Supporting information: A computational investigation of the decomposition of acetic acid in the H-SSZ-13 zeolite and its role in the initiation of the MTO process

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S1 Additional mechanisms:

Barriers for additional reaction pathways (Fig. S1) were calculated comprising hydration reactions of acetylketene and the formation of diketene.

Acetylketene (C3) can be protonated yielding D5 with a barrier of 180 kJ/mol. Three pathways for the hydration of D5 have been computed. D5 can react with the zeolite forming the surface ester of 3-oxobutanoic acid. For this reaction, an insignificant DFT free energy barrier of 3 kJ/mol relative to D5 was found. Including the ab initio corrections, the transition state becomes 1 kJ/mol lower in free energy than D5. We therefore conclude that the barrier D5-D7 is insignificant. D7 is 63 kJ/mol lower in free energy than D5. D7 then is hydrated, forming C5 with a barrier of 209 kJ/mol. Further reactions of C5 including the reaction to 3-oxobutanoic acid are discussed in the main article. D5 can also be hydrated directly to C5 with a barrier of 197 kJ/mol. Another hydration reaction (TS(D5-D8)) yields a 3-oxobutanoic acid that is protonated at its acidic OH group. The DFT energy of TS(D5-D8) is by 25 kJ/mol higher than that of D8. Taking thermodynamic contributions into account, the DFT free energy of TS(D5-D8) is by 5 kJ/mol lower than that of D8. The cluster model corrected free energy of TS(D5-D8) is by 10 kJ/mol lower that of D8. The subsequent deprotonation to 3-oxobutanoic acid has a barrier of 211 kJ/mol.

D5 can also react to a protonated diketene (D6). The DFT free energy of TS(D5-D6) is by 11 kJ/mol higher than that of D6. After adding the cluster model correction term, the free energy of TS(D5-D6) is by 16 kJ/mol lower than that of D6. D6 can be protonated yielding diketene with a barrier of 216 kJ/mol. Another pathway for the formation of diketene starts from two ketene molecules. These can couple to D1 with a barrier of 252 kJ/mol. D1 can directly react to diketene with a barrier of 208 kJ/mol. In the gas phase, a direct dimerization from C2 to D4 was computed with a higher barrier of 291 kJ/mol. D1 can also react with the zeolite to a surface ester with a barrier of 226 kJ/mol. Hydration of D2 yields an enol of 3-oxobutanoic acid with a barrier of 237 kJ/mol. The keto-enol tautomerization to D3 has a barrier of 173 kJ/mol. With a barrier of 272 kJ/mol D3 can be dehydrated to diketene.
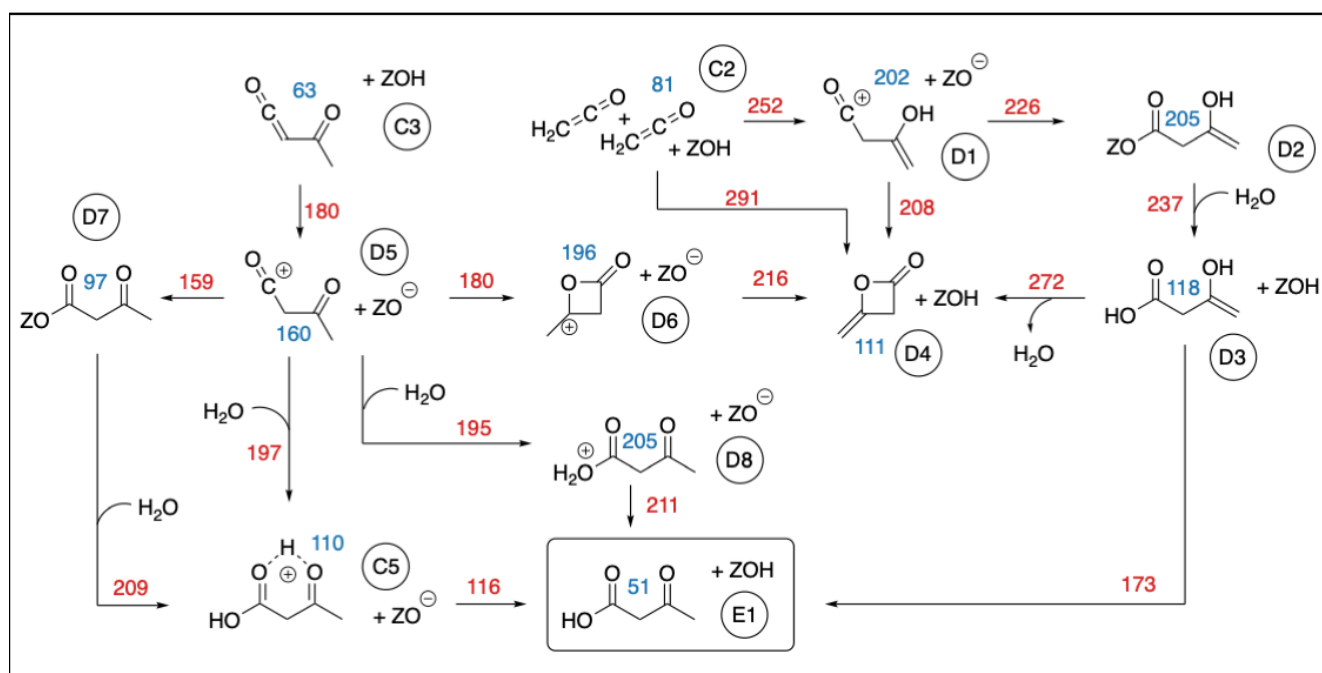

Figure S1: Additional reaction mechanisms for the hydration of acetylketene and for the formation of diketene. Gibbs free energies at 400 °C for transition states (red) and intermediates (blue) are given relative to the reference state A1 (gaseous acetic acid and the empty zeolite).

S2 Summarized values of Gibbs free energy profiles:

Here, the values for the Gibbs free energy profiles depicted in the main article and in Figure S1 are listed.

Table S1: Values for the states in the Gibbs free energy profiles depicted in the main article and Figure S1 in kJ/mol. DFT free energies ΔG_{PBE-D3}^{PBC}, cluster model corrected free energies ΔG, DFT enthalpies ΔH_{PBE-D3}^{PBC}, and cluster model corrected enthalpies ΔH at 400 °C are listed. If the free energy does not correspond to the adsorbed state depicted in the mechanisms, but to a gaseous state, this gaseous state is accordingly labeled in the table.

Fig. 5	state	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
A1	ZOH + 2x AcOH(g)	0	0	0	0
TS(A1-A2)_O3		142	153	35	46
A2_O3		57	50	44	37
TS(A2-A3)		102	99	80	77
A3		87	91	84	88
TS(A3-C1)		78	100	67	89
C1	ZOH + ketene(g) + H2O(g) + AcOH(g)	43	41	142	140
C2		180	190	192	202
TS(C2-C3)		164	202	177	215
C3		72	63	166	157
TS(C3-C4)		143	147	144	147
C4		33	62	-117	-87
TS(C4-C5)		98	139	-60	-19
C5		78	110	-65	-33
TS(C5-E1)		96	116	-46	-26
E1		37	51	-108	-94
TS(A1-E1)		204	214	52	62
Fig. 6	**state**	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
A1	ZOH + 2x AcOH(g)	0	0	0	0
TS(A1-B1)		174	183	58	67
B1	ZOH + AcOH(g) + 1,1-dihydroxyethene(g)	121	118	116	114
TS(B1-B2)		187	244	-75	-19
B2	ZOH + 3,3-dihydroxybutanoic acid(g)	162	143	35	15
TS(B2-B3)		189	217	-80	-52
B3		179	208	-78	-49
TS(B3-C5)		198	242	-55	-11
C5		78	110	-65	-33
TS(C5-E1)		96	116	-46	-26
B4	ZOAc + 1,1-dihydroxyethene(g)	170	158	151	139
TS(B4-E1)		249	259	111	121
E1		37	51	-108	-94
Fig. 7	**state**	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
A1	ZOH + 2x AcOH(g)	0	0	0	0
TS(A1-A2)_O3		137	149	22	35
A2_O3		49	40	35	25
TS(A2-C3)		187	197	181	192
C3		72	63	166	157
TS(C3-C4)		143	147	144	147

	state	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
C4		33	62	-117	-87
TS(C4-C5)		98	139	-60	-19
C5		78	110	-65	-33
TS(C5-E1)		96	116	-46	-26
E1		37	51	-108	-94
Fig. 8	**state**	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
E1		0	0	0	0
A1	ZOH + 2x AcOH(g)	-37	-51	108	94
TS(E1-E2)		72	103	82	113
E2	ZOH + propene-2-ol(g) + H2O(g) + CO2(g)	-39	-66	188	161
TS(E2-E3)		15	6	121	112
E3	ZOH + acetone(g) + H2O(g) + CO2(g)	-95	-118	134	111
Fig. 10	**state**	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
E3	ZOH + 2x acetone(g)	0	0	0	0
E4	ZOH + acetone(g) + propen-2-ol(g)	57	53	54	50
TS(E4-E5)		107	169	-145	-83
E5		78	119	-170	-130
TS(E5-E6)		132	181	-128	-79
E6	ZOH + (Z)-4-methylpent-2-ene-2,4-diol(g)	143	127	12	-4
TS(E6-E7)		164	183	-96	-77
E7		123	154	-148	-117
TS(E7-E8)		142	185	-112	-69
E8		-19	15	-160	-126
TS(E8-E9)		103	153	-43	7
E9		77	144	-55	12
TS(E9-E10)		110	120	-5	6
E9	ZOAc + isobutene(g) + H2O(g)	43	28	22	7
Fig. S1b	**state**	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
A1	ZOH + 2x AcOH(g)	0	0	0	0
C3	ZOH + Acetylketene(g) + 2x H2O(g)	72	63	166	157
TS(C3-D5)		151	180	119	148
D5		146	160	124	138
TS(D5-D7)		148	159	118	128
D7		114	97	79	62
TS(D7-C5)		188	209	72	93
C5		78	110	-65	-33
TS(C5-E1)		96	116	-46	-26
E1		37	51	-108	-94
TS(D5-C5)		188	197	68	78
TS(D5-D8)		170	195	66	92
D8		175	205	44	75
TS(D8-E1)		182	211	87	116
Fig. S1c	**state**	ΔG_{PBE-D3}^{PBC}	ΔG	ΔH_{PBE-D3}^{PBC}	ΔH
A1	ZOH + 2x AcOH(g)	0	0	0	0

C3	ZOH + Acetylketene(g) + 2x H2O(g)	72	63	166	157
TS(C3-D5)		151	180	119	148
D5		146	160	124	138
TS(D5-D6)		183	180	163	161
D6		172	196	143	167
TS(D6-D4)		181	216	134	169
D4		106	111	79	85
C2	ZOH + 2x Ketene(g) + 2x H2O(g)	86	81	285	280
TS(C2-D1)		215	252	210	247
D1		192	202	167	177
TS(D1-D2)		228	226	177	175
D2		215	205	181	171
TS(D2-D3)		231	237	108	114
D3		108	118	-34	-24
TS(D3-D4)		249	272	103	126
TS(D3-E1)		131	173	-14	29
TS(D1-D4)		204	208	165	170

S3 Batch reactor simulation:

During the batch reactor simulation, turnovers are calculated for every elementary reaction for each time step. The total turnovers for a reaction can be obtained by summing over all time steps. The formation of 3-oxobutanoic acid was simulated by several pathways. The relevance of these pathways can be evaluated by comparing the total turnovers for significant elementary reactions. In Table S2, the conversions through these reactions are shown.

Table S2: Total conversion through reaction steps used as benchmark reactions for the different pathways for the formation of 3-oxobutanoic acid.

Reaction	Pressure (bar)	Percentage (%)
A2-C3	0.44	73.2
C2-C3	0.15	25.8
C2-D4	0.00	0.0
C2-D3	0.00	0.0
A1-E1	0.01	0.9
B1-B2	0.00	0.0
B4-E1	0.00	0.0

For the batch reactor simulations, some barriers were modified to achieve a more efficient performance. Some pathways comprising more than one elementary reaction steps were truncated to one elementary reaction taking the highest barrier of the whole pathway. Some low energy barriers regarding the reaction between surface acetate (A2) and ketene (C1) were shifted to a higher value of 80 kJ/mol. As a reference for a barrier, the previous state (adsorbed or gaseous precursor) lowest in free energy was taken. Only for DME, MeOH and H2O adsorption free energy barriers were considered explicitly.

Barriers of the MTO initiation from methanol to surface acetate and further initiation steps via carbonylation as well as methylation and cracking reactions of the hydrocarbon pool were taken from previous work [ACS Catal. 2017, 7, 11, 7987–7994; Catal. Sci. Technol., 2018, 8, 4420-4429; J. Am. Chem. Soc. 2019, 141, 14, 5908–5915]. The reaction barrier from A2 to C1 was already computed previously, but the corresponding barriers for this reaction computed in this study were taken. All barriers are listed in Table S3. The conversion of acetic acid was modeled with the reactions number 105-144. The MTO decarbonylation mechanism was modeled with reactions 1-104, 108 and the decarboxylation mechanism was modeled with the reactions 1-9, 21-144.

Table S3: Gibbs free energy barriers in kJ/mol for elementary reaction steps used for the batch reactor model. Reactions 1-41 were taken from [ACS Catal. 2017, 7, 11, 7987–7994], reactions 42-104 were taken from [Catal. Sci. Technol., 2018, 8, 4420-4429], and reactions 105-140 were computed in this work. Some Carbon species from previous work were renamed from CX to CX-species (X = number) to avoid confusion to species labeled C from our work.

Number	Reaction	Forward barrier	Backward barrier
1	ZOH*MeOH > ZOMe + H2O	169	177
2	MeOH + ZOMe > ZOH*DME	151	160
3	ZOH*DME > ZOCOMe +	220	153
4	MF + ZOH > ZOH*MeOH + CO	135	178
5	ZOCOMe + MeOH > DMM + ZOH	119	121
6	DMM + ZOH > hacetal + ZOMe	145	137
7	hacetal + ZOH > MF + + ZOH	181	249
8	CO + ZOMe > A2_O1_pos1	190	177
9	A2_O1_pos1 + MeOH > MA + ZOH	97	150
10	Ketene + ZOMe > ZO2CEt	159	203
11	ZO2CEt + MeOH > MeO2CEt + ZOH	81	134
12	ZO2CEt > Mketene + ZOH	80	82
13	Mketene + ZOMe > ZO2CiPr	139	192
14	ZO2CiPr + MeOH > MeO2CiPr + ZOH	83	132
15	ZO2CiPr > ZOH + CO + C3-species	130	215
16	ZO2CEt > ZOH + CO + C2-species	172	239
17	ZO2CiPr > Dketene + ZOH	80	82
18	Dketene + ZOMe > ZO2CtBu	136	117

19	ZO2CtBu + MeOH > MeO2CtBu + ZOH	83	203
20	ZO2CtBu > ZOH + CO + C4b-species	10	179
21	ZOH*MeOH > ZOH + + FA	226	206
22	FA + ZOMe > ZOCOMe	173	137
23	ZOH + MeOH > ZOH*MeOH	82	80
24	ZOH + DME > ZOH*DME	80	81
25	ZOH + H2O > ZOH*H2O	109	80
26	ZOMe + MeOH > ZOH + CH4 + FA	237	345
27	ZOMe + DMM > ZOMe + CH4 + MF	205	394
28	ZOMe + hacetal > ZOH + CH4 + MF	215	412
29	ZOMe + DME > ZOCOMe + CH4	232	296
30	ZOH*DME + DME > ZOCOMe + CH4 + MeOH	245	299
31	ZOH*MeOH + DME > ZOCOMe + CH4 + H2O	260	332
32	ZOH*DME + DMM > ZOMe + CH4 + MF + MeOH	235	414
33	ZOH*MeOH + DMM > ZOMe + CH4 + MF + H2O	255	452
34	ZOH*DME + hacetal > ZOH*MeOH + CH4 + MF	208	394
35	ZOH*MeOH + hacetal > ZOH*H2O + CH4 + MF	248	423
36	ZOH*MeOH + DME > ZOH*MeOH + CH4 + FA	228	328
37	ZOH*MeOH + MeOH > ZOH*H2O + CH4 + FA	275	361
38	ZOH*MeOH + MeOH > ZOH*DME + H2O	192	210
39	FA + ZOH > ZOH + CO +	251	322
40	FA + ZOH*DME > s_ch4-fa + ZOH	274	456
41	DME + ZOCOMe > s_ch4-fa + ZOH	244	456
42	C4b-species + ZOMe > C5a-species + ZOH	147	206
43	C2-species + ZOMe > C3-species + ZOH	176	250
44	C3-species + ZOMe > C4a-species + ZOH	155	218
45	C4a-species + ZOMe > C5a-species + ZOH	154	218
46	C5a-species + ZOMe > C6a-species + ZOH	132	196
47	C6a-species + ZOMe > C7a-species + ZOH	146	188
48	C2-species + ZOH*MeOH > C3-species + ZOH*H2O	208	260
49	C6a-species + ZOH*MeOH > C7b-species + ZOH*H2O	140	151
50	C7b-species + ZOH*MeOH > C8b-species + ZOH*H2O	156	193
51	C3-species + ZOH*MeOH > C4a-species + ZOH*H2O	195	236
52	C4a-species + ZOH*MeOH > C5a-species + ZOH*H2O	178	221
53	C5a-species + ZOH*MeOH > C6a-species + ZOH*H2O	157	199
54	C2-species + ZOH*DME > C3-species + ZOH*MeOH	216	276
55	C3-species + ZOH*DME > C4a-species + ZOH*MeOH	208	258
56	C4a-species + ZOH*DME > C5a-species + ZOH*MeOH	195	247
57	C5a-species + ZOH*DME > C6a-species + ZOH*MeOH	165	215
58	C6a-species + ZOH*DME > C7b-species + ZOH*MeOH	173	192
59	C7b-species + ZOH*DME > C8b-species + ZOH*MeOH	165	210
60	C4a-species + ZOH*MeOH > C5b-species + ZOH*H2O	200	232
61	C4a-species + ZOH*DME > C5b-species + ZOH*MeOH	207	247
62	C5b-species + ZOH*MeOH > C6b-species + ZOH*H2O	187	216

63	C5b-species + ZOH*DME > C6b-species + ZOH*MeOH	208	245
64	C5b-species + ZOH*MeOH > C6c-species + ZOH*H2O	176	219
65	C5b-species + ZOH*DME > C6c-species + ZOH*MeOH	183	234
66	C6b-species + ZOH*MeOH > C7c-species + ZOH*H2O	194	227
67	C6b-species + ZOH*DME > C7c-species + ZOH*MeOH	194	235
68	C7c-species + ZOH*MeOH > C8c-species + ZOH*H2O	201	229
69	C6b-species + ZOH*MeOH > C7d-species + ZOH*H2O	173	213
70	C6b-species + ZOH*DME > C7d-species + ZOH*MeOH	190	238
71	C7c-species + ZOH*MeOH > C8d-species + ZOH*H2O	198	238
72	C7c-species + ZOH*DME > C8d-species + ZOH*MeOH	187	234
73	C7a-species + ZOMe > C8a-species + ZOH	115	169
74	C8a-species + ZOMe > C9a-species + ZOH	130	156
75	C5a-species + ZOH > C3-species + C2-species + ZOH	211	185
76	C8a-species + ZOH > C3-species + C5a-species + ZOH	168	183
77	C9a-species + ZOH > C4b-species + C5a-species + ZOH	87	145
78	C7a-species + ZOH > C3-species + C4a-species + ZOH	187	191
79	C7a-species + ZOH > C2-species + C5a-species + ZOH	179	174
80	C6a-species + ZOMe > C7b-species + ZOH	130	162
81	C7b-species + ZOMe > C8b-species + ZOH	110	168
82	C8b-species + ZOMe > C9a-species + ZOH	129	160
83	C8b-species + ZOH > C4b-species + C4a-species + ZOH	111	135
84	C4a-species + ZOMe > C5b-species + ZOH	171	223
85	C5b-species + ZOMe > C6c-species + ZOH	149	213
86	C5b-species + ZOMe > C6b-species + ZOH	159	209
87	C6b-species + ZOMe > C7c-species + ZOH	146	200
88	C7c-species + ZOMe > C8c-species + ZOH	174	222
89	C8c-species + ZOMe > C9b-species + ZOH	171	220
90	C6b-species + ZOMe > C7d-species + ZOH	141	202
91	C7c-species + ZOMe > C8d-species + ZOH	154	214
92	C8c-species + ZOMe > C9c-species + ZOH	142	208
93	C4a-species + ZOH > ZOH + C2-species + C2-species	246	210
94	C5b-species + ZOH > ZOH + C3-species + C2-species	238	224
95	C6c-species + ZOH > ZOH + C4b-species + C2-species	186	177
96	C6c-species + ZOH > ZOH + C3-species + C3-species	199	194
97	C6b-species + ZOH > ZOH + C4a-species + C2-species	211	209
98	C7d-species + ZOH > ZOH + C3-species + C4a-species	209	220
99	C7d-species + ZOH > ZOH + C5a-species + C2-species	168	169
100	C7c-species + ZOH > ZOH + C3-species + C4a-species	215	233
101	C8c-species + ZOH > ZOH + C5b-species + C3-species	200	221
102	C8d-species + ZOH > ZOH + C5b-species + C3-species	236	245
103	C9b-species + ZOH > ZOH + C6b-species + C3-species	201	224
104	C9c-species + ZOH > ZOH + C6b-species + C3-species	233	238
105	acetic_acid + ZOH > A2_O1_pos2 + H2O	161	126
106	acetic_acid + ZOH > A2_O1_pos1 + H2O	149	110

