

Supporting Information

Effect of Substituents and Promoters on Diels-Alder Cycloaddition

Reaction in Biorenewable Synthesis of Trimellitic Acid

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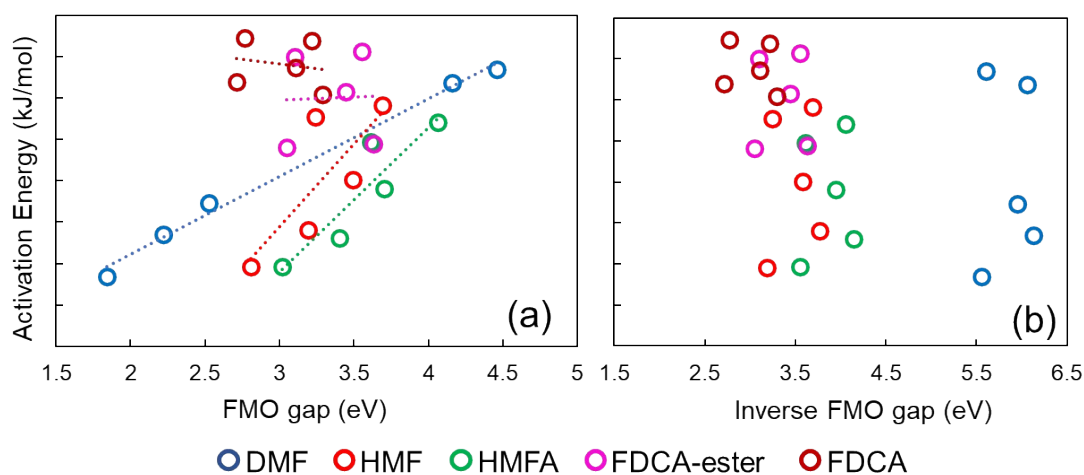


Figure SI-1. Linear scaling relationship between Activation Energy (kJ/mol) and (a) FMO gap and (b) inverse FMO gap for Diels Alder reaction of the molecules included in our scope of study.

$$\text{Normal FMO gap} = \text{HOMO}_{\text{diene}} - \text{LUMO}_{\text{dienophile}}$$

$$\text{Inverse FMO gap} = \text{HOMO}_{\text{dienophile}} - \text{LUMO}_{\text{diene}}$$

$$\text{FMO gap} = \min \{ \text{Normal FMO gap}, \text{Inverse FMO gap} \}$$

Table SI-1. DFT calculated activation barrier for Diels-Alder reaction between HMF+Acrolein, HMFA+Acrolein, HMF+Propylene and HMFA+Propylene using two different exchange-correlation functional, GGA BLYP and hybrid B3LYP. Grimme (G06) DFT+D vdW correction applied in both the method.

Activation Energy (E_a)	BLYP+vdW(Grimme) (kJ/mol)	B3LYP+vdW(Grimme) (kJ/mol)
HMF+Acrolein	39.2	56.3
HMFA+Acrolein	39.3	54.6
HMF+Propylene	75.5	91.1
HMFA+Propylene	69.5	83.6

Table SI-2. The R^2 fitting parameters for the linear scaling correlation of the activation energy with normal FMO gap and FMO gap

Linear Scaling R^2 value	Activation Energy vs Normal FMO gap (Figure 6)	Activation Energy vs FMO gap (Figure SI-1 (a))
DMF	0.99	0.99
HMF	0.92	0.62
HMFA	0.89	0.82
FDCA-ester	0.88	0.01
FDCA	0.87	0.04

Table SI-3. Effect of Solvent in DFT+C₂H₄ Diels-Alder reaction

Solvent	dielectric constant	Activation barrier (kJ/mol)	Reaction energy (kJ/mol)	FMO gap (eV)
gas-phase	0.00	86.6	-28.2	4.19
Water	78.54	88.1	-30.6	4.30
Acetone	20.70	88.0	-30.3	4.30
acetonitrile	37.50	88.0	-30.5	4.30
CCl ₄	2.24	87.3	-28.9	4.24
Diethyl ether	4.34	87.7	-29.5	4.27
Ethanol	24.30	88.0	-30.4	4.30
n-hexane	1.89	87.2	-28.8	4.23

Coordinate of DFT optimized Dienes, Dienophiles, Oxa-norbornene cyclo-adducts and Diels-

Alder reaction transition states

		HMF		
	ATOM	X	Y	Z
1	C	0.415361	-0.10504	0.729463
2	C	1.07682	-1.2077	1.481522
3	C	1.528209	-2.45295	1.106096
4	C	2.048215	-3.06619	2.280177
5	C	1.885563	-2.15794	3.309499
6	H	1.478301	-2.86902	0.106408
7	H	2.490967	-4.05155	2.375751
8	C	2.248132	-2.25233	4.715014
9	O	1.289138	-1.00729	2.824028
10	O	2.076905	-1.37899	5.563541
11	O	-1.02019	-0.17745	0.943334
12	H	0.657638	-0.21745	-0.33994
13	H	0.812502	0.85839	1.084471
14	H	-1.38764	0.696006	0.72124
15	H	2.718719	-3.23237	4.966113

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		HMFA		
	ATOM	X	Y	Z
1	C	0.412344	-0.07201	0.774011
2	C	1.062739	-1.21369	1.472666
3	C	1.553496	-2.42196	1.033173
4	C	2.040658	-3.1104	2.1811
5	C	1.820053	-2.28068	3.257504
6	H	1.553553	-2.76622	0.005295
7	H	2.499948	-4.08968	2.236446
8	C	2.12482	-2.49175	4.671965
9	O	2.663259	-3.5058	5.101623
10	O	1.218998	-1.10642	2.835687
11	O	1.747246	-1.43674	5.471663
12	O	-1.02812	-0.15918	0.953053
13	H	0.67752	-0.12339	-0.2945
14	H	0.795326	0.873445	1.189584
15	H	-1.40033	0.700763	0.689273
16	H	1.996576	-1.69879	6.382425

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FDCA				
	ATOM	X	Y	Z
1	C	0.224546	-0.25672	0.726174
2	C	0.990341	-1.25634	1.481756
3	C	1.774555	-2.29059	1.011733
4	C	2.302859	-2.94523	2.153418
5	C	1.80955	-2.27407	3.253973
6	H	1.932898	-2.52532	-0.03359
7	H	2.963345	-3.80262	2.193101
8	C	2.044886	-2.53163	4.6803
9	O	2.760451	-3.44053	5.081155
10	O	0.999902	-1.23144	2.859352
11	O	1.385172	-1.65329	5.501617
12	O	-0.43123	0.640543	1.529699
13	H	-0.89867	1.251781	0.92227
14	H	1.614247	-1.91909	6.416984
15	O	0.187528	-0.2372	-0.49749

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FDCA-ester				
	ATOM	X	Y	Z
1	C	0.107361	-0.46854	0.705311
2	O	0.108494	-0.43911	-0.52041
3	C	0.950004	-1.39839	1.472336
4	C	1.835992	-2.35048	1.009724
5	C	2.385829	-2.98069	2.155841
6	C	1.804302	-2.3783	3.25269
7	H	2.04342	-2.55062	-0.03407
8	H	3.115056	-3.77983	2.20131
9	C	2.017688	-2.65541	4.681256
10	O	2.785503	-3.5272	5.073453
11	O	0.919022	-1.40119	2.850524
12	O	1.272486	-1.84643	5.48919
13	O	-0.65471	0.330825	1.507364
14	C	-1.51538	1.267171	0.782354
15	C	1.455219	-2.09124	6.920785
16	H	2.499467	-1.90586	7.200344
17	H	1.192715	-3.12886	7.159702
18	H	0.78177	-1.38587	7.414416
19	H	-2.05314	1.814284	1.560869

20	H	-2.20597	0.714772	0.134023
21	H	-0.90293	1.941804	0.171991

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DMF

	ATOM	X	Y	Z
1	C	0.263596	-0.20169	0.659364
2	C	1.068394	-1.25796	1.337444
3	C	1.835527	-2.29672	0.889665
4	C	2.371094	-2.95604	2.053742
5	C	1.899948	-2.2835	3.14612
6	H	1.999553	-2.56121	-0.14951
7	H	3.024398	-3.82172	2.076119
8	C	2.078269	-2.44651	4.617706
9	O	1.092877	-1.23031	2.728006
10	H	-0.78861	-0.22669	0.983277
11	H	0.295609	-0.36091	-0.4259
12	H	2.535114	-1.55082	5.067547
13	H	2.731466	-3.30619	4.812877
14	H	1.114464	-2.61683	5.122739
15	H	0.654492	0.805127	0.875331

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Ethylene

	ATOM	X	Y	Z
1	C	3.299118	-0.75891	2.912178
2	C	2.785321	-0.14972	1.836397
3	H	3.986528	-1.6011	2.817063
4	H	3.048829	-0.43894	3.92499
5	H	3.024407	-0.47872	0.823763
6	H	2.107997	0.700628	1.931271

Propylene

	ATOM	X	Y	Z
1	C	3.369315	-0.71021	2.863173
2	C	2.751865	-0.12268	1.830701
3	C	4.598968	-1.57377	2.749148
4	H	2.970046	-0.56875	3.87129
5	H	3.122525	-0.24286	0.810299
6	H	1.864029	0.494208	1.971898
7	H	4.933977	-1.64907	1.704972
8	H	4.405569	-2.59171	3.125758

