Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Determining Michael Acceptor Reactivity from Kinetic, Mechanistic, and Computational Analysis for the base-catalyzed Thiol-Michael Reaction

Sijia Huang, Kangmin Kim, Grant Musgrave, Marcus Sharp, Jasmine Sinha, Jeffrey W. Stansbury, Charles B. Musgrave, and Christopher N. Bowman

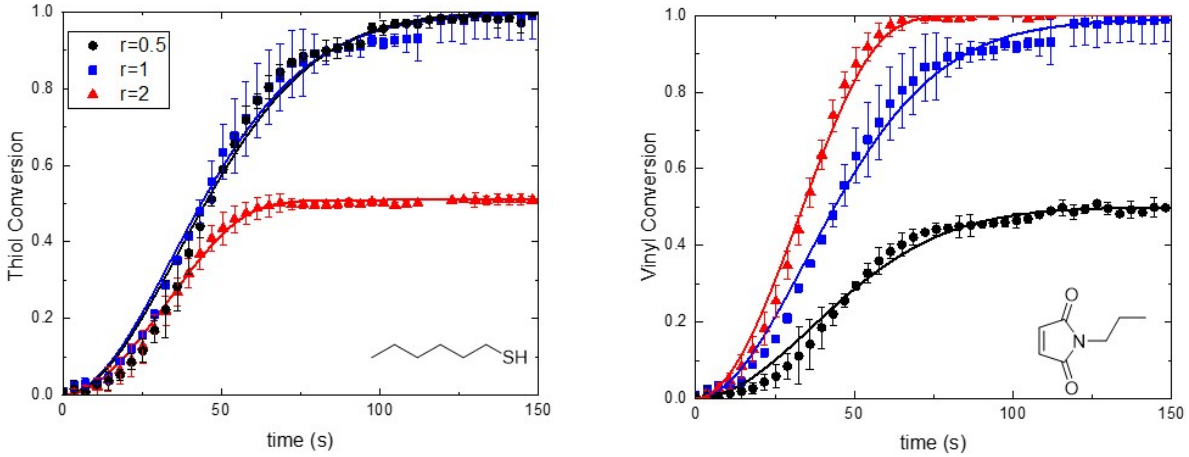


Figure S1 Model predictions and experimental data for functional group conversion vs time for the HT and PMI reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

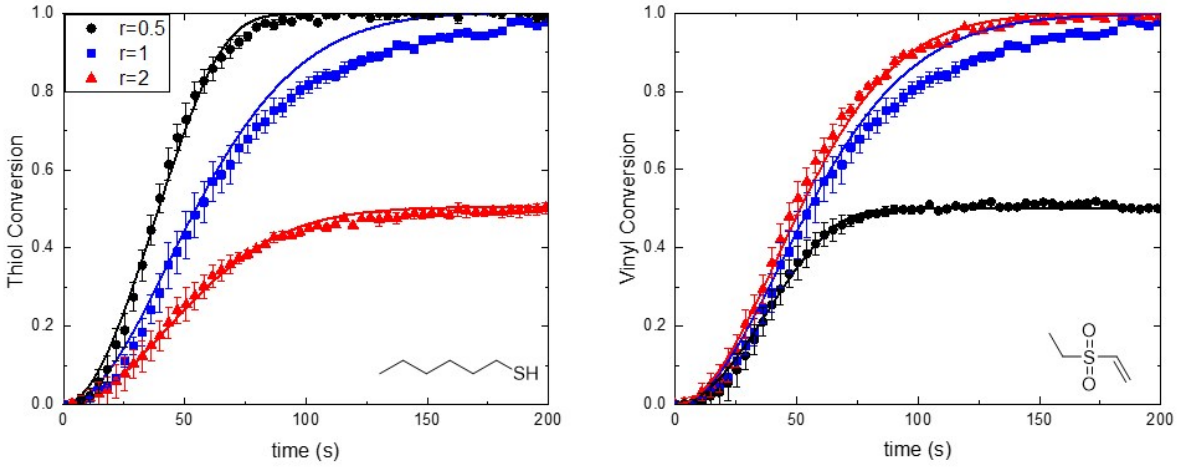


Figure S2 Model predictions and experimental data for functional group conversion vs time for the HT and EVS reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in

2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

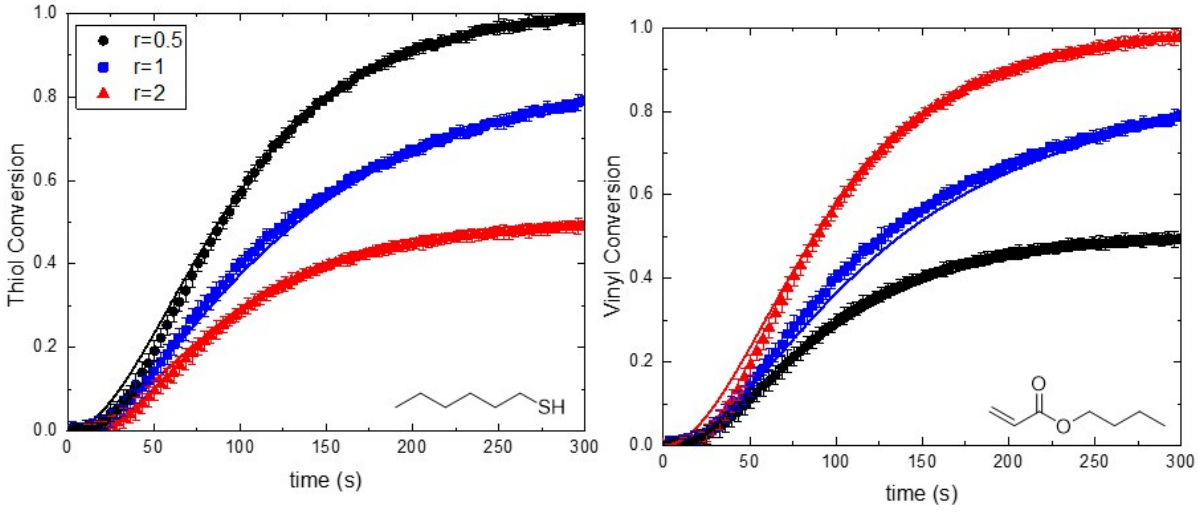


Figure S3 Model predictions and experimental data for functional group conversion vs time for the HT and BA reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

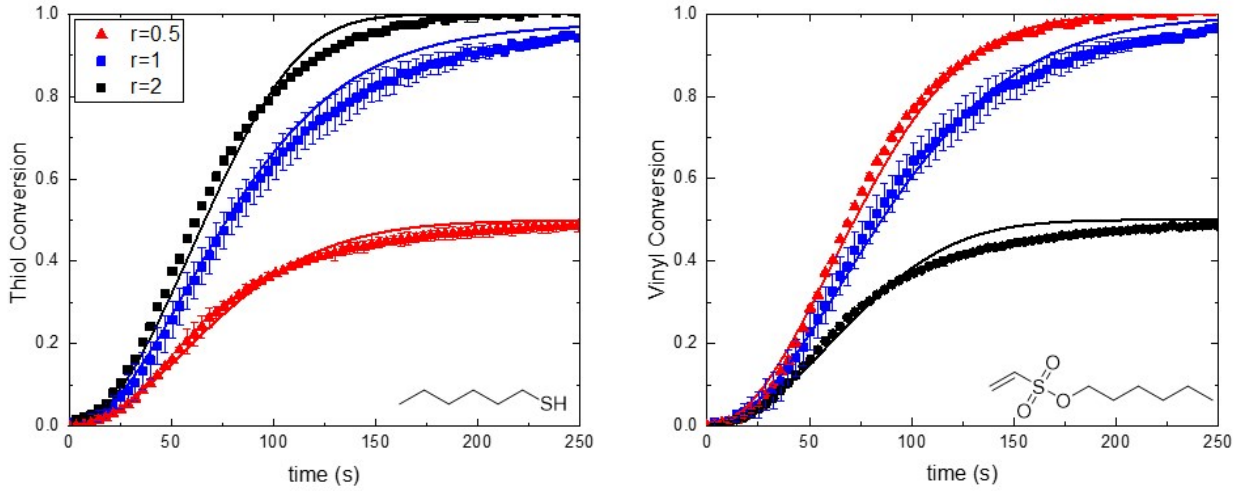


Figure S4 Model predictions and experimental data for functional group conversion vs time for the HT and HVS reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in

2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

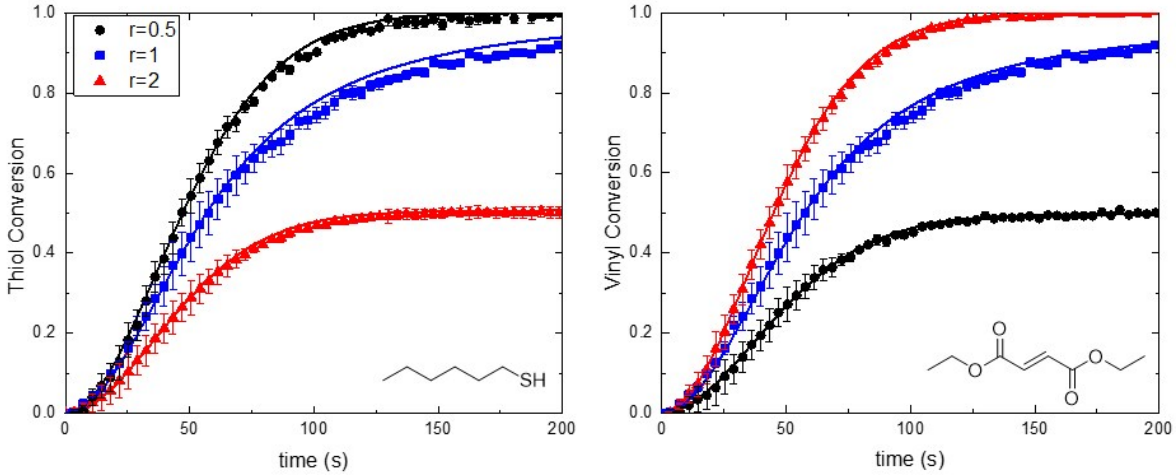


Figure S5 Model predictions and experimental data for functional group conversion vs time for the HT and DEF reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

