Thiol Michael Addition in Polar Aprotic Solvents: Nucleophilic Initiation or Base Catalysis? – Supporting Information

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S1 Analysis of gas chromatography (GC) experiments

Peak assignment is according to Table S1 and is illustrated in Figure S1.

Table S1. Peak assignment for the GC chromatograms.

time (min)	molecule
3.7	ethyl acrylate (EAc)
3.9	n-butanethiol (BT)
10.6	n-decane (internal standard)
16.8	Thiol Michael adduct (P)
14.8	Aza Michael adduct (NP)

Comparison of the chromatogram of the thiol-Michael addition of n-butanethiol to ethyl acrylate catalyzed by n-butylamine to the chromatogram of the aza-Michael addition of n-butylamine to ethyl acrylate shows that traces of aza-Michael product are being formed, however, amounts were too small to reliably determine the concentration. Determination of the concentration of the other species was done via determination of response factors, which were acquired as follows: First, in every chromatogram, all peak areas were standardized using the internal standard, decane. Then, for the reactant molecules EAc and BT, response factors were determined by dividing the starting concentrations by their respective peak areas at time = 0. For the determination of the response factor of the product, the conversion of the limiting reactant was determined for the sample with the highest reaction time. Since the concentration of the aza-Michael product is insignificant, the concentration of the product can thus be related to that conversion. An estimate of the response factor was then taken as the ratio between that estimated concentration and the peak area.

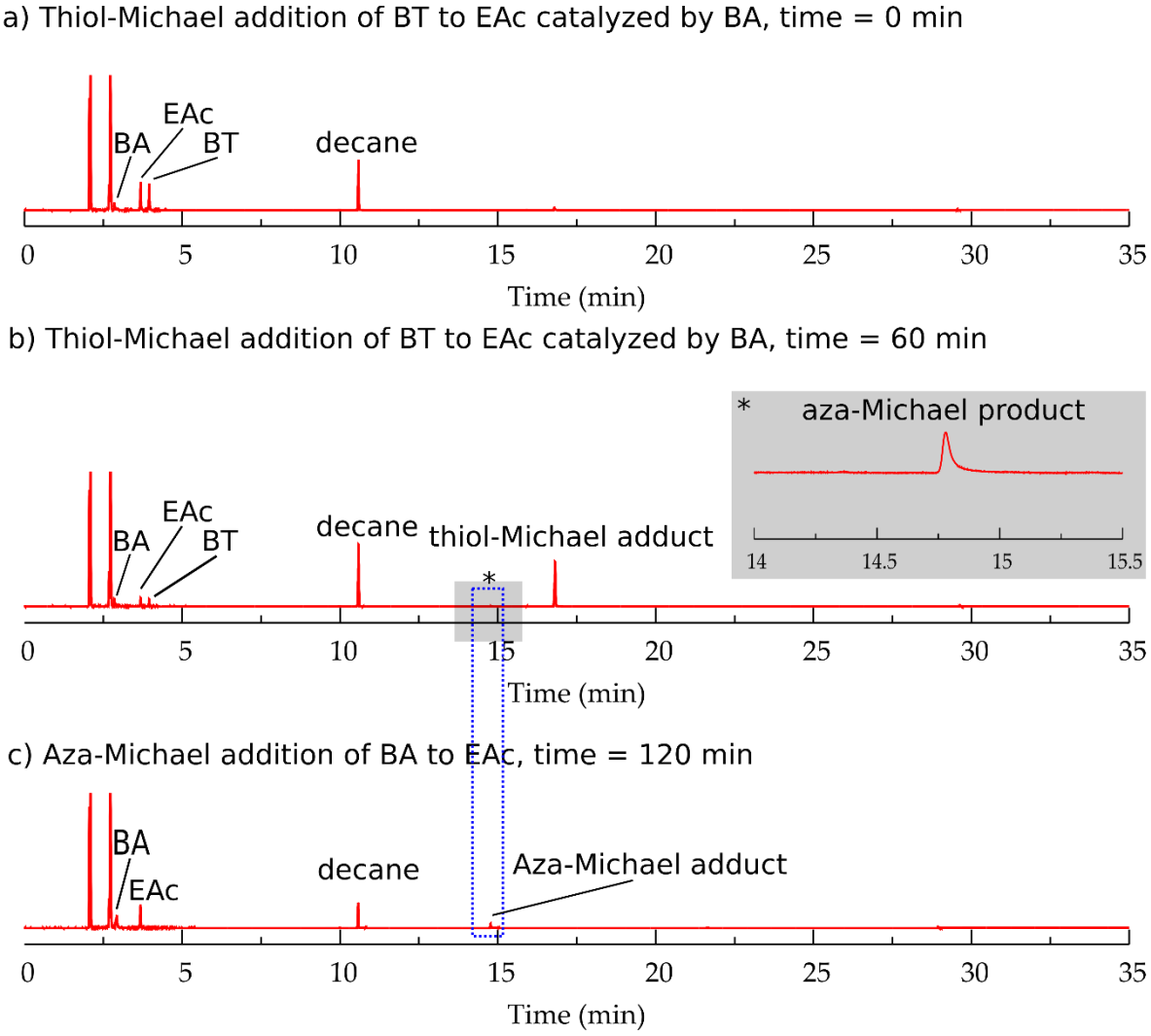

Figure S1. GC chromatograms of a) the Thiol-Michael addition of n-butanethiol (1 mol L^{-1}) to ethyl acrylate (1 mol L^{-1}) catalyzed by n-butylamine (0.3 mol L^{-1}) in THF at the start of the reaction (time = 0 min) and b) after 60 min. GC chromatogram of c) the Aza-Michael addition of ethylamine (1 mol L^{-1}) to ethyl acrylate (1 mol L^{-1}) in THF

S2 Diffusion coefficients

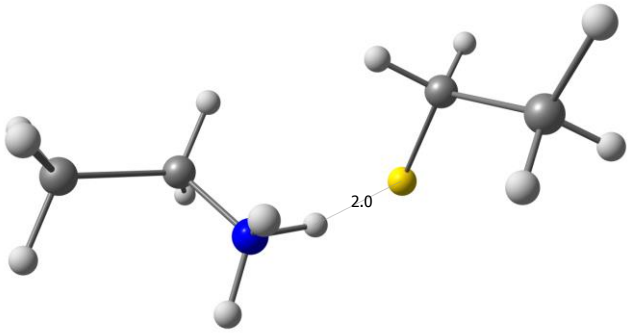

Figure S2. Optimized geometry at the B3LYP/6-31+G(d)//SMD(THF) level of theory of the encounter pair between AC and TA (as in Figure 1 in the main manuscript) in the thiol Michael addition of ethanethiol to ethyl acrylate initiated by ethylamine. The reaction distance is 2.0 Å.

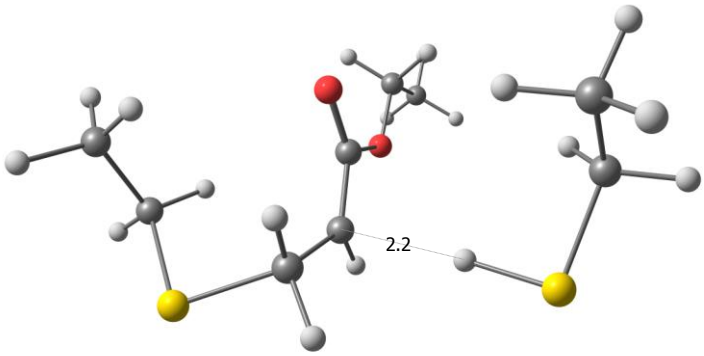

Figure S3. Optimized geometry at the B3LYP/6-31+G(d)//SMD(THF) level of theory of the encounter pair between PA and T (as in Figure 1 in the main manuscript) in the thiol Michael addition of ethanethiol to ethyl acrylate. The reaction distance is 2.2 Å.

Using molecular dynamics to simulate the path of a THF molecule in an NVT ensemble of THF molecules allows monitoring of the root mean square displacement, as shown in Figure S4.

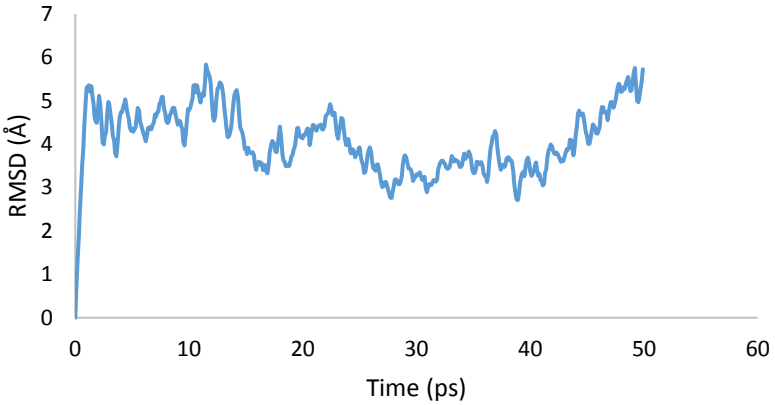

Figure S4. Root mean square displacement of the center of mass of a THF molecule as a function of time in a molecular dynamics simulation according to the specifications described in the computational section in the main manuscripts.

Once the system is equilibrated, application of the Einstein relation then allows the calculation of the diffusion coefficient via taking an average over the last 10 picoseconds, as shown in Figure S5, leading to the diffusion coefficients shown in Table S2.

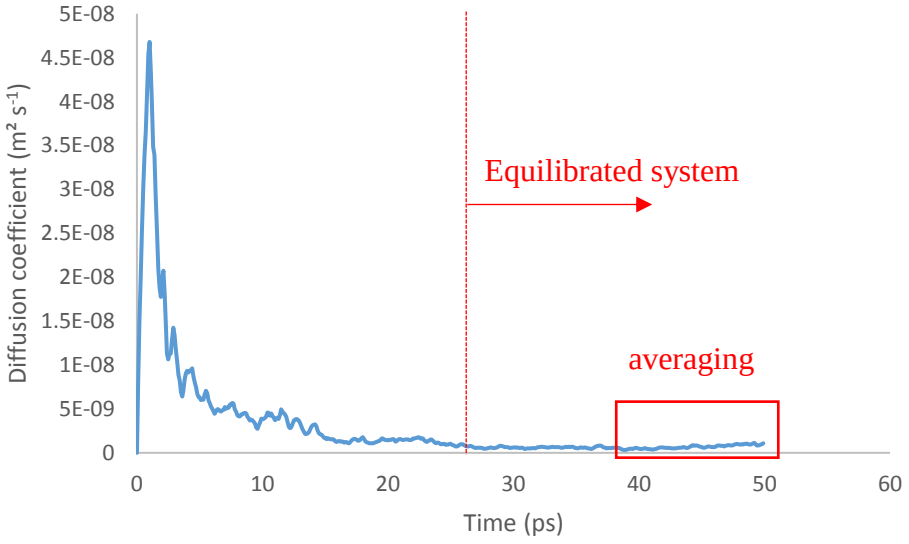

Figure S5. Diffusion coefficient as a function of time via application of the Einstein relation on the result obtained in Figure S4.

Table S2. Diffusion coefficients in THF calculated from NVT molecular dynamics simulations using the MMFF force field.

molecule	Diffusion coefficient $m^2\ s^{-1}$
THF	6.64E-10
T	2.79E-09
TA	1.06E-09
PA-ET-EAc	1.42E-09
AC-EA	4.59E-10
NZ-EA-EAc	5.10E-10
NC-EA-EAc	1.64E-09
AC-DEA	1.07E-09
NZ-DEA-EAc	1.19E-09
NC-DEA-EAc	1.24E-09
AC-TEA	1.29E-09
AC-TEP	6.21E-10
NZ-TEP-EAc	7.88E-10
NC-TEP-EAc	9.4E-10
NZ-ET-MI	5.6E-10
NC-ET-MI	4.9E-10
PA-ET-MI	5.8E-10
NZ-ET-MVS	4.3E-10
NC-ET-MVS	3.6E-10
PA-ET-MVS	8.1E-10

S3 Thiol-Michael addition of ethanethiol to ethyl acrylate initiated by ethylamine

S3.1 Thermodynamic and kinetic data in the gas phase

Table S3. Standard reaction and activation enthalpy, entropy and Gibbs free energy ($\Delta_rH°$, $\Delta_rS°$, $\Delta_rG°$ and $\Delta^‡H°$, $\Delta^‡S°$, $\Delta^‡G°$, in respectively kJ mol^{-1}, J mol^{-1} K^{-1}, kJ mol^{-1}) at 298.15 K in the gas phase (reference state is 1 mol L^{-1}) for the thiol-Michael addition of ethanethiol to various enes (EAc, MVS and MI), using various catalysts (EA, DEA, TEA and TEP). Reactions are labeled according to Figure 1 in the main manuscript.

ene	catalyst	reaction	$\Delta_rH°$	$\Delta^‡H°$	$\Delta_rS°$	$\Delta^‡S°$	$\Delta_rG°$	$\Delta^‡G°$
EAc		4	-55.7	-46.0	-130.9	-141.0	-16.7	-4.0
		7	-24.3	-47.0	-8.1	-140.6	-21.9	-5.1
	EA	1	573.7		-9.1		576.4	
		2	67.8	82.6	-153.8	-144.8	113.6	125.7
		3	364.6	7.3	-10.7	-133.0	367.8	47.0
		5	-598.0		1.0		-598.3	
		6	-533.6		5.6		-535.2	
	DEA	1	532.7		-25.8		540.4	
		2	52.0	68.6	-163.7	-155.6	100.8	115.0
		3	354.7	4.7	-18.3	-136.6	360.2	45.5
		5	-557.0		17.7		-562.3	
		6	-504.3		13.5		-508.3	
	TEA	1	535.9		-5.5		537.5	
		5	-560.2		-2.6		-559.4	
	TEP	1	510.7	94.8	-4.0	-128.2	511.8	133.1
		2	53.7	61.9	-154.6	-155.1	99.8	108.2
		3	306.1	-20.6	-29.1	-133.3	314.8	19.2
		5	-535.0		-4.2		-533.7	
		6	-330.4	-290.8	21.0	-143.6	-336.7	-248.0
MVS		4	-81.3	-80.2	-135.1	-144.5	-41.0	-37.1
		7	-11.1	-48.1	-10.1	-142.3	-8.1	-5.6
	EA	2	60.7	60.0	-152.6	-136.7	106.1	100.8
		3	428.4	-9.5	-2.0	-135.7	429.0	31.0
		6	-587.0		-9.3		-584.2	
MI		4	-103.5	-79.9	-129.7	-130.9	-64.8	-40.9
		7	13.6	-39.0	-5.9	-128.4	15.4	-0.7
	EA	2	81.6	70.7	-144.5	-129.9	124.7	109.4
		3	420.0	33.8	-9.0	-136.5	422.7	74.5
		6	-574.4		9.0		-577.1	

S3.2 Illustration of barrierless transition states

In between **PA** and **AC** (**5**, see Figure S6) and **PA** and **NC** (**6**), no transition states could be located. In order to illustrate this, the electronic energy surface between **PA** and **AC** (**5**) is given in Figure S7.

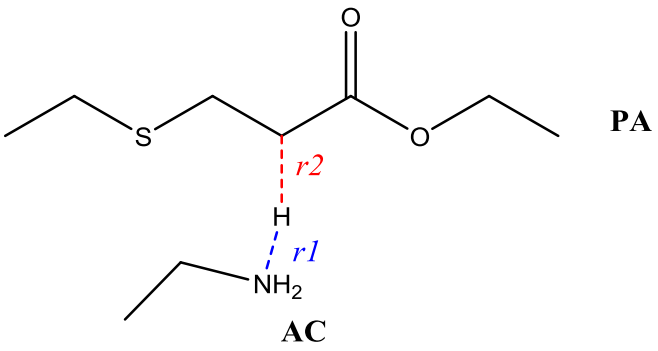

Figure S6. Transition state 5, the proton transfer between PA and AC (cf. Figure 1 in the main manuscript) in the thiol Michael addition of ethanethiol to ethyl acrylate catalyzed by ethylamine.

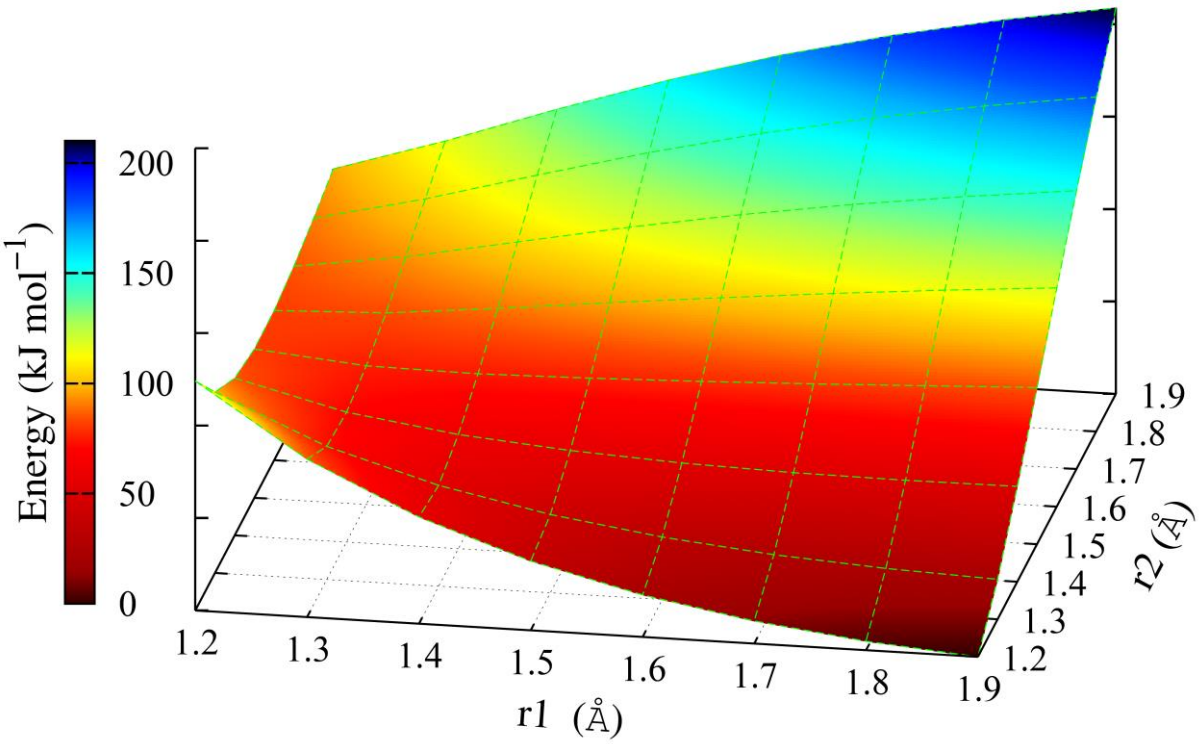

Figure S7. Electronic energy surface of transition state 5 based on the two internal coordinates r1 and r2, shown in Figure S6. This reaction has no barrier. Energies are referred to the minimum energy of the surface.