9 H 5.426764 -1.16668 3.352801

Acrolein

ATOM		X	Y	Z
1	C	3.335623	-0.64772	2.804507
2	C	2.747903	-0.09387	1.729044
3	C	4.622701	-1.38695	2.710468
4	H	2.883683	-0.57881	3.795764
5	H	3.221549	-0.17926	0.75041
6	H	1.803059	0.442838	1.805113
7	O	5.258417	-1.5602	1.674335
8	H	4.999056	-1.79918	3.6763

Acrylic Acid

ATOM		X	Y	Z
1	C	3.421009	-0.65787	2.825015
2	C	2.782842	-0.13403	1.769358
3	C	4.715444	-1.38815	2.657349
4	H	3.005103	-0.56104	3.830164
5	H	3.211489	-0.23937	0.772692
6	H	1.838638	0.396633	1.882851
7	O	5.287946	-1.56862	1.59995
8	O	5.27205	-1.88413	3.826411
9	H	4.703786	-1.66432	4.588758

Methyl Acrylate

ATOM		X	Y	Z
1	C	3.371417	-0.58437	2.746519
2	C	2.641206	-0.07396	1.743683
3	C	4.734542	-1.15712	2.609812
4	H	2.994307	-0.61778	3.76735
5	H	3.026448	-0.04546	0.725639
6	H	1.644206	0.326941	1.925366
7	O	5.21549	-1.11088	1.323207
8	O	5.365935	-1.62421	3.55075
9	C	6.554041	-1.67313	1.156481
10	H	6.791865	-1.53395	0.098052
11	H	6.550216	-2.73693	1.424438
12	H	7.268813	-1.14239	1.796961

Oxa-norbornene (HMF+Ethylene)

ATOM		X	Y	Z
1	C	0.247951	-0.311	0.608825
2	C	1.340884	-0.97087	1.432137
3	C	1.779673	-2.38711	1.059769
4	C	2.227308	-2.94639	2.193224
5	C	2.041403	-1.87084	3.275423
6	H	1.820244	-2.78501	0.049329
7	H	2.71827	-3.90427	2.340672
8	C	1.96438	-2.34128	4.70338
9	O	0.869262	-1.1639	2.813742
10	C	3.17931	-0.77999	3.015638
11	C	2.654565	-0.14105	1.692928
12	H	4.17183	-1.23531	2.926407
13	H	3.178882	-0.05787	3.839892
14	H	3.363131	-0.22371	0.860921
15	H	2.379135	0.908228	1.838019
16	O	1.093762	-2.04299	5.50021
17	O	-0.12382	0.977822	1.128111
18	H	-0.61913	-0.99087	0.57162
19	H	0.60925	-0.14404	-0.41412
20	H	-0.3671	0.835153	2.062165
21	H	2.823324	-2.99789	4.991886

Oxa-norbornene (HMF+Propylene)

ATOM		X	Y	Z
1	C	0.251982	-0.25433	0.626675
2	C	1.338806	-0.96084	1.419277
3	C	1.749611	-2.37279	1.001425
4	C	2.191712	-2.9752	2.115171
5	C	2.029096	-1.93157	3.229975
6	H	1.775645	-2.74009	-0.02108
7	H	2.662065	-3.94748	2.227333
8	C	1.946183	-2.44591	4.640489
9	O	0.867773	-1.19109	2.796092
10	C	3.176146	-0.82299	3.019497
11	C	2.668453	-0.16587	1.696707
12	C	4.611216	-1.35597	2.977481
13	H	3.058635	-0.11352	3.847254

14	H	3.385795	-0.27261	0.873584
15	H	2.425073	0.891914	1.837709
16	O	1.083356	-2.1553	5.44962
17	O	-0.09182	1.022316	1.19346
18	H	-0.62787	-0.9167	0.574757
19	H	0.607202	-0.0589	-0.39335
20	H	-0.32475	0.852116	2.125663
21	H	2.792247	-3.12698	4.907812
22	H	4.732537	-2.07033	2.151341
23	H	4.885182	-1.85466	3.918543
24	H	5.315535	-0.52754	2.817149

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Oxa-norbornene (HMF+Acrolein)

ATOM		X	Y	Z
1	C	0.189868	-0.28758	0.635334
2	C	1.314506	-0.96885	1.397461
3	C	1.726861	-2.37974	0.996062
4	C	2.210065	-2.95898	2.104672
5	C	2.067087	-1.90422	3.202686
6	H	1.740824	-2.75997	-0.0212
7	H	2.711367	-3.91536	2.216135
8	C	2.075214	-2.36901	4.634952
9	O	0.906088	-1.17105	2.803808
10	C	3.217917	-0.75068	2.904066
11	C	2.645061	-0.14457	1.599482
12	C	4.613302	-1.32386	2.839897
13	H	3.149215	-0.05686	3.751141
14	H	3.334903	-0.26804	0.758575
15	H	2.387866	0.910409	1.733789
16	O	1.27583	-2.0324	5.488115
17	O	-0.14576	0.994942	1.191077
18	H	-0.68342	-0.95988	0.623901
19	H	0.508935	-0.10655	-0.39904
20	H	-0.37771	0.838583	2.125601
21	H	2.927371	-3.05714	4.862348
22	O	5.211625	-1.59162	1.808499
23	H	5.07852	-1.52655	3.834834

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Oxa-norbornene (HMF+Acrylic Acid)

ATOM		X	Y	Z
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1	C	0.190664	-0.30923	0.614857
2	C	1.309828	-0.9654	1.405855
3	C	1.784236	-2.35894	0.9959
4	C	2.259027	-2.93082	2.11158
5	C	2.037999	-1.89443	3.223719
6	H	1.82698	-2.73017	-0.02432
7	H	2.779014	-3.87601	2.237376
8	C	1.955972	-2.44584	4.630795
9	O	0.859848	-1.20455	2.787299
10	C	3.173151	-0.74697	2.961779
11	C	2.601448	-0.10242	1.671222
12	C	3.248248	0.210776	4.139863
13	H	3.30372	-0.14172	0.832034
14	H	2.297817	0.931015	1.859461
15	O	1.043756	-2.23183	5.406201
16	O	-0.17144	0.976443	1.141398
17	H	-0.67158	-0.99653	0.601453
18	H	0.522851	-0.14161	-0.41798
19	H	-0.34359	0.852605	2.094058
20	H	2.826987	-3.08784	4.901528
21	O	2.728594	1.306708	4.227566
22	O	3.99014	-0.35272	5.160376
23	H	3.94616	0.27302	5.914425
24	H	4.149403	-1.22308	2.83039

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Oxa-norbornene (HMF+Methyl Acrylate)

ATOM		X	Y	Z
1	C	0.161534	-0.2567	0.675315
2	C	1.241521	-1.04436	1.39742
3	C	1.430345	-2.51769	1.040465
4	C	1.918476	-3.10906	2.140289
5	C	2.013189	-1.99289	3.191075
6	H	1.293434	-2.94211	0.049336
7	H	2.289644	-4.11896	2.276154
8	C	2.025456	-2.40727	4.646483
9	O	0.913522	-1.12905	2.831309
10	C	3.241882	-1.05766	2.768011
11	C	2.674291	-0.39784	1.467075
12	C	4.561306	-1.79701	2.655437
13	H	3.359621	-0.29076	3.544048
14	H	3.279609	-0.62029	0.583077
15	H	2.576401	0.685187	1.581328

16	O	1.333321	-1.89931	5.510943
17	O	0.030232	1.081955	1.184691
18	H	-0.78852	-0.80938	0.758905
19	H	0.423027	-0.16381	-0.38669
20	H	-0.13596	0.99435	2.14217
21	H	2.755269	-3.21865	4.863917
22	O	5.478641	-1.06146	1.961224
23	O	4.798476	-2.89168	3.147329
24	C	6.805682	-1.67664	1.848348
25	H	7.397003	-0.96671	1.264247
26	H	6.72462	-2.64423	1.339306
27	H	7.233282	-1.82541	2.846808

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Oxa-norbornene (HMFA+Ethylene)

ATOM		X	Y	Z
1	C	0.237111	-0.31107	0.63341
2	C	1.345557	-0.97912	1.428319
3	C	1.787359	-2.38766	1.027489
4	C	2.246794	-2.96493	2.146549
5	C	2.080777	-1.91158	3.243853
6	H	1.818553	-2.76518	0.009202
7	H	2.737546	-3.92118	2.294412
8	C	2.04225	-2.41648	4.665308
9	O	2.739878	-3.33502	5.064644
10	O	0.889643	-1.19897	2.813071
11	C	3.197895	-0.80599	2.993259
12	C	2.655061	-0.14454	1.689565
13	H	4.189852	-1.25755	2.889371
14	H	3.200593	-0.10027	3.831268
15	H	3.354501	-0.20955	0.848364
16	H	2.376285	0.900926	1.854898
17	O	1.197619	-1.6986	5.466336
18	O	-0.14099	0.961699	1.188376
19	H	-0.62422	-0.99809	0.590274
20	H	0.584186	-0.11613	-0.38942
21	H	-0.34817	0.79664	2.127404
22	H	1.279371	-2.08831	6.363141

Oxa-norbornene (HMFA+Propylene)