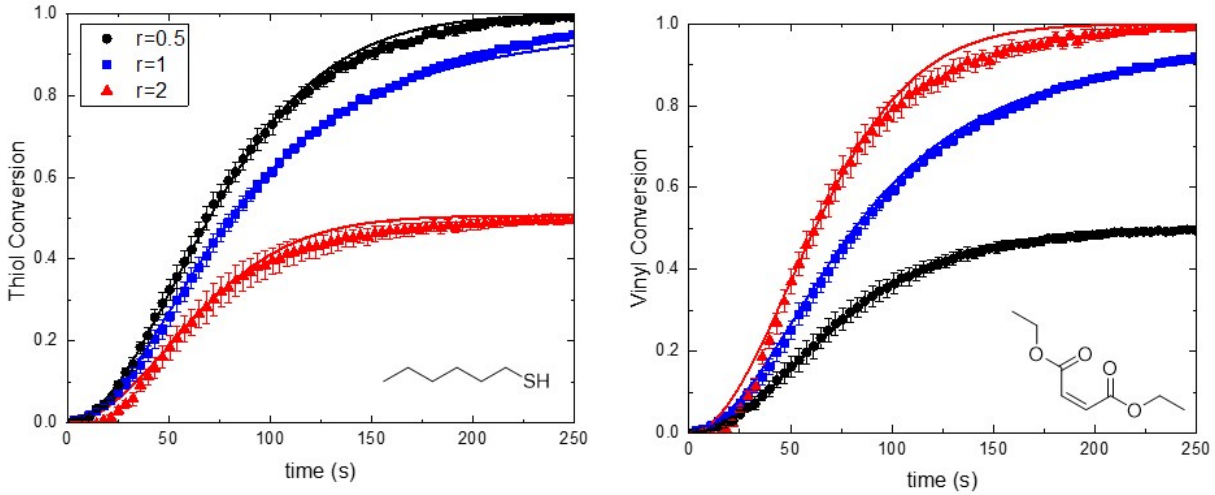


Figure S6 Model predictions and experimental data for functional group conversion vs time for the HT and DEM reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

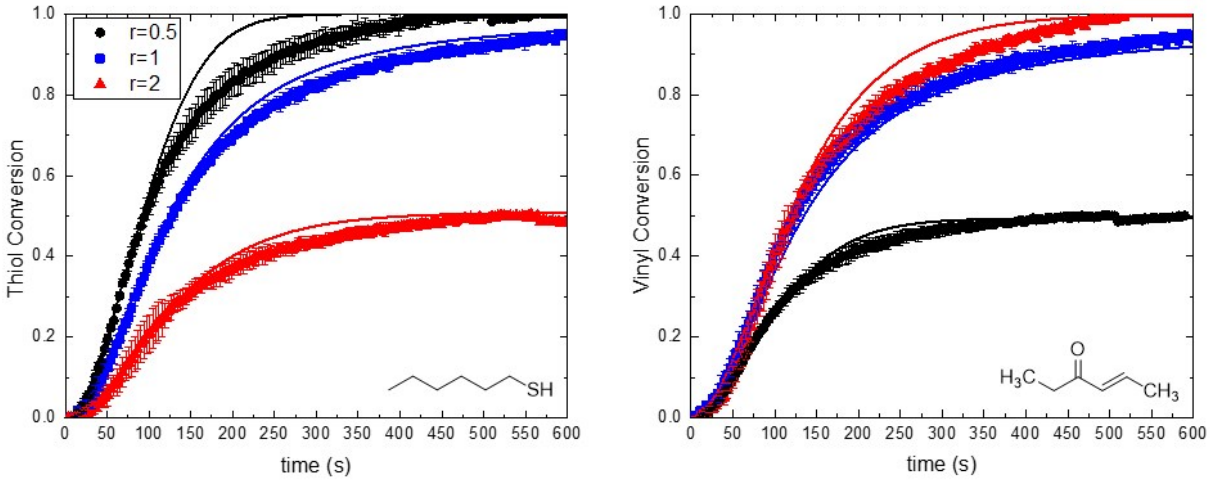


Figure S7 Model predictions and experimental data for functional group conversion vs time for the HT and HEO reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

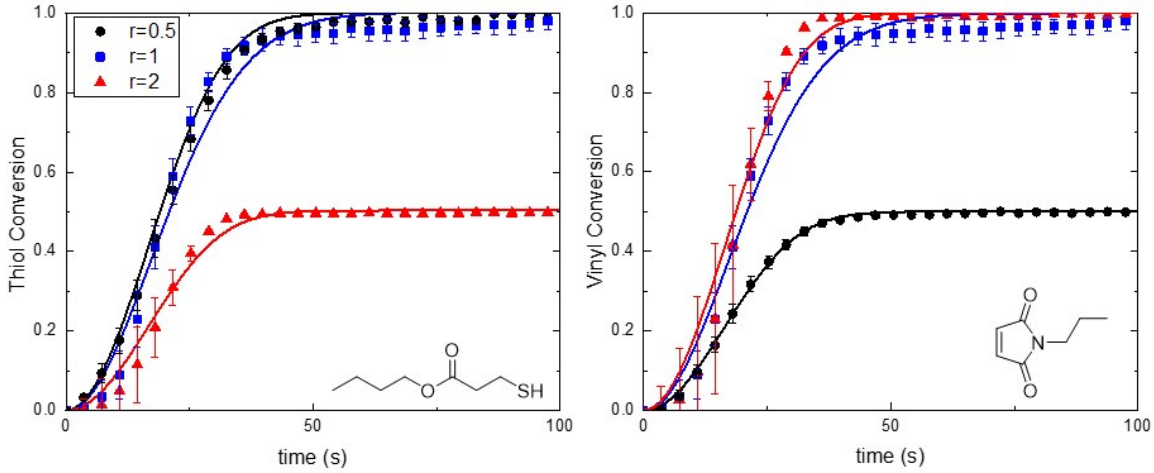


Figure S8 Model predictions and experimental data for functional group conversion vs time for the BMP and PMI reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

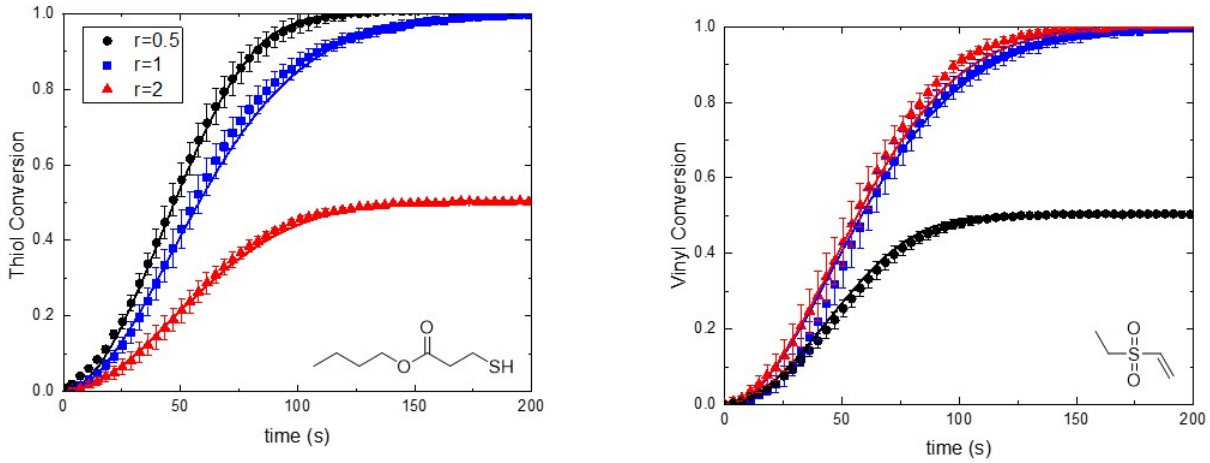


Figure S9 Model predictions and experimental data for functional group conversion vs time for the BMP and EVS reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

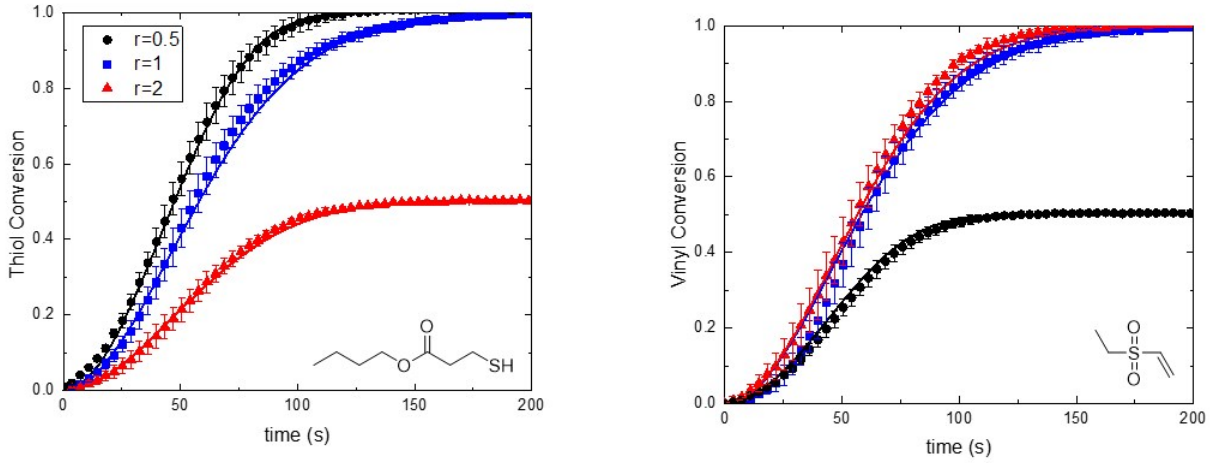


Figure S10 Model predictions and experimental data for functional group conversion vs time for the BMP and BA reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EDGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

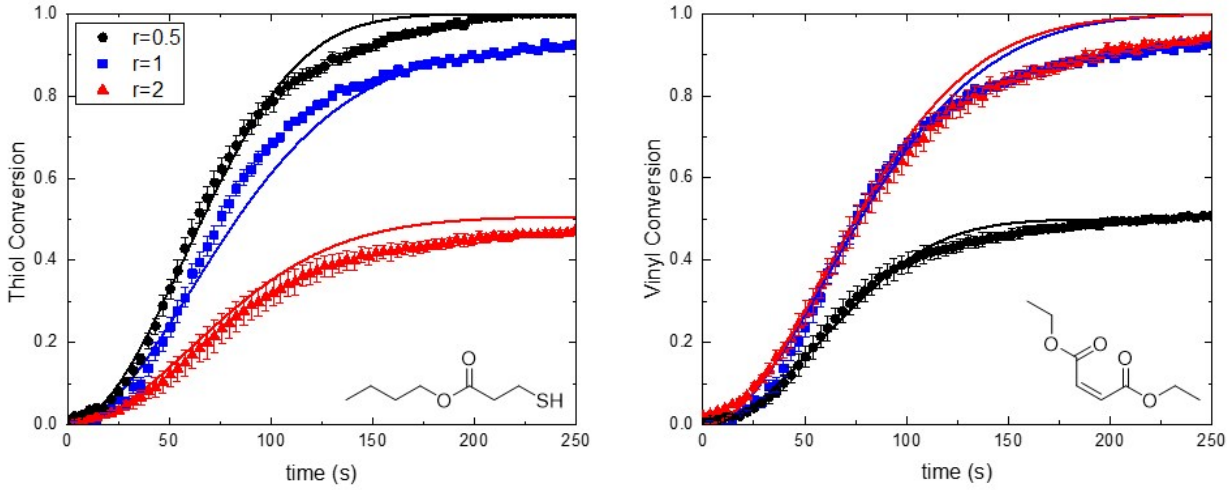


Figure S11 Model predictions and experimental data for functional group conversion vs time for the BMP and DEM reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