S3.3 Competition with the aza-Michael addition

For a detailed assessment of the intrinsic rate coefficients relating to the aza-Michael addition the reader is referred to previous work.[1] Note that reaction **2** in Figure S8 is the same as reaction **2** in Figure 1 in the main manuscript. The parameters reported in the previous work are obtained using a slightly different computational procedure: geometries in this work are optimized at B3LYP/6-31+G(d) and in the previous work at B3LYP/6-31G(d). This difference, however, is well within chemical accuracy ($\Delta\Delta_rG°$ and $\Delta\Delta^{‡}G°$ < 1 kcal mol^{-1}). The combined set of parameters for the reaction mechanism taking into account both thiol- and aza-Michael addition is shown in Table S4.

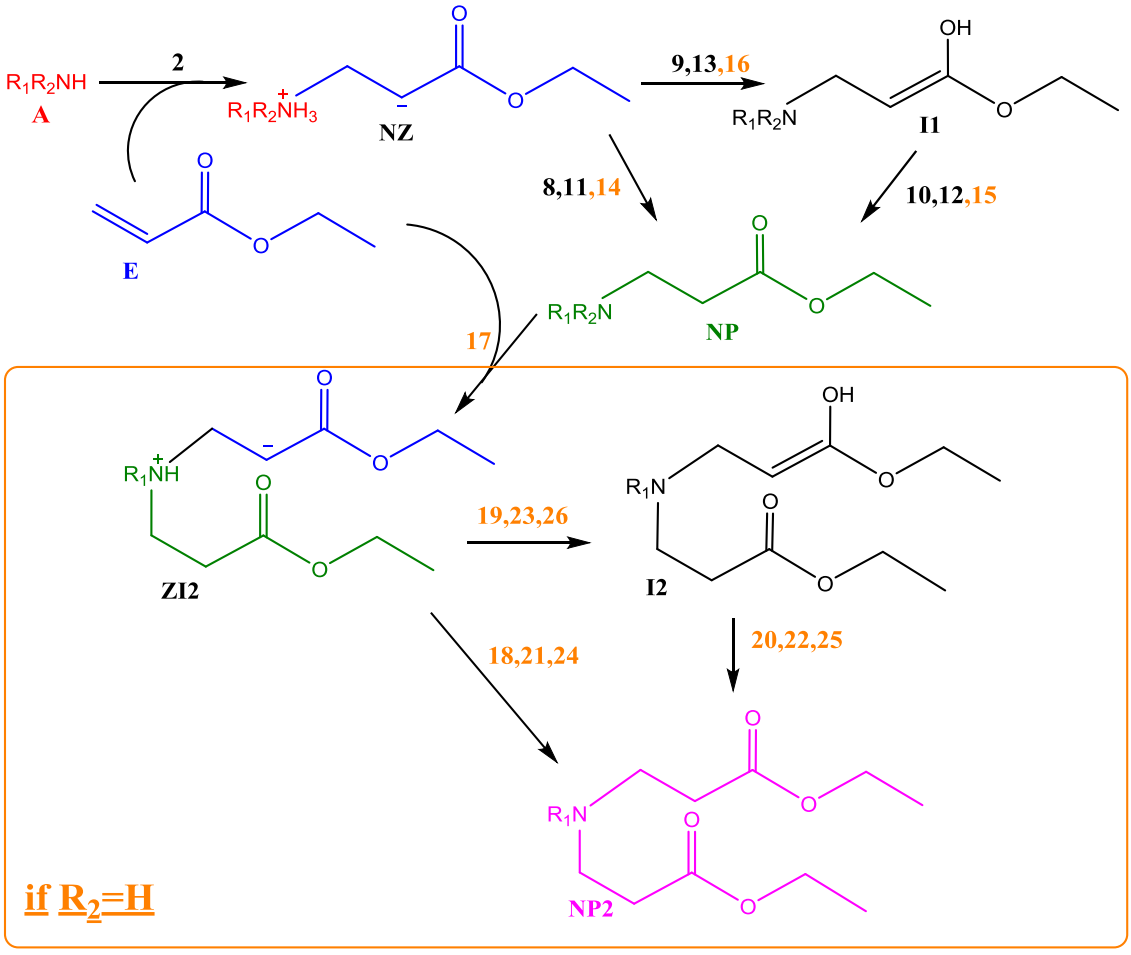

Figure S8. Reaction scheme for the aza Michael addition. Reactions 2, 8 - 10 and 11 - 14 are unassisted. Reactions 11 – 13 and 21 - 23 are assisted by the amine reactant. In case of a primary amine as reactant, reactions 14 – 16 and 24 – 26 are assisted by the product P1, which is a secondary amine.

(1) Desmet, G. B.; D'Hooge, D. R.; Omurtag, P. S.; Espeel, P.; Marin, G. B.; Du Prez, F. E.; Reyniers, M.-F. *J Org Chem* **2016**.

Table S4. Equilibrium coefficients (K_c, dimensionless or in L^{-1} mol^{-1}), intrinsic chemical forward and reverse rate coefficient (k_+ and k_-, in mol L^{-1} s^{-1} or s^{-1}), diffusional limitations (k_{diff}, in mol L^{-1} s^{-1}) (reference state is 1 mol L^{-1}) and apparent forward and reverse rate coefficients ($k_{app,+}$ and $k_{app,-}$, in mol L^{-1} s^{-1} or s^{-1}) at 298.15 K in THF calculated using the encounter pair model for all elementary reactions in both the thiol-Michael addition of ethane thiol to ethyl acrylate catalyzed by ethylamine as shown in Figure 1 in the main manuscript and the aza-Michael addition as shown in Figure S8.

	K_c	k_+	k_-	k_{diff}	$k_{app,+}$	$k_{app,-}$
R1	2.4E-06	2.7E+03	1.1E+09	-	2.7E+03	1.1E+09
R2	1.4E-13	1.5E-04	1.0E+09	-	1.5E-04	1.0E+09
R3	1.7E+09	6.5E+07	3.8E-02	3.6E+09	6.4E+07	3.7E-02
R4	2.2E-09	2.3E+01	1.1E+10	-	2.3E+01	1.1E+10
R5	7.0E+20	6.2E+12	8.9E-09	1.6E+09	1.6E+09	2.3E-12
R6	1.4E+24	6.2E+12	4.3E-12	5.9E+09	5.9E+09	4.1E-15
R7	1.7E+15	1.0E+10	6.0E-06	9.9E+09	5.0E+09	3.0E-06
R8	8.1E+17	5.2E-03	6.4E-21	-	5.2E-03	6.4E-21
R9	6.9E+00	4.8E+12	6.9E+11	-	4.8E+12	6.9E+11
R10	1.2E+17	4.9E-25	4.2E-42	-	4.9E-25	4.2E-42
R11	8.1E+17	4.6E+08	5.7E-10	1.9E+09	3.7E+08	4.6E-10
R12	1.2E+17	4.3E+06	3.7E-11	-	4.3E+06	3.7E-11
R13	6.9E+00	3.7E+12	5.3E+11	1.4E+09	1.4E+09	2.0E+08
R14	8.1E+17	1.6E+07	2.0E-11	-	1.6E+07	2.0E-11
R15	1.2E+17	1.4E+04	1.2E-13	-	1.4E+04	1.2E-13
R16	6.9E+00	5.7E+11	8.2E+10	1.8E+08	1.8E+08	2.6E+07
R17	2.5E-14	6.8E-04	2.7E+10	-	6.8E-04	2.7E+10
R18	1.8E+18	1.6E-02	9.1E-21	-	1.6E-02	9.1E-21
R19	2.3E+01	1.2E+13	5.3E+11	-	1.2E+13	5.2E+11
R20	7.7E+16	5.5E-26	7.2E-43	-	5.5E-26	7.2E-43
R21	1.8E+18	3.6E+08	2.0E-10	1.4E+09	2.9E+08	1.6E-10
R22	7.7E+16	9.0E+06	1.2E-10	-	9.0E+06	1.2E-10
R23	2.3E+01	2.5E+13	1.1E+12	1.2E+09	1.2E+09	5.2E+07
R24	1.8E+18	4.9E+06	2.7E-12	-	4.9E+06	2.7E-12
R25	7.7E+16	1.6E+03	2.1E-14	-	1.6E+03	2.1E-14
R26	2.3E+01	1.2E+06	5.2E+04	-	1.2E+06	5.2E+04

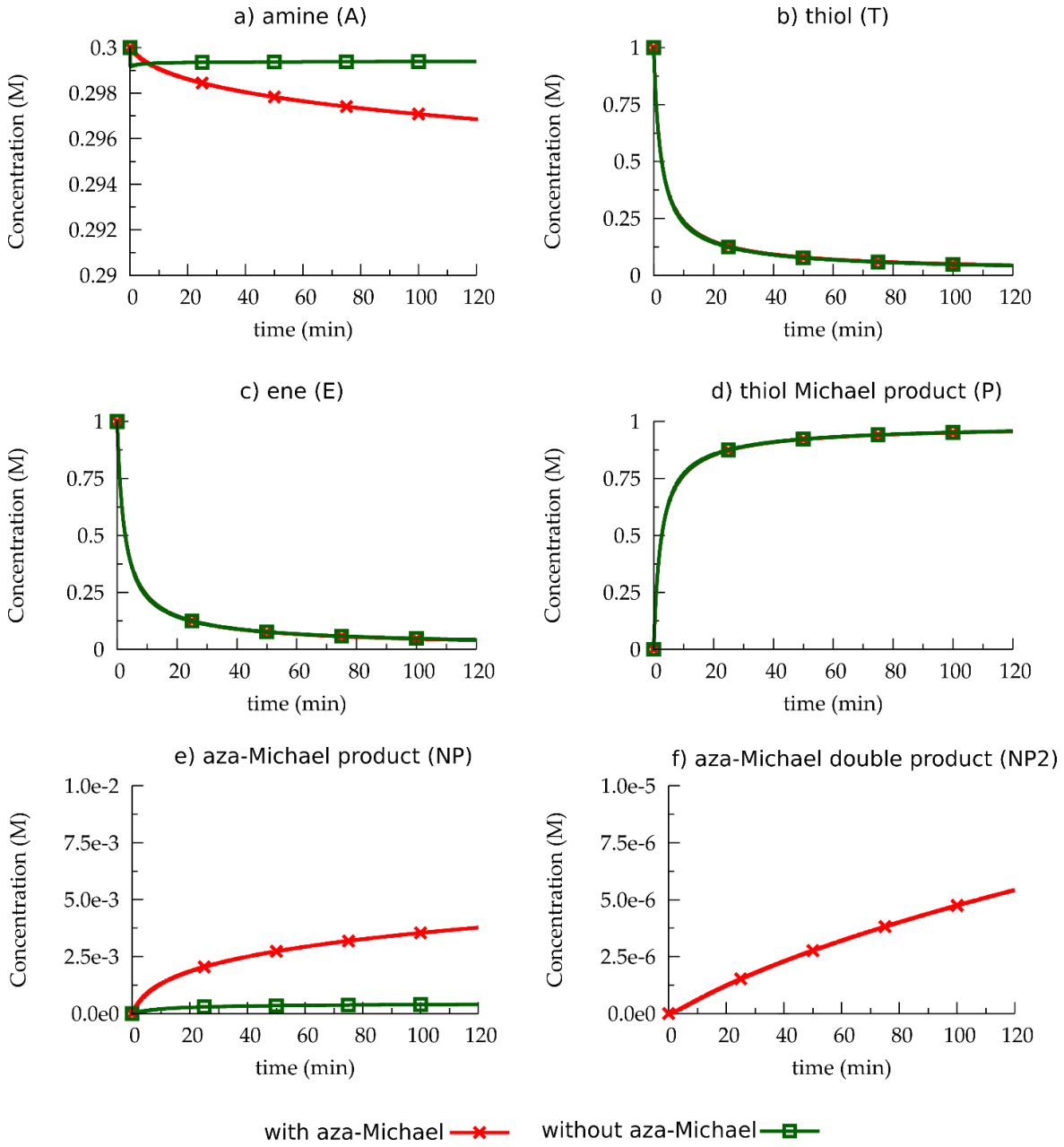

Figure S9. Concentration profiles of amine (a), thiol (b), ene (c), thiol-Michael product (d), aza-Michael product (e) and aza-Michael double product (f) as a function of time in a reaction mixture of ethylamine (0.3 M), ethanethiol (1 M) and ethyl acrylate (1 M) in THF. The red line with cross-symbols is obtained using a kinetic model of the thiol-Michael addition including the aza Michael addition (thus both the schemes in Figure 1 in the main manuscript and Figure S8 in the Supporting Information). The green line with square-symbols is obtained using a kinetic model of the thiol-Michael addition including only the reactions of Figure 1 in the main manuscript.

S3.4 Temkin table

Table S5. Temkin table showing the different theoretically possible reaction mechanism. Numbering and labelling of the reactions is according to Figure 1 in the main manuscript.

		reaction mechanisms			
		base catalysis		nucleophilic initiation	
	elementary reaction	A	B	C	D
1	A + T → AC + TA	1	1	0	0
2	A + E → NZ	0	0	1	1
3	NZ + T → NC + TA	0	0	1	1
4	TA + E → PA	1	1	1	1
5	PA + AC → P + A	1	0	0	0
6	PA + NC → P + NP	0	0	1	0
7	PA + T → P + TA	0	1	0	1

S3.5 Concentration profiles of intermediate species

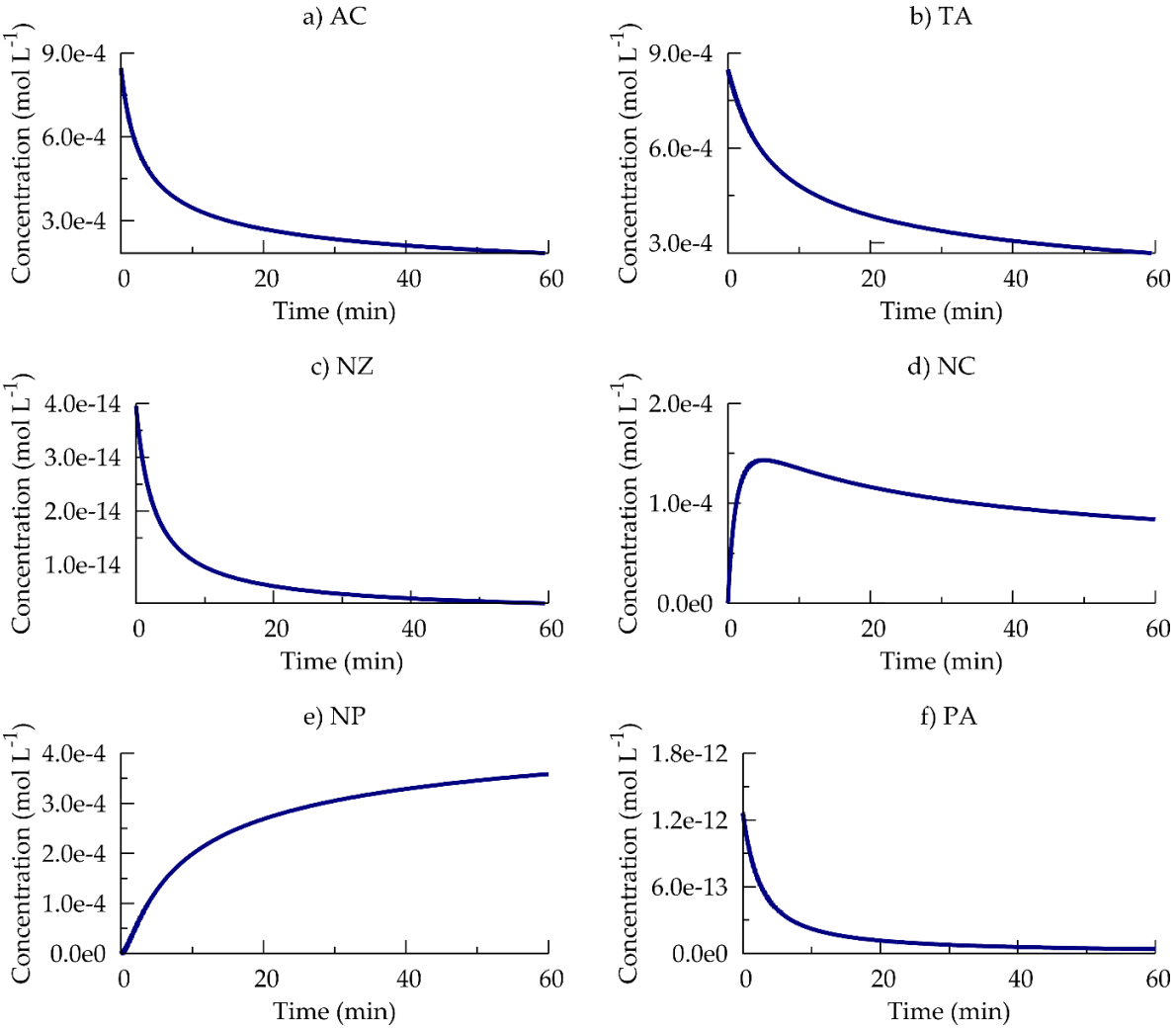

Figure S10. Concentration profiles of intermediate structures in the thiol Michael addition of ethanethiol to ethyl acrylate in THF at 298.15 K, catalyzed by ethylamine. The labels of the different intermediates refer to the structures shown in Figure 1 in the main manuscript. $c_{0,\ ethylamine}$ = 0.3 mol L^{-1}, $c_{0,\ ethanethiol}$ = 1 mol L^{-1}, $c_{0,\ ethyl\ acrylate}$ = 1 mol L^{-1}

S3.6 Influence of changing an ethyl with an n-butyl substituent

Table S6. Standard reaction enthalpy and Gibbs free energy ($\Delta_r H°$ and $\Delta_r G°$) in THF at 298.15 K for the thiol-Michael addition of n-butanethiol (BT) to ethyl acrylate (EAc) catalyzed by n-butylamine (BA) and for the thiol-Michael addition of ethanethiol (EA) to ethyl acrylate (EAc) catalyzed by ethylamine. Numbering of the reactions is according to Figure 1 in the main manuscript.