ATOM		X	Y	Z
1	C	0.239673	-0.25846	0.648603

2	C	1.341036	-0.96701	1.418346
3	C	1.748322	-2.37577	0.983127
4	C	2.203715	-2.98727	2.085701
5	C	2.065248	-1.95669	3.206167
6	H	1.762503	-2.73092	-0.04364
7	H	2.674856	-3.95682	2.205074
8	C	2.035293	-2.48987	4.613884
9	O	2.756732	-3.39963	4.994285
10	O	0.887376	-1.21138	2.801133
11	C	3.199085	-0.841	2.993154
12	C	2.670088	-0.16986	1.685676
13	C	4.629691	-1.37842	2.932818
14	H	3.090065	-0.1415	3.830437
15	H	3.376121	-0.26657	0.851797
16	H	2.426912	0.885992	1.841093
17	O	1.17784	-1.80818	5.43255
18	O	-0.10231	1.012428	1.231
19	H	-0.63809	-0.92425	0.603728
20	H	0.578851	-0.05275	-0.3748
21	H	-0.30515	0.835244	2.168805
22	H	1.272019	-2.21493	6.320571
23	H	4.750894	-2.04791	2.07007
24	H	4.879517	-1.93768	3.845035
25	H	5.341742	-0.5477	2.826218

Oxa-norbornene (HMFA+Acrolein)

	ATOM	X	Y	Z
1	C	0.194859	-0.2889	0.650181
2	C	1.330738	-0.95707	1.40664
3	C	1.754407	-2.36497	0.998255
4	C	2.242531	-2.94659	2.102466
5	C	2.109919	-1.89111	3.201866
6	H	1.766573	-2.73993	-0.02084
7	H	2.747405	-3.89824	2.228715
8	C	2.148343	-2.3876	4.625366
9	O	3.032276	-3.12808	5.028113
10	O	0.925881	-1.17178	2.813626
11	C	3.238977	-0.75151	2.897429
12	C	2.647867	-0.11879	1.61277
13	C	4.636595	-1.3325	2.79332
14	H	3.20927	-0.06072	3.750443
15	H	3.335146	-0.21132	0.765685
16	H	2.376524	0.929121	1.772019

17	O	1.141596	-1.90082	5.405704
18	O	-0.16161	0.985319	1.214014
19	H	-0.66812	-0.97455	0.635867
20	H	0.509485	-0.09656	-0.38343
21	H	-0.37574	0.820189	2.151164
22	H	1.286757	-2.27337	6.302211
23	O	5.27419	-1.42119	1.754648
24	H	5.051862	-1.70947	3.753989

Oxa-norbornene (HMFA+Acrylic Acid)

ATOM		X	Y	Z
1	C	0.215604	-0.30117	0.696482
2	C	1.364566	-0.94261	1.45717
3	C	1.757508	-2.37579	1.103633
4	C	2.259814	-2.9258	2.217786
5	C	2.187719	-1.80098	3.270328
6	H	1.739462	-2.7985	0.103367
7	H	2.756085	-3.88036	2.359197
8	C	2.165585	-2.22549	4.720638
9	O	3.186472	-2.44225	5.373494
10	O	0.996115	-1.09118	2.881041
11	C	3.335871	-0.74418	2.863125
12	C	2.683548	-0.10766	1.602804
13	C	4.735905	-1.34377	2.602349
14	H	3.424987	-0.01719	3.679784
15	H	3.337873	-0.1855	0.73014
16	H	2.410226	0.937114	1.777057
17	O	0.92327	-2.37333	5.23064
18	O	-0.12827	0.994774	1.214972
19	H	-0.64903	-0.98459	0.72124
20	H	0.514693	-0.14959	-0.34852
21	H	-0.33922	0.867792	2.158481
22	H	1.032477	-2.66264	6.162959
23	O	5.358528	-1.16321	1.572204
24	O	5.270499	-2.07927	3.615476
25	H	4.620388	-2.1755	4.360398

Oxa-norbornene (HMFA+Methyl acrylate)

ATOM		X	Y	Z
1	C	-0.13073	-0.45827	0.735937
2	C	1.167709	-0.91189	1.379715

3	C	1.868397	-2.1451	0.816227
4	C	2.545239	-2.68798	1.837041
5	C	2.252363	-1.79798	3.038067
6	H	1.890009	-2.42119	-0.2341
7	H	3.24283	-3.5176	1.852649
8	C	2.436105	-2.41512	4.410391
9	O	3.085894	-3.42421	4.616937
10	O	0.906879	-1.33401	2.771699
11	C	3.045383	-0.39832	2.838103
12	C	2.276706	0.181904	1.614527
13	C	4.54645	-0.59013	2.769864
14	H	2.843016	0.181882	3.741832
15	H	2.913905	0.313118	0.735902
16	H	1.792764	1.128677	1.872588
17	O	1.824511	-1.68046	5.387546
18	O	-0.71801	0.665198	1.416349
19	H	-0.82476	-1.31414	0.708285
20	H	0.067464	-0.13196	-0.29299
21	H	-0.83226	0.393549	2.346157
22	H	2.030546	-2.12695	6.236245
23	O	5.017617	-0.69284	1.488948
24	O	5.253454	-0.68885	3.762105
25	C	6.452488	-0.96996	1.390717
26	H	6.664417	-0.99368	0.318175
27	H	6.675727	-1.93364	1.863766
28	H	7.022045	-0.17957	1.89342

Oxa-norbornene (FDCA+Ethylene)

	ATOM	X	Y	Z
1	C	0.291911	-0.20508	0.727303
2	C	1.308694	-0.95387	1.555755
3	C	1.663933	-2.36661	1.090043
4	C	2.164382	-2.98155	2.169018
5	C	2.114947	-1.94368	3.28892
6	H	1.592022	-2.69968	0.060472
7	H	2.616219	-3.96196	2.272841
8	C	2.125664	-2.46917	4.705809
9	O	2.700324	-3.49389	5.03551
10	O	0.933281	-1.16017	2.948321
11	C	3.265783	-0.88629	2.988408
12	C	2.681149	-0.16891	1.733798
13	H	4.22762	-1.37798	2.810776
14	H	3.350195	-0.1968	3.834763

15	H	3.30878	-0.24968	0.840973
16	H	2.46695	0.883831	1.94562
17	O	1.481634	-1.64038	5.580045
18	O	-0.54206	0.574665	1.475856
19	H	-1.13286	1.031045	0.838934
20	H	1.569642	-2.05574	6.464649
21	O	0.267187	-0.25728	-0.4919

Oxa-norbornene (FDCA+Propylene)

ATOM		X	Y	Z
1	C	0.263033	-0.21341	0.741632
2	C	1.296778	-0.93827	1.57003
3	C	1.663903	-2.34407	1.08925
4	C	2.162455	-2.96981	2.161784
5	C	2.105573	-1.94341	3.292822
6	H	1.597932	-2.66354	0.054947
7	H	2.618465	-3.94915	2.256225
8	C	2.11418	-2.48473	4.703671
9	O	2.690951	-3.51139	5.023985
10	O	0.919814	-1.16275	2.958831
11	C	3.24677	-0.88015	3.007117
12	C	2.676176	-0.1402	1.752546
13	H	4.215094	-1.36115	2.835444
14	H	3.318036	-0.19415	3.858564
15	H	3.302002	-0.29892	0.867989
16	C	2.464143	1.359259	2.000616
17	O	1.466476	-1.66717	5.586179
18	O	-0.67139	0.442969	1.48861
19	H	-1.26826	0.88658	0.848201
20	H	1.554623	-2.0923	6.466048
21	O	0.299338	-0.19184	-0.47866
22	H	1.778134	1.505733	2.845299
23	H	2.044276	1.849301	1.111002
24	H	3.423051	1.841277	2.236658

Oxa-norbornene (FDCA+Acrolein)

ATOM		X	Y	Z
1	C	0.260467	-0.20388	0.726631
2	C	1.294444	-0.92721	1.563667

3	C	1.668306	-2.33204	1.086626
4	C	2.164643	-2.95276	2.16343
5	C	2.113897	-1.92062	3.288694
6	H	1.598786	-2.65408	0.053469
7	H	2.61634	-3.93353	2.262988
8	C	2.118694	-2.45434	4.704084
9	O	2.712171	-3.47006	5.027934
10	O	0.929801	-1.13639	2.94731
11	C	3.263255	-0.86323	3.001154
12	C	2.697927	-0.13408	1.754807
13	H	4.226618	-1.34999	2.82379
14	H	3.340068	-0.16344	3.839292
15	H	3.298594	-0.26711	0.845417
16	C	2.478103	1.363412	1.939422
17	O	1.446181	-1.64707	5.572263
18	O	-0.64631	0.484469	1.474489
19	H	-1.25155	0.926696	0.840716
20	H	1.535233	-2.05881	6.458469
21	O	0.283229	-0.21481	-0.49336
22	O	2.793243	2.005536	2.925744
23	H	1.999623	1.860688	1.063149

Oxa-norbornene (FDCA+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.224605	-0.14913	0.75733
2	C	1.279078	-0.84001	1.588411
3	C	1.574683	-2.27554	1.102302
4	C	2.06398	-2.91139	2.172026
5	C	2.091683	-1.87227	3.29033
6	H	1.479893	-2.60282	0.07225
7	H	2.477884	-3.90953	2.264004
8	C	2.114483	-2.39875	4.708098
9	O	2.689776	-3.42895	5.01854
10	O	0.93557	-1.03714	2.97346
11	C	3.279147	-0.87539	2.959811
12	C	2.72333	-0.12728	1.713849
13	H	4.214106	-1.40813	2.764348
14	H	3.409277	-0.17175	3.786643
15	H	3.2992	-0.33343	0.805078
16	C	2.689602	1.406053	1.906439
17	O	1.483315	-1.57234	5.587014
18	O	-1.01028	-0.17089	1.302427