107	acetic_acid + ZOH > A2_O3 + H2O	153	103
108	A2_O1_pos2 > ZOH + Ketene	86	80
109	A2_O3 > ZOH + Ketene	80	89
110	acetic_acid + ZOH > Ethene-1,1-diol + ZOH	183	65
111	A2_O1_pos1 + Ketene > ZOH + Acetylketene	117	134
112	A2_O1_pos2 + Ketene > ZOH + Acetylketene	136	148
113	A2_O3 + Ketene > D5	119	50
114	ZOH + Acetylketene > D5	116	20
115	ZOH + Acetylketene > D7	95	62
116	D7 + H2O > C5	112	99
117	D5 + H2O > E1	36	144
118	D8 > E1	6	160
119	D5 + H2O > C5	37	88
120	C5 > E1	6	64
121	Acetylketene + H2O > 3-hydroxybut-2-enoic_acid	84	77
122	3-hydroxybut-2-enoic_acid + ZOH > C5	69	29
123	3-hydroxybut-2-enoic_acid + ZOH > E1	128	147
124	Ketene + Ketene + ZOH > Acetylketene + ZOH	121	139
125	Ketene + Ketene + ZOH > D4	171	141
126	Ketene + Ketene + ZOH > D2	171	47
127	D2 + H2O > D3	32	119
128	D3 > D4 + H2O	154	161
129	D3 > E1	55	122
130	D4 > D5	105	56
131	ZOH + Ethene-1,1-diol + acetic_acid > ZOH + 3,3-dihydroxybutanoic_acid	126	101
132	ZOH + 3,3-dihydroxybutanoic_acid > B3	74	9
133	B3 > C5 + H2O	34	132
134	ZOH + 3,3-dihydroxybutanoic_acid > E1 + H2O	240	331
135	A2_O1_pos1 + Ethene-1,1-diol > E1	101	208
136	A2_O1_pos2 + Ethene-1,1-diol > E1	114	215
137	A2_O3 + Ethene-1,1-diol > E1	117	233
138	acetic_acid + Ketene + ZOH > E1	173	162
139	E1 > ZOH + Propen-2-ol + CO2	103	169
140	ZOH + Propen-2-ol > ZOH + Acetone	72	125
141	ZOH + Acetone + Propen-2-ol > E6	128	20
142	E6 > E8 + H2O	24	170
143	E8 > A2_O1_pos1 + C4b-species	138	125
144	E8 > A2_O1_pos2 + C4b-species	138	131

S4. The (101) surface reactivity:

Below, reactions catalyzed by the Lewis acid site located at the (101) surface of SSZ-13 are shown. For details regarding the surface and the active site, see [J. Phys. Chem. C 2022, 126, 13, 5896–5905]. The reaction mechanisms at Lewis acid sites often differ from those at Brønsted acid sites (see Fig. S2). Adsorbed acetic acid can be considered as a protonated surface acetate, which is why C-C coupling reactions involving surface acetate were not investigated explicitly.

For all reactions, an oxygen is bonded to the Lewis acid site. Additionally, a hydrogen is often shifted from a product oxygen to a zeolite oxygen adjacent to the aluminum. Subsequent hydrogen shift reactions from the zeolite to the product, which are expected to happen easily, were not computed. The aldol self-condensation of acetone (E4-E6*) yields a deprotonated diacetone instead of its protonated enol (E5) as in the Brønsted-acid-site catalyzed bulk reaction. For the following dehydration to mesityl oxide, diacetone alcohol (E7*) and its enol (E7) are considered as reactants. For the decomposition of mesityl oxide to acetic acid and isobutene, a water molecule is required for an equivalent mechanism to the Brønsted-acid-site catalyzed reaction.
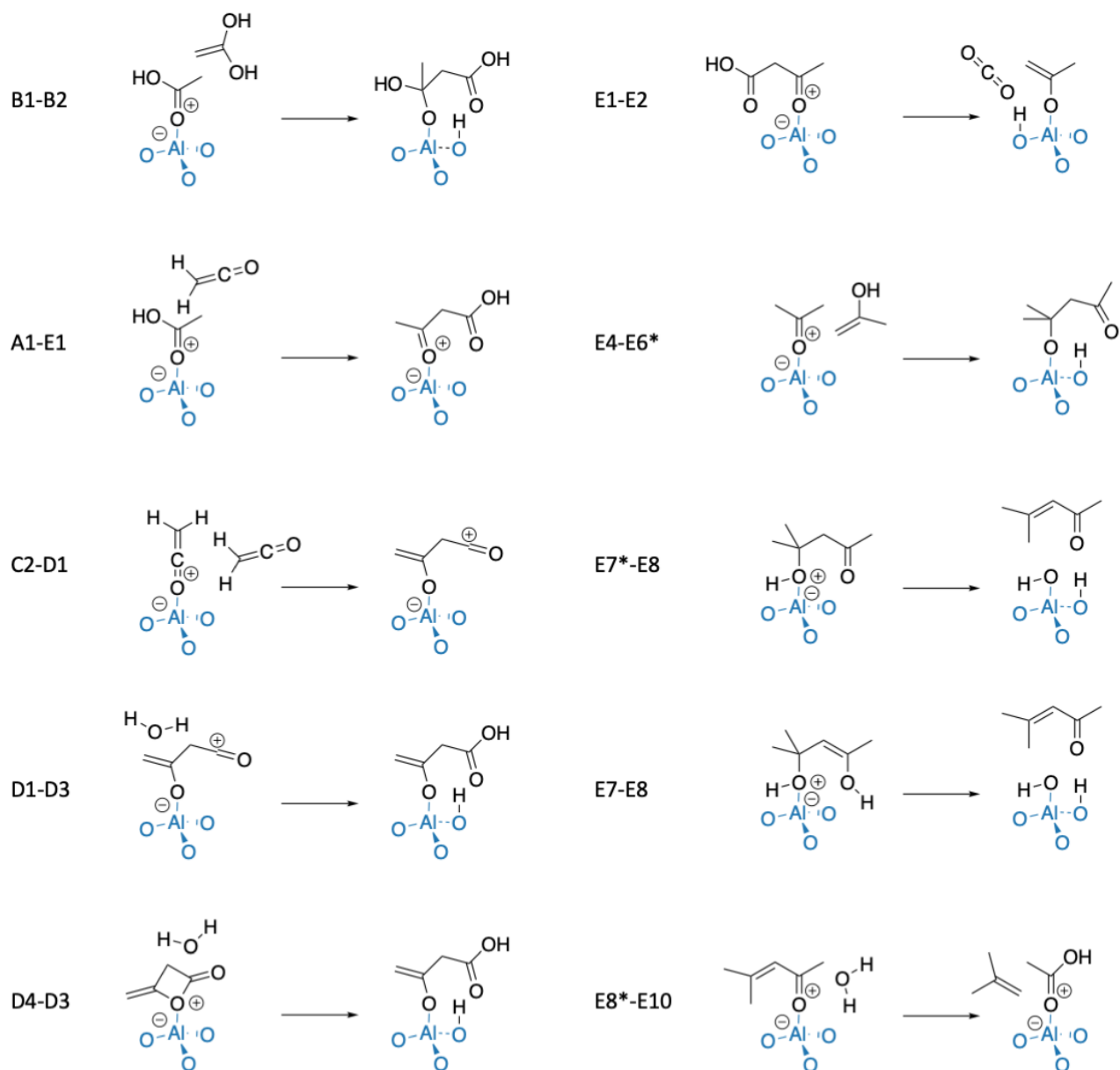
Figure S2: Mechanisms of reactions catalyzed by the (101) surface Lewis acid site.

In Table S1, the free energy barriers of reactions catalyzed by the Lewis acid site are shown. Compared to the Brønsted acid site, these barriers are slightly higher for most transition states. Only the barriers for TS(D4-D3), TS(E1-E2), and TS(E7-E8) are slightly lower at the Lewis acid site. The free energy barrier for TS(E8*-E10) is approximately 150 kJ/mol higher than the barrier for the equivalent reaction at the Brønsted acid site. This might result from the additionally involved water molecule.

Table S4: Free energy barriers in kJ/mol of reactions catalyzed by the (101) surface Lewis acid site. Reference states for the Lewis-acid-site catalyzed reactions are the single adsorbed states (acetic acid or acetone). Reference states for the Brønsted-acid-site catalyzed reactions are gaseous acetic acid or gaseous acetone and the empty zeolite.

Reaction	B1-B2	A1-E1	C2-D1	D1-D3	D4-D3	E1-E2	E4-E6*	E7*-E8	E7-E8	E8*-E10
(101) surface Lewis acid site	270	230	261	254	260	141	177	215	177	305
Bulk Brønsted acid site	243	214	252	237	272	155	169		185	153

S5 Total energies and frequencies:

The periodic PBE-D3 energies, corresponding D3 energies and ZPVE as well as PBE-D3 energies from cluster models are listed in Table S4. For the cluster models, HF/cc-pVXZ (X=D,T,Q) are listed in Table S5. MP2/cc-pVXZ (X=D,T) and CCSD(T)/cc-pVDZ energies are given in Tables S6. The obtained harmonic frequencies are listed in Table S7.

Table S5. Periodic PBE-D3 energies, corresponding D3 contribution, ZPVE and PBE-D3 energies of cluster models in eV.

System	PBE-D3	D3	ZPVE	PBE-D3 CM
Gas phase				
Acetic_acid	-46.814	-0.045	1.623	-6229.555
H2O	-14.225	-0.000	0.563	-2078.416
Ethene-1_1-diol	-45.621	-0.042	1.611	-6228.334
3_3-dihydroxybutanoic_acid	-93.407	-0.209	3.370	-12458.862
3-hydroxybut-2-enoic_acid	-78.899	-0.118	2.654	-10380.109
Ketene	-30.974	-0.013	0.830	-4149.503
3-hydroxybut-3-enoic_acid	-78.173	-0.133	2.643	-10379.529
Diketene	-63.000	-0.070	1.909	-8300.054
Acetylketene	-63.343	-0.078	1.858	-8300.377
CO2	-22.993	-0.002	0.307	-5128.782
3-oxobutanoic_acid	-78.870	-0.128	2.618	-10380.115
Propen-2-ol	-55.508	-0.064	2.224	-5251.031
Mesityl_oxide	-97.692	-0.167	3.825	-8424.545
Acetone	-56.042	-0.067	2.202	-5251.595
(Z)-4-methylpent-2-ene-2_4-diol	-112.136	-0.250	4.588	-10503.194
Isobutene	-65.436	-0.083	2.841	-4273.788
TS(C2-D4)_gas	-61.231	-0.084	1.788	-8298.246
TS(C3-C4)_gas	-77.844	-0.134	2.507	-10379.098
Bulk				
ZOH	-862.579	-5.920	1.254	-509092.732
ZOH*H2O	-877.877	-6.083	1.893	-511172.357
ZOH*AcOH	-910.814	-6.403	2.873	-515323.851
TS(A1-A2_o1_pos1)	-909.200	-6.506	2.851	-515322.282
TS(A1-A2_o1_pos2)	-909.007	-6.481	2.836	-515322.107
TS(A1-A2_o3)	-909.069	-6.445	2.830	-515322.162
A2_o1_is*H2O	-909.316	-6.483	2.848	-515322.400
A2_o1_os*H2O	-909.437	-6.448	2.849	-515322.518
A2_o3_is*H2O	-909.275	-6.466	2.837	-515322.274
A2_o1_is	-894.798	-6.286	2.215	-513243.563
A2_o1_os	-894.832	-6.286	2.214	-513243.646
A2_o3_is	-894.701	-6.276	2.210	-513243.474
TS(A2_o1_pos2-A3)	-894.242	-6.295	1.501	-513242.952
TS(A2_o3-pos1-A3)	-894.228	-6.282	2.142	-513242.968
A3	-894.230	-6.282	2.137	-513242.978
TS(A3-C3)	-894.276	-6.289	2.035	-513243.046
ZOH*Ketene	-894.248	-6.279	2.128	-513243.043
ZOH*2xKetene	-925.705	-6.714	3.005	-517393.034

ZOH*AcOH*Ketene	-942.189	-6.890	3.739	-519473.709
TS(C2-C3)	-925.700	-6.638	2.895	-517393.029
ZOH*Acetylketene	-927.443	-6.700	3.130	-517394.733
TS(C3-C4)_catalyzed	-941.950	-6.818	3.847	-519473.488
ZOH*3-hydroxybut-2-enoic_acid	-943.230	-6.805	3.897	-519474.694
TS(C4-C5)	-942.519	-6.807	3.798	-519474.042
C5	-942.666	-6.771	3.862	-519474.196
TS(C5-E1)	-942.476	-6.798	3.889	-519473.991
TS(C4-E1)	-941.838	-6.886	3.807	-519473.373
TS(A1-E1)	-941.446	-6.810	3.865	-519473.011
TS(A1-B1)	-910.814	-6.403	2.873	-515323.851
ZOH*Ethene-1,1-diol	-909.093	-6.344	2.894	-515322.121
ZOH*AcOH*Ethene-1_1-diol	-957.143	-7.015	4.517	-521552.925
TS(B1-B2)	-957.096	-6.992	4.599	-521552.871
ZOH*3_3-dihydroxybutanoic_acid	-957.245	-6.971	4.627	-521552.976
TS(B2-E1)	-955.337	-6.959	4.505	-521551.056
TS(B2-B3)	-957.137	-6.910	4.605	-521552.799
B3	-957.168	-6.905	4.618	-521552.871
TS(B3-C5)	-956.925	-6.928	4.607	-521552.672
C5*H2O	-957.854	-6.977	4.478	-521553.625
B4_o1_pos1	-941.074	-6.866	3.858	-519472.620
B4_o1_pos2	-941.150	-6.846	3.856	-519472.701
B4_o3	-941.005	-6.863	3.855	-519472.483
TS(B4-E1_o1_pos1)	-940.855	-6.862	3.829	-519472.425
TS(B4-E1_o1_pos2)	-940.793	-6.839	3.813	-519472.359
TS(B4-E1_o3)	-940.641	-6.856	4.149	-519472.196
A2_o1_pos1*Ketene	-926.169	-6.634	3.071	-517393.491
A2_o1_pos2*Ketene	-926.250	-6.676	3.073	-517393.592
A2_o3*Ketene	-926.136	-6.670	3.069	-517393.423
TS(A2-C3_o1_pos1)	-925.768	-6.683	3.035	-517393.127
TS(A2-C3_o1_pos2)	-925.595	-6.663	3.033	-517392.962
TS(A2-D5_o3)	-925.695	-6.674	3.043	-517393.052
TS(E1-E2)	-942.267	-6.814	3.849	-519473.814
ZOH*Propen-2-ol*CO2	-942.366	-6.770	3.852	-519473.978
ZOH*Propen-2-ol	-919.290	-6.525	3.528	-514345.066
TS(E2-E3)	-918.830	-6.505	3.519	-514344.656
ZOH*Acetone	-919.960	-6.563	3.472	-514345.482
ZOH*Acetone*Propen-2-ol	-976.378	-7.258	5.736	-519597.728
TS(E4-E5)	-976.319	-7.247	5.799	-519597.678
E5	-976.629	-7.191	5.832	-519597.990
TS(E5-E6)	-976.101	-7.236	5.766	-519597.456
ZOH*Z-4-methylpent-2-ene-2-4-diol	-976.180	-7.244	5.875	-519597.560
TS(E6-E7)	-975.878	-7.191	5.872	-519597.252
E7	-976.360	-7.223	5.816	-519597.651

TS(E7-E8)	-976.023	-7.214	5.842	-519597.253
ZOH*MO	-962.229	-7.135	5.146	-517519.195
TS(E8-E9)	-960.853	-7.050	4.986	-517517.932
E9	-961.091	-7.000	5.067	-517518.188
TS(E9-10_pos2)	-960.418	-7.046	5.018	-517517.581
TS(E9-10_pos1)	-960.548	-7.067	5.028	-517517.650
A2*Isobutene_pos2	-960.975	-7.036	5.085	-517518.127
A2*Isobutene_pos1	-960.871	-7.061	5.084	-517518.026
TS(C3-D5)	-926.342	-6.661	3.036	-517393.650
D5	-926.406	-6.641	3.115	-517393.714
D5*H2O	-941.334	-6.784	3.755	-519472.922
TS(D5-D7)	-926.428	-6.589	3.128	-517393.813
D7	-926.919	-6.650	3.197	-517394.237
D7*H2O	-941.567	-6.876	3.844	-519473.143
TS(D7-C5)	-941.262	-6.794	3.800	-519472.862
TS(D5-C5)	-941.287	-6.785	3.795	-519472.740
TS(D5-D8)	-941.289	-6.791	3.741	-519472.902
D8	-941.551	-6.782	3.836	-519473.137
TS(D8-E1)	-941.468	-6.812	4.027	-519473.039
TS(D5-D6)	-925.957	-6.574	3.104	-517393.077
D6	-926.209	-6.577	3.143	-517393.468
TS(D6-D4)	-926.196	-6.577	3.090	-517393.459
ZOH*Diketene	-926.891	-6.554	3.180	-517394.155
TS(C2-D1)	-925.452	-6.645	3.022	-517392.790
D1	-925.975	-6.644	3.146	-517393.134
TS(D1-D4)	-925.916	-6.716	3.112	-517393.093
ZOH*Diketene*H2O	-941.626	-6.787	3.823	-519473.149
TS(D4-D3)	-940.870	-6.877	3.791	-519472.384
ZOH*3-hydroxy-but-2-enoic-acid	-942.398	-6.859	3.907	-519473.894
TS(D1-D2)	-925.844	-6.655	3.180	-517393.193
D2	-925.875	-6.636	3.203	-517393.228
D2*H2O	-941.065	-6.855	3.854	-519472.638
TS(D2-D3)	-940.895	-6.802	3.830	-519472.480
TS(D2-E1)	-942.077	-6.876	3.815	-519473.597
TS(DAA_dehydration)	-975.784	-7.226	5.732	-519597.014
Z(101)				
Z(101)	-1792.635	-11.166	0.737	-732986.127
Z*AcOH	-1841.375	-11.367	2.398	-739217.618
Z*Ketene	-1824.442	-11.302	1.615	-737136.464
Z*Diketene	-1856.826	-11.481	2.673	-741287.370
Z*E1	-1873.457	-11.647	3.415	-743368.199
Z*Acetone	-1850.379	-11.403	3.000	-738239.454
Z*Mesityl_oxide	-1892.362	-11.819	4.614	-741412.726
TS(C2-D1)	-1855.824	-11.525	2.510	-741286.367

TS(D1-D3)	-1871.320	-11.699	3.271	-743366.049
TS(D4-D3)	-1871.400	-11.647	3.322	-743366.199
TS(A1-E1)	-1871.814	-11.691	3.330	-743366.557
TS(B1-B2)	-1887.207	-11.754	4.079	-745446.178
TS(E1-E2)	-1872.686	-11.655	3.321	-743367.497
TS(E4-E6*)	-1906.531	-11.845	5.308	-743491.182
TS(E7*-E8)	-1905.856	-11.924	5.136	-743490.445
TS(E7-E8)	-1906.375	-11.893	5.324	-743491.003
TS(E8*-E10)	-1905.173	-11.897	5.178	-743489.726

Table S6. HF energies of cluster models in eV.

