80	1182.85	1240.83	1359.52	1421.78	
	1479.23	1519.91	1601.54	1735.33	1960.68	3152.78	
	3257.19	3834.19	3906.03				
PC9	41.85	58.73	88.55	120.53	181.19	370.06	-305.246643
	443.94	522.58	545.04	613.16	667.50	893.09	
	1029.12	1079.94	1245.16	1363.84	1432.46	1478.26	
	1485.25	1615.26	1851.80	3085.18	3157.56	3198.69	
	3782.52	3830.06	3968.28				
RCS1	25.49	47.97	76.10	108.82	160.71	175.63	-418.415823
	178.92	203.81	215.15	331.88	431.77	440.92	
	574.37	605.32	648.41	688.10	860.76	1006.12	
	1088.70	1168.75	1237.32	1368.74	1399.79	1429.22	
	1621.28	1835.61	2273.25	3104.61	3194.94	3307.02	
	3459.10	3775.39	3963.25				
TSS1	-610.85	67.26	90.63	178.64	261.58	318.86	-418.390846
	410.87	485.21	509.51	583.36	608.61	662.06	
	710.97	768.74	942.83	1001.31	1083.44	1093.31	
	1251.16	1269.48	1299.07	1390.92	1436.03	1455.89	
	1519.40	1662.63	1770.16	2021.12	2148.35	3113.84	
	3167.96	3262.05	3848.18				
PCS1	25.33	30.75	93.38	97.37	151.65	167.63	-418.466132
	185.00	436.17	532.35	603.30	644.85	678.72	
	850.01	873.17	1012.01	1077.61	1085.95	1210.35	
	1246.41	1330.49	1369.45	1419.83	1430.44	1479.37	
	1482.41	1853.67	1905.41	3080.87	3096.84	3152.08	

Table S5. Equilibrium constant (K_{eq} , molecules/cm³) of all relevant complexes, rate constants (k , cm³/molecules·s) for the main reaction pathway and the rate ratio at the temperature range 210-298 K.

reaction	210 K	230 K	250 K	270 K	290 K	298 K
$K_{\text{eq}1}(\text{CH}_2=\text{C}=\text{O}\cdots\text{H}_2\text{O})^{\text{A}}$	1.47×10^{-23}	1.14×10^{-23}	9.34×10^{-24}	8.02×10^{-24}	7.12×10^{-24}	6.85×10^{-24}
$K_{\text{eq}2}(\text{HNO}_3\cdots\text{H}_2\text{O})^{\text{B}}$	5.76×10^{-18}	1.03×10^{-18}	2.45×10^{-19}	7.30×10^{-20}	2.59×10^{-20}	1.78×10^{-20}
$K_{\text{eq}3}(\text{H}_2\text{O}\cdots\text{H}_2\text{O})^{\text{C}}$	2.27×10^{-21}	1.23×10^{-21}	7.39×10^{-22}	4.86×10^{-22}	3.41×10^{-22}	3.01×10^{-22}
$K_{\text{eq}4}(\text{2H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O})^{\text{D}}$	3.64×10^{-23}	1.59×10^{-23}	8.06×10^{-24}	4.57×10^{-24}	2.83×10^{-24}	2.39×10^{-24}
$K_{\text{eq}5}(\text{3H}_2\text{O})^{\text{E}}$	7.59×10^{-19}	1.39×10^{-19}	3.33×10^{-20}	9.90×10^{-21}	3.49×10^{-21}	2.40×10^{-21}
$K_{\text{eq}6}(\text{3H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O})^{\text{F}}$	1.34×10^{-23}	8.10×10^{-24}	5.41×10^{-24}	3.90×10^{-24}	2.98×10^{-24}	2.72×10^{-24}
$K_{\text{eq}7}(\text{3H}_2\text{O}\cdots\text{HNO}_3)^{\text{G}}$	2.26×10^{-14}	1.71×10^{-15}	1.97×10^{-16}	3.16×10^{-17}	6.57×10^{-18}	3.73×10^{-18}
k_1^{H}	2.82×10^{-44}	1.46×10^{-43}	8.48×10^{-43}	5.48×10^{-42}	3.93×10^{-41}	8.87×10^{-41}
k_2^{I}	2.04×10^{-46}	3.87×10^{-45}	8.03×10^{-44}	1.78×10^{-42}	4.08×10^{-41}	1.41×10^{-40}
k_{31}^{J}	3.18×10^{-21}	8.4×10^{-21}	1.92×10^{-20}	3.91×10^{-20}	7.26×10^{-20}	9.10×10^{-20}
k_{32}^{K}	1.33×10^{-27}	1.39×10^{-26}	1.01×10^{-25}	5.49×10^{-25}	2.38×10^{-24}	4.06×10^{-24}
k_4^{L}	1.06×10^{-21}	2.28×10^{-21}	4.33×10^{-21}	7.41×10^{-21}	1.18×10^{-20}	1.39×10^{-20}
k_{51}^{M}	3.65×10^{-18}	4.90×10^{-18}	6.27×10^{-18}	7.73×10^{-18}	9.26×10^{-18}	9.89×10^{-18}
k_{52}^{N}	2.16×10^{-27}	2.33×10^{-26}	1.73×10^{-25}	9.56×10^{-25}	4.21×10^{-24}	7.21×10^{-24}
k_{61}^{O}	8.77×10^{-19}	8.64×10^{-19}	8.43×10^{-19}	8.17×10^{-19}	7.88×10^{-19}	7.75×10^{-19}
k_{62}^{P}	5.19×10^{-28}	4.10×10^{-27}	2.32×10^{-26}	1.01×10^{-25}	3.58×10^{-25}	5.65×10^{-25}
k_{OH}^{Q}	7.03×10^{-11}	5.69×10^{-11}	4.77×10^{-11}	4.10×10^{-11}	3.60×10^{-11}	3.43×10^{-11}