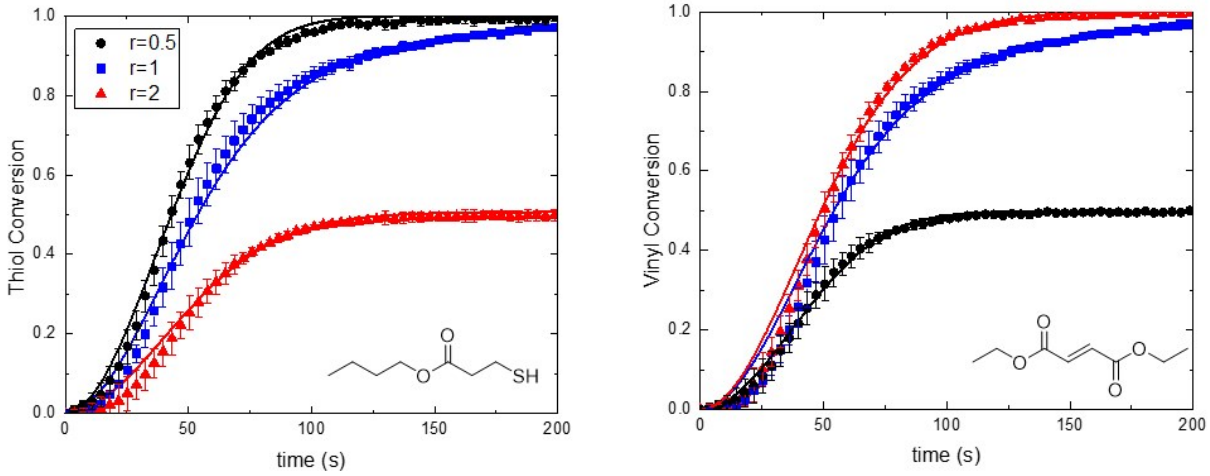


Figure S12 Model predictions and experimental data for functional group conversion vs time for the BMP and DEF reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

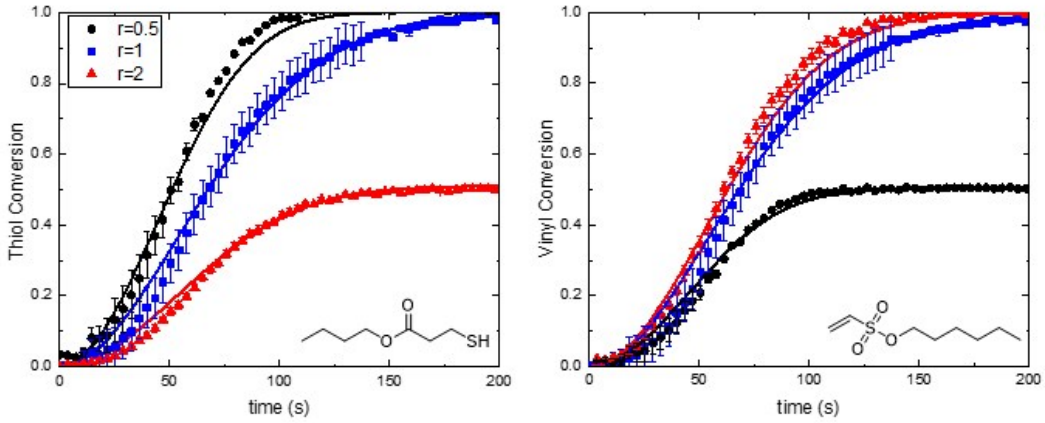


Figure S13 Model predictions and experimental data for functional group conversion vs time for the BMP and HVS reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

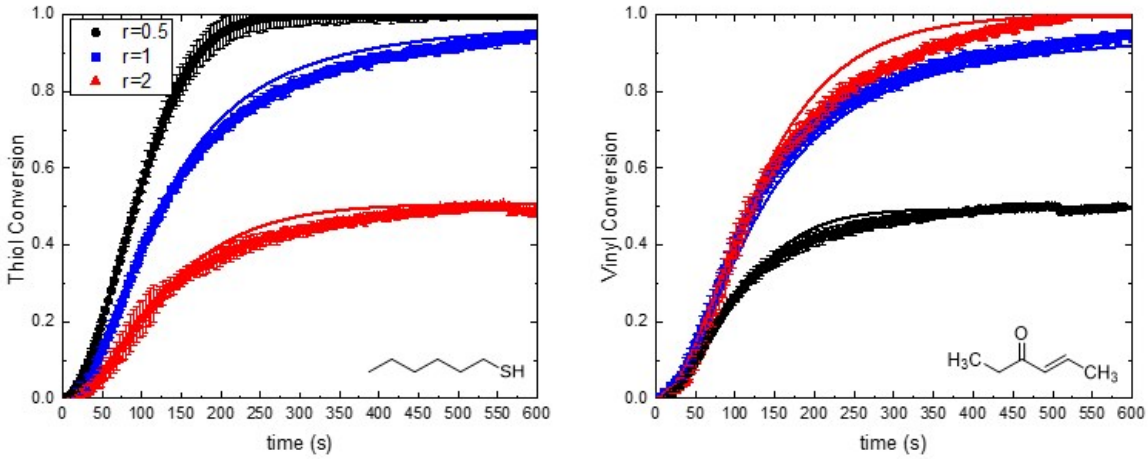


Figure S14 Model predictions and experimental data for functional group conversion vs time for the BMP and HEO reaction: (a) thiol conversion for initial stoichiometric ratios r=0.5, r=1, r=2 of thiol:vinyl functional group concentrations; (b) vinyl conversion for r=0.5, 1 and 2. All reactions were conducted in 2M solution of EGDE and contains 0.06 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW /cm^2 365 nm wavelength at ambient temperature.

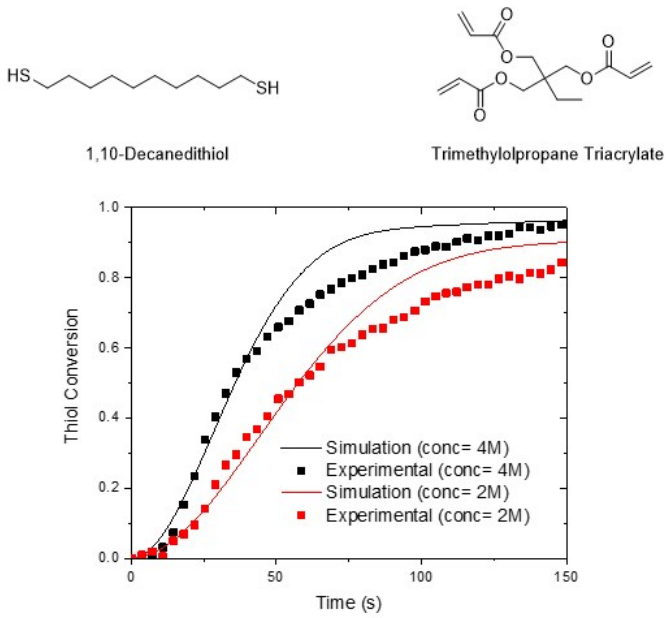


Figure S15. Comparisons of simulations with the cross-linking thiol–Michael polymerization under solution condition. Thiol functional group conversion vs time for the dithiol and triacrylate at initial stoichiometric ratio of 1:1 of thiol:vinyl functional group concentrations. All reactions were conducted in 2M and 4M solution of EGDE and contains 0.2 mol/L NPPOC-TMG. Each sample was stabilized in the dark for 1 min and then irradiated with 10 mW/cm^2 365 nm wavelength at ambient temperature.

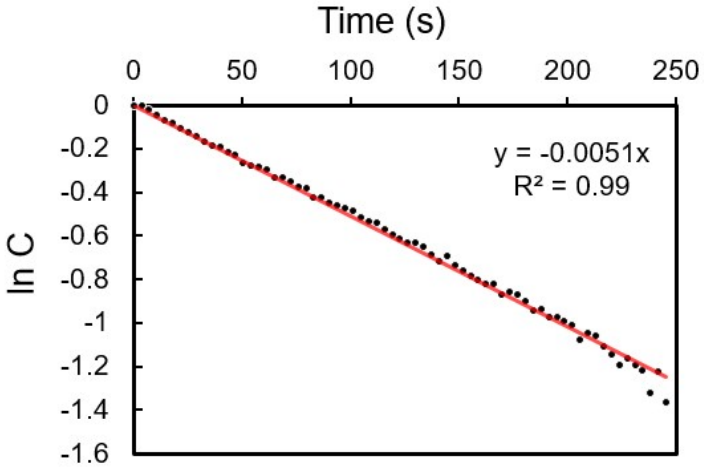


Figure S16. Linear fits of NPPOC-TMG photodecay upon 10 mW/cm^2, 365 nm LED light irradiation.

Table S1 Experimentally determined kinetic constants, corresponding Mayr's and Parr's electrophilicities, for the seven monomers reacting with butyl 3-mercaptopropionate (BMP).

	k_p[a]	k_{CT}[a]	k_{-P}[b]	Mayr's E	Parr's ω

PMI	23	21	2.6	-14.1	2.6
EVS	2.3	5.1	0.1	-18.4	1.6
HVS	1.8	6.4	0.2	N/A	N/A
BA	0.5	1.2	0.1	-19.6	1.5
DEM	1.4	2.4	4.9	-19.5	1.7
DEF	3.4	6.6	5.4	-17.8	2.2
HEO	0.8	4.7	9.2	N/A	N/A

[a] the unit of kinetic constants is M-1s-1 [b] the unit of kinetic constants is s-1

2. Computational Methods.

2.1 Benchmarking of Computational Methods

We conducted a benchmarking study to identify DFT functionals that best reproduce the reaction energetics calculated with the accurate, but highly computationally demanding CBS-QB3 level of theory. The reactions considered for the benchmarking effort were elementary steps involved in the thiol-Michael mechanism, using N-methylmaleimide and methanethiol as the model chemistry. The density functionals were considered based on their known ability to accurately predict the energetics of organic systems: B3LYP, B3PW91, BMK, M062X, M06, M08HX, M11, MN15, O3LYP, PBE1PB E, LC-wHPBE, and WB97XD.[1] We referenced their results against those of the CBS-QB3[2,3] method that produces highly accurate energy profiles. (Table S1). The MN15[4] density functional performed the best of the considered functionals; it produced reaction enthalpies and free energies with the lowest root mean square errors (RMSE) against CBS-QB3 of 0.5 and 0.4 kcal/mol, respectively. The RMSE of other functionals are 2-9 times larger than those of MN15. After confirming the small sensitivity of MN15 energies to the choice of basis set, MN15/6-31+g(d,p)[5] was selected and used throughout this study in conjunction with the SMD solvation model[6] of diethyl ether.

Table S2. Root mean square errors (kcal/mol) of enthalpies (H) and Gibbs free energies (G) computed by several DFT density functionals against the compound CBS-QB3 reference method.