	BA-BT-EAc		EA-ET-EAc		deviation	
	ΔrH° kJ mol^{-1}	**ΔrG°** kJ mol^{-1}	**ΔrH°** kJ mol^{-1}	**ΔrG°** kJ mol^{-1}	**ΔΔrH°** kJ mol^{-1}	**ΔΔrG°** kJ mol^{-1}
TS1	6.1	33.1	2.2	32.0	-3.9	-1.1
TS2	22.6	75.0	22.4	73.3	-0.1	-1.7
TS3	-44.9	-51.9	-47.9	-52.7	-3.1	-0.8
TS4	12.6	53.4	13.0	49.5	0.3	-4.0
TS5	-91.0	-122.2	-87.5	-119.0	3.5	3.2
TS6	-130.7	-141.3	-127.9	-137.9	2.8	3.4
TS7	-84.9	-89.1	-85.3	-86.9	-0.4	2.1

S4 Influence of the initiation agent on the thiol-Michael addition to ethyl acrylate

S4.1 Diethylamine

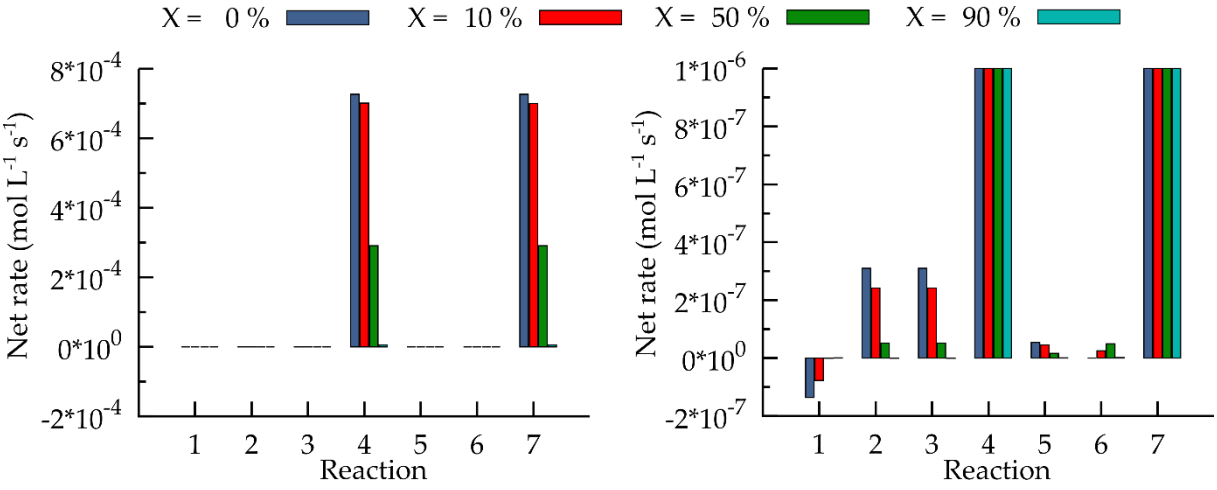

Figure S11. Net rates (different scales, left: [$-2*10^{-4}$: $8*10^{-4}$]; right: [$-2*10^{-7}$: $1*10^{-6}$]) at different conversion levels (0% blue, 10% red, 50% green and 90% cyan) for the thiol Michael addition of ethanethiol to ethyl acrylate catalyzed by diethylamine in THF at 298.15 K. $c_{0,\,amine}$ = 0.3 mol L^{-1}, $c_{0,\,ethanethiol}$ = 1 mol L^{-1}, $c_{0,\,ethyl\ acrylate}$ = 1 mol L^{-1}

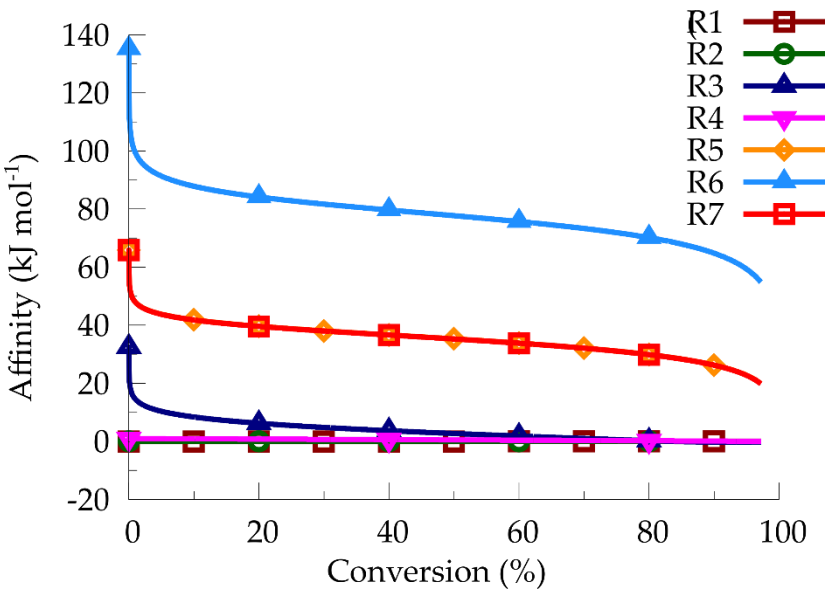

Figure S12. Affinities as a function of conversion for the thiol Michael addition of ethanethiol to ethyl acrylate catalyzed by diethylamine in THF at 298.15 K. $c_{0,\ amine}$ = 0.3 mol L^{-1}, $c_{0,\ ethanethiol}$ = 1 mol L^{-1}, $c_{0,\ ethyl\ acrylate}$ = 1 mol L^{-1}

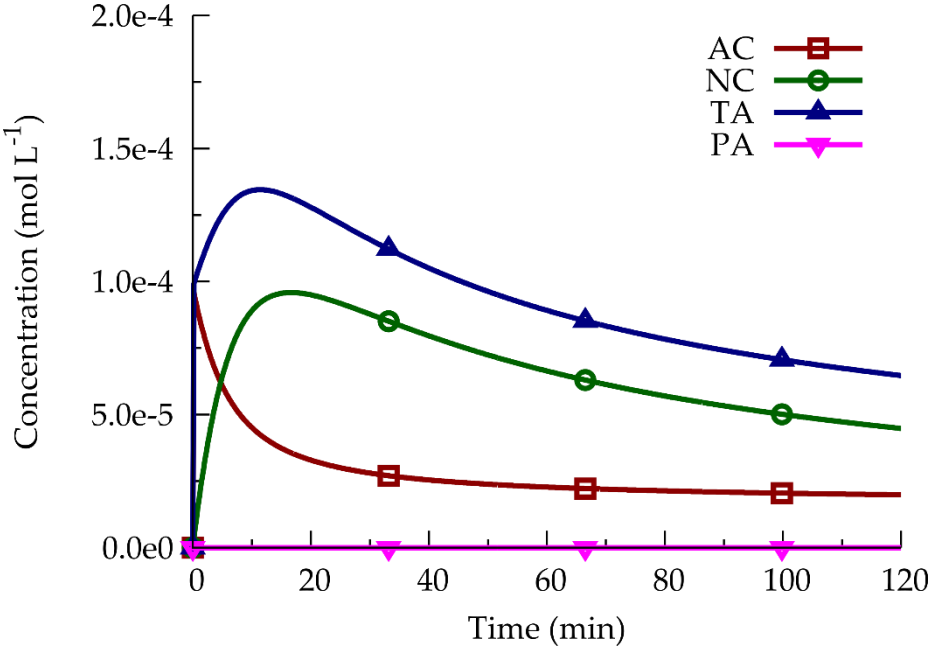

Figure S13. Concentration as a function of time for the cations generated by base catalysis (AC, brown) and nucleophilic initiation (NC, dark green) and for the thiolate anion (TA, dark blue) and the product anion (PA, pink), as shown in Figure 1 in the main text, for the thiol Michael addition of ethanethiol to ethyl acrylate in THF at 298.15 K, catalyzed by diethylamine. $c_{amine,0}$ = 0.3 M, $c_{thiol,0}$ = 1.0 M, $c_{ene,0}$ = 1.0 M

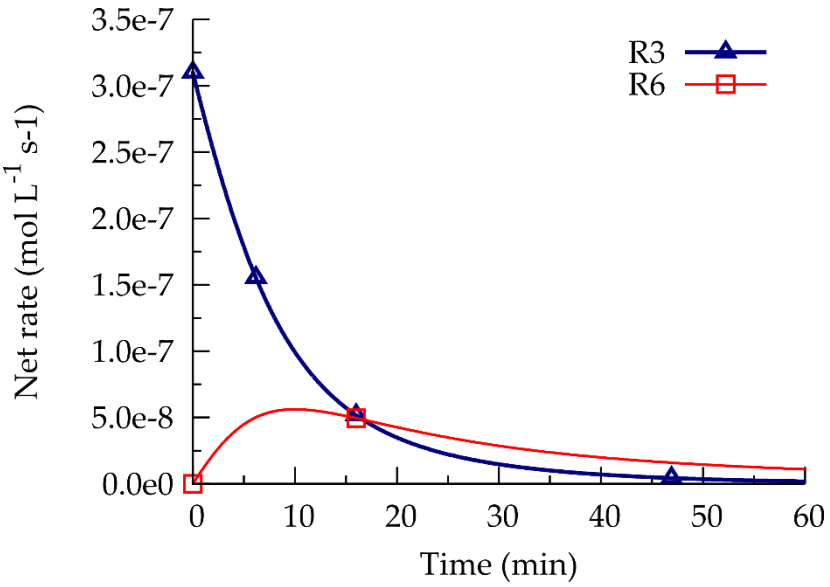

Figure S14. Net rate as a function of conversion for the thiol Michael addition of ethanethiol to ethyl acrylate catalyzed by diethylamine in THF at 298.15 K. $c_{0,\ amine}$ = 0.3 mol L^{-1}, $c_{0,\ ethanethiol}$ = 1 mol L^{-1}, $c_{0,\ ethyl\ acrylate}$ = 1 mol L^{-1}

S4.2 Triethylamine

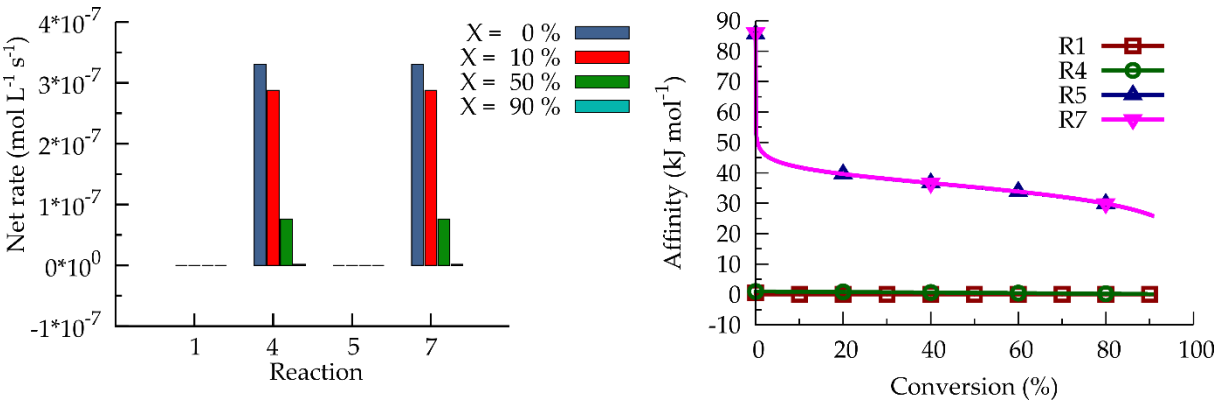

Figure S15. Results from the microkinetic simulation of the thiol-Michael addition of ethanethiol to ethyl acrylate catalyzed by triethylamine in THF at 298.15 K using the apparent parameters of Table 1. Left: Net rates at different conversion levels (0% blue, 10% red, 50% green and 90% cyan). Right: Thermodynamic affinities as a function of the conversion. Elementary reactions are labeled according to Figure 1. $c_{0,\ triethylamine}$ = 0.3 mol L^{-1}, $c_{0,\ ethanethiol}$ = 1 mol L^{-1}, $c_{0,\ ethyl\ acrylate}$ = 1 mol L^{-1}

S4.3 Triethylphosphine

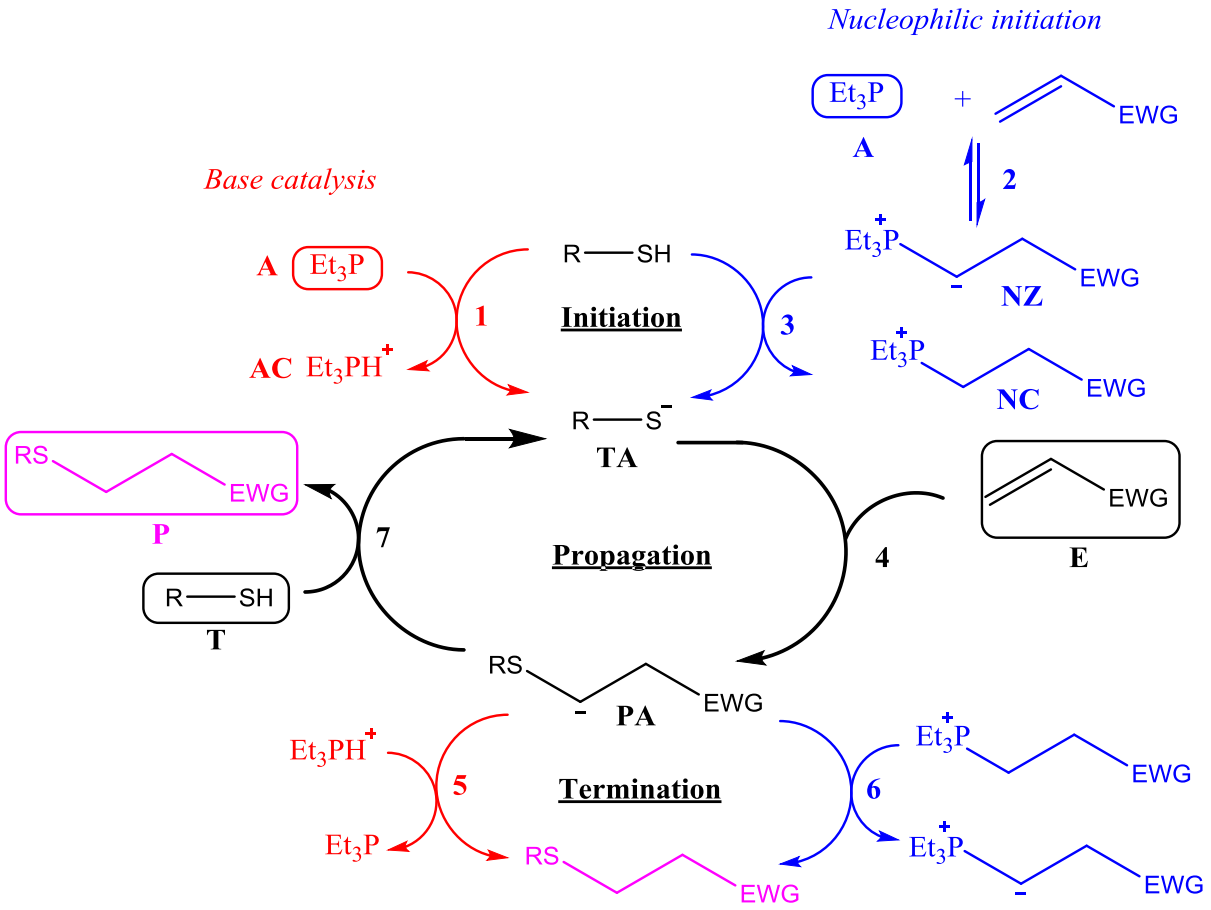

Figure S16. The two reaction mechanisms for the thiol-Michael addition, with a tertiary phosphine as an initiating agent. The base catalyzed mechanism is shown on the left side in red and the mechanism corresponding to nucleophilic initiation is presented on the right side in blue.