System	HF/cc-pVDZ	HF/cc-pVTZ	HF/cc-pVQZ
Gas phase			
Acetic_acid	-6199.558	-6201.446	-6201.910
H2O	-2068.762	-2069.584	-2069.792
Ethene-1_1-diol	-6198.208	-6200.162	-6200.633
3_3-dihydroxybutanoic_acid	-12398.671	-12402.373	-12403.280
3-hydroxybut-2-enoic_acid	-10329.343	-10332.339	-10333.082
Ketene	-4129.006	-4130.195	-4130.493
3-hydroxybut-3-enoic_acid	-10328.855	-10331.891	-10332.643
Diketene	-8258.804	-8261.176	-8261.749
Acetylketene	-8259.347	-8261.628	-8262.209
CO2	-5106.133	-5107.646	-5108.032
3-oxobutanoic_acid	-10329.432	-10332.432	-10333.180
Propen-2-ol	-5223.168	-5224.763	-5225.143
Mesityl_oxide	-8378.521	-8380.781	-8381.341
Acetone	-5223.922	-5225.449	-5225.818
(Z)-4-methylpent-2-ene-2_4-diol	-10447.332	-10450.326	-10451.049
Isobutene	-4248.335	-4249.515	-4249.799
TS(C2-D4)_gas	-8256.289	-8258.698	-8259.310
TS(C3-C4)_gas	-10328.193	-10331.215	-10331.973
Bulk			
ZOH	-507910.158	-508016.896	-508040.489
ZOH*H2O	-509979.932	-510087.047	-510110.763
ZOH*AcOH	-514110.667	-514218.849	-514242.840
TS(A1-A2_o1_pos1)	-514108.946	-514216.857	-514240.846
TS(A1-A2_o1_pos2)	-514108.894	-514216.812	-514240.797
TS(A1-A2_o3)	-514108.905	-514216.854	-514240.847
A2_o1_is*H2O	-514109.334	-514217.437	-514241.430
A2_o1_os*H2O	-514109.461	-514217.657	-514241.666
A2_o3_is*H2O	-514109.110	-514217.430	-514241.449
A2_o1_is	-512040.299	-512147.852	-512171.702
A2_o1_os	-512040.438	-512147.924	-512171.770
A2_o3_is	-512040.108	-512147.749	-512171.609
TS(A2_o1_pos2-A3)	-512039.859	-512147.155	-512170.994

TS(A2_o3-pos1-A3)	-512039.683	-512146.988	-512170.841
A3	-512039.609	-512146.908	-512170.751
TS(A3-C3)	-512039.178	-512146.677	-512170.520
ZOH*Ketene	-512039.658	-512147.337	-512171.196
ZOH*2xKetene	-516168.794	-516277.466	-516301.560
ZOH*AcOH*Ketene	-518239.582	-518348.743	-518372.959
TS(C2-C3)	-516168.259	-516276.824	-516300.922
ZOH*Acetylketene	-516170.326	-516278.757	-516302.815
TS(C3-C4)_catalyzed	-518239.234	-518348.180	-518372.391
ZOH*3-hydroxybut-2-enoic_acid	-518240.483	-518349.668	-518373.893
TS(C4-C5)	-518239.555	-518348.671	-518372.895
C5	-518240.193	-518349.151	-518373.356
TS(C5-E1)	-518240.261	-518349.190	-518373.405
TS(C4-E1)	-518238.946	-518347.931	-518372.133
TS(A1-E1)	-518238.930	-518347.943	-518372.157
TS(A1-B1)	-514110.667	-514218.849	-514242.840
ZOH*Ethene-1,1-diol	-514108.795	-514217.278	-514241.305
ZOH*AcOH*Ethene-1_1-diol	-520309.180	-520418.962	-520443.321
TS(B1-B2)	-520308.608	-520418.424	-520442.791
ZOH*3_3-dihydroxybutanoic_acid	-520309.173	-520419.021	-520443.386
TS(B2-E1)	-520306.610	-520416.552	-520440.920
TS(B2-B3)	-520308.928	-520418.759	-520443.136
B3	-520309.057	-520418.826	-520443.200
TS(B3-C5)	-520308.955	-520418.516	-520442.880
C5*H2O	-520309.664	-520419.489	-520443.858
B4_o1_pos1	-518238.758	-518347.956	-518372.188
B4_o1_pos2	-518238.887	-518348.131	-518372.370
B4_o3	-518238.477	-518347.879	-518372.133
TS(B4-E1_o1_pos1)	-518238.354	-518347.343	-518371.582
TS(B4-E1_o1_pos2)	-518238.405	-518347.331	-518371.551
TS(B4-E1_o3)	-518238.009	-518347.094	-518371.338
A2_o1_pos1*Ketene	-516169.489	-516278.120	-516302.218
A2_o1_pos2*Ketene	-516169.578	-516278.167	-516302.258
A2_o3*Ketene	-516169.307	-516277.960	-516302.062
TS(A2-C3_o1_pos1)	-516168.882	-516277.207	-516301.295
TS(A2-C3_o1_pos2)	-516168.771	-516277.136	-516301.227
TS(A2-D5_o3)	-516168.725	-516277.144	-516301.242
TS(E1-E2)	-518239.255	-518348.620	-518372.865
ZOH*Propen-2-ol*CO2	-518240.294	-518349.694	-518373.948
ZOH*Propen-2-ol	-513134.075	-513241.937	-513265.804
TS(E2-E3)	-513133.766	-513241.834	-513265.751
ZOH*Acetone	-513134.607	-513242.589	-513266.500
ZOH*Acetone*Propen-2-ol	-518358.457	-518467.561	-518491.716
TS(E4-E5)	-518358.041	-518467.062	-518491.221

E5	-518358.552	-518467.574	-518491.727
TS(E5-E6)	-518357.498	-518466.623	-518490.783
ZOH*Z-4-methylpent-2-ene-2-4-diol	-518357.946	-518467.239	-518491.420
TS(E6-E7)	-518357.833	-518467.138	-518491.298
E7	-518357.839	-518466.834	-518490.957
TS(E7-E8)	-518357.678	-518466.499	-518490.638
ZOH*MO	-516289.556	-516397.765	-516421.763
TS(E8-E9)	-516288.031	-516396.379	-516420.399
E9	-516288.455	-516396.676	-516420.690
TS(E9-10_pos2)	-516288.134	-516396.513	-516420.547
TS(E9-10_pos1)	-516288.297	-516396.559	-516420.590
A2*Isobutene_pos2	-516288.853	-516397.393	-516421.432
A2*Isobutene_pos1	-516288.690	-516397.145	-516421.171
TS(C3-D5)	-516168.800	-516277.229	-516301.308
D5	-516169.302	-516277.661	-516301.753
D5*H2O	-518238.768	-518347.829	-518372.075
TS(D5-D7)	-516169.462	-516277.922	-516302.028
D7	-516170.242	-516278.817	-516302.916
D7*H2O	-518239.281	-518348.469	-518372.708
TS(D7-C5)	-518238.879	-518347.864	-518372.090
TS(D5-C5)	-518238.879	-518347.903	-518372.144
TS(D5-D8)	-518238.879	-518347.937	-518372.170
D8	-518238.924	-518347.718	-518371.936
TS(D8-E1)	-518238.832	-518347.710	-518371.937
TS(D5-D6)	-516169.081	-516277.334	-516301.427
D6	-516168.896	-516277.301	-516301.376
TS(D6-D4)	-516168.588	-516277.046	-516301.120
ZOH*Diketene	-516169.814	-516278.566	-516302.652
TS(C2-D1)	-516168.039	-516276.648	-516300.737
D1	-516168.748	-516276.979	-516301.041
TS(D1-D4)	-516168.669	-516276.905	-516300.951
ZOH*Diketene*H2O	-518238.920	-518348.304	-518372.545
TS(D4-D3)	-518237.563	-518346.628	-518370.857
ZOH*3-hydroxy-but-2-enoic-acid	-518239.805	-518349.137	-518373.374
TS(D1-D2)	-516168.546	-516276.922	-516301.000
D2	-516168.864	-516277.254	-516301.316
D2*H2O	-518238.501	-518347.706	-518371.935
TS(D2-D3)	-518238.367	-518347.380	-518371.620
TS(D2-E1)	-518239.078	-518348.267	-518372.478
TS(DAA_dehydration)	-518357.792	-518466.675	-518490.837
(101)			
Z(101)	-731236.971	-731396.448	-731431.562
Z*AcOH	-737438.443	-737599.552	-737635.124
Z*Ketene	-735366.852	-735527.391	-735562.804

Z*Diketene	-739497.019	-739658.582	-739694.263
Z*E1	-741568.236	-741730.225	-741766.035
Z*Acetone	-736462.703	-736623.465	-736658.933
Z*Mesityl_oxide	-739617.451	-739778.657	-739814.251
TS(C2-D1)	-739495.649	-739657.196	-739692.885
TS(D1-D3)	-741565.847	-741727.926	-741763.762
TS(D4-D3)	-741565.709	-741727.664	-741763.490
TS(A1-E1)	-741566.176	-741728.191	-741764.018
TS(B1-B2)	-743635.982	-743798.821	-743834.807
TS(E1-E2)	-741567.380	-741729.427	-741765.232
TS(E4-E6*)	-741685.625	-741847.647	-741883.419
TS(E7*-E8)	-741684.720	-741846.735	-741882.527
TS(E7-E8)	-741685.562	-741847.558	-741883.334
TS(E8*-E10)	-741683.639	-741845.551	-741881.312

Table S7. DLPNO-MP2 and DLPNO-CCSD(T) energies of cluster models in eV.

System	MP2/cc-pVDZ	MP2/cc-pVTZ	CCSD(T)/cc-pVDZ
Gas phase			
Acetic_acid	-6217.031	-6223.327	-6218.242
H2O	-2074.278	-2076.729	-2074.624
Ethene-1_1-diol	-6215.627	-6222.065	-6216.866
3_3-dihydroxybutanoic_acid	-12433.950	-12446.606	-12436.346
3-hydroxybut-2-enoic_acid	-10358.970	-10369.321	-10360.998
Ketene	-4140.950	-4144.931	-4141.806
3-hydroxybut-3-enoic_acid	-10358.476	-10368.839	-10360.557
Diketene	-8282.930	-8290.984	-8284.673
Acetylketene	-8283.405	-8291.322	-8285.059
CO2	-5119.379	-5124.127	-5119.737
3-oxobutanoic_acid	-10359.097	-10369.358	-10361.163
Propen-2-ol	-5239.540	-5245.067	-5241.184
Mesityl_oxide	-8405.953	-8414.431	-8408.792
Acetone	-5240.287	-5245.655	-5241.914
(Z)-4-methylpent-2-ene-2_4-diol	-10480.597	-10491.506	-10483.745
Isobutene	-4263.654	-4268.186	-4265.662
TS(C2-D4)_gas	-8280.892	-8288.964	-8282.472
TS(C3-C4)_gas	-10357.976	-10368.296	-10359.944
Bulk			
ZOH	-508366.066	-508599.555	-508387.946
ZOH*H2O	-510441.906	-510677.419	-510464.084
ZOH*AcOH	-514584.871	-514824.279	-514607.919
TS(A1-A2_o1_pos1)	-514583.620	-514822.847	-514606.603
TS(A1-A2_o1_pos2)	-514583.511	-514822.730	-514606.486
TS(A1-A2_o3)	-514583.521	-514822.751	-514606.507
A2_o1_is*H2O	-514583.679	-514823.061	-514606.747
A2_o1_os*H2O	-514583.702	-514823.117	-514606.758

A2_o3_is*H2O	–514583.342	–514822.895	–514606.395
A2_o1_is	–512508.785	–512745.909	–512531.524
A2_o1_os	–512508.902	–512745.981	–512531.645
A2_o3_is	–512508.594	–512745.805	–512531.317
TS(A2_o1_pos2-A3)	–512508.393	–512745.339	–512531.050
TS(A2_o3-pos1-A3)	–512508.328	–512745.284	–512530.966
A3	–512508.286	–512745.245	–512530.919
TS(A3-C3)	–512508.088	–512745.211	–512530.668
ZOH*Ketene	–512507.934	–512745.236	–512530.665
ZOH*2xKetene	–516649.460	–516890.645	–516673.012
ZOH*AcOH*Ketene	–518726.254	–518969.575	–518750.124
TS(C2-C3)	–516649.517	–516890.538	–516672.897
ZOH*Acetylketene	–516651.413	–516892.341	–516674.852
TS(C3-C4)_catalyzed	–518726.132	–518969.300	–518749.935
ZOH*3-hydroxybut-2-enoic_acid	–518727.104	–518970.521	–518750.969
TS(C4-C5)	–518726.438	–518969.789	–518750.256
C5	–518726.868	–518970.005	–518750.760
TS(C5-E1)	–518726.772	–518969.882	–518750.690
TS(C4-E1)	–518725.990	–518969.197	–518749.825
TS(A1-E1)	–518725.940	–518969.123	–518749.748
TS(A1-B1)	–514584.871	–514824.279	–514607.919
ZOH*Ethene-1,1-diol	–514582.816	–514822.587	–514605.905
ZOH*AcOH*Ethene-1_1-diol	–520801.425	–521047.037	–520825.704
TS(B1-B2)	–520801.157	–521046.830	–520825.365
ZOH*3_3-dihydroxybutanoic_acid	–520801.589	–521047.281	–520825.821
TS(B2-E1)	–520799.550	–521045.286	–520823.708
TS(B2-B3)	–520801.315	–521047.014	–520825.534
B3	–520801.435	–521047.077	–520825.657
TS(B3-C5)	–520801.295	–521046.704	–520825.548
C5*H2O	–520802.154	–521047.771	–520826.349
B4_o1_pos1	–518725.305	–518968.654	–518749.266
B4_o1_pos2	–518725.334	–518968.717	–518749.298
B4_o3	–518724.999	–518968.514	–518748.939
TS(B4-E1_o1_pos1)	–518725.210	–518968.423	–518749.068
TS(B4-E1_o1_pos2)	–518725.239	–518968.371	–518749.077
TS(B4-E1_o3)	–518724.919	–518968.214	–518748.778
A2_o1_pos1*Ketene	–516650.181	–516891.245	–516673.767
A2_o1_pos2*Ketene	–516650.293	–516891.318	–516673.865
A2_o3*Ketene	–516650.064	–516891.144	–516673.628
TS(A2-C3_o1_pos1)	–516650.012	–516890.826	–516673.468
TS(A2-C3_o1_pos2)	–516649.884	–516890.708	–516673.325
TS(A2-D5_o3)	–516649.832	–516890.752	–516673.289
TS(E1-E2)	–518726.151	–518969.619	–518749.904
ZOH*Propen-2-ol*CO2	–518726.649	–518970.093	–518750.474

ZOH*Propen-2-ol	–513607.242	–513845.848	–513630.717
TS(E2-E3)	–513606.681	–513845.443	–513630.159
ZOH*Acetone	–513607.615	–513846.232	–513631.084
ZOH*Acetone*Propen-2-ol	–518848.595	–519092.411	–518873.646
TS(E4-E5)	–518848.392	–519092.170	–518873.434
E5	–518849.002	–519092.762	–518873.998
TS(E5-E6)	–518848.312	–519092.217	–518873.211
ZOH*Z-4-methylpent-2-ene-2-4-diol	–518848.486	–519092.515	–518873.425
TS(E6-E7)	–518848.194	–519092.251	–518873.188
E7	–518848.788	–519092.605	–518873.711
TS(E7-E8)	–518848.308	–519091.978	–518873.280
ZOH*MO	–516774.221	–517015.599	–516798.872
TS(E8-E9)	–516772.667	–517014.155	–516797.330
E9	–516772.835	–517014.162	–516797.580
TS(E9-10_pos2)	–516772.793	–517014.222	–516797.390
TS(E9-10_pos1)	–516772.987	–517014.329	–516797.599
A2*Isobutene_pos2	–516773.225	–517014.762	–516797.947
A2*Isobutene_pos1	–516773.224	–517014.713	–516797.936
TS(C3-D5)	–516650.359	–516891.261	–516673.742
D5	–516650.500	–516891.371	–516673.947
D5*H2O	–518725.629	–518968.819	–518749.403
TS(D5-D7)	–516650.592	–516891.516	–516674.037
D7	–516651.107	–516892.126	–516674.682
D7*H2O	–518725.992	–518969.323	–518749.880
TS(D7-C5)	–518725.752	–518968.874	–518749.546
TS(D5-C5)	–518725.617	–518968.809	–518749.434
TS(D5-D8)	–518725.708	–518968.877	–518749.490
D8	–518726.122	–518969.007	–518749.968
TS(D8-E1)	–518725.956	–518968.923	–518749.796
TS(D5-D6)	–516650.128	–516890.863	–516673.624
D6	–516650.057	–516890.970	–516673.592
TS(D6-D4)	–516649.895	–516890.872	–516673.403
ZOH*Diketene	–516650.523	–516891.789	–516674.125
TS(C2-D1)	–516649.145	–516890.231	–516672.616
D1	–516650.062	–516890.844	–516673.522
TS(D1-D4)	–516650.065	–516890.879	–516673.523
ZOH*Diketene*H2O	–518725.491	–518969.059	–518749.402
TS(D4-D3)	–518725.022	–518968.342	–518748.798
ZOH*3-hydroxy-but-2-enoic-acid	–518726.383	–518969.882	–518750.306
TS(D1-D2)	–516649.948	–516890.948	–516673.442
D2	–516650.070	–516891.036	–516673.637
D2*H2O	–518725.383	–518968.750	–518749.266
TS(D2-D3)	–518725.291	–518968.537	–518749.132
TS(D2-E1)	–518726.031	–518969.394	–518749.839

TS(DAA_dehydration)	-518847.745	-519091.436	-518872.812
(101)			
Z(101)	-731929.590	-732282.107	-731960.239
Z*AcOH	-738148.797	-738507.410	-738180.660
Z*Ketene	-736071.488	-736427.900	-736103.058
Z*Diketene	-740214.065	-740574.414	-740246.446
Z*E1	-742290.998	-742653.397	-742323.707
Z*Acetone	-737171.770	-737529.507	-737204.064
Z*Mesityl_oxide	-740337.816	-740698.459	-740371.301
TS(C2-D1)	-740212.767	-740573.078	-740245.128
TS(D1-D3)	-742288.737	-742651.344	-742321.320
TS(D4-D3)	-742289.014	-742651.473	-742321.624
TS(A1-E1)	-742289.390	-742651.887	-742321.987
TS(B1-B2)	-744364.594	-744729.523	-744397.593
TS(E1-E2)	-742290.439	-742652.796	-742323.023
TS(E4-E6*)	-742412.103	-742775.126	-742445.887
TS(E7*-E8)	-742411.253	-742774.287	-742445.047
TS(E7-E8)	-742412.021	-742775.058	-742445.802
TS(E8*-E10)	-742410.478	-742773.509	-742444.243

Table S8. Harmonic Frequencies in cm^{-1}.