^AThe equilibrium constant of the reaction: $\text{CH}_2=\text{C}=\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{CH}_2=\text{C}=\text{O}\cdots\text{H}_2\text{O}$.

^BThe equilibrium constant of the reaction: $\text{HNO}_3 + \text{H}_2\text{O} \rightleftharpoons \text{HNO}_3\cdots\text{H}_2\text{O}$.

^CThe equilibrium constant of the reaction: $\text{H}_2\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O}\cdots\text{H}_2\text{O}$.

^DThe equilibrium constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O} + \text{CH}_2=\text{C}=\text{O} \rightleftharpoons \text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O}$.

^EThe equilibrium constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O} + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}$.

^FThe equilibrium constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O} + \text{CH}_2=\text{C}=\text{O} \rightleftharpoons \text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O}$.

^GThe equilibrium constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O} + \text{HNO}_3 \rightleftharpoons \text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{HNO}_3$.

^HThe rate constant of the reaction: $\text{CH}_2=\text{C}=\text{O} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH}$.

^IThe rate constant of the reaction: $\text{CH}_2=\text{C}=\text{O} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{C}_2(\text{OH})_2$.

^JThe rate constant of the reaction: $\text{CH}_2=\text{C}=\text{O}\cdots\text{H}_2\text{O} + \text{HNO}_3 \rightarrow \text{CH}_3\text{COOH} + \text{HNO}_3$.

^KThe rate constant of the reaction: $\text{CH}_2=\text{C}=\text{O} + \text{HNO}_3\cdots\text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{HNO}_3$.

^LThe rate constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O} + \text{HNO}_3 \rightarrow \text{CH}_3\text{COOH} + \text{H}_2\text{O} + \text{HNO}_3$.

^MThe rate constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O} + \text{HNO}_3 \rightarrow \text{CH}_3\text{COOH} + 2\text{H}_2\text{O} + \text{HNO}_3$.

^NThe rate constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{HNO}_3 + \text{CH}_2=\text{C}=\text{O} \rightarrow \text{CH}_3\text{COOH} + 2\text{H}_2\text{O} + \text{HNO}_3$.

^OThe rate constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{CH}_2=\text{C}=\text{O} + \text{HNO}_3 \rightarrow \text{H}_2\text{C}_2(\text{OH})_2 + 2\text{H}_2\text{O} + \text{HNO}_3$.

^PThe rate constant of the reaction: $\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{H}_2\text{O}\cdots\text{HNO}_3 + \text{CH}_2=\text{C}=\text{O} \rightarrow \text{H}_2\text{C}_2(\text{OH})_2 + 2\text{H}_2\text{O} + \text{HNO}_3$.

^QThe rate constant of the $\text{CH}_2=\text{C}=\text{O} + \text{OH}$ reaction.