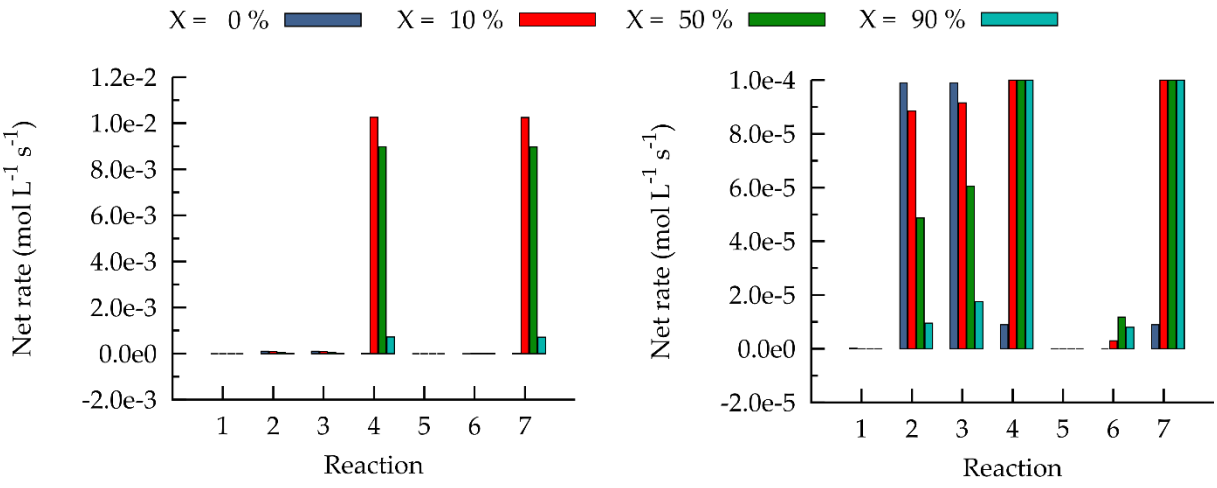

Figure S17: Net rates (different scales, left: [-2*10^{-3} : 1.2*10^{-2}]; right: [-2*10^{-5} : 1*10^{-4}]) at different conversion levels (0% blue, 10% red, 50% green and 90% cyan) for the thiol Michael addition of ethanethiol to ethyl acrylate catalyzed by triethylphosphine in THF at 298.15 K. $c_{0,\ triethylphosphine}$ = 0.3 mol L^{-1}, $c_{0,\ ethanethiol}$ = 1 mol L^{-1}, $c_{0,\ ethyl\ acrylate}$ = 1 mol L^{-1}

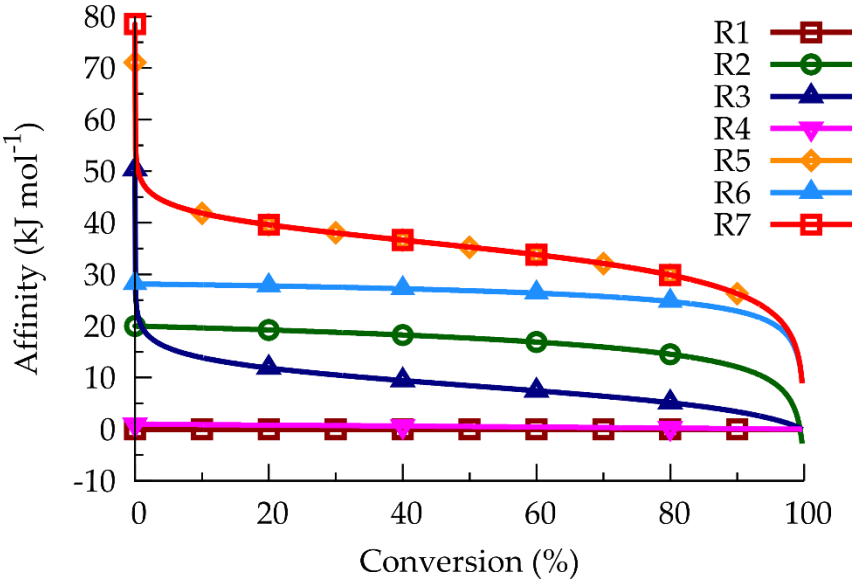

Figure S18. Affinities as a function of conversion for the thiol Michael addition of ethanethiol to ethyl acrylate catalyzed by triethylphosphine in THF at 298.15 K. $c_{0,\text{ triethylphosphine}}$ = 0.3 mol L^{-1}, $c_{0,\text{ ethanethiol}}$ = 1 mol L^{-1}, $c_{0,\text{ ethyl acrylate}}$ = 1 mol L^{-1}

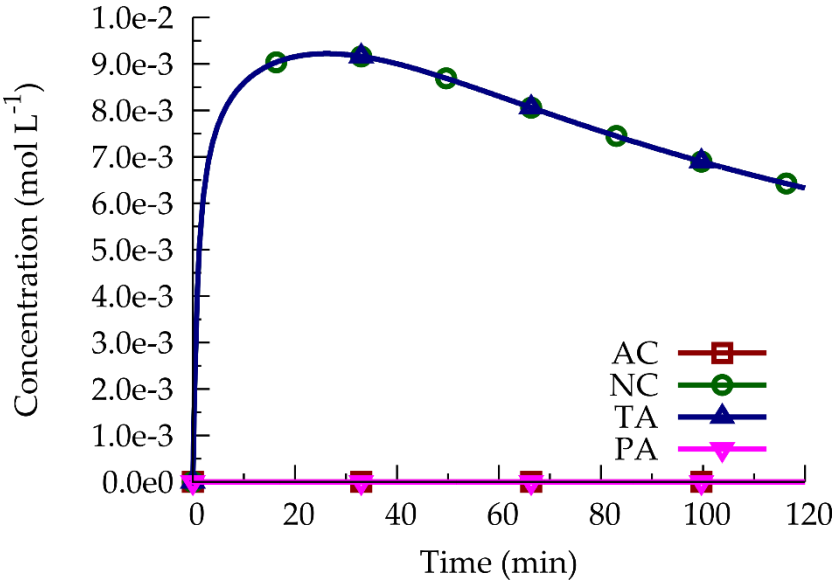

Figure S19. Concentration as a function of time for the cations generated by base catalysis (AC, brown) and nucleophilic initiation (NC, dark green) and for the thiolate anion (TA, dark blue) and the product anion (PA, pink), as shown in Figure 1 in the main text, for the thiol Michael addition of ethanethiol to ethyl acrylate in THF at 298.15 K, catalyzed by triethylphosphine. $c_{\text{phosphine},0}$ = 0.3 M, $c_{\text{thiol},0}$ = 1.0 M, $c_{\text{ene},0}$ = 1.0 M

S5 Influence of the ene on the thiol-Michael addition initiated by ethylamine

S5.1 Methyl vinylsulfone

Analysis of the net rates and affinities for the thiol-Michael addition of ethanethiol to methyl vinylsulfone initiated by ethylamine (Figure S20) gives a similar picture as for the thiol-Michael addition to ethyl acrylate (Figure 5 in the main manuscript). Only for high conversions (90 %), reaction **1** becomes slightly positive again, this to maintain the equilibrium. Analysis of the concentrations of all the species throughout the reaction shows that more side product (**NP)** is being formed (approx. 10 times more than in the case for EAc).

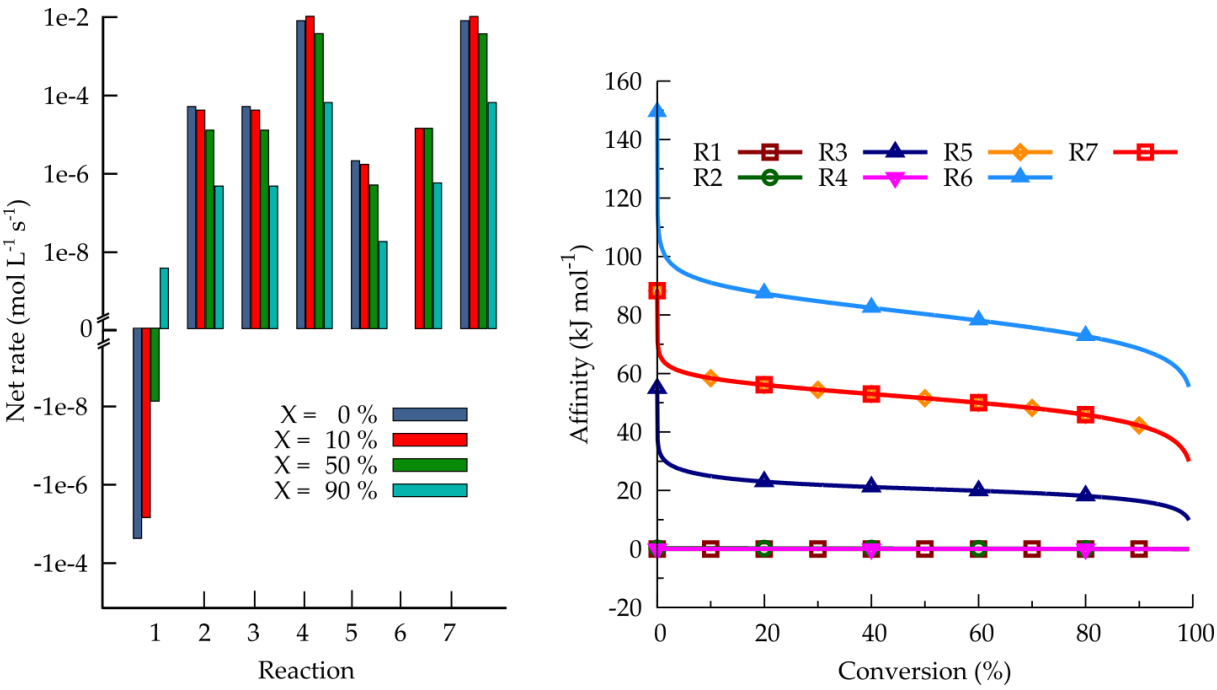

Figure S20. Simulation results for the thiol-Michael addition of ethanethiol to methyl vinylsulfone catalyzed by ethylamine in THF at 298.15 K. Left: Net rates (logarithmic scale) at different conversion levels (0% blue, 10% red, 50% green and 90% cyan). Right: Thermodynamic affinities as a function of the conversion. Elementary reactions are labeled according to Figure 1 in the main manuscript. $c_{0,\text{ethylamine}}$ **= 0.3 mol L^{-1},** $c_{0,\text{ethanethiol}}$ **= 1 mol L^{-1},** $c_{0,\text{methyl vinylsulfone}}$ **= 1 mol L^{-1}**

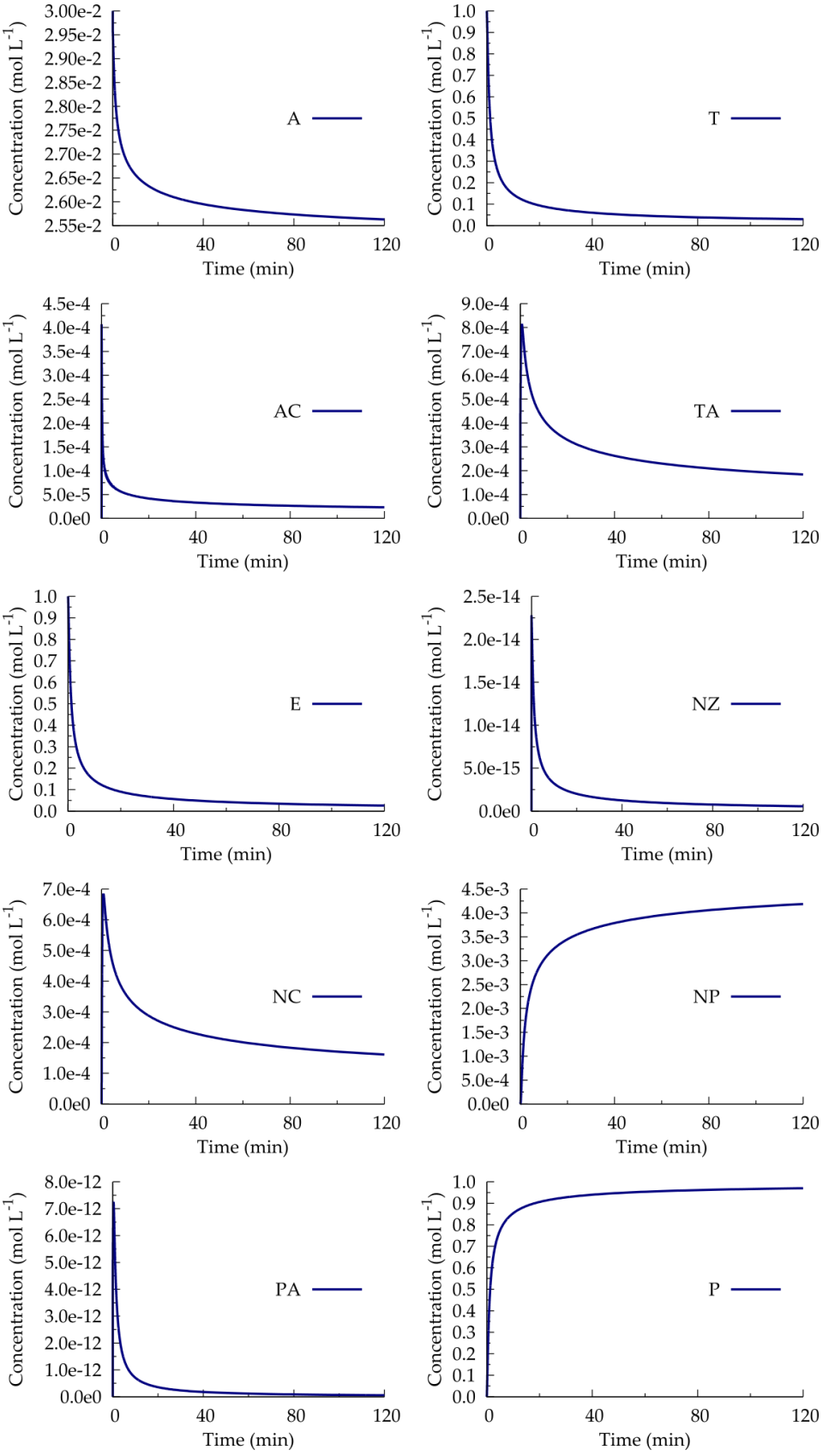

Figure S21. Concentration profiles of all species in the thiol Michael addition of ethanethiol to methyl vinyl sulfone in THF at 298.15 K, catalyzed by ethylamine. The labels of the different intermediates refer to the structures shown in Figure 1 in the main manuscript. $c_{0,\ ethylamine}$ **= 0.3 mol L^{-1},** $c_{0,\ ethanethiol}$ **= 1 mol L^{-1},** $c_{0,\ methyl\ vinylsulfone}$ **= 1 mol L^{-1}**

S5.2 Maleimide

The net rates and affinities for the thiol-Michael addition of ethanethiol to maleimide initiated by ethylamine is shown in Figure S22. Contrary to the thiol-Michael addition to EAc, the net rates of reaction **1** are positive over the whole course of the reaction. This can be explained by the fact consumption of the thiolates by reaction **4**, since this reaction now has a positive driving force and is no longer in a quasi-equilibrium as for EAc and MVS.

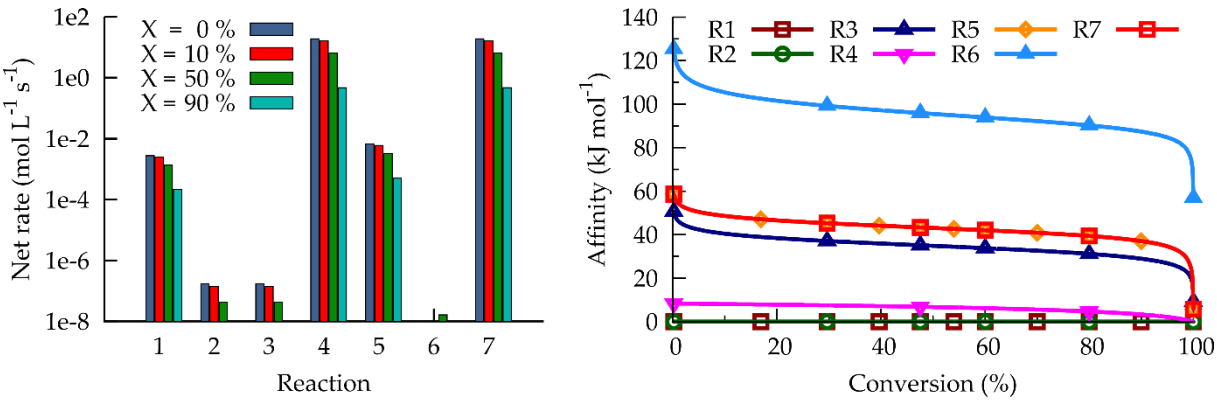

Figure S22. Simulation results for the thiol-Michael addition of ethanethiol to maleimide catalyzed by ethylamine in THF at 298.15 K. Left: Net rates (logarithmic scale) at different conversion levels (0% blue, 10% red, 50% green and 90% cyan). Right: Thermodynamic affinities as a function of the conversion. Elementary reactions are labeled according to Figure 1 in the main manuscript. $c_{0,\,ethylamine}$ = 0.3 mol L^{-1}, $c_{0,\,ethanethiol}$ = 1 mol L^{-1}, $c_{0,\,maleimide}$ = 1 mol L^{-1}

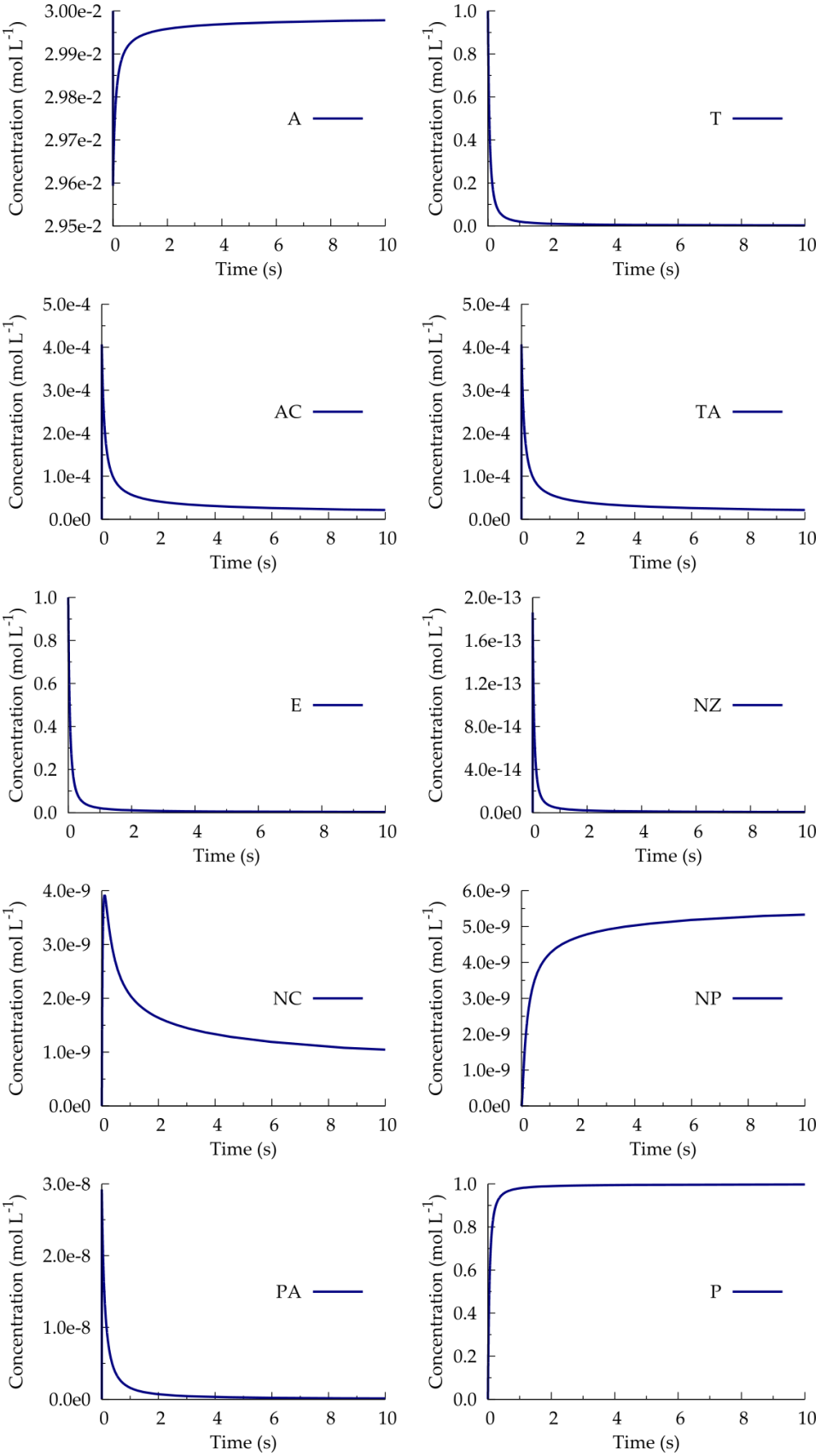

Figure S23. Concentration profiles of all species in the thiol Michael addition of ethanethiol to maleimide in THF at 298.15 K, catalyzed by ethylamine. The labels of the different intermediates refer to the structures shown in Figure 1 in the main manuscript. $c_{0,\ ethylamine}$ **= 0.3 mol** L^{-1}**,** $c_{0,\ ethanethiol}$ **= 1 mol** L^{-1}**,** $c_{0,\ maleimide}$ **= 1 mol** L^{-1}