19	H	-1.60922	0.282451	0.669481
20	H	1.584628	-1.97979	6.473988
21	O	0.482713	0.328635	-0.3448
22	O	3.013446	1.977094	2.927916
23	O	2.318719	2.124266	0.802317
24	H	1.961107	1.528375	0.10473

Oxa-norbornene (FDCA+Methyl acrylate)

ATOM		X	Y	Z
1	C	0.16465	-0.18213	0.862144
2	C	1.262016	-0.89715	1.62946
3	C	1.638358	-2.28229	1.107637
4	C	2.186546	-2.92049	2.147978
5	C	2.160037	-1.917	3.298338
6	H	1.529727	-2.58094	0.071064
7	H	2.658892	-3.89487	2.205744
8	C	2.231979	-2.48577	4.697988
9	O	2.845386	-3.50509	4.969639
10	O	0.955673	-1.1433	3.024087
11	C	3.285135	-0.83637	2.988866
12	C	2.665667	-0.08606	1.771281
13	H	4.242597	-1.31006	2.752574
14	H	3.393128	-0.17146	3.848593
15	H	3.237821	-0.20864	0.848626
16	C	2.41391	1.4089	1.927336
17	O	1.58987	-1.70964	5.618575
18	O	-0.54201	0.684547	1.643469
19	H	-1.18155	1.128552	1.046454
20	H	1.716047	-2.15227	6.485169
21	O	-0.02872	-0.34922	-0.32867
22	O	2.284187	1.800009	3.225552
23	O	2.294972	2.157573	0.968644
24	C	1.909036	3.203727	3.404371
25	H	0.931536	3.380084	2.94096
26	H	2.659243	3.854709	2.940585
27	H	1.867794	3.349066	4.487085

Oxa-norbornene (FDCA-ester+Ethylene)

ATOM		X	Y	Z
1	C	0.506977	-0.49325	1.377571

2	O	0.499874	-0.57555	-0.93165
3	C	2.457675	-1.8687	2.949235
4	C	3.19544	-4.51681	2.057767
5	C	4.161224	-5.66925	4.093022
6	C	4.018047	-3.72428	6.221305
7	H	3.080862	-5.13618	0.107414
8	H	5.054501	-7.50407	4.281768
9	C	4.055662	-4.73896	8.895688
10	O	5.132894	-6.69586	9.48408
11	O	1.752707	-2.29231	5.578484
12	C	6.144335	-1.67254	5.669982
13	C	5.014926	-0.33036	3.303376
14	H	7.986456	-2.55399	5.336807
15	H	6.26264	-0.37639	7.278732
16	H	6.209675	-0.44345	1.618741
17	H	4.562465	1.647445	3.712371
18	O	2.873461	-3.16227	10.54005
19	O	-1.11231	0.892411	2.804616
20	C	-2.99044	2.323653	1.357824
21	C	2.909918	-4.00591	13.17671
22	H	4.866944	-4.18889	13.83302
23	H	1.955265	-5.83745	13.34181
24	H	1.898627	-2.53703	14.21866
25	H	-4.15423	3.262572	2.783317
26	H	-4.11688	1.031208	0.194766
27	H	-2.03817	3.700428	0.136045

Oxa-norbornene (FDCA-ester+Propylene)

	ATOM	X	Y	Z
1	C	0.270231	-0.23526	0.728725
2	O	0.265376	-0.26659	-0.4938
3	C	1.29493	-0.98348	1.551542
4	C	1.651783	-2.39071	1.070249
5	C	2.155888	-3.01758	2.140597
6	C	2.110771	-1.99181	3.270239
7	H	1.575408	-2.71287	0.037388
8	H	2.607293	-3.99924	2.228797
9	C	2.146402	-2.53447	4.679432
10	O	2.766357	-3.54426	4.984368
11	O	0.925389	-1.20957	2.944233
12	C	3.254991	-0.90495	2.992685
13	C	2.664013	-0.1996	1.730821

14	C	4.663333	-1.48054	2.824441
15	H	3.222156	-0.21227	3.841077
16	H	3.300521	-0.2955	0.844589
17	H	2.455485	0.857792	1.926122
18	O	1.483344	-1.73675	5.55627
19	O	-0.5792	0.49869	1.491786
20	C	-1.56707	1.272184	0.734187
21	C	1.523996	-2.19202	6.948373
22	H	2.563879	-2.25902	7.289812
23	H	1.048845	-3.17677	7.031084
24	H	0.967564	-1.43549	7.507693
25	H	-2.17698	1.76868	1.49355
26	H	-2.1711	0.598981	0.114446
27	H	-1.05751	2.000974	0.092421
28	H	4.701214	-2.14669	1.951807
29	H	4.961936	-2.05421	3.712942
30	H	5.390276	-0.67018	2.672264

Oxa-norbornene (FDCA-ester+Acrolein)

	ATOM	X	Y	Z
1	C	0.206724	-0.28968	0.727389
2	O	0.070616	-0.45923	-0.47476
3	C	1.283182	-0.98861	1.531656
4	C	1.652582	-2.40141	1.092847
5	C	2.191257	-2.98704	2.169391
6	C	2.150739	-1.92447	3.267002
7	H	1.56437	-2.75765	0.072747
8	H	2.674819	-3.9518	2.275254
9	C	2.26706	-2.41455	4.692017
10	O	3.111394	-3.23774	5.018106
11	O	0.962428	-1.17026	2.949003
12	C	3.285363	-0.81592	2.887046
13	C	2.637649	-0.1639	1.64123
14	C	4.660923	-1.42756	2.697698
15	H	3.32193	-0.12227	3.737446
16	H	3.259645	-0.27062	0.74779
17	H	2.403576	0.88944	1.82503
18	O	1.39284	-1.81443	5.533314
19	O	-0.52046	0.572024	1.482292
20	C	-1.55139	1.310253	0.744908
21	C	1.496901	-2.24472	6.933082
22	H	2.506549	-2.04412	7.309952

23	H	1.285142	-3.31775	7.004606
24	H	0.745574	-1.65436	7.463509
25	H	-2.04582	1.929103	1.498136
26	H	-2.25338	0.606468	0.283017
27	H	-1.08264	1.923721	-0.03366
28	O	5.259843	-1.47374	1.633894
29	H	5.097729	-1.86683	3.62216

Oxa-norbornene (FDCA-ester+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.218501	-0.31287	0.804116
2	O	0.017867	-0.5861	-0.36941
3	C	1.320776	-0.96611	1.612368
4	C	1.623989	-2.42777	1.293745
5	C	2.205298	-2.93466	2.38832
6	C	2.271675	-1.75629	3.376668
7	H	1.472275	-2.87725	0.318607
8	H	2.673148	-3.90161	2.540464
9	C	2.367642	-2.10375	4.846307
10	O	3.440082	-2.38575	5.388184
11	O	1.079324	-1.00666	3.054565
12	C	3.421114	-0.77646	2.812683
13	C	2.689134	-0.17191	1.579793
14	C	4.7747	-1.43601	2.462935
15	H	3.607058	-0.00885	3.573545
16	H	3.247465	-0.32342	0.652778
17	H	2.478013	0.891635	1.728206
18	O	1.186915	-2.10348	5.478361
19	O	-0.44743	0.631694	1.514251
20	C	-1.49346	1.336909	0.764606
21	C	1.238814	-2.44759	6.908519
22	H	1.897233	-1.7463	7.432385
23	H	1.616007	-3.46944	7.02682
24	H	0.205179	-2.35868	7.250151
25	H	-1.94736	2.016993	1.489853
26	H	-2.22474	0.616891	0.379653
27	H	-1.04279	1.885393	-0.07096
28	O	5.340165	-1.26679	1.397306
29	O	5.339917	-2.20146	3.433187
30	H	4.743662	-2.26304	4.228881

**Oxa-norbornene (FDCA-ester+Methyl
acrylate)**

ATOM		X	Y	Z
1	C	0.125348	-0.25711	0.667736
2	O	-0.00806	-0.3549	-0.54305
3	C	1.241156	-0.9458	1.425909
4	C	1.716998	-2.28955	0.887234
5	C	2.304139	-2.90309	1.922012
6	C	2.177759	-1.9402	3.093628
7	H	1.655744	-2.57643	-0.15647
8	H	2.852152	-3.83695	1.963205
9	C	2.288205	-2.53413	4.485393
10	O	2.849998	-3.59369	4.713204
11	O	0.928337	-1.2542	2.820309
12	C	3.191276	-0.69642	2.855941
13	C	2.538494	-0.03843	1.607203
14	C	4.647277	-1.10873	2.802616
15	H	3.073655	-0.05988	3.735502
16	H	3.173915	-0.06513	0.71876
17	H	2.238632	0.990765	1.829984
18	O	1.755981	-1.71163	5.423348
19	O	-0.6396	0.518963	1.476977
20	C	-1.70736	1.252182	0.789571
21	C	1.902582	-2.18435	6.803761
22	H	2.967014	-2.27052	7.05101
23	H	1.417026	-3.16078	6.916522
24	H	1.410567	-1.42302	7.414704
25	H	-2.2126	1.817186	1.577048
26	H	-2.39037	0.544761	0.305193
27	H	-1.27463	1.918138	0.033476
28	O	5.047057	-1.48484	1.549082
29	O	5.372924	-1.13975	3.785608
30	C	6.427108	-1.9686	1.469266
31	H	6.576009	-2.2317	0.418396
32	H	6.553645	-2.84056	2.121663
33	H	7.117264	-1.17685	1.784094