System	Frequencies
Gas phase	
Acetic_acid	35.7i, 30.2i, 22.6i, 14.1i, 21.3, 55.1, 76.3, 410.9, 528.1, 563.3, 652.0, 842.6, 955.1, 1018.9, 1150.7, 1287.7, 1351.8, 1414.6, 1419.1, 1761.9, 2985.8, 3051.1, 3101.5, 3615.7
H2O	1579.0, 3697.3, 3812.2
Ethene-1_1-diol	43.7i, 32.8i, 3.6i, 68.3, 78.5, 94.0, 246.6, 440.4, 450.9, 529.4, 631.0, 639.2, 665.7, 926.3, 941.0, 1105.4, 1200.0, 1396.3, 1404.1, 1661.2, 3098.0, 3185.8, 3728.9, 3730.6
3_3-dihydroxybutanoic_a-cid	29.7i, 16.7i, 5.4i, 32.4, 47.5, 59.9, 90.2, 106.7, 183.3, 234.1, 284.5, 319.9, 335.9, 385.5, 420.0, 469.4, 504.5, 541.1, 574.6, 607.3, 679.5, 804.0, 838.5, 865.7, 919.5, 931.2, 1041.6, 1054.6, 1089.6, 1149.7, 1213.0, 1265.6, 1276.0, 1312.0, 1348.1, 1393.1, 1401.0, 1431.7, 1440.6, 1777.3, 2976.1, 2997.5, 3052.1, 3066.4, 3071.6, 3600.1, 3618.4, 3685.1
3-hydroxybut-2-enoic_acid	32.3i, 6.9i, 3.2i, 31.3, 51.7, 68.7, 115.0, 145.3, 180.3, 238.2, 368.0, 407.5, 500.0, 526.9, 563.0, 626.1, 702.0, 759.9, 803.5, 844.1, 927.3, 991.7, 1017.0, 1090.5, 1174.8, 1262.0, 1331.6, 1348.8, 1412.8, 1415.2, 1436.1, 1623.0, 1738.5, 2972.5, 3030.5, 3080.9, 3150.4, 3393.6, 3639.6
Ketene	29.1i, 24.0i, 1.6i, 69.1, 73.7, 80.3, 418.5, 500.6, 558.9, 937.9, 1138.4, 1347.8, 2175.4, 3108.8, 3201.2
3-hydroxybut-3-enoic_acid	22.7i, 5.5i, 4.1i, 15.8, 52.4, 59.6, 83.5, 90.2, 200.7, 350.2, 403.3, 458.9, 473.4, 511.0, 541.3, 604.6, 697.8, 708.2, 801.8, 847.2, 873.5, 923.0, 952.5, 1071.8, 1175.7, 1219.3, 1252.3, 1288.0, 1303.9, 1386.0, 1399.8, 1681.3, 1783.3, 2952.1, 3079.0, 3097.3, 3192.8, 3607.4, 3619.0
Diketene	35.2i, 26.5i, 9.3i, 40.0, 66.1, 79.2, 147.1, 311.2, 444.3, 489.9, 511.9, 655.3, 707.2, 795.9, 816.7, 859.7, 937.6, 962.6, 983.1, 1072.3, 1154.5, 1219.2, 1365.5, 1383.0, 1714.8, 1897.8, 3009.9, 3062.4, 3099.7, 3192.1
Acetylketene	31.5i, 20.3i, 8.4i, 53.1, 63.5, 66.7, 86.6, 114.6, 141.3, 346.7, 447.1, 508.8, 543.1, 593.9, 625.6, 864.0, 932.9, 991.4, 1085.9, 1134.1, 1315.7, 1353.2, 1410.7, 1416.9, 1679.3, 2174.2, 2965.3, 3031.5, 3085.9, 3127.4
CO2	31.7i, 6.4i, 1.2i, 44.0, 58.4, 632.1, 633.4, 1318.3, 2365.7
3-oxobutanoic_acid	18.4i, 13.2i, 9.8i, 32.2, 45.0, 59.8, 68.5, 105.3, 124.5, 251.0, 351.4, 390.5, 442.9, 550.5, 559.7, 667.7, 801.3, 840.6, 874.7, 887.3, 955.4, 998.7, 1146.1, 1149.3, 1199.7, 1291.6, 1335.9, 1362.0, 1401.2, 1412.4, 1414.3, 1682.3, 1782.3, 2954.6, 2963.7, 3025.7, 3038.5, 3086.0, 3120.2
Propen-2-ol	23.4i, 21.6i, 8.6i, 24.6, 43.1, 65.0, 193.8, 275.0, 406.5, 460.2, 485.2, 707.3, 792.4, 840.9, 942.9, 984.8, 1025.8, 1193.2, 1280.2, 1354.5, 1384.0, 1423.8, 1431.2, 1689.4, 2942.5, 2993.4, 3063.0, 3096.0, 3190.6, 3720.2
Mesityl_oxide	36.5i, 23.6i, 14.1i, 3.4i, 23.9, 37.1, 59.8, 78.9, 115.7, 133.0, 192.6, 209.7, 332.9, 369.0, 432.5, 452.5, 577.3, 613.2, 815.4, 816.5, 894.5, 927.1, 938.0, 959.5, 993.2, 1055.4, 1057.4, 1153.4, 1214.1, 1318.2, 1328.8, 1350.4, 1364.5,

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	1401.9, 1409.2, 1412.2, 1416.3, 1429.0, 1443.2, 1611.3, 1683.5, 2942.4, 2948.1, 2958.1, 2990.5, 2997.3, 3020.0, 3048.8, 3058.7, 3081.8, 3090.8
Acetone	39.0i, 22.6i, 17.2i, 27.9, 43.9, 62.0, 77.5, 132.2, 371.8, 472.7, 523.1, 775.6, 841.4, 853.4, 1041.2, 1068.7, 1197.8, 1324.8, 1329.1, 1401.3, 1405.5, 1413.7, 1429.8, 1725.9, 2958.6, 2965.1, 3020.8, 3027.0, 3079.7, 3081.3
(Z)-4-methylpent-2-ene-2_4-diol	21.7i, 7.8i, 3.3i, 47.9, 52.6, 70.6, 81.8, 133.3, 175.5, 229.0, 246.0, 276.0, 285.3, 311.2, 349.1, 370.2, 411.1, 451.5, 467.8, 580.5, 599.3, 708.7, 761.5, 779.1, 873.3, 891.1, 905.9, 942.4, 978.9, 1001.5, 1019.3, 1091.2, 1119.9, 1157.4, 1188.5, 1290.5, 1334.8, 1340.0, 1349.6, 1357.6, 1406.2, 1413.8, 1420.2, 1426.8, 1431.6, 1442.1, 1451.7, 1673.5, 2940.6, 2959.2, 2961.8, 3016.6, 3021.9, 3031.7, 3051.9, 3057.2, 3068.2, 3112.7, 3367.1, 3692.3
Isobutene	48.7i, 25.9i, 4.2i, 20.3, 26.7, 52.9, 167.9, 203.7, 375.4, 426.3, 428.3, 676.4, 809.8, 872.3, 929.1, 957.6, 979.8, 1045.7, 1058.8, 1259.6, 1353.1, 1355.2, 1388.4, 1412.1, 1425.4, 1431.6, 1446.2, 1665.0, 2940.5, 2945.3, 2990.8, 2992.0, 3043.5, 3045.2, 3056.3, 3139.5
TS(C2-D4)_gas	360.9i, 26.8i, 13.5i, 8.8i, 38.8, 52.4, 63.9, 120.6, 222.7, 368.4, 399.9, 464.6, 493.3, 589.6, 642.0, 686.3, 845.1, 937.1, 981.2, 1013.6, 1042.3, 1161.9, 1359.4, 1396.0, 1665.0, 2149.6, 2962.5, 3061.0, 3091.9, 3192.2
TS(C3-C4)_gas	63.1i, 20.8i, 18.9i, 3.6i, 46.8, 64.6, 67.5, 72.1, 91.1, 127.5, 187.7, 236.6, 242.5, 370.2, 402.6, 438.8, 525.8, 535.5, 610.1, 627.5, 730.0, 869.3, 943.9, 994.5, 1108.7, 1138.1, 1323.8, 1395.9, 1413.3, 1419.7, 1588.1, 1646.8, 2158.2, 2966.6, 3031.1, 3084.4, 3087.3, 3309.0, 3764.8
Bulk	
ZOH	184.8, 192.9, 207.8, 233.7, 240.4, 272.8, 308.9, 322.6, 333.6, 351.5, 368.2, 381.5, 498.7, 598.7, 627.3, 636.9, 652.1, 666.4, 673.5, 687.8, 689.1, 722.0, 739.0, 745.4, 772.4, 1048.8, 1096.7, 1125.2, 1196.7, 3656.8
ZOH*H2O	64.1, 124.1, 180.0, 199.8, 206.3, 222.4, 247.1, 256.6, 288.2, 315.9, 319.7, 333.0, 351.8, 358.4, 385.8, 451.6, 554.6, 606.8, 622.8, 630.4, 639.3, 645.0, 654.1, 668.9, 682.7, 693.4, 707.7, 732.4, 736.5, 859.7, 957.8, 1085.5, 1139.6, 1174.5, 1428.5, 1562.2, 2218.5, 3488.9, 3734.5
ZOH*AcOH	38.4, 58.7, 66.2, 94.1, 121.0, 128.6, 157.7, 202.2, 221.4, 238.2, 244.6, 259.6, 299.8, 322.1, 336.8, 351.6, 372.1, 401.5, 489.6, 566.9, 583.2, 611.6, 634.7, 649.0, 655.5, 662.1, 666.9, 672.5, 686.7, 692.3, 706.0, 722.9, 739.8, 865.1, 912.4, 977.2, 1007.4, 1021.9, 1049.4, 1100.7, 1124.9, 1152.6, 1291.8, 1334.1, 1364.8, 1401.7, 1417.8, 1444.7, 1546.5, 1755.3, 2771.4, 2985.8, 3058.8, 3102.4
TS(A1-A2_o1_pos1)	141.2i, 37.2, 82.3, 95.2, 128.4, 168.1, 179.8, 198.0, 218.0, 226.5, 233.8, 244.7, 253.7, 264.2, 305.6, 321.5, 338.5, 345.0, 372.5, 378.4, 407.1, 427.3, 444.9, 494.6, 557.0, 626.5, 636.8, 647.0, 648.7, 656.3, 662.8, 671.6, 681.2, 692.4, 706.6, 715.9, 742.5, 879.9, 923.5, 984.8, 1006.4, 1082.8, 1107.1, 1149.8, 1323.6, 1363.6, 1396.4, 1601.4, 2074.7, 2983.4, 3067.5, 3107.0, 3415.8, 3710.5
TS(A1-A2_o1_pos2)	118.8i, 60.7, 76.2, 83.4, 115.1, 142.0, 170.9, 199.5, 217.0, 218.3, 235.2, 240.3, 250.1, 257.1, 301.8, 308.0, 328.4, 341.3, 351.0, 366.9, 384.0, 395.7, 426.9, 458.1, 556.7, 627.6, 633.1, 642.1, 646.5, 658.3, 663.9, 667.8, 680.7, 694.4, 703.3, 712.2, 737.1, 904.3, 940.1, 977.4, 1002.2, 1082.1, 1102.5, 1145.8, 1326.9, 1351.2, 1389.3, 1607.0, 2172.3, 2944.2, 3037.4, 3090.6, 3400.7, 3727.0
TS(A1-A2_o3)	57.4i, 37.2, 80.0, 99.4, 104.2, 125.8, 164.9, 180.2, 192.0, 207.2, 219.5, 239.7, 253.7, 260.4, 311.6, 323.3, 336.7, 339.9, 373.1, 375.4, 397.3, 425.7, 438.9, 464.2, 538.9, 562.2, 624.0, 636.3, 642.2, 647.9, 653.1, 676.5, 682.3, 685.2, 695.9, 714.3, 734.6, 872.1, 930.3, 997.9, 1026.7, 1028.2, 1054.4, 1151.0, 1321.6, 1375.6, 1405.5, 1606.7, 2055.9, 2970.3, 3051.9, 3090.8, 3563.0, 3708.5
A2_o1_is*H2O	52.1, 58.2, 81.8, 100.5, 123.5, 131.0, 149.6, 160.7, 190.3, 204.9, 231.3, 242.5, 251.9, 257.6, 271.6, 286.2, 320.5, 332.1, 342.1, 357.7, 406.1, 453.0, 480.3, 534.6, 538.1, 584.7, 615.0, 636.0, 650.1, 657.2, 663.8, 669.3, 691.4, 698.2, 713.6, 724.4, 742.4, 756.3, 962.5, 1014.9, 1074.6, 1094.8, 1113.8, 1162.5, 1334.4, 1388.3, 1408.2, 1590.3, 1880.0, 2992.5, 3071.7, 3117.0, 3609.7, 3760.7
A2_o1_os*H2O	43.6, 61.5, 66.8, 91.2, 110.1, 142.5, 156.3, 175.5, 197.4, 211.4, 236.9, 243.0, 251.0, 257.1, 268.9, 313.6, 330.9, 346.4, 353.9, 366.6, 411.3, 451.7, 457.8, 531.2, 548.3, 583.1, 615.8, 641.5, 650.0, 655.1, 664.2, 667.1, 692.5, 702.6, 712.7, 725.7, 738.6, 780.2, 960.4, 1017.7, 1074.4, 1094.9, 1112.1, 1170.5, 1347.8, 1399.1, 1416.7, 1596.2, 1903.8, 2931.7, 3022.3, 3091.3, 3625.7, 3737.1
A2_o3_is*H2O	26.0, 40.1, 87.5, 89.7, 104.2, 115.1, 137.7, 158.4, 179.4, 204.8, 214.1, 234.1, 257.7, 259.5, 293.0, 305.8, 324.6, 343.4, 362.5, 364.8, 394.1, 410.7, 463.8, 513.4, 521.9, 581.4, 620.8, 641.5, 646.7, 656.6, 662.2, 679.5, 686.1, 689.2, 720.2, 733.1, 748.3, 801.6, 951.1, 1019.5, 1045.6, 1057.7, 1073.6, 1143.8, 1339.6, 1396.0, 1408.4, 1599.7, 1936.1, 2982.3, 3055.5, 3099.5, 3632.3, 3752.7
A2_o1_is	58.6, 83.1, 113.2, 157.6, 169.4, 176.2, 201.0, 234.8, 245.6, 250.2, 260.4, 315.9, 331.6, 343.9, 356.1, 401.5, 471.2, 529.3, 568.3, 585.2, 618.9, 627.8, 640.6, 645.4, 667.7, 670.0, 685.7, 702.6, 714.6, 734.7, 740.3, 779.1, 958.0, 1023.3, 1076.8, 1089.9, 1137.3, 1172.6, 1340.2, 1402.8, 1409.2, 1893.9, 2985.4, 3060.1, 3100.7
A2_o1_os	46.3, 78.9, 105.7, 149.5, 158.5, 178.0, 205.5, 238.9, 247.3, 253.4, 265.5, 315.5, 333.0, 347.0, 360.7, 416.5, 440.4, 533.2, 575.1, 586.7, 624.0, 633.2, 647.2, 649.9, 663.3, 670.3, 688.9, 708.3, 718.0, 737.9, 739.0, 774.9, 957.1, 1024.1, 1077.4, 1087.7, 1130.2, 1164.6, 1338.1, 1402.6, 1412.0, 1887.1, 2986.9, 3058.9, 3101.7
A2_o3_is	47.4, 92.0, 104.9, 139.1, 164.9, 180.3, 205.1, 211.2, 236.3, 258.0, 302.7, 327.7, 342.0, 357.2, 368.9, 401.9, 460.8, 517.5, 531.6, 582.5, 619.7, 636.9, 642.5, 652.2, 664.2, 677.1, 684.6, 686.7, 722.8, 730.8, 752.8, 804.0, 953.2, 1019.8, 1052.7, 1068.4, 1097.1, 1144.9, 1341.5, 1396.0, 1406.1, 1929.4, 2983.0, 3055.9, 3101.5
TS(A2_o1_pos2-A3)	81.5i, 35.0, 58.7, 106.2, 134.8, 186.6, 269.7, 317.9, 334.4, 363.1, 376.5, 560.0, 583.2, 628.6, 659.6, 684.8, 923.8, 957.7, 985.4, 1025.5, 1272.8, 1312.2, 1342.3, 2266.1, 2771.8, 2997.2, 3059.3
TS(A2_o3-pos1-A3)	8.4i, 45.0, 82.0, 139.3, 168.9, 190.8, 210.2, 218.0, 253.6, 277.3, 300.9, 320.3, 335.7, 347.4, 358.0, 374.5, 393.2, 398.0, 422.1, 560.0, 630.3, 633.6, 640.6, 644.4, 656.7, 662.0, 668.9, 676.3, 684.3, 703.6, 723.7, 940.8, 976.6, 993.0, 1039.0, 1056.9, 1077.9, 1127.8, 1304.8, 1322.2, 1331.2, 2219.5, 2449.2, 2951.7, 3051.1

A3	32.0, 58.2, 75.5, 145.9, 169.9, 191.0, 206.9, 214.2, 251.4, 281.7, 299.9, 322.5, 334.6, 342.8, 359.8, 376.9, 396.8, 414.2, 451.4, 559.1, 629.4, 633.0, 639.8, 642.9, 657.6, 659.6, 669.9, 676.3, 683.9, 703.9, 724.2, 928.3, 989.6, 1001.4, 1021.8, 1058.5, 1091.3, 1137.7, 1310.3, 1321.7, 1325.6, 2161.0, 2328.5, 2952.7, 3041.5
TS(A3-C3)	687.0i, 29.8, 65.2, 86.6, 134.1, 187.4, 197.3, 207.4, 246.6, 261.6, 264.4, 311.0, 333.6, 344.9, 362.7, 373.1, 387.3, 484.6, 524.2, 547.1, 584.9, 625.8, 638.8, 647.0, 656.1, 664.2, 679.4, 684.1, 686.1, 706.0, 717.9, 740.5, 879.6, 934.8, 1011.5, 1071.2, 1073.4, 1090.5, 1143.1, 1225.5, 1328.3, 1391.9, 2222.1, 2984.4, 3082.8
ZOH*Ketene	42.1, 54.0, 67.6, 95.8, 144.9, 195.7, 198.1, 209.7, 223.7, 241.2, 248.4, 286.5, 319.2, 332.6, 349.3, 350.9, 390.9, 407.9, 514.1, 541.2, 602.6, 606.2, 630.0, 636.3, 643.3, 661.5, 669.0, 687.5, 695.5, 714.5, 720.4, 739.6, 748.8, 815.5, 922.7, 1088.0, 1134.0, 1138.9, 1165.4, 1200.1, 1338.8, 2151.3, 3088.4, 3128.3, 3185.2
ZOH*2xKetene	41.2, 55.7, 61.4, 65.7, 78.0, 83.4, 106.7, 111.9, 140.6, 171.1, 196.8, 197.4, 204.1, 215.6, 242.3, 246.8, 276.1, 285.6, 321.2, 331.4, 348.2, 351.3, 391.5, 421.2, 424.1, 515.3, 518.3, 548.1, 592.2, 605.2, 627.6, 635.2, 639.4, 643.5, 657.2, 665.7, 684.5, 699.7, 709.0, 720.7, 741.4, 752.7, 822.1, 924.6, 935.8, 1091.0, 1136.0, 1141.5, 1144.2, 1170.3, 1211.7, 1340.8, 1346.9, 2135.3, 2168.4, 3048.9, 3078.2, 3090.7, 3173.9, 3186.2
ZOH*AcOH*Ketene	40.6, 64.1, 66.2, 73.8, 83.2, 88.0, 103.1, 123.9, 140.7, 146.8, 152.2, 194.7, 211.9, 214.3, 215.7, 242.9, 252.3, 263.5, 300.2, 325.8, 342.7, 358.9, 399.5, 414.6, 420.2, 474.5, 515.7, 545.6, 576.3, 593.3, 601.3, 621.8, 630.8, 644.0, 657.9, 661.5, 665.3, 679.1, 685.6, 697.6, 712.9, 733.7, 907.7, 912.5, 931.7, 990.1, 1006.0, 1021.3, 1102.1, 1121.5, 1141.7, 1157.7, 1173.9, 1327.0, 1342.6, 1345.3, 1354.1, 1399.9, 1417.0, 1497.9, 1577.8, 1762.8, 2166.1, 2251.7, 3000.5, 3066.8, 3095.5, 3116.4, 3188.8
TS(C2-C3)	742.3i, 14.3, 27.7, 42.2, 56.0, 63.5, 82.6, 91.6, 106.6, 155.0, 186.0, 204.1, 211.7, 235.8, 253.5, 267.3, 280.9, 302.5, 320.0, 344.0, 356.9, 362.9, 363.3, 422.9, 481.5, 513.1, 527.8, 560.0, 577.8, 611.2, 629.2, 640.6, 645.4, 650.4, 657.9, 676.5, 684.3, 686.2, 705.1, 719.4, 732.2, 877.5, 916.5, 943.2, 998.7, 1065.8, 1084.9, 1114.9, 1138.0, 1165.6, 1231.0, 1327.1, 1341.8, 1377.6, 2165.1, 2209.2, 2989.8, 3066.4, 3073.3, 3175.0
ZOH*Acetylketene	37.8, 42.3, 53.8, 67.8, 87.1, 118.4, 125.9, 150.6, 165.7, 196.7, 204.5, 237.2, 243.3, 259.1, 307.0, 323.5, 336.0, 351.8, 356.8, 377.0, 407.2, 502.3, 517.6, 552.6, 584.1, 615.4, 632.8, 640.4, 645.2, 657.5, 660.1, 666.9, 681.0, 684.8, 691.0, 712.2, 730.6, 736.2, 835.8, 860.5, 994.3, 1006.6, 1073.0, 1099.5, 1116.7, 1146.3, 1151.8, 1258.0, 1343.2, 1376.5, 1403.1, 1445.4, 1446.0, 1473.5, 1742.9, 2188.0, 2966.7, 3035.2, 3067.3, 3100.6
TS(C3-C4)_catalyzed	75.2i, 42.4, 49.6, 82.4, 90.6, 99.4, 135.1, 139.4, 156.0, 177.0, 194.6, 206.5, 218.0, 237.2, 244.7, 269.7, 283.9, 315.3, 325.4, 339.6, 357.6, 385.8, 398.6, 407.6, 409.5, 420.3, 520.4, 550.0, 559.8, 585.6, 622.8, 632.6, 634.5, 635.1, 642.2, 646.8, 650.6, 654.6, 670.4, 678.2, 695.1, 697.9, 727.3, 737.6, 905.0, 950.7, 988.9, 1002.2, 1042.1, 1083.8, 1090.3, 1107.4, 1160.1, 1177.7, 1335.0, 1342.3, 1391.6, 1432.3, 1462.7, 1584.9, 1605.5, 2104.8, 2577.0, 2968.7, 3048.2, 3096.6, 3106.4, 3299.6, 3676.7
ZOH*3-hydroxybut-2-enoic_acid	37.1, 40.3, 72.7, 90.8, 92.3, 113.5, 129.5, 147.4, 185.2, 197.6, 208.4, 228.8, 242.3, 267.5, 275.1, 311.4, 317.8, 335.8, 350.0, 356.1, 382.8, 388.6, 471.2, 540.9, 561.8, 571.0, 627.0, 636.4, 641.6, 653.0, 662.3, 673.7, 680.9, 685.4, 692.8, 697.0, 716.4, 720.8, 749.7, 793.9, 845.6, 862.6, 906.1, 931.2, 969.0, 1008.3, 1023.4, 1047.0, 1068.3, 1084.9, 1159.0, 1164.6, 1230.8, 1262.6, 1318.2, 1349.8, 1386.0, 1416.6, 1422.3, 1463.7, 1542.7, 1618.1, 1747.4, 2984.1, 2989.5, 3050.8, 3093.4, 3155.8, 3219.5
TS(C4-C5)	960.9i, 48.5, 59.9, 74.2, 79.0, 92.7, 102.4, 129.6, 163.9, 192.3, 206.6, 221.9, 234.4, 249.9, 263.9, 309.6, 322.4, 337.7, 356.5, 364.4, 371.3, 375.6, 435.2, 482.8, 537.0, 570.6, 594.9, 631.0, 635.6, 641.8, 654.8, 660.0, 670.9, 675.7, 679.6, 682.6, 693.5, 719.7, 721.5, 733.6, 758.1, 891.4, 921.6, 939.6, 952.8, 994.8, 1006.3, 1060.0, 1078.4, 1084.0, 1137.4, 1143.9, 1164.4, 1185.4, 1319.1, 1333.6, 1364.7, 1393.0, 1411.0, 1427.7, 1484.1, 1570.6, 1660.3, 2473.4, 2953.8, 3038.6, 3077.7, 3089.8, 3376.5
C5	41.3, 46.7, 51.6, 62.8, 73.4, 81.9, 145.1, 164.2, 173.1, 193.1, 208.1, 217.7, 246.7, 253.5, 305.1, 306.3, 327.9, 339.8, 361.8, 363.4, 387.8, 398.9, 436.3, 468.9, 531.0, 561.3, 573.3, 622.9, 627.9, 635.5, 638.9, 652.2, 658.0, 671.6, 675.9, 685.1, 694.4, 714.0, 722.0, 774.8, 812.6, 871.5, 898.5, 967.9, 1002.9, 1032.7, 1057.8, 1069.7, 1090.9, 1140.9, 1165.7, 1191.2, 1230.2, 1244.9, 1316.8, 1329.1, 1360.6, 1382.1, 1416.3, 1460.8, 1623.3, 1701.3, 1815.8, 2729.3, 2933.5, 3001.5, 3020.1, 3094.7, 3236.2
TS(C5-E1)	211.6i, 12.7, 51.0, 66.3, 75.8, 77.6, 87.0, 111.7, 132.9, 191.3, 201.9, 209.8, 222.9, 249.1, 266.4, 307.8, 329.0, 340.7, 351.7, 357.6, 365.9, 381.5, 391.7, 446.5, 502.7, 552.7, 558.7, 607.0, 627.6, 635.6, 638.9, 640.4, 648.6, 665.1, 672.3, 678.6, 682.1, 698.8, 707.9, 720.1, 736.5, 835.3, 875.0, 906.0, 970.5, 993.4, 1050.8, 1070.0, 1084.0, 1132.0, 1140.8, 1149.2, 1176.6, 1272.5, 1311.6, 1337.1, 1385.3, 1393.0, 1395.9, 1448.2, 1572.4, 1733.5, 2841.0, 2910.2, 2956.0, 3005.5, 3063.7, 3093.8, 3423.4
TS(C4-E1)	861.1i, 51.3, 56.3, 79.2, 100.6, 109.4, 116.6, 132.7, 141.2, 181.0, 194.8, 213.6, 220.8, 241.2, 258.3, 280.9, 316.7, 328.9, 346.1, 359.2, 362.9, 382.4, 421.4, 498.3, 535.4, 545.7, 573.8, 610.7, 629.2, 641.9, 647.7, 648.9, 655.2, 660.9, 670.0, 686.4, 688.2, 696.6, 703.3, 724.1, 740.3, 748.7, 853.2, 879.6, 931.7, 945.4, 998.0, 1014.1, 1074.0, 1091.4, 1102.1, 1151.4, 1172.2, 1189.5, 1259.0, 1334.1, 1349.8, 1367.8, 1395.5, 1430.1, 1488.8, 1503.6, 1721.9, 2964.6, 3038.6, 3078.4, 3129.7, 3171.1, 3570.0
TS(A1-E1)	223.4i, 31.8, 53.0, 63.3, 72.7, 100.7, 115.6, 143.9, 209.5, 215.3, 221.0, 224.3, 243.8, 257.4, 258.3, 305.6, 318.8, 330.8, 343.8, 359.1, 365.3, 392.5, 405.0, 415.7, 444.4, 506.8, 558.7, 590.5, 629.0, 639.8, 644.9, 652.2, 656.1, 659.8, 662.5, 674.4, 686.9, 691.3, 699.6, 723.6, 774.7, 798.4, 841.5, 872.0, 949.3, 967.7, 990.1, 1041.9, 1064.1, 1074.9, 1105.9, 1129.9, 1143.5, 1152.9, 1207.3, 1318.5, 1341.2, 1355.9, 1418.4, 1434.0, 1474.9, 2199.2, 2935.2, 2982.6, 2986.2, 3005.2, 3060.7, 3066.5, 3089.3
TS(A1-B1)	38.4, 58.7, 66.2, 94.1, 121.0, 128.6, 157.7, 202.2, 221.4, 238.2, 244.6, 259.6, 299.8, 322.1, 336.8, 351.6, 372.1, 401.5, 489.6, 566.9, 583.2, 611.6, 634.7, 649.0, 655.5, 662.1, 666.9, 672.5, 686.7, 692.3, 706.0, 722.9, 739.8, 865.1, 912.4, 977.2, 1007.4, 1021.9, 1049.4, 1100.7, 1124.9, 1152.6, 1291.8, 1334.1, 1364.8, 1401.7, 1417.8, 1444.7, 1546.5, 1755.3, 2771.4, 2985.8, 3058.8, 3102.4
ZOH*Ethene-1,1-diol	15.2, 39.5, 50.5, 83.0, 120.8, 167.4, 192.3, 216.9, 221.3, 262.9, 276.0, 298.2, 305.7, 328.0, 345.8, 362.5, 386.4, 403.8, 449.6, 523.8, 545.4, 609.2, 618.4, 638.5, 649.8, 653.5, 668.2, 674.5, 681.0, 684.9, 690.1, 707.9, 725.5, 734.5,