	H; G (TS1)	H; G (INT1)	H; G (TS2)	H; G (INT2)	H;G (RMSE)
B3LYP	3.2; 3.4	0.6; 0.6	3.1; 3.4	0.1; 0.2	2.3; 2.4
B3PW91	5.5; 5.3	3.5; 3.4	5.5; 3.2	0.2; 0.2	4.2; 3.5
BMK	1.2; 1.1	1.7; 1.4	6.0; 6.8	4.7; 4.7	4.0; 4.3
M062X	0.1; 0.6	1.1; 0.5	2.6; 1.6	1.2; 1.8	1.5; 1.3
M06	3.4; 3.8	2.2; 2.4	0.7; 0.5	1.0; 1.0	2.1; 2.3
M08HX	0.4; 2.2	2.1; 3.5	0.2; 0.4	0.1; 0.6	1.1; 2.1
M11	1.3; 0.1	2.9; 4.1	1.1; 0.2	0.8; 0.5	1.7; 2.1
MN15	0.2; 0.3	0.3; 0.2	0.1; 0.3	0.9; 0.7	0.5; 0.4
O3LYP	4.0; 3.4	7.5; 7.3	2.7; 2.6	0.8; 0.8	4.5; 4.3
PBE1PBE	Not Converged	4.2; 4.1	Not Converged	0.3; 0.4	N/A
LC-WHPBE	5.5; 5.4	1.9; 1.6	0.9; 0.3	1.9; 2.2	3.1; 3.0
WB97XD	2.1; 2.0	0.6; 0.7	1.9; 2.0	2.3; 2.3	1.9; 1.9
DFT ENERGIES ARE CALCULATED WITH THE 6-31+G(D,P) BASIS SET.					

2.2. Influence of alkyl length within thio-Michael reactions.

We tested a common practice of alkyl group truncation in simulation reactions for the sake of reduced computational costs by systematically varying the number of carbon on either thiolate and monomer within thio-Michael framework. The model chemistry was propagation reaction between N-alkyl maleimide and alkyl thiol with varying alkyl length, whose reaction enthalpy and free energy were compared to chemicals used in experiments: hexane thiol and N-propane maleimide.

Reaction enthalpy for hexane thiolate was -10.1 kcal/mol for the propagation reaction with N-methyl maleimide. Except for methyl thiolate with -11.6 kcal/mol, thiolates with 2-5 carbon deviated less than 2% from hexane thiolate. Reaction free energy change for hexane thiolate was 1.7 kcal/mol. Again, methyl thiolate was inaccurate (-0.2 kcal/mol) to replicate hexane thiolate. Ethane and propane thiolate deviated about 18%. Butane and pentane thiolate nearly reproduced hexane thiolate. Balancing between computational costs and accuracy, ethane thiolate was chosen for further computations to reproduce experiments. When a similar study was conducted for monomer, we found that N-ethyl maleimide produced very closed to it. Reaction enthalpy was -10 kcal/mol for both ethane and propane maleimide

while reaction free energy was 1.8 and 1.7 kcal/mol, respectively. Especially, enthalpies were near constant regardless of alkyl length. Therefore, we used ethyl group to replace alkyl groups in other monomers as well.

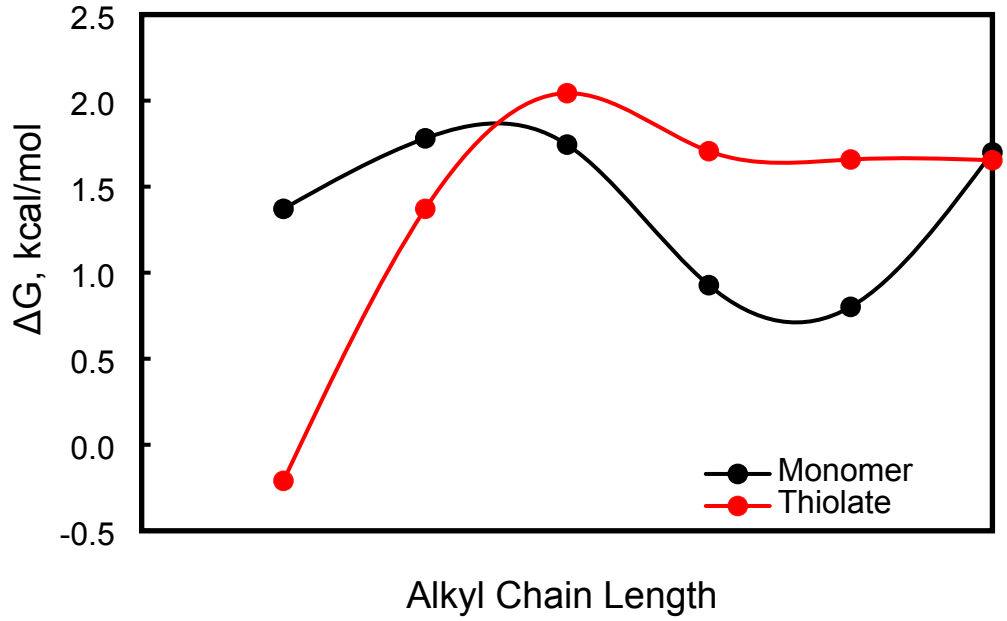


Figure S17 The effect of alkyl chain on the free energy

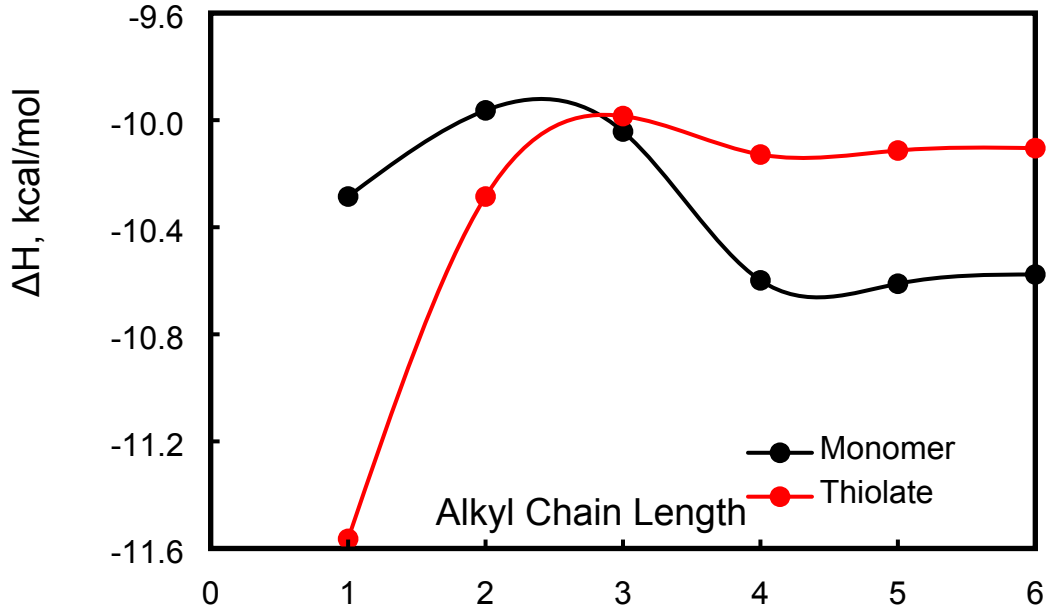
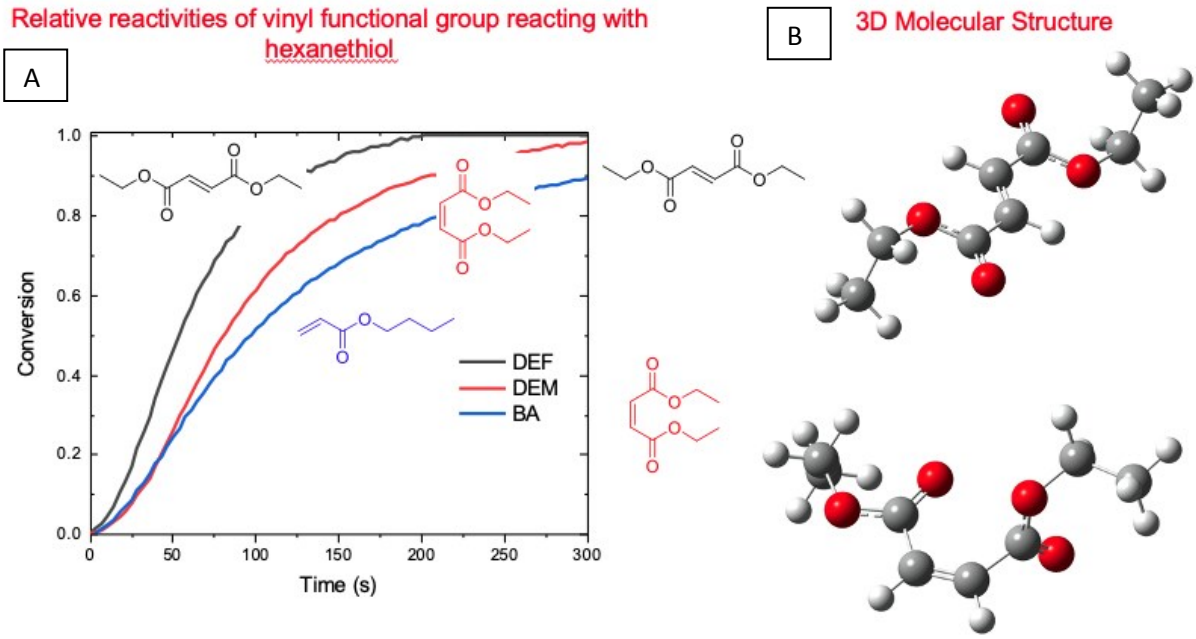


Figure S18 The effect of alkyl chain on the entropy

Table S3. Detailed energetics of all the reactions with ethyl thiol in the study calculated at MN15/6-31+g(d,p)/SMD-diethylether

	$\Delta H_{Prop}^{\neq}$	$-T\Delta S_{Prop}^{\neq}$	$\Delta G_{Prop}^{\neq}$	ΔH_{Prop}°	$-T\Delta S_{Prop}^{\circ}$	ΔG_{Prop}°	$\Delta H_{CT}^{\neq}$	$-T\Delta S_{CT}^{\neq}$	$\Delta G_{CT}^{\neq}$	ΔH_{CT}°	$-T\Delta S_{CT}^{\circ}$	ΔG_{CT}°
PMI	-3.3	12.1	8.8	-9.9	11.6	1.7	-5.6	11.9	6.3	-11.5	0.3	-11.2
DEF	-1.8	12.2	10.4	-2.1	12.8	10.7	-7.4	12.0	4.6	-17.2	0.5	-16.6
EVS	-0.8	11.8	11.0	-1.6	11.1	9.5	-8.8	12.3	3.5	-21.0	1.1	-19.9
HEO	5.1	12.4	17.5	2.7	11.8	14.6	-8.8	13.1	4.2	-16.5	2.1	-14.4
DEM	-2.9	11.6	8.6	-6.2	13.5	7.3	-7.2	13.4	6.2	-15.0	0.4	-14.6
BA	4.1	12.9	17.0	-0.2	12.8	12.6	-9.8	16.3	1.6	-20.1	-0.6	-20.7
HVS	-4.0	11.7	7.8	-10.0	11.4	1.4	-4.8	12.0	7.2	-14.3	1.4	-12.9