S6 Ordinary differential equations

$y(1)=c_A$, $y(2)=c_T$, $y(3)=c_{AC}$, $y(4)=c_{TA}$, $y(5)=c_E$, $y(6)=c_{NZ}$, $y(7)=c_{NC}$, $y(8)=c_{NP}$, $y(9)=c_{PA}$, $y(10)=c_P$

```
dy(1)/dt=
        - kf( 1)*y( 1)*y( 2)
        - kf( 2)*y( 1)*y( 5)
        + kr( 1)*y( 3)*y( 4)
        + kr( 2)*y( 6)
        + kf( 5)*y( 3)*y( 9)
        - kr( 5)*y( 1)*y(10)
dy(2)/dt=
        - kf( 1)*y( 1)*y( 2)
        - kf( 3)*y( 2)*y( 6)
        - kf( 7)*y( 2)*y( 9)
        + kr( 1)*y( 3)*y( 4)
        + kr( 3)*y( 4)*y( 7)
        + kr( 7)*y( 4)*y(10)
dy(3)/dt =
        - kf( 5)*y( 3)*y( 9)
        + kr( 5)*y( 1)*y(10)
        + kf( 1)*y( 1)*y( 2)
        - kr( 1)*y( 3)*y( 4)
dy(4)/dt=
        - kf( 4)*y( 4)*y( 5)
        + kr( 4)*y( 9)
        + kf( 1)*y( 1)*y( 2)
        + kf( 3)*y( 2)*y( 6)
        + kf( 7)*y( 2)*y( 9)
        - kr( 1)*y( 3)*y( 4)
        - kr( 3)*y( 4)*y( 7)
        - kr( 7)*y( 4)*y(10)
dy(5)/dt=
        - kf( 2)*y( 1)*y( 5)
        - kf( 4)*y( 4)*y( 5)
        + kr( 2)*y( 6)
        + kr( 4)*y( 9)
dy(6)/dt=
        - kf( 3)*y( 2)*y( 6)
        + kr( 3)*y( 4)*y( 7)
        + kf( 2)*y( 1)*y( 5)
        - kr( 2)*y( 6)
dy(7)/dt=
        - kf( 6)*y( 7)*y( 9)
        + kr( 6)*y( 8)*y(10)
        + kf( 3)*y( 2)*y( 6)
        - kr( 3)*y( 4)*y( 7)
dy(8)/dt=
        + kf( 6)*y( 7)*y( 9)
        - kr( 6)*y( 8)*y(10)
dy(9)/dt=
        - kf( 5)*y( 3)*y( 9)
        - kf( 6)*y( 7)*y( 9)
```

```
            - kf( 7)*y( 2)*y( 9)
            + kr( 5)*y( 1)*y(10)
            + kr( 6)*y( 8)*y(10)
            + kr( 7)*y( 4)*y(10)
            + kf( 4)*y( 4)*y( 5)
            - kr( 4)*y( 9)
      ydot(10)/dt=
            + kf( 5)*y( 3)*y( 9)
            + kf( 6)*y( 7)*y( 9)
            + kf( 7)*y( 2)*y( 9)
            - kr( 5)*y( 1)*y(10)
            - kr( 6)*y( 8)*y(10)
            - kr( 7)*y( 4)*y(10)
```

S7 Cartesian coordinates of the optimized geometries

The Cartesian coordinates for the minimum energy conformations and the Cartesian coordinates and imaginary frequencies for the transition states for the reactions studied in this work are given below. The structures are labelled according to Figure 1 in the main text.

S7.1 ET EAc EA

```
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 H  1.217008 -1.000797 -0.888499
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 H -1.389652 -0.699085 -0.814971

Ac
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 H -1.590245 -1.284857 -0.887670
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 O  2.222726  0.511308 -0.594125
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 C -3.768812  0.545258  0.096731
 C -5.144314 -0.108239 -0.015124
 O  1.597840  1.607183 -0.060227
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 H  4.002685  0.986183  0.828511
 H  4.973351 -1.468864 -0.773389
 H  4.961321 -1.337312  1.002292
 H  6.020095 -0.286730  0.038536
```

```
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 H -3.628843  1.281991 -0.702456
 H -5.314439 -0.833409  0.789551
 H -5.267955 -0.624422 -0.974594
 H -0.985023  0.926360  1.001376
 H  0.374558 -1.186954  0.769558
 H -5.923483  0.660900  0.055703

TS2
 C -3.547602  1.614431 -0.320539
 C -3.527711  0.148654  0.090943
 O -2.417011 -0.557220 -0.494560
 C -1.222221 -0.572109  0.203057
 C -0.197338 -1.269561 -0.506292
 C  1.090238 -1.404747  0.036463
 N  2.210607  0.080306 -0.329145
 C  3.589376  0.015643  0.197362
 C  4.413015  1.268881 -0.092919
 O -1.128922 -0.032816  1.317268
 H -2.663900  2.141931  0.055270
 H -4.439603  2.104942  0.091000
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 H  1.756318 -2.140108 -0.411110
 H  1.196433 -1.319919  1.116365
 H  2.197430  0.178318 -1.345988
 H  1.698219  0.875612  0.056532
 H  3.511932 -0.153286  1.276866
 H  4.061587 -0.868519 -0.244523
 H  4.508819  1.440701 -1.172189
 H  3.954282  2.157273  0.358434
 H  5.422445  1.161606  0.323310

Imaginary Frequency:  266i

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 C  0.263812 -1.046248 -0.086849
 C  0.105525  0.244112  0.498319
 C  1.195147  1.234097  0.216707
 N  2.584815  0.622628  0.388237
 C  3.741967  1.478020 -0.028156
 C  5.061242  0.743479  0.161139
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 H -1.583455 -5.169494  0.017128
 H -2.618492 -3.753426  0.298025
 H  0.441677 -3.700108 -0.093132
 H -0.752384 -3.218143 -1.311058
 H -0.353781  0.276555  1.484664
 H  1.144418  2.101888  0.877807
 H  1.191325  1.588807 -0.820836
 H  2.700127  0.328133  1.363974
 H  2.546803 -0.243596 -0.180995
 H  3.573897  1.739315 -1.075818
 H  3.696406  2.391223  0.571424
 H  5.230764  0.486666  1.213696
 H  5.096273 -0.176362 -0.434390
 H  5.885256  1.387845 -0.164297
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 H -4.435895  1.399011 -0.430467
 C -3.511186  2.521204  1.171525
 H -4.327628  2.337776  1.885743
 H -2.571475  2.556563  1.736021
 H -3.669721  3.509164  0.722243
 H -1.057046  0.915975 -0.365674
 S -2.157133  1.646213 -1.171920

Imaginary Frequency:  817i

TS4
 O  2.074874  0.031016 -0.452024
 O  1.076527 -1.208687  1.188897
 C  1.016071 -0.743515  0.034263
 C -0.012619 -0.906237 -0.927166
 C -1.200728 -1.638772 -0.648244
 H -1.736630 -2.029425 -1.511059
 C  3.185940  0.226533  0.430104
 H  2.849750  0.729807  1.345384
 H  3.604126 -0.744647  0.723105
 C  4.222922  1.064857 -0.298385
 H  3.813765  2.041531 -0.584372
 H  4.574089  0.559369 -1.206276
 H  5.088364  1.234758  0.355057
 C -2.064061  1.084000  0.550984
 H -2.124543  1.259723  1.632084
 H -1.001019  0.936383  0.302389
 C -2.605790  2.295829 -0.210651
 S -2.891641 -0.497829  0.149262
 H -1.126374 -2.363779  0.159107
 H  0.085686 -0.365964 -1.866088
 H -2.054983  3.205463  0.073745
 H -2.499053  2.159250 -1.293889
 H -3.668552  2.467999  0.002196

Imaginary Frequency:  83i

TS7
 C -0.723977  4.245458 -0.983735
 C -0.104552  3.325291  0.055202
 O -0.188265  1.981870 -0.435127
 C  0.356429  0.982610  0.379252
 C  0.070020 -0.319494 -0.103565
 O  0.945693  1.306174  1.430449
 H -0.187641  4.182809 -1.938563
 H -0.678183  5.284889 -0.633831
 H -1.775962  3.991986 -1.162596
 H  0.943883  3.590943  0.237724
 H -0.635377  3.403986  1.012603
 H -0.302853 -0.384404 -1.125481
 C -3.696164 -0.887196 -0.410999
 H -3.312619 -0.049410 -1.004646
 H -4.751954 -0.677566 -0.206199
 C -3.561493 -2.196883 -1.186313
 H -4.106229 -2.134756 -2.140059
 H -2.512512 -2.421481 -1.412249
 H -3.971434 -3.038929 -0.615447
```

H	-1.489129	-0.580227	0.674016
S	-2.831603	-0.876781	1.223185
C	0.798948	-1.496476	0.433382
H	0.178951	-2.402469	0.462262
H	1.153953	-1.305340	1.449925
S	2.284722	-2.138323	-0.572478
C	3.353296	-0.650410	-0.705472
H	2.702205	0.198114	-0.945890
H	3.992014	-0.827276	-1.578950
H	3.575638	-0.168843	1.406694
C	4.203198	-0.351657	0.528012
H	4.883601	-1.181739	0.753914
H	4.810074	0.549571	0.358304

Imaginary Frequency: 288i

S7.2 ET EAc DEA

A

C	-0.131886	0.499378	1.225274
H	-1.142097	0.930092	1.238190
H	0.575698	1.351065	1.237926
C	0.080884	-0.357549	2.470343
H	-0.024077	0.247888	3.379169
H	-0.649700	-1.174551	2.515837
H	1.086079	-0.800295	2.479303
N	-0.000000	-0.295783	-0.000000
H	0.919970	-0.739919	-0.000000
C	-0.131886	0.499378	-1.225274
H	-1.142097	0.930092	-1.238190
H	0.575698	1.351065	-1.237926
C	0.080884	-0.357549	-2.470343
H	-0.649700	-1.174551	-2.515837
H	1.086079	-0.800295	-2.479303
H	-0.024077	0.247888	-3.379169

Ac

C	-2.487141	-0.000000	-0.362163
C	-1.274164	-0.000000	0.552558
N	-0.000000	-0.000000	-0.253843
C	1.274164	0.000000	0.552558
C	2.487141	0.000000	-0.362163
H	-1.238093	0.889525	1.185560
H	-1.238093	-0.889525	1.185560
H	-3.396332	-0.000000	0.249218
H	-2.510586	0.891979	-0.999292
H	-2.510586	-0.891979	-0.999292
H	1.238093	0.889525	1.185560
H	1.238093	-0.889525	1.185560
H	2.510586	0.891979	-0.999292
H	2.510586	-0.891979	-0.999292
H	3.396332	0.000000	0.249218
H	-0.000000	-0.818442	-0.875682
H	-0.000000	0.818442	-0.875682

E

O	0.190832	-0.684240	0.000000
O	-1.102969	1.175211	0.000000
C	0.000000	0.650228	0.000000
C	1.300900	1.367798	0.000000
H	2.196806	0.752471	0.000000
C	1.366323	2.704031	0.000000
H	0.466876	3.315297	0.000000
H	2.322778	3.220165	0.000000
C	-0.996074	-1.524386	0.000000
H	-1.590245	-1.284857	0.887670
H	-1.590245	-1.284857	-0.887670
C	-0.538938	-2.968783	0.000000
H	0.057925	-3.197385	0.890432
H	0.057925	-3.197385	-0.890432
H	-1.417984	-3.624550	0.000000

T

C	0.508197	0.646269	0.091932
H	0.561378	1.169385	1.051656
H	0.549951	1.404560	-0.697257
C	1.649191	-0.354429	-0.054427
H	2.612845	0.166439	0.027473
H	1.614141	-1.118475	0.731767
H	1.614857	-0.861048	-1.025520
H	-1.086459	-0.948270	0.966915
S	-1.175690	-0.097727	-0.080004

TA

C	0.461799	0.640270	0.000007
H	0.557549	1.293592	0.879172
H	0.557589	1.293541	-0.879188
C	1.626276	-0.354237	0.000050
H	2.597911	0.166578	0.000002
H	1.589371	-1.002079	0.885776
H	1.589340	-1.002193	-0.885593
S	-1.213763	-0.154103	-0.000032

NZ

C	4.736713	0.305158	-0.308076
C	3.321817	-0.068817	-0.715780
O	2.523440	-0.129361	0.474048
C	1.175524	-0.431958	0.319045
C	0.409980	-0.348694	1.476228
C	-1.032052	-0.683819	1.386479
N	-1.734960	0.083717	0.224911
C	-3.060857	-0.526767	-0.148944
C	-2.926652	-1.728621	-1.076587
O	0.732352	-0.727114	-0.835856
H	4.759719	1.278133	0.197660
H	5.375256	0.366948	-1.198440
H	5.165512	-0.444252	0.368185
H	2.905240	0.675497	-1.406351
H	3.305396	-1.039218	-1.225891
H	0.816870	0.069595	2.390235
H	-1.584858	-0.429257	2.295419
H	-1.241327	-1.731399	1.139776
H	-1.051250	-0.067487	-0.547456
H	-3.557113	-0.794055	0.789635
H	-3.655701	0.249472	-0.634587
H	-2.453472	-1.446982	-2.024305
H	-2.347339	-2.542686	-0.630097
H	-3.928444	-2.112409	-1.301312
C	-1.834056	1.556013	0.507441
H	-2.698280	1.694598	1.165136
H	-0.928334	1.815430	1.060527
H	-1.065312	2.254403	-1.401315

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 C -1.940325  2.399400 -0.756965
 H -2.842252  2.180198 -1.339153
 H -1.976473  3.457888 -0.474638

NC
 C -4.900062 -0.023290 -0.197621
 C -3.487267  0.080327 -0.729104
 O -2.576063 -0.067302  0.409426
 C -1.270741 -0.020731  0.166482
 C -0.441664 -0.248576  1.414304
 C  0.940808  0.406009  1.367376
 N  1.790218 -0.016721  0.186689
 C  2.930704  0.957982 -0.050982
 C  2.486085  2.269064 -0.683597
 O -0.787071  0.154004 -0.948021
 H -5.077687 -0.995624  0.275136
 H -5.603076  0.084782 -1.031984
 H -5.110332  0.767828  0.530687
 H -3.258024 -0.708975 -1.450301
 H -3.291690  1.050801 -1.193548
 H -0.382391 -1.332219  1.577011
 H  1.506808  0.163223  2.269704
 H  0.832200  1.489495  1.306050
 H  1.156271  0.020049 -0.630003
 H  3.407070  1.110019  0.921463
 H  3.640339  0.449642 -0.704522
 H  1.993487  2.104437 -1.648743
 H  1.816899  2.849694 -0.041303
 H  3.379290  2.877249 -0.864140
 C  2.299172 -1.439723  0.325962
 H  3.146322 -1.394650  1.015631
 H  1.504979 -2.017994  0.798632
 H  1.817253 -2.081474 -1.695460
 C  2.673041 -2.065685 -1.010153
 H  3.508648 -1.558600 -1.502048
 H  2.975771 -3.102970 -0.829763
 H -0.969047  0.156455  2.283432

NP
 C  3.983058  1.216901 -0.687742
 C  3.122639 -0.029751 -0.677258
 O  2.109737  0.138521  0.353833
 C  1.239823 -0.873777  0.529356
 C  0.247242 -0.590388  1.637967
 C -1.206035 -0.795801  1.184035
 N -1.626741  0.139179  0.130576
 C -2.773998 -0.392332 -0.627974
 C -2.396071 -1.465337 -1.649565
 O  1.276153 -1.907182 -0.117788
 C -1.919944  1.476792  0.676314
 C -1.821975  2.593558 -0.363993
 H  0.457569 -1.300272  2.449452
 H -1.865893 -0.723375  2.069327
 H  3.707121 -0.926140 -0.447137
 H  2.617121 -0.183013 -1.635749
 H  4.484159  1.362674  0.276216
 H  3.387285  2.109130 -0.911901
 H  4.753633  1.117632 -1.461912
 H -2.919627  1.489043  1.153938
 H -1.196890  1.686214  1.470509
 H -2.539280  2.468858 -1.183399
 H -2.027123  3.563097  0.107952
 H -0.814937  2.629564 -0.796837
 H -1.300032 -1.814497  0.800292
 H  0.412931  0.414133  2.034812
 H -3.545640 -0.784424  0.063896
 H -3.235944  0.442803 -1.162910
 H -1.966891 -2.359249 -1.183360
 H -1.666068 -1.075492 -2.369063
 H -3.289859 -1.780849 -2.203351

PA
 H -5.223258  0.944815 -0.471276
 C -4.396353  0.292170 -0.780644
 C -3.204956  0.488065  0.145010
 O -2.156063 -0.371866 -0.297788
 C -0.958858 -0.356164  0.460823
 C -0.035044 -1.304700  0.006255
 C  1.297869 -1.442308  0.592923
 S  2.811523 -0.703421 -0.429960
 C  2.219691  0.995702 -0.788071
 C  2.601570  2.046783  0.254274
 H  2.208756  1.789262  1.244266
 H -4.136775  0.539433 -1.817518
 H -4.751789 -0.745303 -0.754813
 H -2.870544  1.533904  0.129753
 H -3.477645  0.249770  1.182045
 H -0.294774 -1.895983 -0.869598
 H  1.651422 -2.476910  0.671958
 H  1.362944 -0.971190  1.576433
 H  2.622065  1.271213 -1.769999
 H  1.128967  0.922152 -0.891825
 H  2.189006  3.027445 -0.025119
 H  3.690580  2.150094  0.337004
 O -0.872291  0.446710  1.422116