	749.8, 821.9, 850.5, 885.1, 930.9, 948.6, 1042.3, 1071.7, 1110.3, 1158.9, 1199.5, 1329.3, 1394.6, 1431.8, 1702.8, 2560.5, 3108.9, 3159.5, 3206.5, 3680.8
ZOH*AcOH*Ethene-1_1-diol	41.1, 45.0, 58.3, 62.9, 68.5, 75.8, 81.6, 87.2, 95.8, 121.9, 135.8, 149.0, 163.9, 215.0, 218.6, 245.3, 258.1, 278.1, 309.0, 331.7, 352.8, 377.9, 393.4, 402.9, 412.6, 450.3, 467.1, 526.0, 544.5, 568.4, 598.4, 614.6, 626.9, 636.1, 645.3, 648.5, 654.1, 666.1, 674.6, 682.6, 693.1, 704.5, 706.4, 714.1, 735.5, 736.7, 911.1, 912.4, 924.1, 944.1, 954.7, 993.2, 1012.1, 1026.7, 1047.2, 1123.5, 1169.7, 1176.5, 1241.7, 1283.1, 1320.0, 1340.4, 1375.5, 1384.8, 1394.7, 1420.0, 1523.8, 1585.1, 1701.4, 1817.3, 2553.0, 2976.6, 3056.2, 3105.5, 3111.1, 3210.8, 3374.1, 3619.9
TS(B1-B2)	186.1i, 31.1, 45.6, 52.0, 79.2, 103.8, 118.7, 130.2, 139.2, 145.5, 214.8, 220.6, 236.2, 248.2, 254.2, 257.6, 266.0, 280.0, 314.3, 332.0, 355.4, 377.2, 395.6, 421.3, 433.6, 445.5, 476.0, 512.1, 554.6, 567.6, 588.9, 641.2, 643.2, 649.9, 654.6, 655.6, 664.1, 672.3, 679.8, 692.7, 697.2, 699.2, 729.8, 744.6, 813.8, 830.7, 870.5, 878.1, 923.0, 963.5, 982.3, 983.0, 997.9, 1005.9, 1011.0, 1054.3, 1116.7, 1173.6, 1222.4, 1260.4, 1321.4, 1348.1, 1372.0, 1401.9, 1420.6, 1440.7, 1458.9, 1524.3, 1604.6, 2856.2, 2896.1, 2951.1, 2970.6, 3058.7, 3103.8, 3108.3, 3204.4, 3634.6
ZOH*3_3-dihydroxybutanoic_acid	34.0, 45.8, 50.6, 81.7, 91.9, 99.0, 128.5, 158.7, 181.2, 208.3, 214.8, 232.0, 239.6, 252.5, 296.5, 307.7, 318.9, 322.9, 330.2, 355.7, 364.5, 390.7, 420.4, 429.7, 442.5, 466.8, 505.8, 521.3, 557.1, 576.4, 581.7, 632.5, 641.6, 645.8, 653.0, 659.0, 665.8, 670.5, 680.7, 683.4, 686.9, 698.4, 711.0, 730.1, 780.5, 843.8, 888.5, 911.7, 926.1, 936.5, 1018.0, 1053.6, 1066.7, 1072.8, 1103.6, 1137.9, 1156.2, 1184.3, 1225.5, 1251.8, 1293.1, 1317.0, 1345.6, 1415.9, 1430.3, 1439.8, 1471.3, 1478.7, 1570.3, 1749.9, 2979.3, 3011.2, 3058.0, 3076.2, 3079.5, 3359.9, 3387.0, 3646.2
TS(B2-E1)	1348.5i, 42.8, 48.2, 62.7, 72.7, 75.1, 87.9, 109.2, 138.6, 196.8, 204.0, 214.8, 220.7, 227.1, 247.3, 251.2, 293.6, 306.2, 309.7, 330.6, 334.4, 349.1, 359.9, 383.9, 390.9, 399.0, 433.3, 515.3, 530.7, 546.2, 588.1, 601.0, 642.4, 656.4, 660.1, 670.8, 677.6, 679.2, 687.5, 695.1, 708.4, 715.7, 726.7, 743.1, 757.0, 785.6, 798.5, 849.0, 896.5, 904.1, 954.7, 972.4, 1025.0, 1061.9, 1083.4, 1096.1, 1133.1, 1162.1, 1192.5, 1235.4, 1310.1, 1322.4, 1344.2, 1352.1, 1393.0, 1406.7, 1422.4, 1435.4, 1704.3, 2008.1, 2932.4, 2954.6, 2978.9, 3019.1, 3053.2, 3086.5, 3262.8, 3641.2
TS(B2-B3)	80.6i, 27.3, 53.9, 56.9, 80.8, 103.4, 114.3, 145.5, 177.6, 195.8, 206.2, 211.8, 228.8, 242.1, 253.7, 291.2, 304.7, 328.4, 334.4, 340.0, 359.5, 363.8, 382.7, 389.1, 403.9, 422.9, 460.2, 508.4, 549.2, 566.4, 569.9, 627.5, 634.9, 636.8, 639.4, 641.0, 649.7, 658.4, 669.1, 677.6, 694.1, 703.1, 713.4, 768.5, 841.2, 886.7, 912.8, 949.8, 958.5, 1022.6, 1049.0, 1065.7, 1083.3, 1088.7, 1124.5, 1148.8, 1166.2, 1222.4, 1238.0, 1271.2, 1293.2, 1361.1, 1380.0, 1382.4, 1391.8, 1432.5, 1439.8, 1496.4, 1610.1, 1928.7, 2876.1, 2937.5, 2986.5, 3047.2, 3071.8, 3078.4, 3477.9, 3665.3
B3	40.2, 50.8, 56.5, 75.5, 83.4, 99.8, 122.1, 155.5, 159.3, 193.4, 208.5, 210.3, 239.2, 241.7, 252.0, 273.7, 305.8, 325.5, 331.5, 338.6, 358.9, 366.3, 385.3, 386.1, 417.7, 449.2, 504.3, 539.6, 550.1, 565.3, 603.2, 615.4, 629.8, 634.6, 636.1, 639.0, 652.7, 659.4, 664.3, 676.2, 702.5, 704.5, 714.1, 784.5, 846.5, 892.8, 909.0, 929.4, 950.8, 1027.7, 1066.7, 1067.5, 1089.3, 1106.5, 1138.3, 1149.2, 1168.9, 1213.6, 1224.8, 1254.8, 1265.0, 1361.3, 1379.9, 1385.0, 1398.4, 1432.4, 1439.7, 1530.0, 1602.8, 2014.9, 2881.6, 2987.3, 3012.6, 3046.8, 3071.4, 3080.1, 3280.7, 3673.5
TS(B3-C5)	96.8i, 26.2, 38.1, 56.0, 83.2, 87.2, 107.4, 119.8, 195.1, 198.3, 205.2, 207.3, 210.4, 221.0, 238.2, 249.0, 260.2, 291.1, 304.9, 321.8, 336.7, 358.9, 362.3, 364.1, 386.4, 387.6, 405.2, 456.2, 528.4, 554.8, 559.3, 588.4, 624.4, 633.7, 635.8, 638.0, 642.4, 652.7, 664.4, 675.9, 679.2, 699.2, 703.0, 716.0, 764.0, 773.3, 842.8, 852.9, 886.9, 901.8, 981.9, 1001.0, 1058.8, 1087.6, 1105.2, 1118.3, 1162.9, 1178.8, 1226.1, 1254.8, 1345.3, 1354.0, 1365.9, 1368.6, 1414.9, 1440.4, 1458.0, 1514.0, 1704.8, 2939.9, 2969.1, 2976.5, 3043.0, 3088.1, 3222.5, 3305.8, 3356.2, 3585.3
C5*H2O	34.6, 42.9, 60.2, 68.9, 81.9, 94.6, 109.3, 122.5, 132.9, 140.2, 151.2, 176.5, 191.9, 208.4, 221.6, 242.3, 256.2, 277.3, 305.1, 317.6, 333.2, 342.8, 345.5, 362.8, 376.2, 406.0, 411.8, 428.9, 439.6, 540.6, 563.3, 577.7, 598.4, 631.2, 636.9, 640.9, 649.3, 660.2, 669.9, 684.3, 687.7, 704.9, 711.6, 725.8, 747.1, 828.2, 851.7, 868.4, 904.5, 961.9, 1012.3, 1017.6, 1062.7, 1096.3, 1109.6, 1165.6, 1175.3, 1178.1, 1214.7, 1307.5, 1323.5, 1350.7, 1359.0, 1399.8, 1406.2, 1442.9, 1535.4, 1609.5, 1641.5, 1727.3, 2388.8, 2869.7, 2950.4, 3001.1, 3015.1, 3093.3, 3552.2, 3705.2
B4_o1_pos1	27.5, 37.5, 51.8, 56.7, 68.9, 84.6, 90.2, 109.0, 125.3, 157.2, 159.4, 185.2, 220.7, 239.2, 246.6, 260.7, 264.4, 318.6, 334.2, 340.4, 383.1, 399.5, 407.2, 449.9, 466.5, 524.1, 540.9, 548.4, 583.7, 613.5, 614.5, 640.5, 649.1, 654.6, 668.6, 673.6, 684.3, 695.3, 696.3, 705.7, 721.1, 736.7, 742.9, 745.4, 758.4, 910.2, 943.6, 958.4, 1019.7, 1059.4, 1076.4, 1118.8, 1154.5, 1187.9, 1247.7, 1279.2, 1335.8, 1376.4, 1392.1, 1404.8, 1704.3, 1880.1, 2993.1, 3063.1, 3110.6, 3112.7, 3210.1, 3387.2, 3620.5
B4_o1_pos2	35.9, 46.5, 54.3, 57.9, 64.3, 79.8, 85.2, 118.0, 131.5, 155.1, 168.2, 181.0, 217.9, 240.6, 248.2, 255.5, 266.1, 317.3, 335.2, 348.3, 373.8, 406.8, 412.9, 450.1, 455.2, 523.1, 533.0, 551.8, 580.2, 608.2, 612.9, 632.8, 639.4, 650.8, 668.3, 671.0, 673.9, 694.1, 697.5, 707.1, 714.6, 732.5, 739.4, 744.3, 768.7, 911.4, 944.0, 956.0, 1016.4, 1064.4, 1078.4, 1107.5, 1152.9, 1187.0, 1237.1, 1271.7, 1342.0, 1376.3, 1403.8, 1407.8, 1705.3, 1897.9, 2985.2, 3054.7, 3100.3, 3112.2, 3211.9, 3403.1, 3617.7
B4_o3	23.3, 36.2, 53.8, 64.3, 78.2, 95.6, 107.4, 109.8, 110.9, 136.7, 164.3, 187.3, 212.4, 220.7, 245.4, 261.0, 306.9, 331.1, 345.6, 356.9, 384.4, 398.4, 430.9, 449.1, 469.2, 513.2, 523.0, 529.4, 578.7, 613.1, 617.4, 643.3, 650.1, 653.3, 664.9, 671.9, 676.5, 689.9, 696.0, 711.2, 716.8, 727.6, 744.8, 748.1, 800.6, 912.9, 942.2, 951.3, 1020.4, 1039.0, 1060.3, 1070.1, 1112.5, 1191.0, 1237.4, 1286.9, 1341.4, 1373.9, 1395.5, 1404.2, 1704.8, 1936.5, 2981.9, 3052.1, 3100.5, 3112.5, 3211.9, 3398.9, 3597.4
TS(B4-E1_o1_pos1)	142.1i, 50.1, 61.6, 75.8, 82.6, 101.0, 122.2, 137.4, 143.9, 160.2, 179.0, 209.1, 210.3, 218.0, 236.0, 252.8, 271.7, 304.9, 312.3, 345.2, 346.7, 365.7, 385.7, 402.6, 429.0, 442.8, 506.6, 537.5, 557.0, 604.3, 632.8, 637.2, 637.5, 644.5, 653.9, 656.5, 668.5, 679.4, 680.2, 700.2, 712.7, 715.4, 732.0, 737.3, 907.1, 917.6, 924.0, 948.4, 975.9, 989.9, 1049.8, 1078.9, 1159.4, 1207.5, 1262.5, 1303.1, 1312.4, 1341.1, 1376.3, 1377.8, 1674.0, 2127.0, 2968.0, 3054.8, 3066.1, 3108.7, 3214.6, 3350.6, 3527.6
TS(B4-E1_o1_pos2)	42.7i, 51.7, 58.2, 67.6, 85.9, 88.9, 111.1, 121.5, 133.2, 145.4, 198.1, 211.0, 223.2, 228.5, 243.5, 262.5, 268.7, 315.3, 321.8, 337.9, 357.5, 361.7, 383.6, 401.5, 406.9, 445.3, 538.5, 559.2, 609.4, 623.4, 630.2, 633.9, 640.9, 649.7, 652.2, 662.6, 667.2, 669.6, 680.4, 696.8, 714.6, 730.5, 745.0, 763.1, 899.2, 949.6, 950.0, 958.0, 986.8, 1011.1, 1045.7, 1088.7, 1152.6, 1219.0, 1256.7, 1307.4, 1322.7, 1330.1, 1364.8, 1383.4, 1682.6, 2241.0, 2680.5, 2961.7, 3017.5, 3109.8, 3210.9, 3274.7, 3398.6