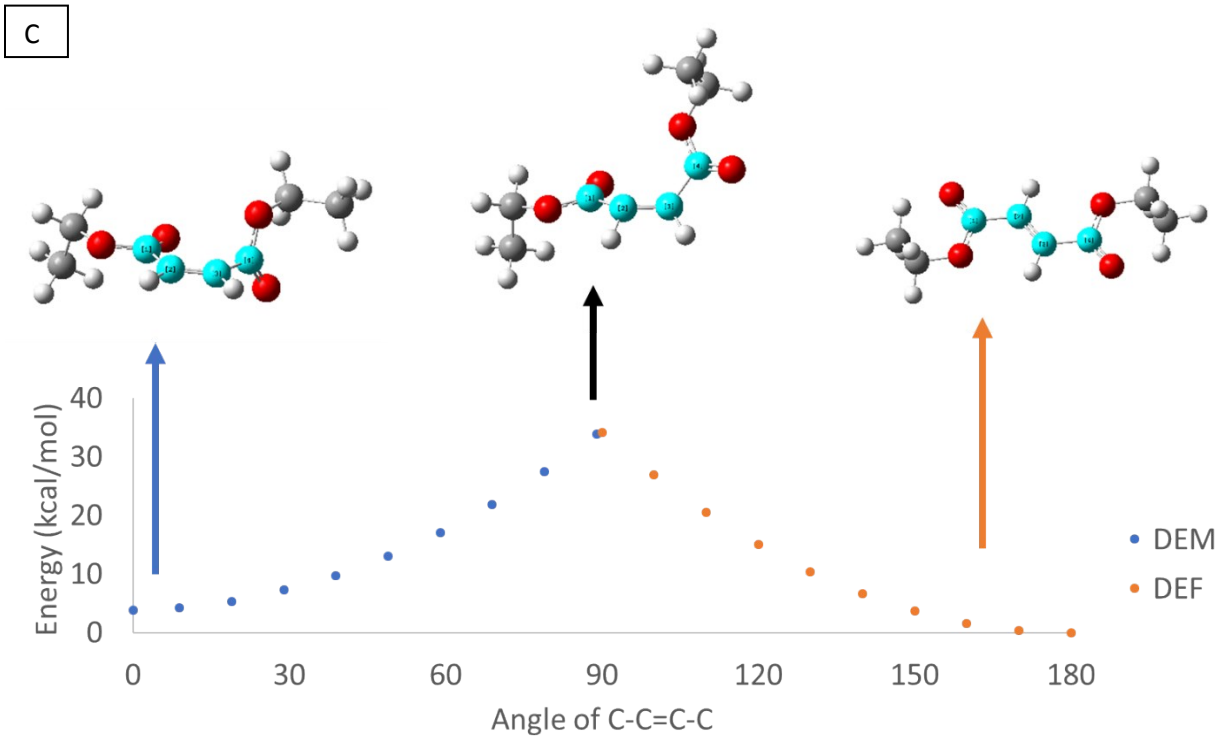


Figure S19 A. Experimental kinetic profiles of DEF, DEM, and BA. Note that the reaction of DEF proceeds more rapidly than that of DEM despite the identical functional groups. B. 3D molecular structure of DEF and DEM that respectively have trans and cis conformation. Trans conformation allows resonance throughout the molecule. C. Conformation search along C-C=C-C between DEM and DEF. DEM is 3.8 kcal/mol higher in energy than DEF while the rotational barrier from DEM to DEF is nearly 30 kcal/mol preventing interconversion between two conformers from occurring at room temperature.

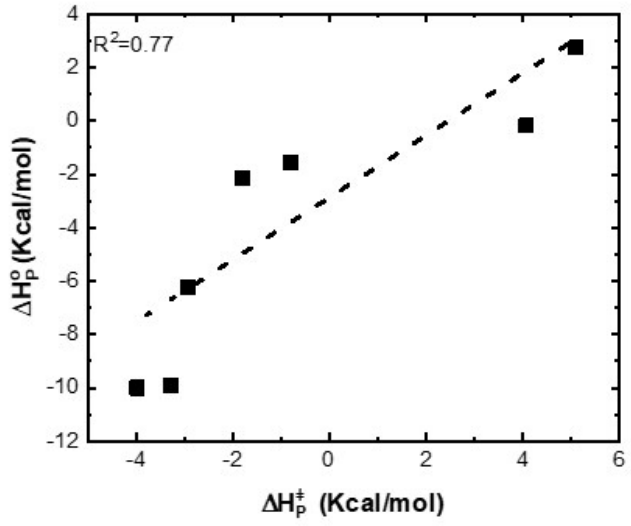


Figure S20 Plot of propagation step reaction enthalpy versus transition-state enthalpy (R^2=0.77) for the addition of ethyl thiolate to alkenes.

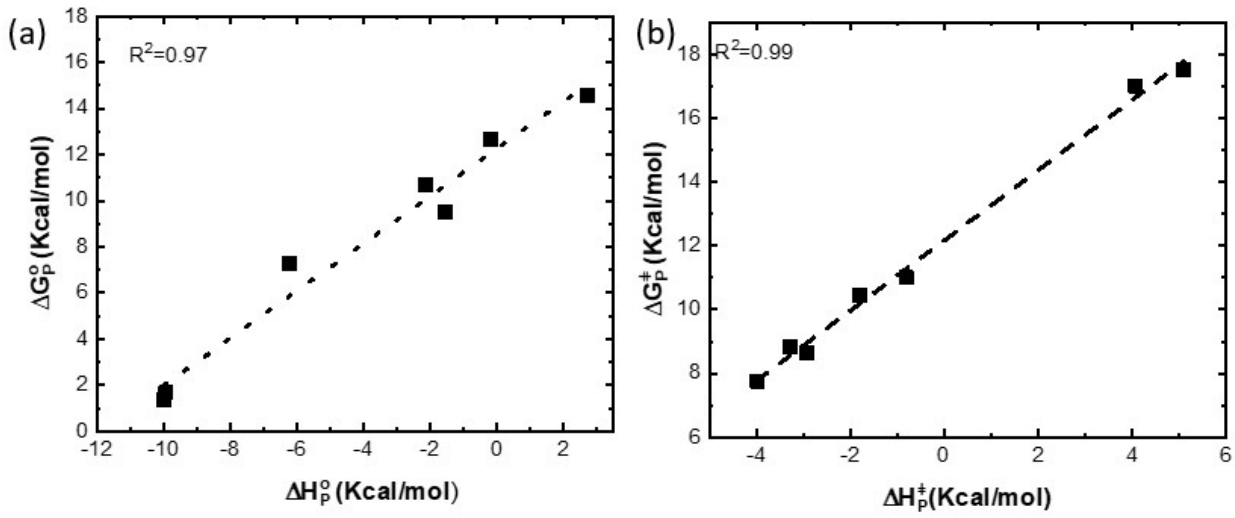


Figure S21 (a) Plot of propagation step reaction enthalpy versus reaction free energies (R^2=0.97). (b)plot of transition state enthalpy versus transition-state free energy (R^2=0.99) for the addition of ethyl thiolate to alkenes.

3. Molecular Coordinates

PMI

ZPE = -437.48

C	1.0177	-1.1395	0.0727
C	2.3889	-0.6677	-0.3110
C	2.3888	0.6683	-0.3107
C	1.0175	1.1397	0.0731
H	3.1936	-1.3566	-0.5376
H	3.1934	1.3574	-0.5371
O	0.6183	2.2863	0.1715
O	0.6186	-2.2862	0.1708
N	0.2559	0.0000	0.3063
C	-1.1604	-0.0002	0.6513
H	-1.3407	-0.8873	1.2656
H	-1.3408	0.8867	1.2659
C	-2.0463	0.0000	-0.5883
H	-1.8578	-0.8900	-1.1986
H	-1.8580	0.8903	-1.1983
H	-3.1023	-0.0001	-0.2987

PMI TS1

ZPE = -914.69

C	1.6691	-0.4910	0.1129

C	0.8393	-1.4234	0.8264
C	-0.4194	-0.8530	0.9917
C	-0.3111	0.5849	0.5804
H	1.1422	-2.4386	1.0493
H	-1.1726	-1.1493	1.7109
O	-1.0926	1.5107	0.8016
O	2.8312	-0.5788	-0.3068
N	0.9096	0.7024	-0.0477
S	-1.8190	-1.2753	-0.8788
C	-3.2438	-0.1563	-0.7304
H	-2.8855	0.8807	-0.7583
H	-3.8761	-0.3033	-1.6165
C	1.4376	1.9362	-0.5924
H	2.1429	1.6630	-1.3838
H	0.6028	2.4803	-1.0471
C	-4.0570	-0.3804	0.5398
H	-4.4213	-1.4136	0.5955
H	-3.4383	-0.1886	1.4247
C	2.1244	2.7893	0.4704
H	1.4161	3.0555	1.2630
H	2.9588	2.2384	0.9190
H	2.5174	3.7144	0.0327
H	-4.9225	0.2956	0.5836

PMI Intermediate

ZPE = -914.70

C	-3.1217	-1.4747	0.3352
C	-2.0989	-2.1276	-0.3381
C	-1.0691	-1.1450	-0.7780
C	-1.6892	0.2075	-0.4282
H	-2.0041	-3.2041	-0.4201
H	-0.7871	-1.1542	-1.8412
O	-1.2423	1.3218	-0.7311
O	-4.1725	-1.8350	0.9203
N	-2.8148	-0.0395	0.2790
S	0.5080	-1.3324	0.1645
C	1.6202	-0.1958	-0.7173
H	1.2840	0.8330	-0.5597
H	1.5489	-0.4091	-1.7918
C	-3.7166	0.9818	0.7649
H	-4.2144	0.5741	1.6506
H	-3.1135	1.8469	1.0624
C	-4.7497	1.3793	-0.2866

H	-4.2557	1.7728	-1.1826
H	-5.3481	0.5070	-0.5725
C	3.0502	-0.3882	-0.2261
H	3.3973	-1.4128	-0.4036
H	3.1296	-0.1852	0.8484
H	3.7289	0.2967	-0.7477
H	-5.4255	2.1508	0.1015

PMI TS2

ZPE = -1392.40

S	3.4273	-2.0391	0.2587
C	3.7908	-2.6146	-1.4234
H	3.3015	-3.5864	-1.5668
H	3.3667	-1.9126	-2.1497
C	5.2969	-2.7350	-1.6192
H	5.7302	-3.4608	-0.9218
S	-1.0898	-3.7906	-1.5312
H	-0.2298	-2.5809	-1.2611
C	-2.0184	-3.5300	0.0153
H	-2.4407	-4.4926	0.3244
H	-1.3072	-3.2298	0.7986
C	-3.1176	-2.4842	-0.1270
H	-3.8354	-2.7830	-0.9002
H	-2.6933	-1.5163	-0.4226
H	5.5209	-3.0656	-2.6397
C	0.8185	-1.4706	-0.7468
C	1.6041	-2.2881	0.2418
H	1.4458	-3.3747	0.1632
C	1.0864	-1.8122	1.5990
H	1.2133	-1.2459	-1.7361
C	0.1768	-0.4214	-0.0280
O	-0.4524	0.5851	-0.3918
O	1.3164	-2.3202	2.6960
N	0.3192	-0.7086	1.3762
C	-0.3457	0.0429	2.4233
H	0.2532	-0.0717	3.3326
H	-0.3352	1.0959	2.1242
C	-1.7767	-0.4338	2.6487
H	-2.2389	0.1120	3.4793
H	-1.7937	-1.5042	2.8884
H	-2.3776	-0.2649	1.7489
H	5.7945	-1.7710	-1.4609
H	-3.6628	-2.3493	0.8173