Table S6. tunneling coefficient (κ) of the reaction $\text{H}_2\text{C}_2(\text{OH})_2$ transfer to CH_3COOH base on Eckart potential, and total rate constant (k , s^{-1}) for the individual reaction pathway of the free reactants and complexes at the temperature range 210-298 K.

reaction	210 K	230 K	250 K	270 K	290 K	298 K
k_7^A	8.51×10^{-17}	3.19×10^{-16}	1.27×10^{-15}	5.31×10^{-15}	2.36×10^{-14}	4.35×10^{-14}
κ_7^B	1.56×10^{18}	4.82×10^{14}	7.12×10^{11}	3.59×10^9	4.84×10^7	1.09×10^7
k_8^C	2.05×10^{-10}	5.43×10^{-11}	1.86×10^{-11}	7.69×10^{-12}	3.69×10^{-12}	2.84×10^{-12}
κ_8^D	1.24×10^{01}	8.20	5.98	4.69	3.88	3.64
k_7^E	2.32×10^{-24}	4.13×10^{-24}	7.68×10^{-24}	1.48×10^{-23}	2.94×10^{-23}	3.89×10^{-23}
κ_9^F	6.27×10^{04}	6.74×10^{03}	1.19×10^{03}	3.11×10^{02}	1.10×10^{02}	7.82×10^{01}

^AThe rate constant of the reaction: $\text{H}_2\text{C}_2(\text{OH})_2 \rightarrow \text{CH}_3\text{COOH}$.

^BThe tunneling coefficient of the reaction: $\text{H}_2\text{C}_2(\text{OH})_2 \rightarrow \text{CH}_3\text{COOH}$.

^CThe rate constant of the reaction: $\text{H}_2\text{C}_2(\text{OH})_2 + \text{HNO}_3 \rightarrow \text{CH}_3\text{COOH} + \text{HNO}_3$.

^DThe tunneling coefficient of the reaction: $\text{H}_2\text{C}_2(\text{OH})_2 + \text{HNO}_3 \rightarrow \text{CH}_3\text{COOH} + \text{HNO}_3$.

^EThe rate constant of the reaction: $\text{H}_2\text{C}_2(\text{OH})_2 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{H}_2\text{O}$.

^FThe tunneling coefficient of the reaction: $\text{H}_2\text{C}_2(\text{OH})_2 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{H}_2\text{O}$.

Table S7. The unimolecular reaction rate constants (s^{-1}) for certain reaction pathway at the temperature range 210-298 K.

reaction	210 K	230 K	250 K	270 K	290 K	298 K
$k_2\text{-uni}^A$	8.85×10^{-08}	2.17×10^{-06}	3.10×10^{-05}	2.93×10^{-04}	2.00×10^{-03}	3.98×10^{-03}
$k_3\text{-uni}^B$	2.66×10^{-01}	2.40	1.46×10^{01}	7.15×10^{01}	2.71×10^{02}	4.38×10^{02}
$k_4\text{-uni}^C$	2.77×10^{-06}	5.48×10^{-05}	6.61×10^{-04}	5.42×10^{-03}	3.28×10^{-02}	6.29×10^{-02}
$k_5\text{-uni}^D$	6.16×10^{-03}	8.64×10^{-02}	7.84×10^{-01}	5.08	2.52×10^{01}	4.50×10^{01}
$k_6\text{-uni}^E$	1.81×10^{-02}	1.99×10^{-01}	1.45	7.75	3.23×10^{01}	5.40×10^{01}

^AThe rate constant of the reaction: $\text{RC}_2 \rightarrow \text{H}_2\text{C}_2(\text{OH})_2$.

^BThe rate constant of the reaction: $\text{RC}_3 \rightarrow \text{CH}_3\text{COOH} + \text{HNO}_3$.

^CThe rate constant of the reaction: $\text{RC}_4 \rightarrow \text{CH}_3\text{COOH} + \text{H}_2\text{O} + \text{HNO}_3$.

^DThe rate constant of the reaction: $\text{RC}_5 \rightarrow \text{CH}_3\text{COOH} + 2\text{H}_2\text{O} + \text{HNO}_3$.

^EThe rate constant of the reaction: $\text{RC}_6 \rightarrow \text{H}_2\text{C}_2(\text{OH})_2 + 2\text{H}_2\text{O} + \text{HNO}_3$.