Oxa-norbornene (DMF+Ethylene)

ATOM		X	Y	Z
1	C	0.209339	-0.24518	0.673986
2	C	1.314663	-0.95403	1.428384
3	C	1.69638	-2.37721	1.003474

4	C	2.213239	-2.96315	2.092437
5	C	2.157979	-1.91056	3.20692
6	H	1.642792	-2.75474	-0.01468
7	H	2.687855	-3.9371	2.183794
8	C	2.097907	-2.38478	4.643455
9	O	0.957441	-1.15809	2.835645
10	C	3.273811	-0.84791	2.86303
11	C	2.67229	-0.16476	1.595315
12	H	4.25102	-1.31482	2.68908
13	H	3.311862	-0.24446	0.707673
14	H	2.446974	0.892611	1.781578
15	H	-0.70734	-0.84943	0.681193
16	H	0.515309	-0.07438	-0.36805
17	H	1.981058	-1.52479	5.316943
18	H	3.027616	-2.91044	4.903686
19	H	1.25042	-3.06814	4.787188
20	H	0.00276	0.726623	1.142484
21	H	3.359476	-0.13902	3.695703

Oxa-norbornene (DMF+Propylene)

	ATOM	X	Y	Z
1	C	0.22097	-0.20404	0.685034
2	C	1.320381	-0.93209	1.429829
3	C	1.704816	-2.3422	0.965472
4	C	2.208662	-2.96267	2.041161
5	C	2.144925	-1.94396	3.184572
6	H	1.659224	-2.68817	-0.06435
7	H	2.676901	-3.9414	2.103878
8	C	2.075729	-2.46284	4.604379
9	O	0.945833	-1.1824	2.82581
10	C	3.256731	-0.84815	2.906163
11	C	2.675898	-0.15193	1.632523
12	C	4.683837	-1.38813	2.761227
13	H	3.210525	-0.15088	3.752411
14	H	3.338544	-0.23804	0.761397
15	H	2.46119	0.908271	1.815673
16	H	-0.69738	-0.80584	0.676204
17	H	0.532122	-0.01349	-0.35202
18	H	1.933982	-1.62449	5.300021
19	H	3.012656	-2.97751	4.859941
20	H	1.240953	-3.16703	4.718502
21	H	0.014974	0.759016	1.171511
22	H	4.748881	-2.07159	1.902734

23	H	4.994694	-1.93251	3.665664
24	H	5.395292	-0.56541	2.599574

Oxa-norbornene (DMF+Acrolein)

1	H	0.438727	-3.95021	1.387416
2	C	0.921877	-3.08115	0.92141
3	H	1.583219	-3.4307	0.11619
4	C	1.726246	-2.30981	1.945238
5	C	2.783819	-3.05628	2.759289
6	C	2.910904	-2.38848	3.913827
7	C	1.928797	-1.21919	3.831895
8	H	3.378452	-3.88664	2.38793
9	H	3.632315	-2.53821	4.71241
10	C	1.406151	-0.61017	5.114586
11	H	2.233803	-0.17109	5.689172
12	H	0.921525	-1.38265	5.726137
13	O	0.866919	-1.77314	3.013491
14	C	2.548354	-0.1722	2.753916
15	C	2.413182	-0.98044	1.439265
16	C	3.929527	0.299921	3.128827
17	H	1.87106	0.69266	2.777391
18	H	3.385212	-1.16109	0.967555
19	H	1.746743	-0.47356	0.731404
20	H	0.150753	-2.43289	0.4839
21	H	0.675882	0.17855	4.889901
22	O	4.969591	-0.01015	2.565139
23	H	3.953801	0.968997	4.024409

Oxa-norbornene (DMF+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.205607	-0.24925	0.677429
2	C	1.314132	-0.95721	1.426735
3	C	1.697435	-2.37648	1.005666
4	C	2.207312	-2.96847	2.09366
5	C	2.141191	-1.92212	3.207201
6	H	1.661648	-2.74758	-0.01475
7	H	2.693836	-3.93564	2.180397
8	C	2.094754	-2.39325	4.645024
9	O	0.961301	-1.16115	2.841687
10	C	3.264529	-0.8074	2.866746

11	C	2.670409	-0.16334	1.586736
12	C	4.663949	-1.38522	2.722904
13	H	3.246685	-0.09847	3.704778
14	H	3.334191	-0.28163	0.724383
15	H	2.451232	0.898604	1.747755
16	H	-0.70847	-0.8568	0.682867
17	H	0.511636	-0.07494	-0.36354
18	H	2.025022	-1.53446	5.327552
19	O	5.245269	-1.60512	1.681401
20	O	5.275358	-1.71887	3.925518
21	H	4.685801	-1.47825	4.66565
22	H	2.996433	-2.97558	4.880996
23	H	1.220174	-3.03782	4.80055
24	H	-0.00328	0.72059	1.148352

Oxa-norbornene (DMF+Methyl acrylate)

	ATOM	X	Y	Z
1	C	0.337906	-0.1841	0.632773
2	C	1.394007	-0.9108	1.437763
3	C	1.789122	-2.32685	1.01122
4	C	2.226708	-2.94382	2.117204
5	C	2.106891	-1.91711	3.246541
6	H	1.803136	-2.67941	-0.0168
7	H	2.685511	-3.9234	2.220091
8	C	1.979804	-2.40379	4.671146
9	O	0.956878	-1.1365	2.821045
10	C	3.269179	-0.82525	2.982038
11	C	2.738101	-0.12552	1.697104
12	C	4.639608	-1.46948	2.978248
13	H	3.244061	-0.14769	3.842107
14	H	3.428892	-0.18254	0.851428
15	H	2.49893	0.924812	1.902295
16	H	-0.58298	-0.77993	0.585968
17	H	0.701798	-0.01004	-0.38962
18	H	1.78102	-1.55256	5.335937
19	O	5.243366	-1.47573	1.747408
20	O	5.148034	-1.974	3.971651
21	H	2.919544	-2.87667	4.982404
22	H	1.154508	-3.12358	4.752623
23	H	0.115202	0.786138	1.0967
24	C	6.534771	-2.16285	1.705659
25	H	6.859254	-2.09176	0.663445

26	H	6.410543	-3.20822	2.012594
27	H	7.245887	-1.67074	2.379729

TS (HMF+Ethylene)

ATOM		X	Y	Z
1	C	0.423331	-0.15942	0.534732
2	C	1.319127	-1.02215	1.397935
3	C	1.802128	-2.34389	1.025415
4	C	2.089208	-2.98651	2.199847
5	C	1.709315	-2.08994	3.26047
6	H	2.047273	-2.65194	0.014214
7	H	2.602457	-3.93212	2.342648
8	C	1.670691	-2.36439	4.698201
9	O	0.85625	-1.13242	2.727365
10	C	3.414316	-0.63965	3.043935
11	C	2.962282	-0.07958	1.811257
12	H	4.265528	-1.3168	3.060631
13	H	3.181568	-0.13474	3.97895
14	H	3.574068	-0.26014	0.926056
15	H	2.528708	0.920594	1.853179
16	O	1.025551	-1.73189	5.529031
17	O	0.190374	1.148212	1.084493
18	H	-0.53105	-0.69075	0.378479
19	H	0.901846	-0.01057	-0.44081
20	H	-0.18151	1.017706	1.976539
21	H	2.332769	-3.21495	4.990143

TS (HMF+Propylene)

ATOM		X	Y	Z
1	C	0.484247	-0.14212	0.509095
2	C	1.38684	-0.98505	1.390773
3	C	1.865048	-2.3146	1.018948
4	C	2.113676	-2.96743	2.198025
5	C	1.708644	-2.08561	3.253412
6	H	2.12829	-2.6204	0.011719
7	H	2.61141	-3.92034	2.344872
8	C	1.703066	-2.32345	4.688481
9	O	0.889111	-1.10209	2.710988
10	C	3.494529	-0.57367	2.992008
11	C	2.953471	-0.02718	1.78451

12	C	4.748787	-1.40326	2.968168
13	H	3.201903	-0.11655	3.935197
14	H	3.567154	-0.15243	0.888123
15	H	2.493649	0.959818	1.860655
16	O	1.09668	-1.65682	5.527136
17	O	0.186604	1.146629	1.070016
18	H	-0.44249	-0.70841	0.317146
19	H	0.986701	0.038944	-0.44898
20	H	-0.20111	0.988242	1.950924
21	H	2.355716	-3.1814	4.981593
22	H	4.723197	-2.10387	2.119281
23	H	4.889129	-1.9713	3.897579
24	H	5.636733	-0.76086	2.827994

		TS (HMF+Acrolein)		
	ATOM	X	Y	Z
1	C	0.404593	-0.51809	1.204217
2	C	2.529039	-1.88087	2.611842
3	C	3.504872	-4.33586	1.809334
4	C	4.383265	-5.50584	3.938049
5	C	3.686444	-3.92702	6.01972
6	H	3.692043	-4.97492	-0.14263
7	H	5.560661	-7.19351	4.089623
8	C	3.974556	-4.47701	8.709906
9	O	1.948626	-2.15626	5.25107
10	C	6.680468	-0.72793	5.331227
11	C	5.447151	0.071951	3.030394
12	C	8.983732	-2.22337	5.316451
13	H	6.107271	0.111607	7.121036
14	H	6.578458	-0.28602	1.34073
15	H	4.579233	1.948231	3.135847
16	O	2.65081	-3.60332	10.39497
17	O	-0.10381	1.954317	2.184249
18	H	-1.34166	-1.68317	1.251875
19	H	0.948993	-0.28576	-0.78297
20	H	-0.49367	1.740702	3.982837
21	H	5.594404	-5.78327	9.090742
22	O	10.04172	-3.04964	3.39829
23	H	9.737245	-2.66599	7.242838