PMI Product
ZPE = -915.21

C	1.6702	-0.7007	0.2455
C	0.4157	-1.3993	0.7268
C	-0.6729	-0.3216	0.7019
C	0.0900	0.9728	0.4652
H	0.2035	-2.2641	0.0903
H	-1.2435	-0.2536	1.6331
O	-0.3505	2.1084	0.5284
O	2.7559	-1.2022	0.0145
N	1.3949	0.6548	0.1272
S	-1.8180	-0.6198	-0.6794
H	0.5961	-1.7719	1.7405
C	-3.0710	0.6664	-0.3993
H	-2.6261	1.6499	-0.5714
H	-3.3890	0.6115	0.6485
C	2.3987	1.6507	-0.2359
H	3.0829	1.1701	-0.9409
H	1.8742	2.4607	-0.7502
C	-4.2463	0.4243	-1.3384
H	-4.7107	-0.5508	-1.1547
H	-3.9314	0.4633	-2.3873
C	3.1416	2.1649	0.9908
H	2.4466	2.6369	1.6936
H	3.6584	1.3451	1.5016
H	3.8883	2.9088	0.6947
H	-5.0064	1.1981	-1.1879

BA
ZPE = -345.29

C	4.3118	-0.1840	0.0182
H	4.4586	-1.2623	0.0234
H	5.1935	0.4510	0.0186
C	3.0804	0.3334	0.0116
C	1.8891	-0.5526	0.0113
O	1.9152	-1.7727	0.0169
O	0.7512	0.1559	0.0038
C	-0.4752	-0.6007	0.0029
H	-0.4837	-1.2497	-0.8795

H	-0.4908	-1.2402	0.8922
C	-1.6227	0.3835	-0.0070
H	-1.5947	1.0259	0.8792
H	-1.5876	1.0161	-0.8999
H	2.8951	1.4044	0.0063
H	-2.5724	-0.1613	-0.0078

BA TS1

ZPE = -822.49

C	2.3873	0.6593	0.3269
H	1.7783	0.8326	-0.5551
C	3.5052	-0.1573	0.2353
H	3.9366	-0.3622	-0.7381
H	4.1864	-0.1925	1.0789
S	2.9772	-2.5246	0.5086
C	1.2273	-2.2631	0.8666
H	0.9155	-2.9223	1.6866
H	1.1101	-1.2285	1.2336
C	0.3205	-2.4648	-0.3447
H	-0.7367	-2.2919	-0.0935
H	0.6019	-1.7719	-1.1492
C	1.9731	1.1561	1.6156
O	2.5364	0.9101	2.6860
O	0.8887	1.9986	1.6982
C	0.1163	2.3628	0.5567
H	-0.3881	3.2917	0.8432
H	0.7718	2.5977	-0.2911
C	-0.9122	1.3027	0.1979
H	-0.4334	0.3605	-0.0892
H	-1.5675	1.1072	1.0541
H	0.4174	-3.4834	-0.7407
H	-1.5308	1.6446	-0.6403

BA Intermediate

ZPE = -822.50

C	-3.0332	-2.1850	1.8297
H	-3.8280	-2.9384	1.9018
H	-3.0075	-1.6250	2.7719
C	-3.1895	-1.2598	0.6886
C	-2.8549	0.0830	0.8201
O	-2.4241	0.6956	1.8327
O	-3.0662	0.8254	-0.3590

C	-2.4034	2.0760	-0.4235
H	-2.8895	2.6283	-1.2368
H	-2.5520	2.6290	0.5117
H	-3.4891	-1.6375	-0.2870
S	-1.4895	-3.2572	1.8260
C	-0.9174	1.9066	-0.7049
H	-0.7616	1.3628	-1.6444
H	-0.4485	1.3414	0.1090
C	-0.2213	-1.9675	1.7489
H	-0.1657	-1.4509	2.7147
H	-0.5559	-1.2359	1.0026
C	1.1335	-2.5541	1.3722
H	1.4648	-3.3032	2.1018
H	1.0901	-3.0372	0.3891
H	-0.4199	2.8818	-0.7809
H	1.8948	-1.7656	1.3312

BA TS2

ZPE = -1300.20

C	-0.7081	-2.8658	2.4048
H	-0.9091	-3.9136	2.1426
H	-1.5132	-2.5334	3.0719
C	-0.6561	-2.0004	1.1914
C	-0.8317	-0.6022	1.3627
O	-1.2937	-0.0073	2.3541
O	-0.4956	0.1219	0.2291
C	-0.7003	1.5298	0.2820
H	-0.8239	1.8467	-0.7597
H	-1.6253	1.7481	0.8284
S	0.7876	-2.8889	3.4982
C	0.4783	2.2427	0.9246
H	0.5967	1.9159	1.9627
H	1.4040	2.0246	0.3793
C	2.0068	-3.5292	2.3216
H	2.1011	-2.8205	1.4906
H	1.6407	-4.4797	1.9113
S	-3.4356	-2.9802	0.0978
H	-2.0697	-2.5153	0.4754
C	-4.2038	-1.6570	1.0925
H	-5.2127	-1.9838	1.3688
H	-3.6257	-1.5528	2.0189
H	0.0024	-2.2989	0.3740

C	-4.2549	-0.3207	0.3624
H	-4.6778	0.4637	1.0051
H	-3.2467	-0.0108	0.0637
C	3.3547	-3.7259	3.0048
H	4.0979	-4.0975	2.2896
H	3.7262	-2.7806	3.4177
H	-4.8667	-0.3946	-0.5451
H	0.3204	3.3282	0.9159
H	3.2820	-4.4481	3.8262

BA Product

ZPE = -823.02

S	0.1363	0.8882	-1.3441
C	-0.8045	2.3468	-0.8214
C	1.6272	1.0645	-0.3215
C	-1.1096	2.3793	0.6783
H	-1.7348	2.3157	-1.3967
H	-0.2635	3.2556	-1.1081
C	2.6910	0.0813	-0.7935
H	1.3729	0.8729	0.7269
H	1.9880	2.0972	-0.4071
C	-1.7170	1.0840	1.1586
H	-0.2062	2.5577	1.2675
H	-1.8135	3.1959	0.8841
H	2.9806	0.2782	-1.8315
H	2.3296	-0.9514	-0.7288
O	-2.8190	0.7639	0.4698
O	-1.2735	0.3997	2.0644
C	-3.4269	-0.5042	0.7844
C	-4.6090	-0.6891	-0.1396
H	-2.6741	-1.2888	0.6489
H	-3.7264	-0.4981	1.8381
H	-4.2884	-0.6887	-1.1865
H	-5.3456	0.1086	0.0024
H	3.5852	0.1634	-0.1663
H	-5.0941	-1.6475	0.0721

HVS

ZPE = -780.36

C	-1.5862	-2.1054	-0.5396
H	-2.3861	-2.2554	-1.2691
H	-1.4239	-3.0384	0.0041
O	-3.8472	0.3735	1.0761
C	-1.5823	1.3835	0.2435
H	-1.8862	2.3295	-0.2006
C	-0.4320	1.1807	0.8802
C	-0.3157	-1.6058	-1.1906
H	0.0301	-2.3568	-1.9092
H	-0.4854	-0.6704	-1.7344
S	-2.8232	0.1450	0.0751
O	-3.2028	0.0604	-1.3271
H	0.2870	1.9903	0.9745
H	-0.1790	0.2206	1.3219
O	-2.0765	-1.2008	0.4965
H	0.4756	-1.4506	-0.4499

HVS TS1

ZPE = -1257.57

C	-3.5134	1.6853	1.2237
H	-2.7073	1.9767	1.9091
H	-4.2657	1.1215	1.7868
O	-2.9479	-1.1131	1.6986
C	-1.8759	-1.3363	-0.6967
H	-2.7269	-1.9600	-0.9535
C	-0.6960	-1.2748	-1.4034
C	-4.1177	2.8941	0.5432
H	-4.5596	3.5596	1.2927
H	-3.3540	3.4505	-0.0098
S	-2.0859	-0.4313	0.7287
O	-0.8223	0.1237	1.2134
H	-0.6742	-1.6591	-2.4157
H	0.0347	-0.5120	-1.1584
S	0.9378	-3.0412	-0.7677
C	-0.1901	-3.7817	0.4330
H	0.3832	-4.2000	1.2700
H	-0.8188	-2.9805	0.8588
C	-1.1004	-4.8479	-0.1696
H	-1.7980	-5.2549	0.5771
H	-1.6888	-4.4213	-0.9925
O	-2.9720	0.8365	0.1919
H	-0.5108	-5.6763	-0.5820
H	-4.9037	2.5898	-0.1560

HVS Intermediate
ZPE = -1257.57

C	2.7633	0.0774	-1.0737
H	1.9347	0.1663	-1.7913
H	2.4238	-0.5609	-0.2444
O	3.1060	1.3661	-0.5801
O	2.6102	3.3546	0.6356
C	0.4715	2.0288	-0.0103
H	0.2594	2.7977	-0.7483
C	-0.5066	0.9732	0.3347
C	3.9894	-0.5157	-1.7393
H	3.7533	-1.5002	-2.1596
H	4.3378	0.1326	-2.5512
S	2.0236	2.0104	0.5387
O	2.1679	1.0934	1.6877
H	-0.1635	0.4169	1.2143
H	-1.4903	1.4033	0.5666
S	-0.8524	-0.2856	-1.0011
C	-2.3464	-1.0525	-0.3067
H	-2.4134	-2.0609	-0.7300
H	-2.1892	-1.1727	0.7737
C	-3.6271	-0.2726	-0.5851
H	-3.5652	0.7483	-0.1907
H	-3.8118	-0.2041	-1.6630
H	4.8036	-0.6309	-1.0156
H	-4.4917	-0.7615	-0.1176

HVS TS2
ZPE = -1735.28

C	1.6236	-2.5241	0.4117
C	0.8028	-1.5993	-0.4346
H	1.3286	-1.1206	-1.2662
H	1.0039	-3.0208	1.1674
S	3.0369	-1.8251	1.3877
C	3.8227	-0.8014	0.1164
H	3.9827	-1.4102	-0.7832
H	3.1395	0.0161	-0.1415
C	5.1467	-0.2484	0.6295
H	4.9960	0.3503	1.5354
H	5.8500	-1.0547	0.8682

S	-1.1541	-3.8371	-1.5583
H	-0.3056	-2.7125	-1.1716
C	-2.0100	-3.8944	0.0524
H	-2.3000	-4.9350	0.2377
H	-1.2873	-3.6110	0.8270
C	-3.2237	-2.9771	0.1240
H	-3.9671	-3.2499	-0.6352
H	-3.6999	-3.0372	1.1124
H	2.0360	-3.3079	-0.2362
O	-1.2513	-0.1135	-0.6530
C	-2.1174	0.9884	-0.3231
H	-3.1368	0.6295	-0.5044
H	-2.0288	1.2221	0.7450
C	-1.7946	2.1954	-1.1808
H	-0.7723	2.5322	-0.9839
H	-1.8867	1.9455	-2.2436
S	-0.0568	-0.4157	0.4250
O	0.5915	0.8962	0.6232
O	-0.6790	-0.9825	1.6303
H	5.6097	0.3963	-0.1266
H	-2.4872	3.0154	-0.9571
H	-2.9190	-1.9392	-0.0478