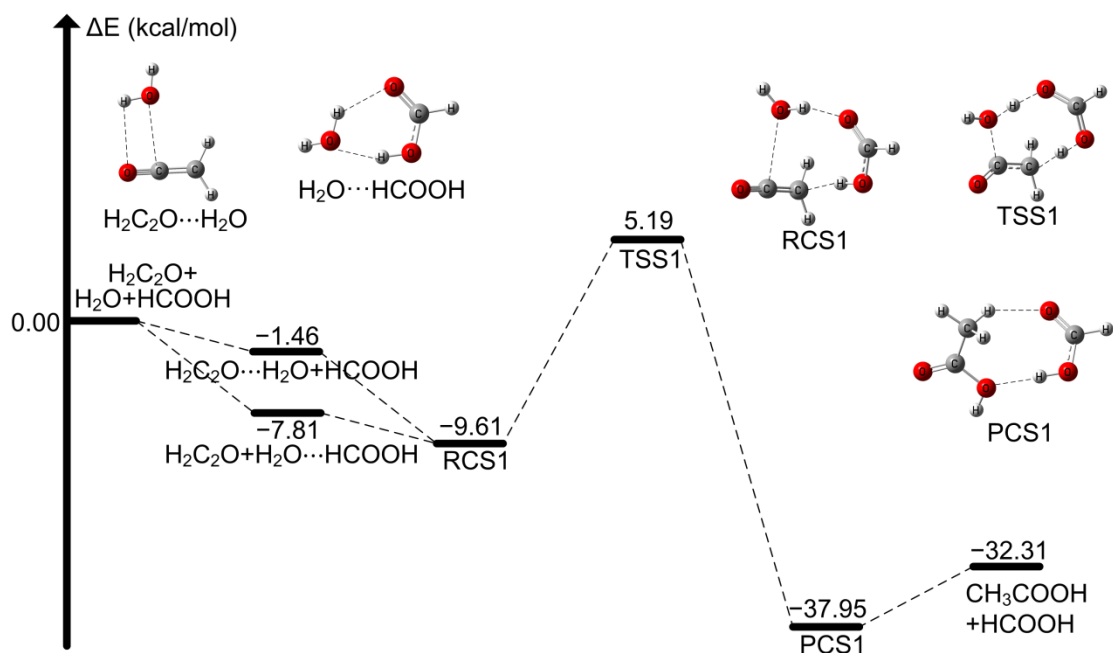


Figure S1 Optimized geometries and potential energy surface diagram for the directly forming of CH_3COOH through hydrolysis of ketene catalyzed by HCOOH . All the relative energies here corrected by zero-point energy were obtained at the CCSD(T)-F12a/cc-pVTZ-F12//M06-2X/6-311++G(d,p) level of theory (in kcal/mol).

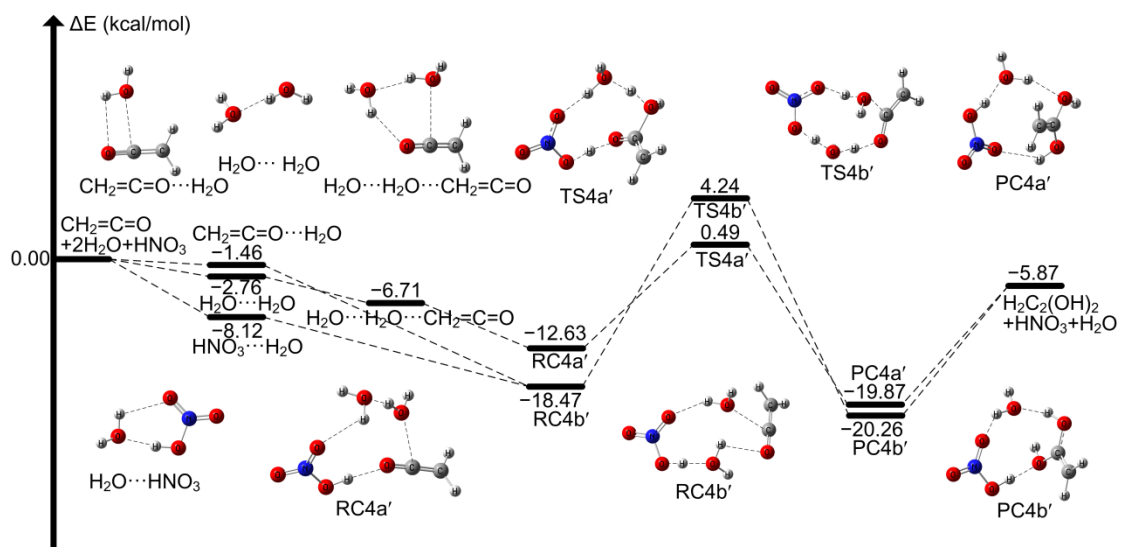


Figure S2. Potential energy surface diagram for the forming of 1,1-enediol through hydrolysis of ketene catalyzed by HNO_3 and one additional water molecule together. All the relative energies here corrected by zero-point energy were obtained at the CCSD(T)-F12a/VTZ-F12//M06-2X/6-311++G(d,p) level of theory (in kcal/mol).