TS(B4-E1_o3)	77.5i, 47.8, 63.4, 71.8, 84.3, 95.9, 116.5, 129.4, 142.2, 161.3, 186.9, 203.1, 207.0, 219.4, 243.5, 252.7, 257.4, 261.9, 303.7, 313.0, 319.1, 329.4, 342.2, 364.8, 372.6, 377.0, 393.6, 396.3, 413.7, 421.3, 438.5, 446.0, 525.4, 550.9, 560.0, 621.2, 635.2, 635.6, 640.9, 645.4, 657.2, 665.8, 680.2, 682.5, 688.0, 695.0, 705.6, 712.4, 729.9, 734.9, 912.8, 919.2, 921.9, 948.6, 972.9, 990.2, 992.9, 1009.9, 1018.8, 1042.3, 1061.1, 1134.9, 1206.5, 1256.9, 1289.4, 1314.1, 1358.5, 1374.1, 1394.8, 1684.5, 2106.0, 2953.9, 3031.0, 3068.3, 3114.2, 3223.1, 3363.3, 3520.4
A2_o1_pos1*Ketene	22.3, 46.9, 49.9, 61.4, 71.6, 85.6, 105.3, 107.6, 137.3, 150.1, 167.9, 175.4, 204.4, 235.0, 245.3, 251.8, 258.8, 315.9, 332.3, 345.4, 358.4, 400.9, 419.6, 468.3, 507.2, 532.5, 563.2, 572.4, 588.1, 627.2, 637.1, 641.5, 648.3, 660.4, 674.2, 688.9, 704.4, 719.0, 735.1, 737.6, 774.8, 937.4, 959.0, 1022.6, 1079.1, 1090.3, 1126.5, 1137.8, 1164.5, 1339.6, 1346.7, 1399.8, 1408.6, 1879.1, 2165.5, 2986.2, 3061.4, 3101.3, 3102.9, 3195.7
A2_o1_pos2*Ketene	28.0, 32.1, 53.2, 57.3, 76.3, 79.6, 85.3, 116.8, 156.4, 161.6, 176.4, 181.4, 211.4, 240.6, 249.2, 252.5, 266.1, 318.5, 334.3, 347.6, 358.9, 416.1, 428.8, 443.0, 509.6, 533.7, 568.5, 572.8, 584.7, 622.3, 634.5, 646.7, 649.1, 664.4, 674.6, 689.1, 705.1, 716.8, 733.3, 737.5, 770.9, 942.0, 956.8, 1023.9, 1077.3, 1089.6, 1120.0, 1142.3, 1158.0, 1339.7, 1351.0, 1402.3, 1412.7, 1888.1, 2165.4, 2984.3, 3054.7, 3088.5, 3099.5, 3186.0
A2_o3*Ketene	22.1, 38.8, 45.1, 58.6, 72.5, 94.1, 100.8, 117.3, 138.7, 163.9, 167.9, 185.0, 209.2, 215.1, 237.1, 257.7, 303.4, 326.5, 342.0, 360.8, 371.3, 405.9, 429.4, 462.2, 511.8, 521.3, 542.0, 582.7, 590.5, 620.8, 639.0, 644.2, 654.3, 662.5, 680.5, 684.7, 686.8, 723.7, 732.2, 748.6, 795.1, 932.1, 955.0, 1019.7, 1050.9, 1068.4, 1082.8, 1138.6, 1147.1, 1339.7, 1350.6, 1395.7, 1407.4, 1915.3, 2159.7, 2981.4, 3053.8, 3084.8, 3099.9, 3177.6
TS(A2-C3_o1_pos1)	123.9i, 31.8, 46.9, 53.7, 62.8, 74.0, 86.4, 137.8, 169.0, 170.1, 205.6, 210.7, 219.9, 234.2, 253.9, 258.5, 294.5, 314.3, 330.0, 331.0, 350.8, 357.3, 362.6, 370.7, 409.7, 425.0, 532.4, 557.8, 629.2, 634.8, 644.8, 645.8, 649.0, 655.2, 656.6, 670.2, 682.1, 691.5, 710.6, 723.5, 908.9, 936.5, 944.6, 970.0, 987.6, 1096.3, 1097.8, 1135.8, 1148.6, 1300.4, 1331.5, 1336.4, 1364.0, 2155.8, 2177.9, 2938.0, 3022.2, 3033.9, 3062.0, 3158.4
TS(A2-C3_o1_pos2)	82.9i, 30.2, 45.1, 56.5, 70.3, 83.9, 90.8, 106.2, 131.1, 173.0, 203.5, 209.6, 221.5, 242.0, 248.1, 253.5, 305.3, 311.6, 322.0, 329.4, 353.1, 360.1, 368.0, 386.9, 402.4, 432.1, 533.2, 561.2, 626.8, 632.6, 637.2, 646.7, 652.2, 659.3, 659.9, 666.4, 682.0, 692.2, 702.8, 721.4, 917.7, 941.4, 957.9, 976.6, 1000.7, 1091.2, 1095.1, 1136.2, 1149.5, 1313.0, 1339.2, 1343.9, 1355.3, 2160.5, 2239.2, 2878.5, 2995.0, 3031.1, 3043.2, 3147.0
TS(A2-D5_o3)	110.9i, 25.2, 54.2, 59.6, 71.7, 105.3, 120.0, 144.0, 165.9, 181.2, 197.5, 212.7, 224.3, 242.0, 256.2, 270.8, 316.0, 319.6, 330.9, 345.6, 352.5, 370.3, 370.8, 390.7, 412.9, 429.2, 535.5, 556.1, 631.5, 635.3, 643.6, 648.0, 654.0, 664.7, 672.7, 678.1, 681.6, 683.0, 707.5, 723.0, 909.8, 932.2, 968.9, 977.1, 1007.5, 1047.8, 1065.1, 1121.9, 1141.4, 1312.2, 1340.5, 1349.2, 1379.6, 2149.2, 2163.4, 2891.7, 2989.6, 3047.2, 3058.0, 3156.7
TS(E1-E2)	157.0i, 28.5, 48.7, 51.9, 71.5, 93.6, 107.7, 110.3, 124.2, 142.1, 155.4, 204.2, 208.1, 217.6, 242.8, 272.1, 287.0, 309.1, 316.2, 336.3, 355.6, 366.8, 388.8, 420.5, 498.1, 524.9, 550.8, 575.1, 605.5, 610.5, 640.3, 644.0, 653.1, 667.5, 675.2, 687.7, 696.8, 707.5, 719.0, 746.1, 788.2, 825.0, 841.9, 851.5, 872.8, 902.1, 968.2, 1007.9, 1019.2, 1056.1, 1076.4, 1158.0, 1224.7, 1240.1, 1267.7, 1341.0, 1379.5, 1412.9, 1421.0, 1440.2, 1568.6, 2073.3, 2694.3, 2967.4, 3035.1, 3078.2, 3082.9, 3172.3, 3261.1
ZOH*Propen-2-ol*CO2	31.6, 41.5, 49.2, 60.0, 65.2, 74.6, 82.3, 90.3, 104.2, 113.4, 126.7, 177.1, 190.9, 202.8, 212.9, 234.0, 260.6, 297.3, 313.5, 330.0, 353.2, 361.6, 392.5, 410.2, 481.3, 500.7, 531.1, 547.4, 565.0, 595.1, 609.4, 611.4, 635.6, 640.9, 651.0, 662.0, 680.0, 683.3, 697.5, 716.2, 718.8, 730.3, 747.8, 762.5, 801.8, 851.7, 953.7, 989.2, 1025.6, 1065.4, 1089.8, 1144.4, 1171.5, 1192.2, 1323.8, 1336.0, 1360.5, 1403.4, 1415.3, 1433.3, 1641.5, 2372.6, 2961.3, 3016.0, 3071.1, 3081.7, 3173.2, 3392.5, 3531.1
ZOH*Propen-2-ol	57.5, 72.3, 87.5, 92.8, 121.3, 171.0, 199.9, 205.1, 213.1, 223.3, 241.7, 252.7, 299.5, 318.6, 333.3, 352.4, 354.8, 385.2, 416.0, 481.6, 495.8, 559.8, 614.5, 629.8, 638.5, 642.2, 659.2, 668.5, 682.4, 686.0, 688.0, 713.1, 731.1, 732.2, 739.6, 820.3, 824.4, 845.4, 934.9, 954.5, 989.6, 1031.9, 1085.8, 1129.2, 1169.1, 1186.7, 1286.8, 1363.6, 1392.0, 1419.7, 1420.7, 1441.0, 1680.0, 2402.5, 2968.2, 3028.2, 3076.3, 3094.9, 3184.2, 3428.6
TS(E2-E3)	24.2i, 51.3, 70.1, 75.1, 82.0, 99.8, 184.7, 188.4, 200.7, 208.4, 226.6, 243.6, 301.7, 306.4, 328.5, 353.2, 362.4, 374.0, 405.4, 409.7, 482.7, 503.6, 528.2, 605.0, 640.8, 646.4, 653.1, 665.8, 668.5, 683.9, 689.1, 693.6, 709.1, 730.6, 733.1, 751.0, 765.5, 799.2, 855.9, 951.7, 987.5, 1026.9, 1031.0, 1070.6, 1088.5, 1136.0, 1200.0, 1336.7, 1358.4, 1405.3, 1414.0, 1433.9, 1642.4, 2962.1, 3020.6, 3071.3, 3089.8, 3180.1, 3477.9, 3609.9
ZOH*Acetone	33.6, 53.0, 57.7, 93.7, 110.7, 117.5, 145.3, 155.3, 197.8, 211.0, 217.2, 239.2, 256.2, 288.1, 319.5, 331.1, 350.6, 360.5, 378.6, 400.2, 483.2, 535.6, 582.3, 625.4, 628.9, 632.4, 639.6, 659.7, 669.4, 678.9, 696.4, 702.4, 722.3, 739.7, 812.3, 849.1, 865.0, 885.6, 1050.8, 1071.1, 1078.9, 1122.7, 1138.7, 1169.5, 1248.9, 1330.2, 1346.1, 1389.4, 1396.0, 1400.0, 1412.0, 1432.5, 1601.5, 1894.3, 2963.2, 2970.5, 3023.6, 3032.0, 3101.4, 3101.8
ZOH*Acetone*Propen-2-ol	34.9, 47.7, 55.9, 61.8, 65.1, 72.4, 77.7, 87.0, 95.8, 99.3, 114.4, 130.3, 138.5, 140.8, 189.3, 199.2, 208.5, 239.1, 251.7, 267.7, 308.4, 325.7, 332.6, 355.9, 370.2, 383.1, 407.8, 413.2, 467.1, 481.3, 507.9, 538.9, 587.2, 620.5, 636.5, 638.1, 640.7, 650.2, 660.6, 671.5, 682.8, 687.4, 716.2, 721.0, 725.5, 740.5, 780.4, 806.4, 853.7, 854.1, 860.8, 913.8, 953.1, 988.8, 1025.3, 1050.7, 1058.1, 1061.7, 1080.7, 1148.9, 1156.2, 1180.7, 1258.0, 1324.5, 1330.2, 1341.0, 1359.9, 1384.9, 1396.5, 1401.6, 1405.7, 1415.6, 1433.3, 1435.9, 1474.7, 1525.8, 1646.1, 1768.6, 2954.6, 2960.5, 2963.7, 3021.9, 3027.3, 3036.1, 3067.9, 3081.6, 3086.6, 3097.5, 3172.9, 3535.5
TS(E4-E5)	44.7i, 37.3, 45.5, 51.6, 81.9, 85.3, 95.5, 111.0, 118.5, 136.0, 159.4, 190.4, 202.9, 209.9, 212.8, 218.9, 224.2, 247.2, 253.8, 267.1, 302.6, 324.4, 340.3, 356.5, 386.4, 390.1, 410.5, 421.9, 455.0, 497.4, 513.9, 544.2, 554.3, 630.7, 638.3, 645.4, 648.5, 653.6, 658.9, 667.2, 677.1, 689.9, 700.9, 722.3, 751.3, 797.4, 844.1, 860.7, 862.7, 878.6, 938.2, 952.8, 967.8, 998.7, 1016.0, 1019.9, 1043.8, 1044.3, 1123.1, 1139.9, 1160.6, 1205.1, 1233.0, 1330.7, 1341.5, 1343.2, 1367.8, 1375.0, 1388.3, 1401.6, 1411.4, 1418.9, 1431.0, 1432.1, 1436.0, 1504.4, 1592.2, 2409.7, 2938.6, 2956.6, 2964.6, 3021.0, 3031.6, 3044.6, 3072.5, 3088.6, 3101.0, 3103.4, 3200.3, 3211.5
E5	21.1, 33.9, 54.9, 58.4, 69.4, 82.1, 122.7, 132.8, 140.1, 179.5, 201.0, 211.4, 224.2, 248.2, 268.4, 276.2, 283.6, 300.5, 302.4, 323.9, 329.5, 331.3, 356.5, 368.7, 389.8, 414.5, 428.2, 451.7, 465.8, 493.0, 553.1, 568.7, 620.0, 627.0, 639.7, 647.4, 653.9, 659.3, 666.1, 668.7, 680.5, 689.9, 695.7, 711.9, 723.8, 810.0, 851.2, 869.5, 907.5, 937.7, 964.4, 971.0, 987.2, 998.5, 1007.2, 1099.4, 1110.1, 1117.9, 1138.8, 1146.9, 1186.2, 1239.6, 1251.1, 1323.9, 1336.9, 1342.0,

	1359.1, 1371.2, 1384.6, 1400.2, 1415.4, 1422.6, 1434.3, 1440.4, 1444.7, 1457.5, 1552.9, 1665.1, 2952.6, 2970.0, 2975.4, 3007.9, 3031.5, 3047.9, 3051.1, 3058.6, 3062.8, 3085.3, 3087.4, 3432.2
TS(E5-E6)	868.1i, 22.8, 47.3, 53.3, 74.3, 84.4, 104.5, 114.6, 125.0, 180.9, 195.5, 207.3, 226.5, 243.3, 262.2, 265.3, 275.7, 300.9, 309.0, 317.6, 326.8, 339.1, 353.2, 366.0, 370.5, 378.3, 393.5, 415.0, 447.5, 468.8, 514.0, 571.2, 604.1, 626.9, 632.6, 643.7, 648.5, 656.7, 663.6, 670.3, 680.7, 683.3, 697.3, 717.7, 734.2, 762.4, 860.4, 870.8, 903.8, 912.7, 936.7, 965.8, 976.9, 993.7, 1006.7, 1021.5, 1081.1, 1083.4, 1097.3, 1121.8, 1139.3, 1152.3, 1186.7, 1202.4, 1296.2, 1339.9, 1343.8, 1351.5, 1368.0, 1378.5, 1412.6, 1416.9, 1425.3, 1432.6, 1445.1, 1452.0, 1461.0, 1594.7, 2936.8, 2955.1, 2981.6, 2999.6, 3031.8, 3048.5, 3050.5, 3059.2, 3081.2, 3091.9, 3093.0, 3676.6
ZOH*Z-4-methylpent-2-ene-2-4-diol	43.1, 51.1, 64.0, 73.6, 74.9, 98.0, 104.8, 158.9, 181.9, 195.2, 207.9, 220.5, 233.1, 245.6, 252.9, 256.3, 295.3, 301.0, 312.0, 318.2, 335.2, 341.3, 358.3, 366.9, 373.8, 383.8, 395.8, 417.1, 456.7, 470.9, 550.4, 593.5, 602.3, 624.3, 633.6, 643.8, 650.3, 663.8, 673.0, 680.4, 683.5, 701.8, 725.5, 738.6, 749.1, 788.1, 819.4, 844.0, 857.7, 883.0, 907.9, 914.2, 949.6, 980.9, 1002.2, 1021.5, 1077.8, 1079.2, 1097.2, 1117.3, 1135.7, 1176.8, 1198.2, 1258.0, 1293.0, 1336.4, 1347.0, 1353.0, 1368.3, 1402.3, 1418.6, 1424.3, 1429.9, 1430.8, 1445.5, 1452.2, 1624.3, 2566.8, 2956.3, 2975.9, 2993.1, 3031.8, 3041.6, 3051.3, 3075.0, 3080.9, 3082.2, 3098.5, 3212.9, 3671.1
TS(E6-E7)	31.9i, 16.1, 50.6, 57.3, 66.9, 88.9, 96.7, 137.0, 183.9, 195.5, 206.7, 229.2, 233.3, 245.3, 245.9, 262.1, 279.9, 284.2, 307.9, 311.2, 325.9, 338.1, 347.6, 352.5, 367.0, 384.7, 404.9, 408.0, 450.7, 465.8, 527.0, 559.1, 587.3, 600.8, 609.8, 638.7, 642.1, 649.6, 656.0, 657.3, 685.0, 691.3, 715.0, 733.9, 736.9, 742.4, 782.1, 791.6, 862.0, 889.5, 905.1, 915.0, 936.2, 980.7, 985.5, 1000.1, 1079.9, 1091.8, 1096.1, 1112.2, 1136.2, 1171.3, 1175.3, 1202.4, 1304.6, 1326.7, 1340.0, 1349.2, 1359.8, 1396.5, 1412.8, 1423.5, 1425.3, 1441.8, 1449.6, 1459.1, 1676.0, 2928.5, 2957.2, 2964.9, 3001.4, 3036.6, 3038.1, 3045.7, 3048.3, 3087.6, 3101.1, 3205.1, 3479.2, 3566.9
E7	44.3, 58.7, 78.9, 89.3, 111.0, 123.5, 129.8, 159.4, 182.1, 201.4, 215.6, 231.8, 237.8, 241.1, 256.8, 263.8, 278.2, 304.3, 312.8, 327.2, 340.3, 352.7, 358.5, 370.1, 399.8, 404.2, 448.9, 450.7, 471.6, 540.8, 568.8, 600.4, 617.3, 631.1, 636.3, 637.1, 647.3, 652.8, 663.5, 668.6, 681.6, 698.5, 719.8, 730.5, 766.2, 799.2, 831.7, 891.8, 905.9, 908.2, 929.9, 983.3, 993.0, 1020.5, 1071.8, 1083.7, 1092.9, 1104.9, 1148.2, 1162.6, 1172.9, 1191.7, 1205.3, 1296.8, 1310.1, 1347.0, 1365.8, 1368.8, 1405.3, 1416.1, 1423.4, 1424.5, 1429.5, 1443.1, 1451.6, 1462.7, 1659.5, 1741.1, 1980.7, 2961.3, 2975.5, 2992.5, 3038.8, 3052.7, 3055.8, 3064.0, 3065.5, 3115.1, 3153.4, 3409.3
TS(E7-E8)	222.9i, 13.5, 46.3, 62.2, 73.1, 92.3, 98.5, 144.8, 156.3, 176.0, 195.9, 201.4, 206.6, 230.9, 235.0, 249.3, 256.1, 279.6, 298.4, 311.3, 313.0, 321.4, 337.7, 340.7, 358.7, 369.4, 399.5, 400.7, 413.0, 448.1, 466.4, 557.6, 583.5, 595.2, 627.2, 632.0, 633.4, 645.9, 647.2, 651.2, 661.3, 675.3, 687.6, 715.5, 721.1, 729.6, 774.0, 834.1, 892.9, 902.4, 931.8, 965.3, 974.0, 995.8, 1013.3, 1019.4, 1022.4, 1063.3, 1097.1, 1113.5, 1159.4, 1164.8, 1256.6, 1272.4, 1332.1, 1347.9, 1357.6, 1360.8, 1373.9, 1409.4, 1415.4, 1421.4, 1429.8, 1439.6, 1448.4, 1572.8, 1642.3, 2819.7, 2970.5, 2975.3, 2982.5, 3040.5, 3043.4, 3047.6, 3052.9, 3074.9, 3080.7, 3114.9, 3123.8, 3642.3
ZOH*MO	23.7, 49.5, 62.5, 75.2, 95.3, 119.1, 123.3, 140.3, 165.3, 183.4, 200.4, 206.0, 216.5, 224.9, 239.4, 250.8, 260.4, 309.8, 326.7, 342.2, 354.6, 358.8, 365.9, 379.1, 438.2, 468.5, 478.9, 544.3, 599.0, 616.7, 625.6, 630.5, 633.1, 636.0, 650.8, 653.7, 669.3, 677.2, 695.2, 715.8, 730.4, 813.4, 823.8, 909.7, 929.8, 958.7, 968.3, 998.5, 1005.3, 1038.6, 1041.1, 1093.7, 1107.5, 1150.9, 1176.8, 1235.3, 1244.8, 1316.6, 1331.0, 1338.4, 1366.6, 1395.6, 1400.2, 1407.2, 1413.6, 1425.6, 1433.5, 1453.9, 1542.2, 1590.6, 2165.1, 2955.3, 2968.4, 2976.9, 3005.3, 3017.9, 3049.9, 3077.8, 3088.3, 3113.9, 3136.3
TS(E8-E9)	520.7i, 40.7, 58.8, 69.1, 77.6, 94.2, 107.3, 124.6, 132.7, 174.9, 189.5, 198.8, 204.6, 208.1, 216.3, 236.6, 247.6, 309.7, 315.6, 339.6, 352.9, 357.5, 365.2, 365.5, 376.1, 443.6, 477.9, 499.4, 580.2, 604.5, 619.3, 630.6, 633.2, 643.0, 645.8, 665.6, 672.8, 678.1, 678.8, 714.8, 721.6, 774.4, 804.7, 840.8, 853.1, 890.8, 944.8, 968.8, 974.3, 982.4, 1025.7, 1041.5, 1061.3, 1089.7, 1131.6, 1138.2, 1146.4, 1208.6, 1291.8, 1310.4, 1329.4, 1340.7, 1347.9, 1391.5, 1405.8, 1406.5, 1411.3, 1413.8, 1437.8, 1501.5, 1718.8, 2939.0, 2961.8, 2967.9, 2992.2, 3007.6, 3028.4, 3030.3, 3076.2, 3077.9, 3096.5
E9	42.0, 52.3, 61.0, 67.7, 72.6, 85.5, 88.5, 105.0, 145.7, 184.0, 199.0, 209.5, 213.1, 217.1, 247.6, 255.4, 301.1, 307.0, 325.3, 338.1, 338.6, 362.7, 366.7, 385.5, 400.1, 448.4, 487.8, 507.2, 560.7, 595.9, 628.6, 634.9, 637.2, 642.0, 649.8, 656.0, 669.3, 675.7, 685.1, 690.1, 700.0, 708.6, 731.3, 822.4, 839.7, 934.2, 956.4, 987.7, 1010.2, 1040.8, 1048.8, 1067.5, 1090.7, 1103.2, 1137.1, 1150.7, 1184.7, 1258.5, 1283.7, 1300.6, 1329.2, 1330.7, 1359.7, 1389.0, 1405.8, 1412.2, 1430.0, 1450.1, 1468.1, 1755.4, 2657.8, 2713.8, 2910.0, 2925.5, 2973.2, 2987.0, 3020.7, 3054.7, 3079.1, 3092.0, 3093.1
TS(E9-10_pos2)	59.5i, 10.6, 39.7, 43.2, 53.4, 57.3, 68.4, 83.9, 105.7, 153.7, 161.6, 165.4, 196.0, 204.2, 207.5, 209.9, 239.6, 253.2, 266.8, 307.4, 318.0, 325.8, 344.1, 360.4, 366.3, 382.6, 393.8, 400.9, 436.6, 447.1, 565.2, 627.5, 634.1, 640.4, 651.6, 652.6, 662.5, 670.0, 678.5, 681.1, 696.4, 718.1, 724.7, 814.2, 887.3, 931.1, 935.3, 955.5, 972.3, 978.8, 984.3, 1032.8, 1049.8, 1058.1, 1066.8, 1092.1, 1136.2, 1271.2, 1310.1, 1324.4, 1344.1, 1356.0, 1359.1, 1387.6, 1408.1, 1421.0, 1430.8, 1449.4, 1633.5, 2239.3, 2706.2, 2942.2, 2948.6, 2971.7, 2993.9, 2997.6, 3046.1, 3051.3, 3055.8, 3058.4, 3141.2
TS(E9-10_pos1)	107.9i, 17.1, 32.3, 53.4, 56.8, 59.1, 77.6, 103.6, 129.8, 141.5, 173.1, 180.9, 202.2, 204.6, 213.1, 216.4, 234.3, 245.1, 262.9, 285.0, 313.8, 326.1, 353.3, 356.1, 361.9, 373.0, 379.1, 409.0, 428.2, 447.1, 559.2, 627.0, 635.0, 642.0, 643.3, 653.5, 657.5, 670.0, 677.7, 690.0, 705.6, 712.3, 720.2, 810.5, 894.6, 917.2, 926.6, 947.1, 962.7, 971.8, 975.4, 998.6, 1044.2, 1057.5, 1097.9, 1101.7, 1152.7, 1266.4, 1298.5, 1322.9, 1345.1, 1354.4, 1357.6, 1389.1, 1408.3, 1423.0, 1430.0, 1447.7, 1641.3, 2213.9, 2896.1, 2944.5, 2951.8, 2999.0, 2999.7, 3004.8, 3047.0, 3047.7, 3051.1, 3054.4, 3135.4
A2*Isobutene_pos2	30.9, 47.4, 47.6, 60.4, 67.5, 75.8, 81.4, 91.8, 127.3, 156.9, 166.6, 176.2, 176.7, 208.5, 209.2, 240.3, 246.6, 252.0, 266.0, 317.8, 334.0, 347.8, 358.8, 381.1, 417.6, 432.1, 435.3, 441.6, 532.5, 570.8, 585.6, 621.0, 633.3, 646.1, 647.3, 662.6, 673.2, 685.8, 690.5, 705.2, 716.8, 736.6, 738.1, 776.2, 815.8, 875.6, 934.3, 955.3, 965.6, 983.6, 1023.6, 1049.9, 1061.5, 1076.4, 1088.7, 1129.2, 1164.3, 1263.6, 1338.3, 1354.4, 1357.2, 1389.7, 1403.7, 1410.6, 1411.8, 1424.5, 1431.3, 1446.9, 1662.5, 1889.1, 2942.1, 2947.1, 2982.0, 2992.3, 2996.3, 3043.4, 3049.6, 3052.5, 3053.2, 3097.3, 3140.4
A2*Isobutene_pos1	19.3, 34.3, 48.4, 57.7, 66.8, 80.4, 86.1, 110.8, 137.0, 155.5, 162.0, 182.7, 190.6, 206.0, 215.0, 240.7, 247.0, 255.9, 269.4, 316.2, 333.9, 344.4, 355.6, 379.4, 416.6, 428.4, 434.7, 449.5, 541.9, 564.3, 586.6, 625.0, 634.8, 643.4, 647.3,