HVS Product

ZPE = -1258.09

C	-1.1024	1.4061	-1.9861
H	-1.2482	1.8232	-2.9851
H	-0.6737	2.1801	-1.3421
O	-0.1092	0.3645	-2.1905
O	0.5284	-1.5512	-0.7896
C	3.0407	1.4408	-1.3538
C	-2.3790	0.8308	-1.4127
H	-3.1316	1.6227	-1.3305
H	-2.7743	0.0406	-2.0588
S	0.7814	-0.1309	-0.9604
O	0.5813	0.7703	0.1685
H	3.0033	1.6756	-0.2842
H	4.0947	1.3972	-1.6449
S	2.2160	2.7874	-2.2563
C	1.7273	3.8636	-0.8755
H	1.0097	4.5714	-1.3057
H	1.1879	3.2510	-0.1434
C	2.8935	4.6026	-0.2342

H	3.6303	3.9032	0.1789
H	3.4029	5.2394	-0.9654
C	2.4421	0.0621	-1.5966
H	3.0232	-0.7014	-1.0667
H	2.3974	-0.2122	-2.6557
H	-2.2074	0.4177	-0.4128
H	2.5373	5.2349	0.5880

DEF

ZPE = -612.14

C	-0.1929	-0.2703	-0.9437
H	0.4394	-0.2528	-1.8270
C	0.3211	-0.3626	0.2886
H	-0.3112	-0.3801	1.1719
C	1.7790	-0.4542	0.5636
C	-1.6508	-0.1786	-1.2187
O	2.2256	-0.5652	1.6936
O	-2.0974	-0.0677	-2.3487
O	-2.4065	-0.2360	-0.1182
O	2.5347	-0.3969	-0.5369
C	3.9640	-0.5085	-0.3605
H	4.3872	-0.0480	-1.2558
H	4.2544	0.0771	0.5168
C	4.3809	-1.9595	-0.2287
H	5.4713	-2.0209	-0.1454
H	3.9431	-2.4129	0.6660
H	4.0701	-2.5328	-1.1082
C	-3.8358	-0.1243	-0.2946
H	-4.2590	-0.5849	0.6007
H	-4.1262	-0.7100	-1.1719
C	-4.2527	1.3266	-0.4264
H	-3.8149	1.7801	-1.3211
H	-5.3431	1.3881	-0.5097
H	-3.9419	1.8999	0.4531

DEF TS1

ZPE = -1089.35

O	2.3775	-1.3169	0.0387
C	2.8902	0.6751	-1.1815
H	3.7089	1.2988	-1.5284
C	1.5630	1.1269	-1.2559
H	0.7828	0.3775	-1.1211

C	-0.4535	1.1709	1.0214
H	-0.6831	1.4018	2.0692
H	0.0129	0.1766	1.0113
C	-1.7357	1.1641	0.1951
H	-1.5229	0.9209	-0.8526
H	-2.2107	2.1533	0.2133
S	0.7753	2.3819	0.4463
C	3.1814	-0.5424	-0.5065
O	4.5241	-0.8439	-0.5043
C	4.8946	-2.0487	0.1589
H	4.3968	-2.9024	-0.3186
H	4.5533	-2.0154	1.2012
C	6.4024	-2.1749	0.0774
H	6.7313	-3.0926	0.5779
H	6.7341	-2.2126	-0.9662
H	6.8899	-1.3226	0.5633
C	1.2303	2.1716	-2.2618
O	-0.0122	2.0128	-2.7588
O	1.9742	3.0660	-2.6354
C	-0.5091	3.0782	-3.5777
H	0.0884	3.1401	-4.4948
H	-0.3884	4.0218	-3.0320
C	-1.9640	2.7832	-3.8712
H	-2.3884	3.5771	-4.4952
H	-2.0695	1.8315	-4.4030
H	-2.5400	2.7282	-2.9406
H	-2.4528	0.4265	0.5816

DEF Intermediate

ZPE = -1089.35

C	2.1890	-0.2563	-1.1683
H	1.7486	-0.2909	-2.1617
C	0.3200	1.0741	-0.3101
C	3.5534	-0.5188	-1.0480
O	-0.5487	1.0499	-1.1658
O	4.3836	-0.7480	-1.9605
O	4.0162	-0.4950	0.2774
O	0.5335	2.1505	0.4751
C	-0.3072	3.2948	0.2532
H	0.2555	4.1396	0.6592
H	-0.4379	3.4376	-0.8241

C	-1.6420	3.1323	0.9564
H	-2.2378	4.0453	0.8442
H	-2.2066	2.2979	0.5283
H	-1.4916	2.9478	2.0262
C	5.3462	-0.9399	0.4893
H	5.6459	-0.5213	1.4576
H	6.0033	-0.5326	-0.2880
C	5.4326	-2.4582	0.5122
H	5.1350	-2.8617	-0.4611
H	6.4579	-2.7851	0.7271
H	4.7682	-2.8705	1.2808
S	0.3341	-1.5522	0.4934
C	-0.6999	-0.8630	1.8210
H	-0.0575	-0.2901	2.5032
H	-1.4315	-0.1674	1.3879
C	-1.4186	-1.9754	2.5754
H	-2.0575	-2.5583	1.9018
H	-0.7013	-2.6615	3.0400
C	1.2961	-0.0389	-0.0018
H	1.8796	0.2498	0.8765
H	-2.0539	-1.5583	3.3657

DEF TS2

ZPE = -1567.06

C	0.3872	-0.8390	1.0778
H	0.0287	-1.3076	1.9960
C	-0.6802	-0.3868	0.1272
H	-0.2406	-0.0005	-0.7973
C	-1.5911	-1.5485	-0.2227
C	1.5866	-0.0893	1.2356
O	-2.1497	-2.2717	0.5836
O	2.4088	-0.1927	2.1614
O	1.8537	0.7498	0.1724
O	-1.7278	-1.6876	-1.5523
C	-2.5061	-2.8070	-2.0098
H	-2.1509	-2.9977	-3.0258
H	-2.2722	-3.6740	-1.3834
C	-3.9887	-2.4851	-1.9925
H	-4.5575	-3.3280	-2.4012
H	-4.3336	-2.3008	-0.9700
H	-4.1980	-1.6003	-2.6044
C	3.0248	1.5560	0.2700
H	3.2747	1.8304	-0.7604

H	3.8459	0.9622	0.6858
C	2.7707	2.7937	1.1137
H	2.5177	2.5057	2.1392
H	3.6633	3.4305	1.1402
H	1.9401	3.3761	0.6985
S	-1.7120	0.9621	0.8484
C	-2.9668	1.1905	-0.4479
H	-2.4599	1.2869	-1.4162
H	-3.6106	0.3024	-0.4932
C	-3.8023	2.4303	-0.1513
H	-4.3032	2.3446	0.8201
H	-3.1779	3.3306	-0.1329
S	1.2759	-3.5269	-0.2425
H	0.9603	-2.1494	0.2920
C	0.7762	-4.2668	1.3472
H	-0.2050	-3.8539	1.6153
H	0.6430	-5.3437	1.1920
C	1.7855	-4.0049	2.4592
H	1.9372	-2.9270	2.5994
H	2.7582	-4.4478	2.2120
H	1.4431	-4.4326	3.4119
H	-4.5739	2.5652	-0.9178

DEF Product

ZPE = -1089.87

C	0.0455	0.4766	0.6426
H	0.0719	0.7015	-0.4286
C	-1.3235	-0.0505	1.0075
C	2.5213	0.0576	0.6748
O	-1.5353	-0.9049	1.8482
O	3.5030	-0.0413	1.3863
O	2.5335	0.6502	-0.5292
O	-2.2808	0.5754	0.3119
C	-3.6441	0.3642	0.7393
H	-4.2521	0.6401	-0.1250
H	-3.7869	-0.6988	0.9547
C	-3.9503	1.2314	1.9438
H	-4.9975	1.1049	2.2384
H	-3.3179	0.9539	2.7938
H	-3.7804	2.2881	1.7092
C	3.7508	1.3186	-0.9210
H	3.7049	1.3659	-2.0115

H	4.6039	0.7016	-0.6245
C	3.8172	2.7014	-0.3029
H	3.8198	2.6393	0.7904
H	4.7348	3.2069	-0.6229
H	2.9612	3.3080	-0.6203
S	0.2778	2.0626	1.5230
C	-0.1101	3.2323	0.1893
H	0.5101	2.9714	-0.6773
H	-1.1633	3.1188	-0.0891
C	0.1831	4.6502	0.6603
H	-0.4258	4.9139	1.5323
H	1.2386	4.7665	0.9332
C	1.1576	-0.4972	1.0156
H	1.0203	-1.4415	0.4724
H	1.1408	-0.7260	2.0845
H	-0.0439	5.3644	-0.1383

DEM

ZPE = -612.14

C	-0.0564	1.7985	2.7169
H	-0.8150	1.0227	2.6676
C	1.2191	1.5002	2.9833
C	-0.4969	3.1922	2.4610
C	2.3380	2.4963	3.0345
O	0.2495	4.1543	2.3837
O	3.1336	2.6390	2.1252
O	2.3992	3.1227	4.2084
O	-1.8260	3.2641	2.3221
C	3.4337	4.1203	4.3623
H	1.5183	0.4657	3.1430
H	3.5181	4.6775	3.4247
C	4.7499	3.4833	4.7604
H	3.0577	4.7865	5.1419
H	5.5012	4.2642	4.9209
H	4.6397	2.9164	5.6908
C	-2.3863	4.5635	2.0343
H	5.1138	2.8134	3.9753
H	-1.8725	5.3098	2.6476
C	-2.2780	4.8841	0.5568
H	-3.4279	4.4909	2.3547
H	-2.7838	4.1201	-0.0428
H	-2.7536	5.8502	0.3559

H	-1.2307	4.9458	0.2457

DEM TS1

ZPE = -1089.35

O	2.8022	2.6303	0.8850
C	1.8859	1.0935	-0.7376
H	2.1903	0.1603	-1.2070
C	0.5252	1.4246	-0.7899
H	-0.0714	0.7770	-1.4280
C	0.5843	-0.0983	1.8898
H	0.6234	0.1216	2.9639
H	1.5487	0.2278	1.4646
C	0.4119	-1.5949	1.6482
H	0.4297	-1.8103	0.5719
H	-0.5471	-1.9520	2.0431
S	-0.6929	0.9112	1.1218
C	2.9078	1.7483	0.0313
O	4.1511	1.2250	-0.2600
C	5.2391	1.7431	0.5010
H	5.0475	1.5863	1.5702
H	5.3189	2.8255	0.3402
C	6.4976	1.0265	0.0566
H	7.3607	1.3992	0.6191
H	6.4128	-0.0521	0.2293
H	6.6836	1.1920	-1.0103
C	-0.0034	2.8209	-0.8279
O	-1.3238	2.8169	-1.1279
O	0.6198	3.8592	-0.7013
C	-1.9698	4.0945	-1.1439
H	-1.4914	4.7310	-1.8979
H	-1.8323	4.5730	-0.1668
C	-3.4335	3.8662	-1.4524
H	-3.9627	4.8250	-1.4737
H	-3.5556	3.3831	-2.4280
H	-3.8964	3.2317	-0.6893
H	1.2167	-2.1718	2.1253