P
 C  5.035872 -0.769317  0.067918
 C  3.958497  0.292487 -0.016546
 O  2.668200 -0.382559  0.005834
 C  1.567168  0.388815 -0.031599
 C  0.310221 -0.459349 -0.048651
 C -0.963150  0.377708  0.054256
 S -2.436637 -0.719552 -0.038341
 C -3.768812  0.545258  0.096731
 C -5.144314 -0.108239 -0.015124
 O  1.597840  1.607183 -0.060227
 H  0.320407 -1.042353 -0.979412
 H -1.010717  1.103753 -0.762887
 H  4.028481  0.870228 -0.943642
 H  4.002685  0.986183  0.828511
 H  4.973351 -1.468864 -0.773389
 H  4.961321 -1.337312  1.002292
 H  6.020095 -0.286730  0.038536
 H -3.665452  1.062291  1.057540
 H -3.628843  1.281991 -0.702456
 H -5.314439 -0.833409  0.789551
 H -5.267955 -0.624422 -0.974594
 H -0.985023  0.926360  1.001376
 H  0.374558 -1.186954  0.769558
 H -5.923483  0.660900  0.055703
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TS2

C	4.928407	0.696942	-0.369865
C	3.721171	-0.202303	-0.570640
O	2.676807	0.257739	0.304597
C	1.485545	-0.444562	0.283237
C	0.528739	0.084221	1.199205
C	-0.746739	-0.501064	1.324471
N	-2.002528	0.118128	0.082291
C	-3.222757	-0.729646	0.084843
C	-3.068655	-1.966842	-0.793863
O	1.344896	-1.419482	-0.475072
C	-2.242503	1.559912	0.316448
C	-2.821377	2.298402	-0.888888
H	0.779485	0.991186	1.741077
H	-1.338468	-0.235929	2.200332
H	3.961909	-1.245732	-0.336027
H	3.370299	-0.166763	-1.608891
H	5.288433	0.652437	0.664895
H	4.690064	1.740458	-0.608394
H	5.743328	0.373465	-1.029550
H	-2.904050	1.640340	1.186248
H	-1.274773	1.995461	0.588972
H	-3.798452	1.905037	-1.192239
H	-2.952088	3.358934	-0.641134
H	-2.142157	2.236847	-1.748322
H	-0.838753	-1.548651	1.046523
H	-3.412724	-1.011432	1.128353
H	-4.079914	-0.137390	-0.253972
H	-2.224212	-2.591401	-0.482966
H	-2.919633	-1.688002	-1.844624
H	-3.978303	-2.575177	-0.733315
H	-1.496903	0.002992	-0.798884

Imaginary Frequency: 237i

TS3

C	2.448390	4.009154	0.688058
C	1.353563	3.327578	-0.110955
O	1.237726	1.971134	0.368338
C	0.281843	1.183586	-0.210363
C	0.244260	-0.153810	0.279336
C	-0.904773	-0.994756	-0.185454
N	-2.263269	-0.262938	-0.133138
C	-3.304056	-0.950151	-0.976905
C	-4.587359	-0.143408	-1.124658
O	-0.457753	1.638836	-1.117206
H	2.209072	4.023320	1.758135
H	2.557757	5.046371	0.347710
H	3.411165	3.502287	0.554110
H	0.392361	3.838878	0.014247
H	1.591713	3.313503	-1.180077
H	0.604436	-0.306579	1.294869
H	-1.006163	-1.914074	0.393916
H	-0.811511	-1.270661	-1.241921
H	-2.027922	0.632293	-0.602984
H	-2.837263	-1.098167	-1.953896
H	-3.486599	-1.933933	-0.537910
H	-5.143882	-0.058142	-0.186132
H	-4.382575	0.864639	-1.505323
H	-5.234030	-0.648612	-1.850915
C	3.613102	-1.853358	0.231037
H	3.521889	-0.951558	0.848340
H	4.651016	-1.895090	-0.117904
C	3.291855	-3.097121	1.058596
H	3.970518	-3.170545	1.921394
H	2.263596	-3.069251	1.439542
H	3.403700	-4.009858	0.460620
H	1.424279	-0.873729	-0.527313
S	2.548732	-1.636149	-1.266357
C	-2.709767	0.084440	1.266624
H	-1.842499	0.548001	1.742141
H	-3.484087	0.848665	1.167693
C	-3.210005	-1.098352	2.084395
H	-2.455596	-1.885493	2.185671
H	-4.122721	-1.539115	1.670591
H	-3.445577	-0.736784	3.091759

Imaginary Frequency: 816i

TS4

O	2.074874	0.031016	-0.452024
O	1.076527	-1.208687	1.188897
C	1.016071	-0.743515	0.034263
C	-0.012619	-0.906237	-0.927166
C	-1.200728	-1.638772	-0.648244
H	-1.736630	-2.029425	-1.511059
C	3.185940	0.226533	0.430104
H	2.849750	0.729807	1.345384
H	3.604126	-0.744647	0.723105
C	4.222922	1.064857	-0.298385
H	3.813765	2.041531	-0.584372
H	4.574089	0.559369	-1.206276
H	5.088364	1.234758	0.355057
C	-2.064061	1.084000	0.550984
H	-2.124543	1.259723	1.632084
H	-1.001019	0.936383	0.302389
C	-2.605790	2.295829	-0.210651
S	-2.891641	-0.497829	0.149262
H	-1.126374	-2.363779	0.159107
H	0.085686	-0.365964	-1.866088
H	-2.054983	3.205463	0.073745
H	-2.499053	2.159250	-1.293889
H	-3.668552	2.467999	0.002196

Imaginary Frequency: 83i

TS7

C	-0.723977	4.245458	-0.983735
C	-0.104552	3.325291	0.055202
O	-0.188265	1.981870	-0.435127
C	0.356429	0.982610	0.379252
C	0.070020	-0.319494	-0.103565
O	0.945693	1.306174	1.430449
H	-0.187641	4.182809	-1.938563
H	-0.678183	5.284889	-0.633831
H	-1.775962	3.991986	-1.162596
H	0.943883	3.590943	0.237724
H	-0.635377	3.403986	1.012603
H	-0.302853	-0.384404	-1.125481
C	-3.696164	-0.887196	-0.410999
H	-3.312619	-0.049410	-1.004646
H	-4.751954	-0.677566	-0.206199

```
 C -3.561493 -2.196883 -1.186313
 H -4.106229 -2.134756 -2.140059
 H -2.512512 -2.421481 -1.412249
 H -3.971434 -3.038929 -0.615447
 H -1.489129 -0.580227  0.674016
 S -2.831603 -0.876781  1.223185
 C  0.798948 -1.496476  0.433382
 H  0.178951 -2.402469  0.462262
 H  1.153953 -1.305340  1.449925
 S  2.284722 -2.138323 -0.572478
 C  3.353296 -0.650410 -0.705472
 H  2.702205  0.198114 -0.945890
 H  3.992014 -0.827276 -1.578950
 H  3.575638 -0.168843  1.406694
 C  4.203198 -0.351657  0.528012
 H  4.883601 -1.181739  0.753914
 H  4.810074  0.549571  0.358304

Imaginary Frequency:  288i
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S7.3 ET EAc TEA

```
A
 C -0.812211  2.337738 -0.426786
 C  0.039368  1.406060  0.437010
 N  0.000694  0.000590 -0.001783
 C  1.199319 -0.735073  0.436057
 C  2.427700 -0.468109 -0.435487
 C -1.237252 -0.668516  0.432900
 C -1.615907 -1.872055 -0.431932
 H  1.078251  1.746985  0.387875
 H -0.266469  1.489946  1.498879
 H -0.732523  3.368791 -0.058382
 H -0.470109  2.317907 -1.468775
 H -1.874132  2.065602 -0.414245
 H -1.161572 -0.974930  1.495279
 H -2.051687  0.060770  0.379521
 H -0.851837 -2.658040 -0.414571
 H -1.763824 -1.566997 -1.475125
 H -2.551879 -2.315783 -0.068319
 H  1.430347 -0.506270  1.495472
 H  0.975103 -1.805429  0.394392
 H  2.721843  0.588088 -0.429954
 H  2.233463 -0.759267 -1.474942
 H  3.283186 -1.050288 -0.068997

Ac
 C -0.677057  2.397693 -0.400734
 C  0.135596  1.444241  0.462325
 N  0.001084 -0.002795  0.019922
 C  1.188906 -0.837599  0.467574
 C  2.415577 -0.620164 -0.405796
 C -1.317840 -0.610176  0.466315
 C -1.747526 -1.772462 -0.415857
 H  1.196025  1.693943  0.408044
 H -0.171373  1.467769  1.511018
 H -0.502836  3.418990 -0.045097
 H -0.361731  2.350495 -1.449940
 H -1.753674  2.207423 -0.345908
 H -1.177855 -0.906356  1.509090
 H -2.062434  0.186396  0.430549
 H -1.039459 -2.607020 -0.396742
 H -1.884138 -1.450608 -1.455273
 H -2.711129 -2.146464 -0.053342
 H  1.369164 -0.569300  1.511792
 H  0.875855 -1.881709  0.429052
 H  2.784687  0.409776 -0.371455
 H  2.212822 -0.887698 -1.449802
 H  3.217862 -1.272309 -0.043953
 H -0.000291 -0.005528 -1.007662

E
 O  0.190832 -0.684240  0.000000
 O -1.102969  1.175211  0.000000
 C  0.000000  0.650228  0.000000
 C  1.300900  1.367798  0.000000
 H  2.196806  0.752471  0.000000
 C  1.366323  2.704031  0.000000
 H  0.466876  3.315297  0.000000
 H  2.322778  3.220165  0.000000
 C -0.996074 -1.524386  0.000000
 H -1.590245 -1.284857  0.887670
 H -1.590245 -1.284857 -0.887670
 C -0.538938 -2.968783  0.000000
 H  0.057925 -3.197385  0.890432
 H  0.057925 -3.197385 -0.890432
 H -1.417984 -3.624550  0.000000

T
 C  0.508197  0.646269  0.091932
 H  0.561378  1.169385  1.051656
 H  0.549951  1.404560 -0.697257
 C  1.649191 -0.354429 -0.054427
 H  2.612845  0.166439  0.027473
 H  1.614141 -1.118475  0.731767
 H  1.614857 -0.861048 -1.025520
 H -1.086459 -0.948270  0.966915
 S -1.175690 -0.097727 -0.080004

TA
 C  0.461799  0.640270  0.000007
 H  0.557549  1.293592  0.879172
 H  0.557589  1.293541 -0.879188
 C  1.626276 -0.354237  0.000050
 H  2.597911  0.166578  0.000002
 H  1.589371 -1.002079  0.885776
 H  1.589340 -1.002193 -0.885593
 S -1.213763 -0.154103 -0.000032

Imaginary Frequency:  -271i

PA
 H -5.223258  0.944815 -0.471276
 C -4.396353  0.292170 -0.780644
 C -3.204956  0.488065  0.145010
 O -2.156063 -0.371866 -0.297788
 C -0.958858 -0.356164  0.460823
 C -0.035044 -1.304700  0.006255
 C  1.297869 -1.442308  0.592923
 S  2.811523 -0.703421 -0.429960
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 C  2.219691  0.995702 -0.788071
 C  2.601570  2.046783  0.254274
 H  2.208756  1.789262  1.244266
 H -4.136775  0.539433 -1.817518
 H -4.751789 -0.745303 -0.754813
 H -2.870544  1.533904  0.129753
 H -3.477645  0.249770  1.182045
 H -0.294774 -1.895983 -0.869598
 H  1.651422 -2.476910  0.671958
 H  1.362944 -0.971190  1.576433
 H  2.622065  1.271213 -1.769999
 H  1.128967  0.922152 -0.891825
 H  2.189006  3.027445 -0.025119
 H  3.690580  2.150094  0.337004
 O -0.872291  0.446710  1.422116
```

P

```
 C  5.035872 -0.769317  0.067918
 C  3.958497  0.292487 -0.016546
 O  2.668200 -0.382559  0.005834
 C  1.567168  0.388815 -0.031599
 C  0.310221 -0.459349 -0.048651
 C -0.963150  0.377708  0.054256
 S -2.436637 -0.719552 -0.038341
 C -3.768812  0.545258  0.096731
 C -5.144314 -0.108239 -0.015124
 O  1.597840  1.607183 -0.060227
 H  0.320407 -1.042353 -0.979412
 H -1.010717  1.103753 -0.762887
 H  4.028481  0.870228 -0.943642
 H  4.002685  0.986183  0.828511
 H  4.973351 -1.468864 -0.773389
 H  4.961321 -1.337312  1.002292
 H  6.020095 -0.286730  0.038536
 H -3.665452  1.062291  1.057540
 H -3.628843  1.281991 -0.702456
 H -5.314439 -0.833409  0.789551
 H -5.267955 -0.624422 -0.974594
 H -0.985023  0.926360  1.001376
 H  0.374558 -1.186954  0.769558
 H -5.923483  0.660900  0.055703
```

TS4

```
 O  2.074874  0.031016 -0.452024
 O  1.076527 -1.208687  1.188897
 C  1.016071 -0.743515  0.034263
 C -0.012619 -0.906237 -0.927166
 C -1.200728 -1.638772 -0.648244
 H -1.736630 -2.029425 -1.511059
 C  3.185940  0.226533  0.430104
 H  2.849750  0.729807  1.345384
 H  3.604126 -0.744647  0.723105
 C  4.222922  1.064857 -0.298385
 H  3.813765  2.041531 -0.584372
 H  4.574089  0.559369 -1.206276
 H  5.088364  1.234758  0.355057
 C -2.064061  1.084000  0.550984
 H -2.124543  1.259723  1.632084
 H -1.001019  0.936383  0.302389
 C -2.605790  2.295829 -0.210651
 S -2.891641 -0.497829  0.149262
 H -1.126374 -2.363779  0.159107
 H  0.085686 -0.365964 -1.866088
 H -2.054983  3.205463  0.073745
 H -2.499053  2.159250 -1.293889
 H -3.668552  2.467999  0.002196
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Imaginary Frequency: 83i

TS7

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 C -0.723977  4.245458 -0.983735
 C -0.104552  3.325291  0.055202
 O -0.188265  1.981870 -0.435127
 C  0.356429  0.982610  0.379252
 C  0.070020 -0.319494 -0.103565
 O  0.945693  1.306174  1.430449
 H -0.187641  4.182809 -1.938563
 H -0.678183  5.284889 -0.633831
 H -1.775962  3.991986 -1.162596
 H  0.943883  3.590943  0.237724
 H -0.635377  3.403986  1.012603
 H -0.302853 -0.384404 -1.125481
 C -3.696164 -0.887196 -0.410999
 H -3.312619 -0.049410 -1.004646
 H -4.751954 -0.677566 -0.206199
 C -3.561493 -2.196883 -1.186313
 H -4.106229 -2.134756 -2.140059
 H -2.512512 -2.421481 -1.412249
 H -3.971434 -3.038929 -0.615447
 H -1.489129 -0.580227  0.674016
 S -2.831603 -0.876781  1.223185
 C  0.798948 -1.496476  0.433382
 H  0.178951 -2.402469  0.462262
 H  1.153953 -1.305340  1.449925
 S  2.284722 -2.138323 -0.572478
 C  3.353296 -0.650410 -0.705472
 H  2.702205  0.198114 -0.945890
 H  3.992014 -0.827276 -1.578950
 H  3.575638 -0.168843  1.406694
 C  4.203198 -0.351657  0.528012
 H  4.883601 -1.181739  0.753914
 H  4.810074  0.549571  0.358304
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Imaginary Frequency: 288i

S7.4 ET EAc TEP

A

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 C  1.944798  2.063521 -0.293190
 C  1.511057  0.699772  0.258304
    0.017400 -0.023400 -0.614422
 C -0.148044 -1.651022  0.301675
 C  0.804649 -2.739841 -0.207326
 C -1.351595  0.963398  0.202433
 C -2.748340  0.649329 -0.347989
 H  2.330486 -0.020966  0.137774
 H  1.305089  0.770712  1.336462
 H  2.836596  2.428804  0.232754
 H  2.188393  2.004263 -1.361455
 H  1.159943  2.820338 -0.172188
```

```
 H -1.321872  0.801147  1.289983
 H -1.122552  2.023528  0.031999
 H -3.024567 -0.400007 -0.186222
 H -2.806054  0.846522 -1.425807
 H -3.508954  1.268329  0.145687
 H  0.001585 -1.481819  1.378033
 H -1.186034 -1.984634  0.172756
 H  1.856440 -2.453483 -0.083240
 H  0.639186 -2.948208 -1.271818
 H  0.653658 -3.677539  0.343494

Ac
 C  1.903577  2.089645 -0.190258
 C  1.607134  0.664332  0.297351
    0.018830 -0.002789 -0.306210
 C -0.250447 -1.718602  0.254535
 C  0.857930 -2.690491 -0.173240
 C -1.375919  1.086439  0.142958
 C -2.745311  0.570869 -0.318453
 H  2.381712 -0.034931 -0.038007
 H  1.576245  0.615160  1.392702
 H  2.898178  2.387657  0.158887
 H  1.899538  2.151668 -1.284469
 H  1.180271  2.812281  0.201546
 H -1.343247  1.212961  1.231965
 H -1.154598  2.062101 -0.304664
 H -3.014717 -0.367225  0.177199
 H -2.775195  0.413394 -1.402507
 H -3.509237  1.314228 -0.066250
 H -0.354306 -1.685838  1.345966
 H -1.218873 -2.028466 -0.154595
 H  1.819455 -2.441312  0.286733
 H  0.986799 -2.703553 -1.261482
 H  0.587118 -3.703378  0.143807
 H  0.086496 -0.033548 -1.708300