TS (HMF+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.071208	-0.48571	0.842313
2	C	1.289141	-1.11058	1.509688
3	C	1.885706	-2.36473	1.014556
4	C	2.419381	-2.99474	2.100163
5	C	2.071105	-2.19812	3.24438
6	H	2.048125	-2.59867	-0.0318
7	H	3.092368	-3.84468	2.114051
8	C	2.420179	-2.42627	4.649688
9	O	1.045072	-1.34808	2.912341
10	C	3.477397	-0.36732	2.709607
11	C	2.602142	0.017733	1.613131
12	C	4.750897	-1.03332	2.428192
13	H	3.303842	0.062384	3.694355
14	H	3.09793	-0.00702	0.639507
15	H	2.064859	0.953381	1.790035
16	O	1.927825	-1.83375	5.606643
17	O	-0.34915	0.730561	1.477356
18	H	-0.74211	-1.22809	0.830308
19	H	0.327704	-0.22881	-0.19271
20	H	-0.57861	0.507384	2.398454
21	H	3.224167	-3.18707	4.77487
22	O	5.064594	-1.49112	1.3353
23	O	5.619497	-1.19759	3.502936
24	H	5.24126	-0.77308	4.296671

TS (HMF+Methyl Acrylate)

	ATOM	X	Y	Z
1	C	0.918363	-0.45016	-0.2033
2	C	1.640379	-1.13991	0.944788
3	C	2.172367	-2.50203	0.835077
4	C	2.144747	-3.02646	2.097646
5	C	1.503327	-2.05242	2.932701
6	H	2.676843	-2.89773	-0.0395
7	H	2.603984	-3.94168	2.455151
8	C	1.200162	-2.12283	4.366801
9	O	0.848607	-1.14077	2.139411
10	C	3.308214	-0.49425	2.883941
11	C	3.01582	-0.14416	1.511172
12	C	4.453569	-1.30323	3.303986

13	H	2.839215	0.063157	3.688951
14	H	3.819772	-0.34592	0.801755
15	H	2.580106	0.850146	1.386971
16	O	0.401829	-1.39457	4.948201
17	O	0.489732	0.880331	0.120281
18	H	0.066007	-1.07799	-0.50888
19	H	1.608834	-0.36053	-1.0509
20	H	-0.10627	0.810688	0.889069
21	H	1.792405	-2.90073	4.898388
22	O	5.101683	-1.89341	2.226064
23	O	4.810164	-1.4766	4.467042
24	C	6.218141	-2.75381	2.597674
25	H	6.60571	-3.14727	1.653168
26	H	5.872576	-3.56468	3.251781
27	H	6.98342	-2.17282	3.126733

TS (HMFA+Ethylene)

ATOM		X	Y	Z
1	C	0.525987	-0.07657	0.530629
2	C	1.380264	-1.00187	1.365344
3	C	1.880221	-2.29452	0.943374
4	C	2.137392	-3.00083	2.090053
5	C	1.756867	-2.1492	3.180764
6	H	2.146817	-2.55291	-0.07628
7	H	2.636922	-3.95496	2.211094
8	C	1.658992	-2.55207	4.592052
9	O	2.234267	-3.52821	5.056591
10	O	0.904367	-1.16441	2.679032
11	C	3.441808	-0.73144	3.106834
12	C	3.079372	-0.07718	1.897555
13	H	4.269475	-1.4368	3.126483
14	H	3.195153	-0.26224	4.057825
15	H	3.704534	-0.24032	1.01946
16	H	2.645451	0.920338	1.965593
17	O	0.896954	-1.69038	5.347918
18	O	0.302913	1.204672	1.146067
19	H	-0.43537	-0.57669	0.319971
20	H	1.032366	0.114872	-0.42313
21	H	-0.07279	1.030846	2.028773
22	H	0.929429	-2.04476	6.261186

TS (HMFA+Propylene)

	ATOM	X	Y	Z
1	C	0.490446	-0.12565	0.507665
2	C	1.391299	-0.99973	1.353917
3	C	1.868061	-2.31531	0.958048
4	C	2.159056	-2.98154	2.120633
5	C	1.80148	-2.10229	3.190612
6	H	2.102799	-2.6094	-0.05955
7	H	2.662461	-3.93107	2.257155
8	C	1.843983	-2.40273	4.618378
9	O	2.517453	-3.3125	5.094972
10	O	0.943932	-1.123	2.686849
11	C	3.53645	-0.62969	2.956692
12	C	3.038371	-0.04629	1.753755
13	C	4.76027	-1.50677	2.968735
14	H	3.263054	-0.15025	3.895876
15	H	3.636013	-0.20031	0.852301
16	H	2.588104	0.944423	1.824704
17	O	1.1084	-1.52551	5.386979
18	O	0.239193	1.165676	1.089366
19	H	-0.4575	-0.66147	0.329077
20	H	0.975764	0.053444	-0.45949
21	H	-0.12076	1.006583	1.981477
22	H	1.247866	-1.81315	6.313261
23	H	4.823123	-2.08295	2.034303
24	H	4.747856	-2.20559	3.817501
25	H	5.678086	-0.89735	3.04477

TS (HMFA+Acrolein)

	ATOM	X	Y	Z
1	C	0.290613	-0.36633	0.657364
2	C	1.415841	-1.01414	1.459974
3	C	1.90231	-2.36203	1.114913
4	C	2.248192	-2.97441	2.286893
5	C	1.904513	-2.06871	3.331892
6	H	2.122774	-2.69339	0.106807
7	H	2.792031	-3.89933	2.433003
8	C	2.113233	-2.25638	4.774666
9	O	2.751532	-3.19107	5.2422
10	O	1.055027	-1.10127	2.861325
11	C	3.641642	-0.37769	2.656693
12	C	2.787128	0.007162	1.542385
13	C	4.746645	-1.28251	2.449027

14	H	3.531072	0.107069	3.624141
15	H	3.282509	-0.11942	0.575168
16	H	2.326681	0.992202	1.654109
17	O	1.530812	-1.26895	5.533838
18	O	-0.08486	0.924699	1.158306
19	H	-0.56991	-1.05337	0.643837
20	H	0.637394	-0.21591	-0.37206
21	H	-0.39447	0.796728	2.073826
22	H	1.738403	-1.49417	6.465094
23	O	4.970407	-1.85703	1.365854
24	H	5.378932	-1.49461	3.33903

TS (HMFA+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.395114	-0.08514	0.67572
2	C	1.434759	-0.90338	1.422594
3	C	2.097693	-2.07143	0.847565
4	C	2.43252	-2.88906	1.894258
5	C	1.90265	-2.26655	3.068541
6	H	2.430123	-2.1498	-0.18123
7	H	3.079703	-3.758	1.896244
8	C	1.992927	-2.7009	4.464525
9	O	2.929824	-3.37105	4.902469
10	O	0.964788	-1.32703	2.705062
11	C	3.498021	-0.49529	3.043531
12	C	2.795786	0.195407	2.001035
13	C	4.743313	-1.22299	2.710426
14	H	3.277923	-0.28803	4.088214
15	H	3.386511	0.360605	1.098421
16	H	2.198826	1.054578	2.309274
17	O	0.965807	-2.24802	5.246424
18	O	-0.10915	1.021147	1.43878
19	H	-0.42286	-0.75455	0.363641
20	H	0.860753	0.337537	-0.22272
21	H	-0.5142	0.651704	2.244745
22	H	1.158867	-2.56262	6.155232
23	O	5.304188	-1.13549	1.623941
24	O	5.267167	-2.04799	3.681044
25	H	4.57431	-2.31333	4.325893

TS (HMFA+Methyl Acrylate)

ATOM		X	Y	Z
1	C	0.190384	-0.54002	0.362853
2	C	1.399593	-0.98465	1.167935
3	C	2.435858	-1.85977	0.628628
4	C	2.958767	-2.54618	1.691942
5	C	2.193806	-2.16491	2.833794
6	H	2.834034	-1.79385	-0.37782
7	H	3.842174	-3.17131	1.732801
8	C	2.340589	-2.67757	4.203746
9	O	3.256748	-3.41147	4.547062
10	O	1.023791	-1.56246	2.41934
11	C	3.018203	0.067018	2.994341
12	C	2.322617	0.468879	1.800357
13	C	4.462129	-0.15025	3.085041
14	H	2.531161	0.180825	3.958214
15	H	2.955794	0.773129	0.966289
16	H	1.473861	1.135709	1.966436
17	O	1.360318	-2.22191	5.053043
18	O	-0.67	0.356387	1.083666
19	H	-0.36147	-1.43486	0.03285
20	H	0.537482	0.003638	-0.52404
21	H	-0.9583	-0.11173	1.888837
22	H	1.578078	-2.5966	5.932225
23	O	5.062017	-0.22359	1.834445
24	O	5.089387	-0.27386	4.13353
25	C	6.490475	-0.51338	1.873181
26	H	6.805875	-0.53847	0.825496
27	H	6.666102	-1.47942	2.363724
28	H	7.021475	0.269939	2.427844

TS (FDCA+Propylene)