DEM Intermediate

ZPE = -1089.35

C	0.6283	1.7216	2.0980
H	-0.0800	0.9710	2.4367
C	2.0360	1.3179	1.8293

C	0.2112	3.0237	1.8766
C	3.0342	2.4584	2.0228
O	0.8920	3.9965	1.4549
O	3.8443	2.8671	1.2107
O	2.9794	2.9185	3.2859
O	-1.1383	3.2465	2.2029
C	3.7589	4.0843	3.5765
H	2.3473	0.5404	2.5422
H	3.7373	4.7434	2.7027
C	5.1805	3.7218	3.9661
H	3.2377	4.5759	4.4030
H	5.7391	4.6276	4.2295
H	5.1847	3.0517	4.8332
C	-1.7276	4.3868	1.5999
H	5.6937	3.2277	3.1355
H	-1.0791	5.2606	1.7356
C	-2.0009	4.1594	0.1202
H	-2.6638	4.5589	2.1441
H	-2.6546	3.2907	-0.0238
H	-2.4851	5.0370	-0.3262
H	-1.0574	3.9796	-0.4083
S	2.3343	0.4807	0.1972
C	1.6360	1.7131	-0.9292
H	2.2391	2.6244	-0.8647
H	0.6273	1.9514	-0.5691
C	1.5954	1.1688	-2.3518
H	0.9816	0.2616	-2.4104
H	2.5997	0.9219	-2.7167
H	1.1648	1.9134	-3.0318

DEM TS2

ZPE = -1567.06

C	1.0947	0.6605	-0.9803
C	0.6832	-0.2982	0.1128
H	0.7147	-1.3379	-0.2198
C	1.0834	-0.1707	1.4718
C	1.0691	2.1380	-0.5962
O	1.1517	-1.0879	2.3088
O	2.0139	2.9063	-0.6056
O	-0.1808	2.5286	-0.3137
O	1.3050	1.1358	1.8725
C	1.7310	1.3349	3.2165
H	1.4450	2.3625	3.4672

H	1.1899	0.6479	3.8764
C	3.2329	1.1423	3.3471
H	3.5555	1.3135	4.3812
H	3.5058	0.1194	3.0631
H	3.7683	1.8444	2.6968
C	-0.3658	3.8972	0.0801
H	-1.4423	4.0651	-0.0159
H	0.1589	4.5439	-0.6321
C	0.1062	4.1532	1.4997
H	1.1817	3.9734	1.5856
H	-0.1018	5.1951	1.7698
H	-0.4149	3.4987	2.2074
H	0.3653	0.5736	-1.8013
S	2.6813	0.2434	-1.8123
C	3.8306	0.2569	-0.4027
H	4.7447	0.7525	-0.7489
H	3.3877	0.9059	0.3603
C	4.1467	-1.1277	0.1515
H	4.8721	-1.0527	0.9732
H	3.2438	-1.6144	0.5357
S	-2.4367	-0.2245	0.3659
H	-0.9273	-0.2694	0.2171
C	-2.3366	0.9787	1.7311
H	-1.5360	1.6805	1.4760
H	-3.2771	1.5424	1.7570
C	-2.0589	0.3467	3.0902
H	-1.1315	-0.2376	3.0623
H	-1.9566	1.1204	3.8663
H	4.5799	-1.7708	-0.6238
H	-2.8713	-0.3290	3.3851

DEM Product

ZPE = -1089.87

C	2.0460	1.3338	1.9528
C	0.1316	3.0234	1.8452
C	3.0578	2.4784	1.9982
O	0.8245	3.9645	1.4984
O	3.7789	2.8313	1.0883
O	3.0813	3.0126	3.2266
O	-1.2020	3.0119	1.7503
C	3.9414	4.1535	3.4248
H	2.4276	0.5793	2.6534

H	3.8831	4.7877	2.5349
C	5.3652	3.7220	3.7143
H	3.5042	4.6861	4.2727
H	5.9840	4.6043	3.9114
H	5.4015	3.0737	4.5964
C	-1.8297	4.1851	1.1854
H	5.7917	3.1864	2.8608
H	-1.3440	5.0750	1.5967
C	-1.7621	4.1613	-0.3288
H	-2.8613	4.1419	1.5414
H	-2.2234	3.2488	-0.7220
H	-2.3064	5.0219	-0.7327
H	-0.7255	4.2184	-0.6767
S	2.0184	0.4615	0.3704
C	1.2769	1.6799	-0.7541
H	1.7947	2.6352	-0.6230
H	0.2169	1.8117	-0.5042
C	1.4152	1.1750	-2.1852
H	0.9280	0.2016	-2.3152
H	2.4692	1.0721	-2.4647
C	0.6641	1.7588	2.4762
H	0.7352	1.9642	3.5523
H	-0.0540	0.9452	2.3419
H	0.9457	1.8820	-2.8778

HEO

ZPE = -309.37

C	-6.4624	0.1394	-0.0325
H	-6.2606	0.6216	0.9293
H	-6.0141	0.7622	-0.8130
H	-7.5461	0.1194	-0.1874
C	-5.8956	-1.2730	-0.0662
H	-6.3610	-1.9025	0.7045
H	-6.1171	-1.7637	-1.0240
C	-4.3933	-1.3153	0.1415
O	-3.7488	-0.2822	0.3123
C	-3.6897	-2.6188	0.1384
H	-2.6125	-2.5519	0.2952
C	-4.2818	-3.8116	-0.0383
H	-5.3611	-3.8557	-0.1936
C	-3.5613	-5.1204	-0.0396
H	-2.4871	-4.9895	0.1231

H	-3.9586	-5.7791	0.7429
H	-3.7124	-5.6418	-0.9932

HEO TS1

ZPE = -786.57

C	-6.0253	0.4423	0.8038
H	-5.5122	0.7937	1.7056
H	-5.7334	1.1098	-0.0140
H	-7.1065	0.5409	0.9598
C	-5.6543	-1.0007	0.4878
H	-5.9753	-1.6616	1.3063
H	-6.1897	-1.3553	-0.4060
C	-4.1532	-1.2048	0.2509
O	-3.3858	-0.2173	0.3724
C	-3.7047	-2.5106	-0.0984
H	-2.6444	-2.6099	-0.3417
C	-4.5460	-3.6245	-0.2826
H	-5.5300	-3.5841	0.1888
C	-3.9156	-4.9982	-0.2706
H	-3.5727	-5.2348	0.7476
H	-4.6118	-5.7823	-0.5854
H	-3.0446	-5.0252	-0.9351
S	-5.5716	-3.6832	-2.3452
C	-6.8635	-4.9031	-1.9604
H	-6.8442	-5.0868	-0.8726
H	-7.8507	-4.4756	-2.1781
C	-6.7070	-6.2280	-2.7023
H	-7.4930	-6.9426	-2.4190
H	-6.7620	-6.0731	-3.7865
H	-5.7327	-6.6837	-2.4857

HEO Intermediate

ZPE = -786.57

C	-5.9905	-0.2187	0.7863
H	-5.8402	-1.0027	1.5413
H	-5.3357	0.6225	1.0442
H	-7.0314	0.1235	0.8555
C	-5.6428	-0.7404	-0.6107
H	-6.2912	-1.5864	-0.8739
H	-5.8218	0.0497	-1.3520

C	-4.1522	-1.0977	-0.7012
O	-3.3597	-0.0994	-0.8360
C	-3.7641	-2.4267	-0.5853
H	-2.6956	-2.6481	-0.6630
C	-4.6726	-3.6112	-0.4023
H	-5.5905	-3.3158	0.1317
C	-3.9855	-4.7029	0.4238
H	-3.7209	-4.3056	1.4121
H	-4.6192	-5.5873	0.5685
H	-3.0607	-5.0236	-0.0742
S	-5.1856	-4.2308	-1.9903
C	-6.3446	-5.5686	-1.5607
H	-5.7951	-6.4634	-1.2450
H	-6.9491	-5.2301	-0.7076
C	-7.2395	-5.8967	-2.7504
H	-7.9243	-6.7178	-2.5068
H	-7.8369	-5.0262	-3.0441
H	-6.6436	-6.2038	-3.6183

HEO TS2

ZPE = -1264.28

C	-5.4175	0.1189	1.6455
H	-6.3226	0.2430	2.2528
H	-4.5647	0.5128	2.2090
H	-5.5186	0.7365	0.7460
C	-5.2069	-1.3436	1.2758
H	-5.1254	-1.9645	2.1844
H	-6.0774	-1.7283	0.7267
C	-3.9458	-1.5869	0.4366
O	-3.1567	-0.6238	0.2516
C	-3.6892	-2.9226	0.0144
H	-2.8558	-3.0341	-0.6881
C	-4.7554	-3.9756	-0.0898
H	-5.3871	-3.9808	0.8135
C	-4.1501	-5.3645	-0.2818
H	-3.4883	-5.6052	0.5602
H	-4.9159	-6.1467	-0.3441
H	-3.5547	-5.3894	-1.2037
S	-5.9100	-3.5827	-1.4927
C	-7.1895	-4.8715	-1.3372
H	-7.1158	-5.2814	-0.3208
H	-8.1664	-4.3797	-1.4074
C	-7.0816	-5.9760	-2.3832

H	-7.8696	-6.7273	-2.2415
H	-7.1841	-5.5638	-3.3936
H	-6.1101	-6.4800	-2.3285
S	-2.4952	-3.9521	2.7447
H	-3.0825	-3.4826	1.4472
C	-1.4074	-2.4910	2.8692
H	-0.4679	-2.8081	3.3361
H	-1.1738	-2.1658	1.8479
C	-2.0272	-1.3416	3.6534
H	-2.2676	-1.6501	4.6781
H	-1.3411	-0.4850	3.7014
H	-2.9524	-1.0052	3.1716

HEO Product

ZPE = -787.09

C	-6.2707	0.3015	0.3998
H	-6.0837	0.5708	1.4445
H	-5.7673	1.0450	-0.2262
H	-7.3477	0.3671	0.2143
C	-5.7642	-1.1006	0.0942
H	-6.2900	-1.8565	0.6954
H	-5.9612	-1.3837	-0.9488
C	-4.2796	-1.2623	0.3232
O	-3.5832	-0.3094	0.6496
C	-3.6031	-2.6149	0.1319
H	-3.0201	-2.5462	-0.8002
C	-4.4464	-3.8955	0.1180
H	-5.2769	-3.8058	0.8317
C	-3.5835	-5.0962	0.5020
H	-3.2188	-4.9900	1.5316
H	-4.1459	-6.0339	0.4373
H	-2.7171	-5.1707	-0.1662
S	-5.1858	-4.1194	-1.5367
C	-6.5518	-5.2459	-1.1370
H	-6.1515	-6.1405	-0.6464
H	-7.2255	-4.7423	-0.4328
C	-7.2964	-5.6274	-2.4102
H	-8.1291	-6.2984	-2.1736
H	-7.7060	-4.7424	-2.9100
H	-6.6350	-6.1425	-3.1155

H	-2.8578	-2.6851	0.9347

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