	663.5, 668.5, 684.7, 688.4, 698.1, 716.0, 736.2, 740.4, 760.3, 812.6, 875.3, 932.8, 959.8, 962.8, 982.4, 1016.7, 1049.2, 1061.4, 1079.5, 1095.6, 1132.0, 1167.9, 1262.6, 1330.4, 1352.3, 1355.4, 1387.1, 1391.2, 1404.3, 1410.3, 1425.5, 1430.4, 1446.3, 1660.8, 1865.7, 2937.7, 2950.2, 2990.3, 2993.4, 3001.7, 3042.8, 3049.7, 3051.5, 3062.3, 3116.7, 3134.1
TS(C3-D5)	433.8i, 47.4, 53.5, 66.7, 75.9, 105.9, 107.1, 139.5, 160.9, 186.1, 205.6, 215.2, 240.3, 255.3, 284.0, 311.1, 326.0, 346.4, 354.9, 365.8, 381.2, 451.4, 494.6, 508.6, 533.4, 573.5, 607.4, 632.5, 634.4, 643.0, 658.3, 659.1, 670.8, 684.5, 695.6, 715.2, 731.3, 735.5, 799.2, 851.8, 947.4, 986.7, 1001.3, 1050.6, 1088.5, 1100.7, 1116.6, 1160.4, 1163.3, 1272.5, 1339.9, 1381.2, 1399.7, 1417.2, 1794.7, 2193.1, 2954.2, 2983.7, 3021.2, 3091.1
D5	45.4, 52.3, 68.4, 70.7, 84.9, 113.9, 140.3, 151.9, 171.0, 204.9, 212.8, 218.8, 250.5, 258.8, 307.9, 322.6, 344.2, 352.2, 357.0, 363.0, 401.7, 422.0, 466.4, 490.8, 557.2, 575.3, 627.9, 636.8, 639.4, 643.4, 646.7, 654.6, 659.0, 672.3, 680.6, 688.2, 700.5, 726.7, 803.3, 949.2, 968.5, 992.7, 1028.8, 1078.2, 1089.2, 1099.2, 1104.4, 1148.3, 1177.2, 1307.2, 1324.5, 1390.6, 1399.4, 1816.9, 2199.2, 2383.7, 2915.7, 2961.7, 3028.5, 3095.7
D5*H2O	13.6, 33.0, 45.9, 56.2, 64.8, 77.8, 79.8, 108.8, 130.2, 133.7, 150.8, 192.7, 212.3, 218.0, 240.0, 248.9, 254.2, 304.8, 308.9, 327.7, 338.6, 342.0, 363.3, 368.4, 392.8, 430.9, 438.9, 460.4, 509.3, 563.3, 594.4, 614.5, 631.7, 640.1, 640.3, 650.8, 654.2, 672.3, 676.2, 684.5, 692.2, 707.4, 718.7, 725.8, 865.1, 943.5, 1005.4, 1031.3, 1041.4, 1066.9, 1096.0, 1100.9, 1145.6, 1181.1, 1224.7, 1327.1, 1334.5, 1394.7, 1400.7, 1594.1, 1787.1, 2187.3, 2400.2, 2484.0, 2961.5, 3021.7, 3093.1, 3462.7, 3715.5
TS(D5-D7)	37.4i, 17.5, 37.6, 54.5, 72.2, 106.5, 157.2, 170.8, 187.2, 202.1, 210.0, 218.9, 257.7, 278.6, 306.2, 318.0, 341.9, 350.1, 361.4, 365.2, 396.3, 409.8, 460.6, 472.2, 546.1, 563.0, 634.4, 639.4, 646.1, 651.9, 657.7, 664.5, 671.4, 675.2, 684.8, 693.4, 714.9, 729.2, 798.4, 946.4, 985.2, 1006.1, 1027.1, 1038.6, 1075.4, 1095.1, 1121.3, 1167.8, 1203.3, 1333.1, 1353.8, 1402.5, 1403.0, 1798.6, 2191.6, 2513.1, 2959.3, 2996.2, 3023.5, 3089.6
D7	52.1, 62.2, 78.1, 83.7, 107.6, 123.8, 139.0, 167.9, 184.2, 204.7, 233.6, 245.1, 253.3, 264.8, 316.2, 331.7, 341.2, 353.5, 358.3, 390.8, 434.4, 473.5, 523.0, 541.5, 569.6, 590.6, 641.7, 644.2, 651.9, 664.1, 667.5, 692.3, 698.7, 715.9, 728.0, 732.0, 740.7, 764.3, 796.8, 861.7, 960.5, 983.3, 1003.3, 1091.8, 1116.5, 1142.6, 1154.5, 1192.7, 1295.4, 1331.1, 1375.2, 1403.7, 1407.5, 1738.9, 1899.5, 2956.1, 2959.3, 3020.7, 3021.9, 3090.9
D7*H2O	39.7, 62.6, 78.0, 87.1, 88.3, 101.3, 113.0, 125.1, 161.5, 179.6, 184.5, 191.5, 207.8, 233.7, 247.3, 254.7, 268.4, 297.9, 312.3, 334.5, 343.7, 356.2, 358.9, 388.4, 400.3, 409.3, 443.0, 484.7, 519.8, 539.9, 546.6, 590.4, 640.7, 642.8, 654.3, 665.0, 667.2, 691.5, 697.0, 710.9, 725.6, 730.0, 742.0, 772.7, 801.9, 869.7, 965.5, 982.5, 1000.8, 1087.9, 1118.6, 1136.7, 1153.4, 1175.7, 1305.8, 1329.7, 1378.7, 1401.7, 1411.4, 1587.4, 1729.0, 1908.8, 2896.7, 2959.9, 3024.3, 3030.3, 3092.7, 3636.6, 3734.2
TS(D7-C5)	66.8i, 25.9, 36.7, 52.5, 61.6, 79.4, 82.7, 101.6, 123.3, 150.1, 189.4, 196.2, 203.0, 214.9, 241.2, 248.4, 257.8, 305.9, 322.7, 342.8, 353.8, 357.2, 363.4, 384.8, 389.0, 396.3, 444.4, 481.0, 498.6, 562.4, 607.1, 628.6, 630.1, 637.4, 639.1, 644.9, 647.3, 662.4, 671.7, 678.7, 681.6, 691.9, 720.7, 729.0, 813.0, 941.8, 961.2, 998.6, 1049.3, 1072.0, 1089.2, 1091.3, 1136.6, 1151.1, 1183.5, 1327.0, 1357.5, 1391.8, 1399.7, 1543.6, 1770.6, 2189.9, 2855.0, 2952.2, 3007.8, 3035.6, 3091.5, 3485.2, 3670.7
TS(D5-C5)	61.1i, 25.5, 44.4, 53.5, 62.6, 75.4, 85.7, 108.3, 129.7, 152.1, 189.1, 194.6, 207.1, 213.3, 249.1, 258.7, 267.4, 305.2, 322.9, 329.7, 338.8, 359.8, 368.8, 377.8, 390.3, 406.3, 442.9, 473.0, 531.7, 564.1, 611.0, 624.9, 633.3, 638.0, 643.7, 647.0, 659.1, 662.8, 667.5, 676.5, 683.1, 706.8, 711.7, 757.7, 785.9, 935.9, 969.0, 1005.1, 1054.8, 1074.5, 1092.3, 1125.6, 1148.2, 1157.9, 1212.5, 1330.0, 1352.5, 1396.4, 1412.6, 1580.9, 1752.0, 2181.0, 2645.8, 2962.5, 3020.0, 3027.7, 3095.9, 3361.9, 3697.4
TS(D5-D8)	25.3i, 30.9, 35.1, 41.5, 52.9, 59.2, 70.9, 107.3, 122.6, 139.2, 141.8, 162.3, 194.0, 197.7, 211.6, 219.9, 249.0, 256.3, 307.2, 327.4, 335.6, 337.8, 362.1, 371.3, 371.9, 396.8, 414.8, 457.2, 497.0, 515.9, 559.0, 602.2, 622.9, 642.8, 645.2, 647.3, 652.6, 664.0, 668.1, 675.7, 689.3, 705.2, 719.9, 736.8, 793.3, 942.8, 994.9, 1010.2, 1019.7, 1058.6, 1101.4, 1102.8, 1138.6, 1159.9, 1242.0, 1305.6, 1329.2, 1402.8, 1405.6, 1589.4, 1781.5, 2112.3, 2261.3, 2962.1, 2984.1, 3024.6, 3091.9, 3550.0, 3755.1
D8	34.8, 47.3, 57.8, 63.8, 83.1, 88.4, 105.8, 137.4, 142.7, 186.2, 190.9, 205.6, 217.0, 239.2, 251.9, 304.5, 319.0, 334.8, 340.1, 355.1, 360.5, 375.9, 385.7, 458.7, 511.0, 531.2, 541.1, 559.6, 592.7, 621.5, 630.6, 634.7, 651.7, 666.8, 671.5, 682.0, 688.3, 699.0, 708.7, 716.9, 800.5, 804.3, 818.8, 939.3, 947.1, 980.5, 1010.8, 1054.3, 1087.5, 1104.2, 1131.8, 1151.0, 1169.2, 1218.2, 1288.4, 1330.2, 1375.4, 1406.3, 1413.6, 1641.8, 1754.6, 1920.5, 2307.8, 2817.7, 2913.8, 2960.3, 3020.1, 3029.0, 3086.6
TS(D8-E1)	185.1i, 22.0, 38.2, 45.0, 55.3, 71.5, 92.8, 97.2, 133.1, 186.9, 195.6, 213.6, 244.8, 264.6, 266.9, 273.1, 302.0, 320.6, 322.3, 326.9, 331.1, 336.4, 360.7, 374.5, 381.1, 389.8, 398.3, 413.8, 417.9, 421.8, 458.2, 471.4, 525.5, 531.5, 618.6, 627.8, 634.7, 645.4, 659.9, 667.1, 676.0, 687.9, 701.0, 718.7, 787.3, 800.1, 852.1, 948.5, 970.8, 974.4, 979.2, 1003.8, 1017.8, 1031.0, 1034.6, 1078.7, 1106.5, 1113.9, 1132.8, 1189.7, 1282.1, 1330.3, 1360.4, 1402.7, 1415.2, 1604.2, 1758.7, 1955.9, 2719.5, 2835.4, 2961.8, 3017.7, 3025.2, 3086.9, 3257.6
TS(D5-D6)	281.3i, 27.0, 44.2, 46.7, 63.0, 73.8, 94.1, 124.7, 162.7, 190.7, 199.4, 214.6, 241.3, 242.4, 246.0, 309.9, 319.8, 337.3, 355.5, 362.3, 367.4, 381.2, 422.5, 434.1, 562.3, 603.9, 618.0, 625.4, 628.4, 639.3, 648.0, 653.0, 664.9, 672.7, 692.7, 704.7, 713.2, 758.8, 775.7, 889.8, 967.4, 998.6, 1062.0, 1087.9, 1116.7, 1131.6, 1175.2, 1179.9, 1256.5, 1316.3, 1338.4, 1381.6, 1397.1, 1657.4, 2240.3, 2675.1, 2910.5, 2963.7, 3009.4, 3085.5
D6	30.3, 34.9, 58.5, 68.3, 84.3, 138.7, 164.7, 202.9, 207.1, 219.3, 245.8, 248.0, 272.8, 308.5, 319.7, 348.2, 354.9, 357.3, 394.5, 415.2, 439.5, 468.1, 474.7, 538.1, 563.1, 626.9, 632.6, 635.3, 644.5, 649.9, 652.0, 661.8, 669.3, 675.8, 687.9, 707.7, 722.2, 792.3, 820.2, 956.0, 969.6, 999.7, 1012.3, 1084.3, 1090.3, 1104.7, 1158.8, 1180.1, 1276.5, 1302.5, 1340.5, 1370.5, 1383.4, 1512.5, 2033.2, 2302.9, 2959.8, 3001.8, 3024.0, 3101.8
TS(D6-D4)	202.3i, 27.9, 41.9, 69.4, 86.2, 121.6, 153.2, 197.5, 206.9, 213.7, 240.5, 249.9, 293.6, 306.8, 310.4, 328.2, 348.4, 358.4, 383.1, 458.6, 482.5, 491.5, 527.5, 585.3, 609.9, 626.0, 630.1, 635.4, 640.6, 653.3, 656.2, 668.1, 679.9, 688.3, 706.9, 716.5, 729.7, 803.8, 838.3, 921.5, 955.0, 965.6, 1005.2, 1078.1, 1083.3, 1109.4, 1145.9, 1173.0, 1215.8, 1261.2, 1314.8, 1344.6, 1360.9, 1397.2, 1613.2, 1990.6, 2980.6, 3019.4, 3037.2, 3115.0