ATOM		X	Y	Z
1	C	0.579534	-0.14978	0.514726
2	C	1.355122	-1.01594	1.424516
3	C	2.017893	-2.23319	1.012674
4	C	2.353613	-2.88887	2.160434
5	C	1.91975	-2.02464	3.248564
6	H	2.260031	-2.47375	-0.0157
7	H	2.946007	-3.78553	2.297098
8	C	1.79384	-2.50114	4.652016
9	O	2.48251	-3.40063	5.110189
10	O	0.917594	-1.18653	2.741166

11	C	3.362057	-0.64139	3.252418
12	C	3.069802	0.129808	2.079607
13	H	4.245908	-1.27713	3.258408
14	H	3.14658	-0.16294	4.210097
15	H	3.691041	-0.03717	1.200769
16	C	2.499543	1.524729	2.240551
17	O	0.879613	-1.78967	5.381948
18	O	-0.40641	0.559911	1.150603
19	H	-0.82324	1.114684	0.457858
20	H	0.902892	-2.16959	6.285672
21	O	0.831989	-0.04326	-0.67868
22	H	1.668699	1.516021	2.959484
23	H	2.134262	1.929435	1.28754
24	H	3.274822	2.20996	2.620838

		TS (FDCA+Acrolein)		
	ATOM	X	Y	Z
1	C	1.059831	-0.83029	0.70529
2	O	1.503617	-1.04845	-1.53378
3	C	2.564131	-2.2583	2.659686
4	C	3.1574	-4.93976	2.345806
5	C	3.592489	-5.85881	4.717142
6	C	3.110226	-3.81024	6.436404
7	H	3.455839	-5.83261	0.527422
8	H	4.321561	-7.68253	5.295827
9	C	3.103489	-3.97384	9.224354
10	O	3.947514	-5.79478	10.35881
11	O	1.688552	-1.99428	5.204061
12	C	6.519173	-1.32933	5.563836
13	C	5.650216	-0.69781	3.048601
14	C	8.617129	-3.09435	5.951352
15	H	6.115149	-0.04643	7.120332
16	H	6.773357	-1.43628	1.482295
17	H	5.143794	1.28514	2.77739
18	O	2.128922	-1.85467	10.34873
19	O	-0.74927	0.78345	1.599842
20	H	-0.86471	0.642146	3.443045
21	H	2.276275	-2.12881	12.17574
22	O	9.85182	-3.26882	7.912313
23	H	9.017271	-4.34386	4.294902

TS (FDCA+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.379364	-0.04964	0.637655
2	C	1.103315	-1.02357	1.480704
3	C	1.612707	-2.29834	1.039292
4	C	2.09059	-2.91829	2.154846
5	C	1.93487	-1.95124	3.247852
6	H	1.65824	-2.60881	0.002116
7	H	2.624383	-3.85616	2.25093
8	C	1.920324	-2.41249	4.675231
9	O	2.645878	-3.31173	5.06772
10	O	0.909896	-1.05996	2.842527
11	C	3.39079	-0.82	3.050877
12	C	3.152459	-0.08202	1.834816
13	H	4.228116	-1.51736	3.054786
14	H	3.32611	-0.20153	3.948764
15	H	3.599388	-0.42476	0.90387
16	C	2.785431	1.353434	1.923114
17	O	1.07123	-1.69647	5.462377
18	O	-0.4503	0.76089	1.34247
19	H	-0.78828	1.434161	0.714181
20	H	1.168621	-2.05134	6.371928
21	O	0.579524	0.028733	-0.57086
22	O	2.619255	1.972697	2.960391
23	O	2.61837	2.004397	0.708483
24	H	2.632194	1.359448	-0.02613

TS (FDCA+Methyl Acrylate)

	ATOM	X	Y	Z
1	C	0.111166	0.238609	1.066676
2	C	1.035406	-0.79704	1.583521
3	C	1.415539	-1.98363	0.855118
4	C	2.093064	-2.76828	1.73845
5	C	2.179925	-1.98862	2.979155
6	H	1.238316	-2.12574	-0.20406
7	H	2.614472	-3.7041	1.575971
8	C	2.443279	-2.66839	4.287863
9	O	3.203552	-3.61859	4.383345

10	O	1.112443	-1.05847	2.937626
11	C	3.58912	-0.8218	2.656924
12	C	3.090744	0.127841	1.68554
13	H	4.385449	-1.48785	2.324116
14	H	3.761579	-0.4066	3.650426
15	H	3.351428	0.019285	0.637244
16	C	2.719552	1.510879	2.049455
17	O	1.799023	-2.08493	5.339649
18	O	-0.35444	1.077981	2.040841
19	H	-0.88671	1.75603	1.573514
20	H	2.067262	-2.58835	6.137854
21	O	-0.16649	0.336337	-0.11879
22	O	2.613405	1.684174	3.410712
23	O	2.503578	2.404846	1.236067
24	C	2.120954	2.994127	3.819714
25	H	1.114227	3.151407	3.415054
26	H	2.78982	3.782782	3.454182
27	H	2.10403	2.964174	4.91285

TS (FDCA-ester+Ethylene)

	ATOM	X	Y	Z
1	C	0.14461	-0.32874	0.780628
2	O	0.131201	-0.26788	-0.4423
3	C	1.167575	-1.1066	1.52757
4	C	1.867139	-2.24696	0.971662
5	C	2.468579	-2.86846	2.028669
6	C	2.119517	-2.0912	3.199777
7	H	1.95734	-2.44623	-0.08936
8	H	3.167884	-3.69596	2.035903
9	C	2.307943	-2.57823	4.591388
10	O	3.149488	-3.41656	4.887426
11	O	0.972763	-1.35226	2.8904
12	C	3.376409	-0.46334	2.968894
13	C	2.745877	0.188309	1.865912
14	H	4.335012	-0.95756	2.820573
15	H	3.224135	-0.0413	3.962021
16	H	3.232126	0.182771	0.891834
17	H	2.141611	1.070631	2.075109
18	O	1.487435	-1.94991	5.479518
19	O	-0.71462	0.334133	1.604482
20	C	-1.71536	1.145274	0.90796
21	C	1.656469	-2.38131	6.868909

22	H	2.686802	-2.19644	7.19535
23	H	1.432336	-3.45113	6.955725
24	H	0.942932	-1.78017	7.438481
25	H	-2.32097	1.589574	1.702209
26	H	-2.32196	0.508954	0.25247
27	H	-1.21802	1.916506	0.307236

TS (FDCA-ester+Propylene)

	ATOM	X	Y	Z
1	C	-0.16028	-0.52941	0.806955
2	O	-0.16612	-0.50045	-0.41664
3	C	0.810768	-1.35416	1.580918
4	C	1.365676	-2.59477	1.064485
5	C	1.903912	-3.23743	2.142194
6	C	1.648246	-2.3875	3.281601
7	H	1.423216	-2.84082	0.011068
8	H	2.510204	-4.13425	2.175603
9	C	1.875296	-2.78126	4.686146
10	O	2.700016	-3.63236	5.003553
11	O	0.589775	-1.53526	2.954834
12	C	3.098083	-0.85597	2.928205
13	C	2.441108	-0.22378	1.821824
14	C	4.411735	-1.58	2.738762
15	H	2.943193	-0.39381	3.903732
16	H	2.917218	-0.28608	0.842452
17	H	1.930257	0.719706	2.016062
18	O	1.132344	-2.05104	5.56747
19	O	-0.97456	0.210044	1.60934
20	C	-1.92041	1.066159	0.890082
21	C	1.37176	-2.37333	6.974546
22	H	2.425808	-2.20282	7.225719
23	H	1.117339	-3.42245	7.168018
24	H	0.717226	-1.69875	7.532876
25	H	-2.50211	1.561631	1.671889
26	H	-2.56144	0.454858	0.243767
27	H	-1.37408	1.794027	0.278027
28	H	4.423788	-2.0959	1.768327
29	H	4.577975	-2.31924	3.535064
30	H	5.253823	-0.86792	2.749888

TS (FDCA-ester+Acrolein)

	ATOM	X	Y	Z
1	C	0.936929	-3.40078	1.826903
2	O	1.280449	-4.23152	1.001223
3	C	1.806642	-2.21515	2.172622
4	C	3.261335	-2.42948	2.317572
5	C	3.708999	-1.45268	3.153069
6	C	2.544425	-0.71507	3.563237
7	H	3.826314	-3.13298	1.719054
8	H	4.727367	-1.17121	3.389657
9	C	2.52155	0.399684	4.536055
10	O	3.540395	0.971699	4.902966
11	O	1.416414	-1.46813	3.339456
12	C	2.098987	0.268743	1.500588
13	C	1.595461	-0.99306	0.959635
14	C	3.414636	0.755746	1.118574
15	H	1.40116	0.971517	1.950918
16	H	2.155597	-1.34804	0.091749
17	H	0.514742	-0.99491	0.793456
18	O	1.256766	0.713156	4.934495
19	O	-0.24893	-3.38446	2.485517
20	C	-1.15103	-4.49185	2.147185
21	C	1.180437	1.821752	5.889221
22	H	1.559515	2.739949	5.424641
23	H	1.77774	1.589883	6.778689
24	H	0.11867	1.908526	6.133584
25	H	-2.02575	-4.34339	2.786059
26	H	-0.65936	-5.44915	2.356354
27	H	-1.41578	-4.44026	1.084643
28	O	4.235291	0.094573	0.465804
29	H	3.676659	1.769414	1.495723