E
 O  0.190832 -0.684240  0.000000
 O -1.102969  1.175211  0.000000
 C  0.000000  0.650228  0.000000
 C  1.300900  1.367798  0.000000
 H  2.196806  0.752471  0.000000
 C  1.366323  2.704031  0.000000
 H  0.466876  3.315297  0.000000
 H  2.322778  3.220165  0.000000
 C -0.996074 -1.524386  0.000000
 H -1.590245 -1.284857  0.887670
 H -1.590245 -1.284857 -0.887670
 C -0.538938 -2.968783  0.000000
 H  0.057925 -3.197385  0.890432
 H  0.057925 -3.197385 -0.890432
 H -1.417984 -3.624550  0.000000

T
 C  0.508197  0.646269  0.091932
 H  0.561378  1.169385  1.051656
 H  0.549951  1.404560 -0.697257
 C  1.649191 -0.354429 -0.054427
 H  2.612845  0.166439  0.027473
 H  1.614141 -1.118475  0.731767
 H  1.614857 -0.861048 -1.025520
 H -1.086459 -0.948270  0.966915
 S -1.175690 -0.097727 -0.080004

TA
 C  0.461799  0.640270  0.000007
 H  0.557549  1.293592  0.879172
 H  0.557589  1.293541 -0.879188
 C  1.626276 -0.354237  0.000050
 H  2.597911  0.166578  0.000002
 H  1.589371 -1.002079  0.885776
 H  1.589340 -1.002193 -0.885593
 S -1.213763 -0.154103 -0.000032

NZ
 C  2.218839  2.565904  0.720499
 C  1.823017  1.163160  1.200323
    1.712846 -0.097063 -0.124918
 C  3.307247 -0.173391 -1.038045
 C  4.554108 -0.484827 -0.200221
 C  1.463718 -1.737459  0.660893
 C  0.210030 -1.897540  1.531091
 H  2.533030  0.787842  1.947145
 H  0.836632  1.185954  1.677644
 H  2.230158  3.252037  1.575228
 H  3.217402  2.579543  0.270111
 H  1.506042  2.960941 -0.011370
 H  1.458400 -2.466997 -0.159155
 H  2.368071 -1.928563  1.251914
 H -0.702067 -1.790427  0.936944
 H  0.188944 -1.171966  2.351634
 H  0.213755 -2.900752  1.974542
 H  3.169787 -0.928977 -1.822477
 H  3.417535  0.789592 -1.551305
 H  4.488244 -1.466891  0.280236
 H  4.721472  0.267172  0.578737
 H  5.437596 -0.492316 -0.849553
 C  0.360089  0.352653 -1.332925
 H  0.230735 -0.547504 -1.948193
 H  0.830885  1.113630 -1.972114
 H -1.039554  1.830574 -0.418383
 C -0.934517  0.800097 -0.744106
 C -2.016587 -0.068878 -0.636110
 O -2.081082 -1.284400 -0.959908
 O -3.157326  0.548447 -0.079996
 C -4.355555 -0.228979 -0.041529
 H -4.191957 -1.149914  0.532131
 H -4.645537 -0.524582 -1.059057
 C -5.443408  0.618441  0.599796
 H -6.381909  0.050685  0.644363
 H -5.624943  1.533766  0.023236
 H -5.170038  0.905639  1.622743

NC
 C  0.908563  2.278279 -4.838840
 C  0.183874  1.013701 -4.359494
   -0.315714 -0.131124 -5.697959
 C  1.151074 -0.644632 -6.669522
 C  2.294739 -1.264272 -5.856497
 C -1.101261 -1.623530 -4.975640
 C -2.040289 -1.383852 -3.784490
 H  0.816411  0.433088 -3.677038
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H -0.723820 1.275079 -3.803981
H 1.173016 2.889253 -3.968804
H 1.834274 2.043764 -5.374591
H 0.275332 2.887929 -5.492630
H -1.622682 -2.125700 -5.798475
H -0.276067 -2.278829 -4.672857
H -2.871162 -0.715262 -4.028186
H -1.504880 -0.967433 -2.925468
H -2.468537 -2.343715 -3.475591
H 0.781966 -1.350264 -7.424250
H 1.494144 0.247063 -7.207545
H 2.694669 -0.564340 -5.114881
H 3.110634 -1.530799 -6.537368
H 1.982474 -2.176892 -5.338152
C -1.404296 0.738309 -6.896086
H -1.529284 0.063318 -7.749831
H -0.807436 1.587883 -7.247838
H -2.734908 1.670222 -5.404119
C -2.771897 1.237005 -6.408003
C -3.870776 0.189995 -6.474169
O -3.805333 -0.850885 -7.106056
O -4.947711 0.580673 -5.779684
C -6.121437 -0.288083 -5.810617
H -5.821517 -1.283050 -5.469205
H -6.463887 -0.362606 -6.847326
C -7.171105 0.326796 -4.908952
H -8.064852 -0.308446 -4.914128
H -7.460560 1.325360 -5.255595
H -6.812708 0.402433 -3.875942
H -3.091188 2.053370 -7.070085

PA
H -5.223258 0.944815 -0.471276
C -4.396353 0.292170 -0.780644
C -3.204956 0.488065 0.145010
O -2.156063 -0.371866 -0.297788
C -0.958858 -0.356164 0.460823
C -0.035044 -1.304700 0.006255
C 1.297869 -1.442308 0.592923
S 2.811523 -0.703421 -0.429960
C 2.219691 0.995702 -0.788071
C 2.601570 2.046783 0.254274
H 2.208756 1.789262 1.244266
H -4.136775 0.539433 -1.817518
H -4.751789 -0.745303 -0.754813
H -2.870544 1.533904 0.129753
H -3.477645 0.249770 1.182045
H -0.294774 -1.895983 -0.869598
H 1.651422 -2.476910 0.671958
H 1.362944 -0.971190 1.576433
H 2.622065 1.271213 -1.769999
H 1.128967 0.922152 -0.891825
H 2.189006 3.027445 -0.025119
H 3.690580 2.150094 0.337004
O -0.872291 0.446710 1.422116

P
C 5.035872 -0.769317 0.067918
C 3.958497 0.292487 -0.016546
O 2.668200 -0.382559 0.005834
C 1.567168 0.388815 -0.031599
C 0.310221 -0.459349 -0.048651
C -0.963150 0.377708 0.054256
S -2.436637 -0.719552 -0.038341
C -3.768812 0.545258 0.096731
C -5.144314 -0.108239 -0.015124
O 1.597840 1.607183 -0.060227
H 0.320407 -1.042353 -0.979412
H -1.010717 1.103753 -0.762887
H 4.028481 0.870228 -0.943642
H 4.002685 0.986183 0.828511
H 4.973351 -1.468864 -0.773389
H 4.961321 -1.337312 1.002292
H 6.020095 -0.286730 0.038536
H -3.665452 1.062291 1.057540
H -3.628843 1.281991 -0.702456
H -5.314439 -0.833409 0.789551
H -5.267955 -0.624422 -0.974594
H -0.985023 0.926360 1.001376
H 0.374558 -1.186954 0.769558
H -5.923483 0.660900 0.055703

TS1
C -0.866503 1.311609 2.326724
C -1.867978 0.708794 1.330909
-1.108643 0.061417 -0.224319
C -2.268791 -1.182246 -0.935139
C -2.431554 -2.456257 -0.095043
C -1.042916 1.410257 -1.481057
C -0.257152 2.661236 -1.070157
H -2.389831 -0.135131 1.796868
H -2.635767 1.440717 1.047789
H -1.399651 1.652575 3.222383
H -0.123466 0.570438 2.640558
H -0.334390 2.171789 1.908085
H -0.600353 0.959239 -2.378177
H -2.079812 1.670979 -1.731052
H 0.780397 2.422660 -0.810811
H -0.717414 3.168487 -0.215633
H -0.238244 3.370861 -1.905925
H -3.237464 -0.689866 -1.090385
H -1.871732 -1.431143 -1.927452
H -2.857831 -2.245149 0.892064
H -1.475342 -2.970492 0.049450
H -3.110404 -3.148792 -0.606622
H 0.266026 -0.651500 -0.029363
S 1.940039 -1.563403 0.097735
H 3.258323 -0.104121 1.539283
C 2.879347 -0.024103 0.512594
H 2.182475 0.828295 0.503716
H 4.775493 -0.550489 -0.424070
C 4.044772 0.267895 -0.434229
H 4.567441 1.191222 -0.140047
H 3.695219 0.389514 -1.467253

Imaginary Frequency: 291i

TS2
C 1.742884 2.466232 0.905113
C 1.489872 0.982803 1.207141
1.792000 -0.141098 -0.228984
C 3.512389 0.203826 -0.842078

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 C  4.654923  0.124992  0.180654
 C  1.869714 -1.849869  0.494349
 C  0.568772 -2.317745  1.159512
 H  2.092532  0.651451  2.062101
 H  0.437450  0.835382  1.483137
 H  1.450910  3.078415  1.767139
 H  2.800714  2.666067  0.700596
 H  1.160742  2.811160  0.042873
 H  2.133901 -2.519877 -0.334496
 H  2.698423 -1.885487  1.213567
 H -0.283658 -2.261246  0.473541
 H  0.330592 -1.717210  2.045568
 H  0.675120 -3.359155  1.488387
 H  3.685946 -0.504648 -1.663083
 H  3.481511  1.199306 -1.302486
 H  4.755652 -0.881313  0.602070
 H  4.509139  0.827306  1.009156
 H  5.607296  0.376596 -0.303858
 C  0.096948  0.311865 -1.724298
 H  0.081469 -0.677890 -2.176346
 H  0.696855  1.025117 -2.286458
 H -1.206698  1.831180 -0.890686
 C -1.093993  0.778870 -1.135208
 C -2.124753 -0.114843 -0.720544
 O -2.144185 -1.351790 -0.840594
 O -3.190510  0.550457 -0.140864
 C -4.321526 -0.247409  0.249441
 H -3.998154 -1.018582  0.957989
 H -4.731160 -0.754854 -0.632309
 C -5.349980  0.676179  0.877724
 H -6.227313  0.094770  1.187884
 H -5.682484  1.442878  0.167775
 H -4.942724  1.178366  1.763525
```

Imaginary Frequency: 220i

TS3

```
 C  3.562915  3.440610  0.833935
 C  2.557739  2.956576 -0.196340
 O  1.925091  1.776291  0.322711
 C  0.960345  1.178189 -0.480041
 C  0.532025 -0.076885  0.026524
 O  0.612869  1.722347 -1.546859
 H  3.070926  3.688876  1.782328
 H  4.065743  4.343141  0.464221
 H  4.327947  2.679958  1.030537
 H  1.800935  3.723791 -0.398528
 H  3.052152  2.720059 -1.146486
 H  0.768793 -0.295270  1.065457
 C  3.757271 -2.217822  0.099399
 H  3.849659 -1.191163  0.471265
 H  4.723176 -2.486164 -0.342029
 C  3.424727 -3.171092  1.246170
 H  4.207596 -3.127477  2.017823
 H  2.470221 -2.910243  1.719044
 H  3.354407 -4.207208  0.893043
 H  1.638705 -1.169166 -0.690352
 S  2.523883 -2.219648 -1.279300
 H -4.533926 -3.092414 -0.780616
 C -3.699891 -2.602109 -0.265552
 H -3.832688 -2.765140  0.809398
 H -2.777521 -3.102467 -0.578875
 C -3.690538 -1.109361 -0.624838
 H -3.597377 -0.980106 -1.709532
 H -4.631231 -0.631333 -0.323168
 H -2.003549  1.706141 -2.295786
 C -2.868844  1.974499 -1.682878
 H -3.760242  1.477821 -2.081111
 H -3.020950  3.055767 -1.779790
 C -2.633214  1.634369 -0.205486
 H -1.767424  2.182424  0.181303
 H -3.499615  1.920564  0.404494
 H -1.913135 -1.374734  2.145190
 C -2.400196 -0.410785  1.954638
 H -3.462303 -0.537228  2.199215
 C -1.786609  0.688235  2.834795
 H -2.309047  1.643151  2.714804
 H -1.875874  0.391757  3.886573
 H -0.726615  0.846804  2.618491
   -2.325918 -0.139162  0.136287
 C -0.705358 -0.710343 -0.546700
 H -0.711118 -1.798324 -0.391403
 H -0.766922 -0.543615 -1.629590
```

Imaginary Frequency: 408i

TS4

```
 O  2.074874  0.031016 -0.452024
 O  1.076527 -1.208687  1.188897
 C  1.016071 -0.743515  0.034263
 C -0.012619 -0.906237 -0.927166
 C -1.200728 -1.638772 -0.648244
 H -1.736630 -2.029425 -1.511059
 C  3.185940  0.226533  0.430104
 H  2.849750  0.729807  1.345384
 H  3.604126 -0.744647  0.723105
 C  4.222922  1.064857 -0.298385
 H  3.813765  2.041531 -0.584372
 H  4.574089  0.559369 -1.206276
 H  5.088364  1.234758  0.355057
 C -2.064061  1.084000  0.550984
 H -2.124543  1.259723  1.632084
 H -1.001019  0.936383  0.302389
 C -2.605790  2.295829 -0.210651
 S -2.891641 -0.497829  0.149262
 H -1.126374 -2.363779  0.159107
 H  0.085686 -0.365964 -1.866088
 H -2.054983  3.205463  0.073745
 H -2.499053  2.159250 -1.293889
 H -3.668552  2.467999  0.002196
```

Imaginary Frequency: 83i

TS7

```
 C -0.723977  4.245458 -0.983735
 C -0.104552  3.325291  0.055202
 O -0.188265  1.981870 -0.435127
 C  0.356429  0.982610  0.379252
 C  0.070020 -0.319494 -0.103565
 O  0.945693  1.306174  1.430449
 H -0.187641  4.182809 -1.938563
 H -0.678183  5.284889 -0.633831
```

```
 H -1.775962  3.991986 -1.162596
 H  0.943883  3.590943  0.237724
 H -0.635377  3.403986  1.012603
 H -0.302853 -0.384404 -1.125481
 C -3.696164 -0.887196 -0.410999
 H -3.312619 -0.049410 -1.004646
 H -4.751954 -0.677566 -0.206199
 C -3.561493 -2.196883 -1.186313
 H -4.106229 -2.134756 -2.140059
 H -2.512512 -2.421481 -1.412249
 H -3.971434 -3.038929 -0.615447
 H -1.489129 -0.580227  0.674016
 S -2.831603 -0.876781  1.223185
 C  0.798948 -1.496476  0.433382
 H  0.178951 -2.402469  0.462262
 H  1.153953 -1.305340  1.449925
 S  2.284722 -2.138323 -0.572478
 C  3.353296 -0.650410 -0.705472
 H  2.702205  0.198114 -0.945890
 H  3.992014 -0.827276 -1.578950
 H  3.575638 -0.168843  1.406694
 C  4.203198 -0.351657  0.528012
 H  4.883601 -1.181739  0.753914
 H  4.810074  0.549571  0.358304

Imaginary Frequency:  288i
```

S7.5 ET MVS EA

```
A
 C  0.000000  0.578394  0.000000
 H  0.037866  1.233147  0.880205
 H  0.037866  1.233147 -0.880205
 C  1.215896 -0.354662  0.000000
 H  2.152970  0.219833  0.000000
 H  1.217008 -1.000797  0.888499
 H  1.217008 -1.000797 -0.888499
 H -1.389652 -0.699085  0.814971
 N -1.311255 -0.089823  0.000000
 H -1.389652 -0.699085 -0.814971

Ac
 C -0.050524  0.607683 -0.000041
 H  0.011647  1.237738 -0.889517
 H  0.011654  1.237854  0.889354
 C -1.291171 -0.265585  0.000025
 H -2.178984  0.375467 -0.000006
 H -1.334558 -0.901781 -0.891812
 H -1.334537 -0.901671  0.891940
 H  1.233190 -0.853562 -0.827179
 N  1.194456 -0.245651  0.000010
 H  1.233183 -0.853474  0.827265
 H  2.047378  0.326396 -0.000018

E
 S -0.375714 -0.180613  0.026459
 O -0.185576 -1.004845 -1.188690
 O -1.029167 -0.789914  1.209534
 C  1.211803  0.453692  0.559990
 H  1.166674  1.044264  1.471990
 C  2.329632  0.157165 -0.098380
 H  2.322231 -0.447909 -1.001404
 H  3.290794  0.515393  0.263038
 C -1.304269  1.294261 -0.425660
 H -2.303304  0.960570 -0.722398
 H -1.368438  1.955062  0.442691
 H -0.801585  1.789801 -1.259718

T
 C  0.508197  0.646269  0.091932
 H  0.561378  1.169385  1.051656
 H  0.549951  1.404560 -0.697257
 C  1.649191 -0.354429 -0.054427
 H  2.612845  0.166439  0.027473
 H  1.614141 -1.118475  0.731767
 H  1.614857 -0.861048 -1.025520
 H -1.086459 -0.948270  0.966915
 S -1.175690 -0.097727 -0.080004

TA
 C  0.461799  0.640270  0.000007
 H  0.557549  1.293592  0.879172
 H  0.557589  1.293541 -0.879188
 C  1.626276 -0.354237  0.000050
 H  2.597911  0.166578  0.000002
 H  1.589371 -1.002079  0.885776
 H  1.589340 -1.002193 -0.885593
 S -1.213763 -0.154103 -0.000032

NZ
 C -3.875150 -0.879134 -0.023755
 C -2.992318  0.298498  0.367307
 N -1.657171  0.231153 -0.301189
 C -0.637863  1.372691  0.059457
 C  0.684963  1.189176 -0.557604
 S  1.572020 -0.196720 -0.123045
 C  2.690770  0.181938  1.253982
 O  0.645998 -1.244512  0.469372
 O  2.466285 -0.626839 -1.240920
 H -1.766257  0.215587 -1.320740
 H -1.115459  2.296916 -0.275810
 H -2.800718  0.313798  1.443677
 H -3.444777  1.252858  0.082908
 H -3.413957 -1.833259  0.257205
 H -4.837237 -0.802624  0.495060
 H -4.073186 -0.891016 -1.102286
 H -0.642970  1.354436  1.154463
 H  0.853257  1.488435 -1.588244
 H -1.151743 -0.636822 -0.048868
 H  2.105904  0.573924  2.090613
 H  3.201091 -0.739969  1.549168
 H  3.413252  0.928979  0.915970