ZOH*Diketene	19.7, 25.4, 51.2, 55.0, 81.2, 124.6, 162.1, 199.5, 203.1, 216.6, 241.5, 249.3, 293.0, 318.7, 323.7, 335.5, 349.1, 355.5, 386.8, 433.7, 484.2, 517.7, 558.5, 613.3, 634.1, 638.4, 644.4, 660.7, 665.1, 667.6, 683.3, 690.9, 711.7, 721.7, 725.9, 737.6, 810.3, 835.7, 844.5, 860.5, 934.2, 948.8, 970.3, 1046.7, 1080.6, 1092.5, 1123.3, 1160.7, 1167.1, 1242.1, 1319.1, 1359.3, 1373.0, 1699.2, 1810.2, 2511.1, 3003.7, 3053.3, 3091.8, 3185.7
TS(C2-D1)	161.2i, 34.1, 41.2, 44.9, 54.0, 66.8, 76.9, 103.1, 138.0, 194.0, 199.8, 225.3, 233.1, 248.0, 267.8, 298.2, 317.1, 334.6, 347.4, 352.5, 385.6, 400.6, 414.8, 436.5, 456.7, 531.6, 542.1, 558.0, 609.7, 632.6, 637.7, 643.5, 647.7, 658.9, 670.1, 684.8, 690.8, 710.9, 712.3, 731.9, 738.7, 819.5, 827.9, 924.4, 965.6, 1094.8, 1109.8, 1124.4, 1133.0, 1162.5, 1301.0, 1343.7, 1368.0, 1971.2, 2179.4, 2818.4, 3073.2, 3075.9, 3164.0, 3215.7
D1	31.0, 45.6, 65.5, 77.1, 82.8, 111.6, 129.8, 157.9, 197.9, 213.3, 221.6, 240.2, 248.7, 307.2, 319.3, 344.4, 354.0, 355.1, 358.8, 386.0, 417.2, 439.7, 503.8, 555.7, 616.2, 623.6, 632.0, 634.8, 640.3, 647.3, 651.1, 666.0, 671.3, 677.1, 687.2, 714.6, 720.4, 803.2, 823.9, 848.9, 938.0, 950.4, 970.1, 1035.8, 1096.5, 1116.1, 1122.5, 1168.2, 1176.8, 1195.3, 1325.5, 1393.6, 1408.4, 1631.7, 2213.1, 2597.4, 2897.0, 2998.6, 3094.4, 3188.5
TS(D1-D4)	84.0i, 39.3, 48.4, 68.9, 77.3, 99.1, 107.8, 148.9, 196.5, 204.6, 235.8, 245.8, 262.4, 304.5, 312.8, 326.5, 339.6, 355.4, 359.0, 366.8, 404.7, 436.5, 456.9, 541.4, 603.2, 626.8, 632.4, 633.0, 639.9, 650.4, 654.4, 664.9, 680.3, 686.3, 692.5, 720.0, 726.5, 822.3, 847.7, 852.7, 894.9, 934.7, 947.3, 1098.5, 1112.4, 1114.2, 1122.0, 1169.6, 1195.3, 1229.6, 1329.4, 1350.2, 1387.0, 1696.5, 2105.7, 2224.5, 2911.3, 2999.4, 3101.0, 3196.2
ZOH*Diketene*H2O	16.7, 40.3, 43.6, 60.3, 74.0, 83.1, 110.1, 125.6, 145.5, 166.9, 201.7, 208.7, 216.1, 240.0, 253.0, 289.2, 314.1, 318.9, 325.2, 338.5, 340.2, 374.1, 382.0, 390.9, 455.3, 507.5, 519.4, 560.9, 564.7, 622.7, 637.4, 648.5, 651.9, 664.4, 668.9, 669.3, 689.2, 690.7, 709.5, 712.1, 720.4, 737.8, 815.3, 832.0, 843.9, 849.7, 946.9, 972.1, 1005.2, 1052.9, 1079.0, 1107.1, 1119.8, 1171.7, 1200.8, 1248.0, 1334.3, 1363.1, 1385.9, 1607.5, 1685.3, 1791.7, 2299.8, 2857.2, 3034.7, 3100.2, 3194.3, 3554.1, 3720.5
TS(D4-D3)	216.5i, 21.6, 54.4, 66.1, 95.1, 116.4, 137.4, 165.2, 185.5, 205.4, 214.7, 224.3, 235.2, 240.9, 257.7, 285.2, 307.8, 327.1, 350.8, 351.8, 366.5, 393.5, 404.1, 430.3, 444.2, 463.3, 511.4, 554.6, 589.2, 598.5, 635.9, 642.4, 644.7, 650.9, 654.7, 661.9, 671.8, 688.5, 699.1, 706.8, 712.0, 735.5, 822.5, 836.1, 849.6, 882.9, 906.1, 909.3, 943.7, 1053.9, 1096.0, 1106.6, 1127.7, 1190.8, 1203.0, 1245.9, 1332.1, 1372.2, 1392.8, 1492.3, 1604.1, 1723.8, 2046.3, 2978.4, 3059.3, 3123.6, 3232.0, 3233.1, 3677.7
ZOH*3-hydroxy-but-2-enoic-acid	29.4, 46.5, 54.4, 69.7, 75.9, 93.4, 109.5, 153.1, 200.0, 203.3, 218.0, 234.9, 242.1, 279.7, 312.6, 316.8, 345.0, 352.6, 360.6, 374.9, 382.0, 398.6, 430.6, 474.0, 538.0, 562.0, 588.1, 623.6, 638.3, 641.8, 650.9, 666.3, 674.7, 689.6, 690.6, 696.2, 704.7, 717.9, 721.0, 745.9, 823.3, 844.9, 858.6, 891.8, 917.9, 926.3, 952.6, 1035.2, 1040.7, 1076.4, 1149.5, 1154.3, 1211.5, 1250.5, 1270.2, 1293.4, 1374.1, 1381.8, 1393.6, 1408.2, 1627.8, 1684.7, 2164.9, 2935.7, 3004.0, 3077.4, 3107.0, 3201.8, 3656.9
TS(D1-D2)	17.3i, 37.2, 68.9, 82.9, 96.6, 128.4, 168.8, 189.3, 213.3, 225.9, 234.0, 244.4, 263.5, 321.8, 325.9, 347.3, 364.3, 372.8, 400.5, 415.9, 438.9, 459.7, 476.8, 542.7, 585.6, 608.9, 637.4, 648.3, 654.5, 657.9, 660.4, 681.5, 685.3, 693.9, 698.6, 704.8, 738.5, 755.3, 805.9, 836.5, 878.6, 904.7, 920.1, 963.2, 977.7, 1043.8, 1113.7, 1130.2, 1242.8, 1261.4, 1322.6, 1382.1, 1394.0, 1669.3, 2060.0, 2950.4, 3009.9, 3103.9, 3198.6, 3290.5
D2	26.3, 45.5, 53.5, 79.3, 117.9, 134.0, 177.1, 206.8, 222.5, 232.5, 242.3, 247.1, 312.5, 332.5, 337.0, 356.3, 370.2, 384.2, 390.9, 413.5, 460.7, 472.2, 517.4, 536.8, 555.3, 606.9, 640.4, 651.5, 658.4, 664.3, 679.0, 685.8, 697.4, 709.1, 721.7, 733.3, 741.9, 750.5, 777.5, 801.9, 850.4, 915.7, 957.1, 969.6, 985.0, 1026.4, 1125.1, 1148.6, 1244.2, 1285.1, 1308.6, 1379.9, 1390.4, 1678.2, 1898.4, 2982.7, 3048.7, 3100.0, 3194.1, 3437.7
D2*H2O	49.4, 52.9, 79.4, 84.7, 95.8, 110.4, 134.3, 146.2, 157.8, 179.0, 190.0, 213.1, 213.6, 226.2, 247.0, 254.1, 309.9, 324.6, 330.9, 352.3, 368.4, 374.2, 391.8, 395.7, 437.2, 463.0, 480.6, 502.8, 521.2, 549.0, 604.9, 639.8, 645.2, 652.3, 657.8, 669.2, 684.7, 689.7, 691.1, 708.8, 724.4, 738.4, 745.4, 748.3, 785.9, 814.3, 853.2, 909.3, 956.5, 966.7, 1035.8, 1055.6, 1135.2, 1170.3, 1256.1, 1287.0, 1321.6, 1357.5, 1392.1, 1588.1, 1673.8, 1911.2, 2970.2, 3020.6, 3098.3, 3193.2, 3235.1, 3608.9, 3743.0
TS(D2-D3)	138.8i, 9.7, 37.6, 51.5, 62.9, 79.0, 93.0, 117.8, 156.4, 182.8, 210.7, 217.0, 221.2, 246.0, 251.0, 265.5, 314.6, 321.5, 349.4, 353.3, 364.9, 367.1, 393.9, 404.9, 411.7, 431.8, 463.4, 506.5, 557.8, 608.1, 634.3, 636.0, 641.8, 647.4, 649.3, 653.1, 668.0, 673.0, 681.8, 688.1, 694.3, 712.1, 723.5, 777.1, 820.5, 825.5, 875.7, 895.2, 953.0, 991.5, 1053.8, 1074.8, 1127.8, 1140.9, 1209.3, 1225.9, 1274.3, 1356.1, 1386.5, 1632.1, 1670.8, 2162.5, 2932.6, 3001.7, 3098.8, 3196.3, 3256.4, 3521.7, 3566.1
TS(D2-E1)	877.0i, 34.4, 36.0, 49.1, 55.5, 68.0, 90.8, 114.6, 159.8, 196.5, 206.8, 219.7, 242.6, 266.3, 273.3, 309.4, 323.8, 346.9, 360.5, 362.4, 378.1, 430.2, 491.7, 514.4, 548.9, 559.9, 577.5, 631.1, 638.2, 646.0, 652.1, 657.7, 660.6, 662.5, 675.0, 683.4, 687.8, 703.3, 716.2, 726.5, 741.2, 754.5, 858.6, 885.7, 905.1, 925.1, 938.2, 1006.0, 1053.9, 1074.6, 1096.9, 1148.6, 1154.7, 1168.7, 1216.3, 1259.6, 1307.8, 1355.6, 1395.0, 1416.7, 1430.2, 1578.3, 1768.6, 3019.7, 3024.7, 3085.2, 3140.2, 3294.2, 3578.9
TS(DAA_dehydration)	64.9i, 34.6, 46.1, 54.1, 57.8, 68.1, 70.8, 79.8, 118.4, 121.1, 131.9, 166.7, 183.2, 185.7, 193.4, 210.1, 215.5, 219.8, 248.9, 268.7, 311.8, 316.3, 326.7, 335.5, 342.1, 361.0, 368.0, 392.2, 396.6, 408.5, 439.9, 466.5, 492.4, 544.4, 563.9, 624.2, 626.5, 632.8, 637.7, 641.8, 644.8, 664.6, 666.5, 668.5, 676.1, 701.0, 710.2, 717.7, 790.1, 837.1, 871.0, 919.1, 938.8, 972.4, 999.8, 1031.8, 1043.1, 1071.1, 1075.5, 1091.2, 1102.1, 1149.1, 1194.3, 1272.3, 1288.3, 1310.7, 1325.2, 1344.3, 1372.5, 1386.6, 1396.1, 1406.3, 1432.0, 1444.5, 1460.2, 1610.6, 1784.4, 2911.3, 2929.7, 2962.9, 2972.0, 2986.6, 3002.7, 3036.9, 3074.4, 3079.7, 3085.9, 3096.7, 3338.8, 3709.1
(101)	
Z(101)	182.7, 211.2, 215.0, 223.9, 285.6, 324.4, 348.8, 352.5, 380.7, 598.9, 642.4, 659.3, 667.4, 688.0, 690.3, 705.3, 761.1, 770.8, 1045.2, 1055.3, 1078.9
Z*AcOH	51.0, 67.9, 85.1, 102.1, 155.8, 162.6, 183.1, 208.8, 231.8, 251.6, 293.9, 334.2, 342.9, 355.1, 362.9, 423.4, 528.7, 589.6, 595.2, 634.0, 640.1, 651.1, 664.4, 679.1, 681.1, 687.5, 702.2, 728.5, 922.5, 972.4, 1010.7, 1026.6, 1074.9, 1088.7, 1100.5, 1334.2, 1364.4, 1402.9, 1416.3, 1491.8, 1622.3, 2303.5, 2989.4, 3055.7, 3106.0

Z*Ketene	19.2, 61.1, 109.4, 119.7, 169.7, 193.4, 211.7, 226.9, 238.8, 290.7, 323.7, 338.1, 349.0, 361.9, 383.6, 412.7, 521.0, 598.7, 631.6, 634.6, 646.4, 657.1, 669.5, 684.7, 690.6, 739.4, 756.6, 904.5, 1051.1, 1081.4, 1116.1, 1139.5, 1328.8, 2140.7, 3072.9, 3177.7
Z*Diketene	40.0, 41.0, 56.6, 89.1, 103.2, 118.2, 178.3, 206.0, 215.9, 228.6, 271.9, 306.2, 331.6, 342.3, 347.4, 361.0, 390.2, 433.6, 470.5, 520.0, 594.0, 627.4, 628.5, 642.9, 657.6, 670.7, 680.8, 683.0, 688.9, 721.7, 731.2, 747.1, 837.2, 879.6, 912.1, 927.4, 970.9, 1057.4, 1084.1, 1087.0, 1109.8, 1171.7, 1182.6, 1356.6, 1374.0, 1731.9, 1963.9, 3002.8, 3054.4, 3093.8, 3190.7
Z*E1	43.4, 50.6, 78.7, 114.4, 119.1, 135.6, 146.8, 150.5, 164.4, 192.5, 208.7, 233.0, 240.2, 294.0, 322.8, 337.6, 343.4, 365.1, 398.8, 420.2, 463.2, 503.4, 559.7, 574.1, 614.4, 631.8, 651.9, 669.3, 676.9, 681.5, 693.7, 702.2, 717.3, 738.7, 814.9, 857.1, 903.7, 965.1, 991.1, 1009.7, 1050.4, 1067.6, 1111.0, 1120.8, 1200.4, 1216.7, 1292.3, 1337.5, 1373.8, 1391.8, 1407.8, 1425.2, 1631.8, 1745.9, 2773.2, 2958.6, 3009.3, 3015.6, 3084.7, 3096.1
Z*Acetone	40.4, 56.8, 77.8, 110.8, 132.6, 150.1, 160.2, 179.2, 211.5, 214.8, 234.3, 283.2, 330.9, 339.3, 350.2, 363.9, 379.1, 439.8, 500.3, 577.5, 605.2, 627.8, 643.7, 652.3, 668.3, 677.6, 685.7, 718.5, 733.7, 822.0, 839.4, 934.4, 1042.4, 1062.9, 1066.2, 1074.7, 1111.7, 1247.7, 1323.0, 1333.6, 1394.1, 1399.9, 1409.9, 1432.1, 1637.1, 2950.2, 2964.2, 3005.5, 3020.5, 3086.7, 3097.8
Z*Mesityl_oxide	12.3, 53.2, 55.2, 75.5, 91.3, 111.3, 115.9, 127.2, 148.8, 177.3, 196.3, 207.7, 213.4, 234.0, 239.1, 290.4, 330.6, 343.2, 350.8, 354.7, 370.2, 379.5, 443.4, 472.5, 507.9, 592.6, 600.7, 619.2, 624.1, 640.7, 646.0, 660.8, 668.5, 681.0, 699.3, 728.9, 803.0, 829.5, 904.6, 935.5, 963.0, 987.7, 992.2, 1039.0, 1048.0, 1074.0, 1081.4, 1121.9, 1175.3, 1245.0, 1320.7, 1323.5, 1339.5, 1368.5, 1392.5, 1396.3, 1405.2, 1414.3, 1426.4, 1443.9, 1512.9, 1588.8, 2948.9, 2955.0, 2959.4, 3002.8, 3023.7, 3030.3, 3064.0, 3069.5, 3084.6, 3091.9
TS(C2-D1)	131.1i, 26.2, 57.2, 63.7, 74.7, 105.3, 125.4, 134.5, 172.2, 202.4, 212.4, 230.5, 237.1, 291.4, 325.6, 331.1, 340.6, 356.9, 369.1, 387.1, 424.8, 444.0, 452.6, 535.9, 541.9, 595.3, 634.1, 649.5, 656.8, 663.7, 677.0, 683.1, 693.2, 715.1, 742.1, 765.2, 892.8, 946.9, 1044.7, 1073.9, 1102.4, 1126.3, 1144.9, 1339.6, 1346.7, 2043.4, 2153.8, 2926.8, 3070.4, 3146.8, 3219.4
TS(D1-D3)	55.2i, 27.8, 53.0, 62.0, 82.3, 95.6, 109.7, 131.0, 141.6, 192.6, 214.3, 218.4, 232.7, 239.0, 286.7, 311.0, 330.2, 342.8, 355.4, 373.4, 388.6, 400.5, 430.7, 491.2, 500.5, 522.6, 544.9, 594.6, 626.7, 632.0, 641.5, 652.3, 661.6, 667.3, 679.9, 695.4, 710.8, 715.8, 752.9, 810.9, 837.0, 952.0, 997.1, 1024.4, 1067.4, 1085.8, 1122.1, 1159.8, 1217.2, 1326.0, 1402.5, 1569.9, 1644.3, 2199.3, 2752.3, 3020.1, 3090.9, 3187.5, 3510.5, 3680.5
TS(D4-D3)	152.5i, 24.5, 44.6, 65.5, 82.8, 111.4, 125.6, 176.7, 195.8, 212.9, 225.2, 239.5, 248.6, 258.8, 298.8, 335.0, 337.7, 358.1, 361.6, 402.2, 412.4, 429.8, 455.6, 460.8, 494.0, 582.1, 602.0, 627.4, 646.0, 650.8, 658.8, 672.0, 674.9, 685.1, 701.9, 708.6, 725.0, 833.1, 835.6, 861.4, 898.0, 915.1, 973.3, 1039.1, 1066.5, 1103.4, 1116.2, 1205.4, 1239.2, 1370.2, 1381.1, 1603.9, 1696.5, 2066.1, 2975.5, 3060.4, 3092.0, 3127.2, 3187.3, 3654.0
TS(A1-E1)	246.1i, 33.0, 59.9, 76.8, 88.1, 137.5, 148.9, 180.1, 218.9, 232.3, 235.4, 238.6, 265.0, 294.5, 324.2, 332.0, 345.6, 351.2, 366.8, 387.3, 421.7, 440.9, 490.5, 549.2, 571.0, 628.0, 633.8, 648.6, 650.3, 664.6, 670.6, 677.9, 695.0, 697.8, 721.1, 733.8, 777.6, 838.5, 967.1, 975.1, 1019.2, 1047.7, 1067.6, 1077.3, 1095.9, 1141.0, 1173.3, 1198.6, 1340.6, 1344.8, 1411.1, 1421.6, 1435.8, 2172.9, 2636.6, 2979.5, 3006.0, 3062.8, 3073.8, 3238.0
TS(B1-B2)	266.1i, 33.3, 45.8, 74.5, 102.1, 114.2, 123.7, 127.3, 155.2, 187.5, 213.8, 240.4, 246.1, 261.5, 266.3, 285.8, 320.2, 334.3, 349.0, 353.8, 387.9, 419.6, 458.4, 488.8, 498.8, 517.9, 541.1, 574.7, 591.9, 625.1, 639.8, 647.4, 662.6, 671.1, 676.2, 687.2, 699.0, 711.1, 731.7, 794.1, 852.2, 943.3, 946.8, 959.2, 981.1, 986.7, 1025.5, 1040.5, 1080.0, 1104.3, 1138.1, 1185.6, 1269.4, 1318.8, 1342.3, 1415.6, 1425.7, 1438.5, 1449.8, 1521.1, 1578.6, 2372.2, 2980.2, 3041.4, 3058.8, 3092.2, 3128.6, 3568.9, 3692.0
TS(E1-E2)	95.6i, 33.9, 47.4, 67.6, 81.5, 87.7, 107.9, 126.5, 145.7, 151.4, 176.2, 200.7, 214.7, 226.4, 241.3, 277.2, 311.1, 326.0, 357.3, 377.3, 388.1, 473.3, 495.4, 527.5, 534.4, 583.0, 590.7, 624.7, 641.2, 651.2, 671.3, 683.1, 687.4, 702.6, 719.7, 742.1, 749.0, 811.5, 825.3, 883.0, 975.7, 1016.0, 1062.2, 1067.5, 1122.0, 1250.3, 1261.5, 1316.3, 1364.0, 1388.2, 1414.6, 1430.4, 1586.8, 2245.9, 2967.5, 3027.4, 3069.4, 3085.4, 3181.5, 3193.4
TS(E4-E6*)	170.7i, 41.1, 54.4, 58.0, 94.4, 109.9, 116.8, 132.0, 156.2, 169.7, 180.3, 212.4, 220.0, 230.2, 231.9, 254.6, 263.7, 281.7, 288.2, 317.1, 347.8, 356.7, 364.1, 398.4, 422.0, 457.0, 477.6, 515.4, 555.9, 564.2, 620.5, 626.8, 637.3, 653.3, 662.2, 667.3, 688.7, 700.0, 715.7, 778.4, 813.6, 869.7, 885.8, 902.8, 931.2, 953.1, 976.8, 988.9, 1012.6, 1028.7, 1043.4, 1051.6, 1111.1, 1143.2, 1228.3, 1283.3, 1343.8, 1344.4, 1352.3, 1390.0, 1398.6, 1409.2, 1415.8, 1421.3, 1430.3, 1440.9, 1465.0, 1488.9, 1564.4, 2839.5, 2952.0, 2961.8, 2962.1, 3031.0, 3033.4, 3039.3, 3072.6, 3074.9, 3085.5, 3087.8, 3182.2
TS(E7*-E8)	569.8i, 26.6, 50.4, 69.4, 74.4, 81.7, 90.7, 105.0, 148.1, 165.0, 180.8, 190.2, 196.5, 207.4, 214.7, 217.9, 236.2, 243.8, 282.7, 295.7, 327.9, 344.4, 346.1, 358.1, 365.7, 424.6, 442.6, 450.6, 508.8, 566.3, 612.5, 615.6, 619.3, 631.8, 658.3, 670.7, 680.5, 693.3, 701.2, 742.1, 758.0, 802.8, 814.8, 852.5, 881.6, 893.4, 942.9, 951.2, 989.7, 990.7, 1029.9, 1039.3, 1114.9, 1141.3, 1149.8, 1195.1, 1229.8, 1303.9, 1318.5, 1329.9, 1335.1, 1354.2, 1378.3, 1403.3, 1411.2, 1412.8, 1420.3, 1447.6, 1495.3, 1692.5, 2926.2, 2955.9, 2961.1, 2995.0, 3023.9, 3025.8, 3040.7, 3071.4, 3084.5, 3108.3, 3746.1
TS(E7-E8)	201.0i, 32.1, 56.9, 59.0, 70.9, 104.6, 108.2, 125.4, 156.4, 188.0, 202.6, 212.9, 218.4, 220.6, 230.4, 265.7, 272.5, 295.4, 318.9, 330.2, 334.5, 339.6, 363.7, 371.3, 383.5, 431.6, 451.3, 506.4, 553.0, 586.4, 601.4, 623.1, 627.2, 639.7, 647.3, 661.2, 669.5, 684.8, 713.7, 725.6, 763.6, 778.5, 828.0, 887.0, 901.1, 939.1, 978.9, 980.7, 1011.7, 1022.7, 1056.0, 1072.6, 1084.5, 1125.2, 1150.5, 1218.6, 1282.8, 1341.6, 1344.3, 1359.5, 1363.2, 1389.7, 1411.3, 1418.8, 1419.9, 1425.6, 1447.0, 1451.1, 1614.5, 2963.3, 2966.5, 2967.4, 3025.9, 3028.1, 3039.6, 3071.0, 3073.9, 3088.8, 3109.3, 3388.0, 3705.6
TS(E8*-E10)	1087.1i, 18.8, 35.6, 60.8, 86.8, 115.0, 124.6, 136.8, 171.1, 175.6, 201.6, 214.6, 215.6, 222.9, 239.1, 255.0, 284.5, 295.8, 319.1, 330.2, 348.5, 355.0, 371.6, 387.7, 411.3, 475.5, 489.5, 517.5, 559.9, 578.4, 620.7, 635.7, 639.9, 648.0, 663.5, 667.8, 672.7, 692.4, 707.8, 725.7, 750.5, 807.8, 846.4, 876.4, 894.5, 957.8, 982.6, 1009.1, 1030.2, 1045.6, 1056.3, 1093.3, 1127.8, 1132.7, 1164.6, 1183.1, 1234.9, 1312.6, 1326.0, 1339.0, 1343.7, 1373.1, 1387.2, 1395.5,

	1416.5, 1425.4, 1425.5, 1439.7, 1546.8, 1779.7, 2922.4, 2955.8, 2973.2, 2978.6, 3010.1, 3014.0, 3014.0, 3060.9, 3067.9, 3073.4, 3077.9