TS (FDCA-ester+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.629608	-0.15558	0.602943
2	O	0.79708	-0.15437	-0.60664
3	C	1.466319	-0.99693	1.523375
4	C	1.977417	-2.29835	1.094978
5	C	2.268991	-2.98426	2.237919
6	C	1.875257	-2.12242	3.325787
7	H	2.210401	-2.55046	0.068014
8	H	2.801607	-3.92043	2.354712
9	C	1.881011	-2.44219	4.768531

10	O	2.803574	-3.06933	5.296795
11	O	0.990413	-1.1767	2.851891
12	C	3.573528	-0.66769	3.089319
13	C	2.978395	0.017528	1.971619
14	C	4.771076	-1.52232	2.841647
15	H	3.433867	-0.2784	4.095792
16	H	3.572063	0.017262	1.057438
17	H	2.499016	0.970405	2.200194
18	O	0.812684	-1.94716	5.431069
19	O	-0.25971	0.618582	1.276365
20	C	-1.07689	1.489311	0.42289
21	C	0.817829	-2.18391	6.881194
22	H	1.70718	-1.72412	7.32772
23	H	0.821159	-3.26161	7.079811
24	H	-0.10046	-1.71455	7.24213
25	H	-1.73131	2.025004	1.115018
26	H	-1.65402	0.880469	-0.28288
27	H	-0.42963	2.178904	-0.1318
28	O	5.375064	-1.53617	1.77793
29	O	5.181237	-2.32623	3.875375
30	H	4.447165	-2.47301	4.51946

TS (FDCA-ester+Methyl Acrylate)

ATOM		X	Y	Z
1	C	0.152579	-0.35972	0.720509
2	O	0.127265	-0.3133	-0.50058
3	C	1.267633	-1.03417	1.46609
4	C	1.915373	-2.22639	0.919042
5	C	2.512823	-2.84641	1.976118
6	C	2.168755	-2.07334	3.139921
7	H	2.002995	-2.43274	-0.14043
8	H	3.201126	-3.68211	1.98443
9	C	2.479595	-2.45937	4.536989
10	O	3.241589	-3.37841	4.803936
11	O	1.0658	-1.29079	2.849936
12	C	3.434045	-0.26609	2.762974
13	C	2.645942	0.196917	1.641844
14	C	4.796678	-0.8048	2.646243
15	H	3.223567	0.147036	3.745379
16	H	3.136053	0.200315	6.69E-01
17	H	2.068628	1.102287	1.840933
18	O	1.86334	-1.656358	5.447252
19	O	-0.74933	0.224846	1.549817

20	C	-1.83677	0.933548	0.866036
21	C	2.189548	-1.96839	6.841821
22	H	3.268291	-1.85739	7.002392
23	H	1.88896	-2.99721	7.073123
24	H	1.620455	-1.24539	7.432006
25	H	-2.45753	1.336956	1.669853
26	H	-2.40061	0.231608	0.240649
27	H	-1.42365	1.732036	0.238849
28	O	5.098266	-1.2025	1.355893
29	O	5.580381	-0.91752	3.583887
30	C	6.408614	-1.82803	1.209941
31	H	6.488498	-2.07797	0.147765
32	H	6.466722	-2.72737	1.835819
33	H	7.198219	-1.12948	1.512935

TS (DMF+Ethylene)

	ATOM	X	Y	Z	
	1	H	-0.37669	-0.06187	0.79932
	2	C	0.701911	0.150157	0.800449
	3	H	0.862772	1.101926	1.319566
	4	H	1.027851	0.266155	-0.23945
	5	C	1.469054	-0.95062	1.452702
	6	C	1.716112	-2.26137	0.955236
	7	C	2.102529	-3.02449	2.033654
	8	C	2.08707	-2.16411	3.167369
	9	C	3.911044	-1.11469	2.752807
	10	C	3.518484	-0.33601	1.654911
	11	H	1.739544	-2.53343	-0.09523
	12	H	2.504018	-4.03306	2.02533
	13	H	4.608132	-1.9401	2.61405
	14	H	3.252973	0.708782	1.816845
	15	C	2.076741	-2.54444	4.610321
	16	H	2.870738	-3.27353	4.807964
	17	H	1.117206	-2.99494	4.900456
	18	H	2.250099	-1.66856	5.245766
	19	O	1.333315	-1.05036	2.828661
	20	H	3.944602	-0.65489	3.740553
	21	H	3.909048	-0.55474	0.661921

TS (DMF+Propylene)

	ATOM	X	Y	Z
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1	C	0.186066	-0.23362	0.763177
2	C	1.235982	-1.06555	1.44032
3	C	1.827328	-2.27892	0.944714
4	C	2.391327	-2.91167	2.029665
5	C	2.13757	-2.07972	3.168418
6	H	1.940649	-2.52611	-0.10623
7	H	3.052864	-3.77172	2.027566
8	C	2.238365	-2.4522	4.61627
9	O	1.07832	-1.22757	2.824896
10	C	3.587802	-0.54824	2.776401
11	C	2.952615	0.092027	1.677164
12	C	4.914097	-1.25872	2.58844
13	H	3.431205	-0.09947	3.758925
14	H	3.426753	0.029601	0.696189
15	H	2.405159	1.017663	1.857054
16	H	-0.78646	-0.74946	0.757257
17	H	0.48526	-0.04145	-0.27576
18	H	2.186167	-1.55542	5.247549
19	H	3.200689	-2.94969	4.796802
20	H	1.430371	-3.13808	4.915809
21	H	0.067525	0.73005	1.275551
22	H	4.925788	-1.78377	1.622339
23	H	5.097619	-1.99643	3.384637
24	H	5.756677	-0.54657	2.592552

		TS (DMF+Acrolein)		
ATOM		X	Y	Z
1	H	0.820397	-4.18311	1.668915
2	C	1.01372	-3.30029	1.046664
3	H	1.605157	-3.60084	0.171202
4	C	1.791826	-2.24765	1.821577
5	C	3.055459	-2.61446	2.474447
6	C	3.089283	-1.97858	3.699796
7	C	1.855793	-1.33507	3.882156
8	H	3.856155	-3.15277	1.984714
9	H	3.933218	-1.90042	4.375724
10	C	1.338306	-0.51754	5.015219
11	H	2.169877	-0.14361	5.623912
12	H	0.673946	-1.11966	5.657812
13	O	0.978548	-1.6719	2.903496
14	C	2.661289	0.233072	1.462293
15	C	2.057798	-0.92683	0.812793

16	C	4.051583	0.225409	1.70334
17	H	2.05163	1.076278	1.782273
18	H	2.717963	-1.35918	0.051788
19	H	1.058319	-0.72985	0.412098
20	H	0.060708	-2.88271	0.698102
21	H	0.754057	0.332581	4.63844
22	O	4.797501	-0.76134	1.430625
23	H	4.487948	1.122161	2.195547

TS (DMF+Acrylic Acid)

	ATOM	X	Y	Z
1	C	0.166561	-0.4023	0.788559
2	C	1.308637	-1.08914	1.498539
3	C	1.897917	-2.34456	1.056798
4	C	2.407036	-2.96064	2.172238
5	C	2.051432	-2.15334	3.288389
6	H	2.090174	-2.59946	0.02055
7	H	3.079799	-3.80982	2.209949
8	C	2.220336	-2.41872	4.746394
9	O	1.083597	-1.2581	2.909005
10	C	3.589416	-0.37818	2.679566
11	C	2.73624	0.054745	1.604274
12	C	4.79755	-1.13576	2.387158
13	H	3.450723	0.045069	3.67289
14	H	3.197646	0.009519	0.615861
15	H	2.203969	0.991993	1.785878
16	H	-0.72844	-1.03843	0.77883
17	H	0.462269	-0.191	-0.24762
18	H	2.159021	-1.4849	5.319
19	O	5.110411	-1.58267	1.288329
20	O	5.632182	-1.41649	3.481729
21	H	5.271491	-0.97277	4.271926
22	H	3.195655	-2.89021	4.920998
23	H	1.434769	-3.09925	5.114363
24	H	-0.07149	0.547953	1.283399

TS (DMF+Methyl Acrylate)

	ATOM	X	Y	Z
1	C	0.2278	-0.4026	0.958588

2	C	1.408683	-1.07257	1.615932
3	C	2.065601	-2.26067	1.095667
4	C	2.648057	-2.88921	2.16758
5	C	2.27159	-2.15783	3.334253
6	H	2.234702	-2.45684	0.042342
7	H	3.364728	-3.70312	2.156992
8	C	2.507656	-2.47791	4.770837
9	O	1.219642	-1.33049	3.012121
10	C	3.637941	-0.30683	2.875641
11	C	2.810299	0.152469	1.792971
12	C	4.927892	-0.96163	2.724049
13	H	3.447039	0.0501	3.883114
14	H	3.27437	0.180544	0.807031
15	H	2.220257	1.046051	2.011298
16	H	-0.6405	-1.07533	0.935488
17	H	0.492147	-0.13227	-0.07256
18	H	2.197205	-1.63581	5.400734
19	O	5.256208	-1.19799	1.389789
20	O	5.661271	-1.3166	3.650547
21	H	3.579721	-2.65866	4.926212
22	H	1.944593	-3.37461	5.07732
23	H	-0.04272	0.512226	1.501314
24	C	6.496741	-1.93301	1.202774
25	H	6.639818	-1.98928	0.118772
26	H	6.415282	-2.9372	1.640656
27	H	7.330344	-1.40534	1.682955