NC
 C  4.629628  0.277346  0.032517
 C  3.340051 -0.520327 -0.058550
 N  2.139418  0.396748  0.026706
 C  0.815786 -0.312688 -0.038210
 C -0.321714  0.704785 -0.033466
 S -1.933135 -0.158922  0.021985
 C -3.121607  1.181115 -0.137194
 O -2.019694 -1.028864 -1.171988
```

```
 O -2.078247 -0.772900  1.360334
 H  2.199152  1.087279 -0.732760
 H  0.817501 -0.906429 -0.953638
 H  3.238668 -1.234627  0.761365
 H  3.249662 -1.051625 -1.008277
 H  4.703586  0.816818  0.984011
 H  5.476121 -0.414456 -0.028799
 H  4.720188  0.994638 -0.791375
 H  0.775205 -0.977790  0.826884
 H -0.288048  1.355688  0.845727
 H -0.321226  1.314236 -0.942787
 H -2.978807  1.676751 -1.100402
 H -4.113539  0.722136 -0.089411
 H -2.989209  1.879040  0.693262
 H  2.195639  0.936584  0.900137

NP
 C  3.869273  0.865102 -0.024852
 C  2.955940 -0.303368  0.334835
 N  1.645217 -0.173253 -0.314918
 C  0.762880 -1.306915 -0.043616
 C -0.617097 -1.141162 -0.672434
 S -1.704577  0.102269  0.105060
 C -1.081887  1.719208 -0.385720
 O -3.047190 -0.067844 -0.507513
 O -1.585506 -0.016204  1.579209
 H  1.788320 -0.102836 -1.323876
 H  1.171335 -2.262647 -0.421575
 H  2.787610 -0.325951  1.419095
 H  3.450928 -1.256318  0.068546
 H  3.424254  1.820535  0.278313
 H  4.838482  0.762960  0.477961
 H  4.057884  0.903422 -1.106235
 H  0.659080 -1.415494  1.041730
 H -0.569128 -0.886077 -1.737193
 H -1.196511 -2.065901 -0.572377
 H -1.103681  1.792468 -1.475962
 H -1.759528  2.455145  0.057841
 H -0.065413  1.832364 -0.005645

PA
 C -1.550037 -0.383170  1.670949
 S -1.824869 -0.134601 -0.123070
 O -2.761997 -1.252406 -0.479975
 C -0.403452 -0.274699 -1.046600
 C  0.588441  0.805198 -1.064823
 S  1.819380  1.044150  0.460498
 C  2.510912 -0.651024  0.599924
 C  3.546396 -1.018449 -0.463691
 O -2.357224  1.267141 -0.198959
 H -2.509858 -0.271274  2.186738
 H -0.835370  0.363650  2.025591
 H -1.154393 -1.390380  1.830872
 H -0.079439 -1.310222 -1.135559
 H  1.268033  0.701260 -1.914540
 H  0.133972  1.798199 -1.107990
 H  1.669415 -1.355516  0.577559
 H  2.954486 -0.715755  1.600209
 H  3.122129 -0.970982 -1.473527
 H  3.909620 -2.044017 -0.303649
 H  4.409438 -0.342754 -0.427628

P
 C -2.988600 -1.121419 -1.022090
 S -2.100757 -0.052687  0.125475
 C -0.392177 -0.036415 -0.524015
 C  0.508278  0.870531  0.313692
 S  2.237139  0.904331 -0.304326
 C  2.868418 -0.711992  0.320735
 C  4.344100 -0.872002 -0.038684
 O -2.093923 -0.703785  1.458513
 O -2.660957  1.316288  0.015329
 H -0.059180 -1.078294 -0.511575
 H  0.515112  0.563749  1.364010
 H  0.157212  1.905297  0.267159
 H -4.026464 -1.151157 -0.676958
 H -2.935752 -0.695181 -2.026922
 H -2.551742 -2.122642 -0.994410
 H  2.280169 -1.523736 -0.119673
 H  2.731184 -0.736971  1.407387
 H  4.710156 -1.835782  0.336117
 H  4.956541 -0.081598  0.410890
 H  4.500178 -0.853521 -1.123864
 H -0.460591  0.311286 -1.559099

TS2
 C -4.285621 -0.722695  0.091031
 C -3.241242  0.377101  0.273709
 N -1.931460  0.053404 -0.325814
 C -0.523384  1.302564 -0.070584
 C  0.658742  0.942086 -0.722527
 S  1.710199 -0.248257 -0.045558
 C  3.066778  0.599328  0.805268
 O  0.983271 -1.005056  1.022018
 O  2.358554 -1.025938 -1.142514
 H -1.996654 -0.074178 -1.337540
 H -1.059591  2.159403 -0.475027
 H -3.068315  0.568950  1.338488
 H -3.582106  1.313226 -0.181974
 H -3.958780 -1.659763  0.558203
 H -5.232553 -0.424112  0.557899
 H -4.478288 -0.915687 -0.971564
 H -0.569931  1.236068  1.014208
 H  0.865952  1.182796 -1.760408
 H -1.536017 -0.804831  0.064510
 H  2.651614  1.214757  1.607326
 H  3.736154 -0.162766  1.216282
 H  3.599316  1.222060  0.081811

Imaginary Frequency:  251i

TS3
 C  4.502110 -1.950875 -0.112322
 C  3.125834 -1.919751  0.536631
 N  2.194429 -1.012788 -0.208907
 C  0.764175 -0.907725  0.358127
 C -0.102193  0.078317 -0.350603
 S  0.462229  1.723503 -0.294916
 C -0.249586  2.493531  1.174140
 O  1.957959  1.779904 -0.053007
 O -0.055159  2.479126 -1.470163
 H  2.131484 -1.306814 -1.189950
```

```
 H  0.342042 -1.913862  0.288013
 H  3.173071 -1.542983  1.561561
 H  2.662430 -2.910055  0.549927
 H  4.959151 -0.954579 -0.128342
 H  5.158354 -2.614763  0.461131
 H  4.452675 -2.330201 -1.139948
 H  0.908532 -0.671194  1.417074
 H -0.344507 -0.161688 -1.387713
 H  2.551251 -0.039100 -0.221191
 H  0.031781  1.913895  2.057635
 H  0.157877  3.506216  1.243393
 H -1.335939  2.521838  1.066937
 C -3.777786 -0.868036 -0.498890
 H -3.453636 -0.159830 -1.270427
 H -4.847233 -0.695496 -0.336971
 C -3.541328 -2.305674 -0.958782
 H -2.477018 -2.497109 -1.142236
 H -3.888576 -3.024534 -0.206819
 H -1.603319 -0.124145  0.452755
 S -2.924970 -0.423175  1.080998
 H -4.085325 -2.502296 -1.894229

Imaginary Frequency:  298i

TS4
 C -1.334106 -0.989568  1.415890
 S -1.853769 -0.107768 -0.087114
 O -2.806250 -1.039399 -0.767891
 C -0.503136  0.158294 -1.121183
 C  0.371023  1.243079 -0.927724
 S  2.032340  0.997198  0.614764
 C  2.359234 -0.788204  0.353516
 C  3.494506 -1.101859 -0.624387
 O -2.388726  1.196908  0.409257
 H -2.210172 -1.086010  2.065523
 H -0.551586 -0.408090  1.909884
 H -0.960814 -1.977963  1.136159
 H -0.256197 -0.702650 -1.735294
 H  1.038624  1.459079 -1.756953
 H -0.033775  2.135150 -0.458186
 H  1.422031 -1.238046 -0.009449
 H  2.570003 -1.245429  1.328109
 H  3.291793 -0.680918 -1.617032
 H  3.619958 -2.189628 -0.738758
 H  4.447686 -0.686898 -0.273994

Imaginary Frequency:  147i

TS7
 C -1.329126  2.736446 -0.494982
 S  0.139730  1.703637 -0.150629
 C -0.194091  0.019044 -0.206446
 C -0.986929 -0.598758  0.888090
 S -2.887423 -0.359638  0.973071
 C -3.403580 -0.966750 -0.683039
 C -3.295726 -2.477748 -0.884672
 O  0.544617  2.095028  1.237907
 O  1.076464  2.050873 -1.267960
 H -0.428737 -0.277958 -1.229873
 H -0.666401 -0.234607  1.868872
 H -0.845861 -1.685081  0.882198
 H -1.021470  3.786162 -0.442560
 H -1.695199  2.503096 -1.498731
 H -2.100140  2.523557  0.248688
 H -2.817266 -0.432086 -1.440179
 H -4.443891 -0.640592 -0.796536
 H -3.643236 -2.748991 -1.891758
 H -3.908439 -3.020735 -0.155204
 H -2.261492 -2.827266 -0.786777
 C  3.756444 -1.087935 -0.584242
 H  3.371630 -0.496527 -1.421643
 H  4.456935 -1.820250 -1.000811
 C  4.466045 -0.189938  0.426557
 H  3.780032  0.554037  0.846513
 H  4.881772 -0.776167  1.255247
 H  1.345194 -1.037484  0.007407
 S  2.351242 -2.062182  0.120533
 H  5.292916  0.348466 -0.059630

Imaginary Frequency:  46i
```

S7.6 ET MI EA

```
A
 C  0.000000  0.578394  0.000000
 H  0.037866  1.233147  0.880205
 H  0.037866  1.233147 -0.880205
 C  1.215896 -0.354662  0.000000
 H  2.152970  0.219833  0.000000
 H  1.217008 -1.000797  0.888499
 H  1.217008 -1.000797 -0.888499
 H -1.389652 -0.699085  0.814971
 N -1.311255 -0.089823  0.000000
 H -1.389652 -0.699085 -0.814971

Ac
 C -0.050524  0.607683 -0.000041
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 H  0.011654  1.237854  0.889354
 C -1.291171 -0.265585  0.000025
 H -2.178984  0.375467 -0.000006
 H -1.334558 -0.901781 -0.891812
 H -1.334537 -0.901671  0.891940
 H  1.233190 -0.853562 -0.827179
 N  1.194456 -0.245651  0.000010
 H  1.233183 -0.853474  0.827265
 H  2.047378  0.326396 -0.000018
E
 C -0.000000  0.669455 -1.268093
 C -0.000000  1.149399  0.154836
 N  0.000000  0.000000  0.942174
 C -0.000000 -1.149399  0.154836
 C -0.000000 -0.669455 -1.268093
 H -0.000000  1.354752 -2.107346
 H -0.000000 -1.354752 -2.107346
 H  0.000000  0.000000  1.956997
 O -0.000000  2.297197  0.563848
 O -0.000000 -2.297197  0.563848

T
 C  0.508197  0.646269  0.091932
 H  0.561378  1.169385  1.051656
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 H  0.549951  1.404560 -0.697257
 C  1.649191 -0.354429 -0.054427
 H  2.612845  0.166439  0.027473
 H  1.614141 -1.118475  0.731767
 H  1.614857 -0.861048 -1.025520
 H -1.086459 -0.948270  0.966915
 S -1.175690 -0.097727 -0.080004

TA
 C  0.461799  0.640270  0.000007
 H  0.557549  1.293592  0.879172
 H  0.557589  1.293541 -0.879188
 C  1.626276 -0.354237  0.000050
 H  2.597911  0.166578  0.000002
 H  1.589371 -1.002079  0.885776
 H  1.589340 -1.002193 -0.885593
 S -1.213763 -0.154103 -0.000032

NZ
 C -0.716499 -1.167586  0.360473
 C  0.045954  0.070734  0.625992
 C -0.871625  1.209755  0.116207
 N -2.036461  0.629919 -0.222338
 C -2.001245 -0.836994 -0.085773
 N  1.365472  0.222433 -0.160729
 C  2.504377 -0.609467  0.354503
 C  3.748318 -0.420410 -0.500055
 O -0.529507  2.390548  0.014730
 O -3.029588 -1.489388 -0.346456
 H  0.348309  0.267580  1.663621
 H -0.471969 -2.137681  0.775834
 H -2.818311  1.124693 -0.639037
 H  2.159527 -1.645915  0.344695
 H  2.668946 -0.299837  1.389662
 H  4.557515 -1.039602 -0.097789
 H  4.086161  0.622720 -0.494851
 H  3.572454 -0.727931 -1.537602
 H  1.177956 -0.032876 -1.138828
 H  1.633422  1.216926 -0.158508

NC
 C -0.668945 -1.214498  0.133368
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 C -2.103268 -0.739565 -0.080176
 N  1.420191  0.245173 -0.163454
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 C  3.827947 -0.344017 -0.369127
 O -0.531189  2.382135 -0.017692
 O -3.094028 -1.421325 -0.230169
 H  0.269769  0.138689  1.576872
 H -0.314054 -1.651962 -0.807733
 H -2.916343  1.214080 -0.307186
 H  2.193497 -1.682338  0.172514
 H  2.589176 -0.475824  1.421469
 H  4.609247 -1.006333  0.017942
 H  4.143395  0.690884 -0.193976
 H  3.747274 -0.514822 -1.448758
 H  1.323355  0.113518 -1.179866
 H  1.708807  1.226825 -0.039765
 H -0.630771 -1.987507  0.903498

NP
 N -2.045240  0.639231 -0.152857
 C -2.054699 -0.750694 -0.088476
 C -0.631654 -1.203465  0.193853
 C  0.152623  0.089651  0.493022
 C -0.809650  1.210928  0.085935
 O -3.045306 -1.440755 -0.251773
 N  1.411107  0.219838 -0.232136
 C  2.495672 -0.595883  0.334715
 C  3.800345 -0.364573 -0.420417
 O -0.551208  2.399214 -0.001330
 H  0.291541  0.189986  1.586437
 H -0.625167 -1.932794  1.008373
 H -2.870544  1.185653 -0.388198
 H  2.204077 -1.650768  0.258978
 H  2.639383 -0.379158  1.409400
 H  4.602184 -0.980705  0.003644
 H  4.114742  0.685458 -0.354241
 H  3.692629 -0.621612 -1.481022
 H  1.691355  1.201512 -0.207901
 H -0.244972 -1.694506 -0.707487

PA
 C -0.628149  1.126052  0.103251
 C -0.078013 -0.233980  0.566689
 C -1.286991 -1.100698  0.634167
 C -2.390223 -0.432865  0.111853
 N -1.924622  0.914930 -0.231041
 S  1.153905 -0.875501 -0.726852
 C  2.652656  0.172223 -0.469591
 C  3.486487 -0.193169  0.757211
 O -3.596526 -0.727205 -0.085038
 O -0.013990  2.198326  0.054837
 H  3.844662 -1.228164  0.702000
 H  2.912841 -0.082452  1.685036
 H  4.362376  0.467403  0.827997
 H  3.243654  0.044798 -1.384611
 H  2.328673  1.216835 -0.433502
 H  0.503974 -0.111981  1.486768
 H -1.282562 -2.146677  0.917757
 H -2.554209  1.649392 -0.534393

P
 C -1.370303 -1.177238  0.531926
 C -0.173861 -0.209768  0.638623
 C -0.709353  1.126241  0.113180
 N -2.017334  0.920096 -0.297787
 C -2.495819 -0.365419 -0.089536
 S  1.270287 -0.814180 -0.337095
 C  2.637167  0.226318  0.334965
 C  3.959683 -0.190452 -0.305062
 O -0.126354  2.194762  0.061075
 O -3.622100 -0.740502 -0.363674
 H  0.152169 -0.071068  1.674075
 H -1.690986 -1.545950  1.511635
 H -2.588325  1.662486 -0.695271
 H  2.670208  0.086384  1.421164
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 H  2.417093  1.275558  0.124401
 H  4.769572  0.425614  0.104450
 H  3.945925 -0.045338 -1.391685
 H  4.198582 -1.240506 -0.098838
 H -1.174953 -2.053145 -0.095684

TS2
 C -0.765734 -1.015421  0.808510
 C -0.120416  0.234941  0.873933
 C -0.996061  1.215934  0.085793
 N -1.937803  0.447804 -0.531298
 C -1.876520 -0.927980 -0.082939
 N  1.428213  0.367703 -0.183526
 C  2.509949 -0.505882  0.319410
 C  3.748178 -0.491726 -0.572946
 O -0.846595  2.431104  0.002844
 O -2.717816 -1.752291 -0.454572
 H  0.370846  0.617730  1.765113
 H -0.504874 -1.915694  1.349314
 H -2.703066  0.816514 -1.085234
 H  2.093965 -1.515939  0.391621
 H  2.752666 -0.165668  1.331422
 H  4.514665 -1.154756 -0.153657
 H  4.175358  0.515577 -0.648502
 H  3.512297 -0.845121 -1.584199
 H  1.155238  0.100381 -1.132834
 H  1.718941  1.348729 -0.206016

Imaginary Frequency:  309i

TS3
 C -0.115424  0.306605 -0.939677
 C  1.094944 -0.093709 -0.146378
 C  1.187049  0.977415  0.970529
 N  0.272746  1.930359  0.655588
 C -0.467751  1.641693 -0.550464
 N  2.381209 -0.056350 -0.984934
 C  3.676695 -0.530222 -0.354800
 C  3.685784 -2.030593 -0.110006
 O  1.948721  0.957001  1.931790
 O -1.261697  2.463482 -1.016211
 H  1.062874 -1.095826  0.289523
 H -0.199353  0.027767 -1.988360
 H  0.110802  2.761140  1.217031
 H  3.802899  0.037984  0.567267
 H  4.458971 -0.240511 -1.061266
 H  4.681285 -2.315207  0.248102
 H  3.488713 -2.591729 -1.031342
 H  2.961113 -2.334070  0.651535
 C -4.459700 -0.308686 -0.367910
 H -3.966742  0.194402 -1.208103
 H -4.947481 -1.212306 -0.753543
 H -5.241734  0.363173  0.016064
 H -3.981532 -1.136171  1.572418
 C -3.462843 -0.650065  0.738286
 H -3.009370  0.264924  1.136664
 S -2.104437 -1.792825  0.213774
 H -1.163538 -0.675034 -0.377538
 H  2.506893  0.902273 -1.332402
 H  2.200799 -0.622167 -1.823123

Imaginary Frequency:  975i

TS4
 C -0.637820  1.080442  0.195321
 C -0.388240 -0.185873  0.972507
 C -1.574041 -0.934724  0.914711
 C -2.462304 -0.332979 -0.033208
 N -1.814050  0.861264 -0.487516
 S  1.237590 -1.035945 -0.510536
 C  2.623568  0.177705 -0.578007
 C  3.754062 -0.078911  0.419496
 O -3.591298 -0.654948 -0.438055
 O  0.018368  2.122715  0.194533
 H  4.215278 -1.061238  0.257358
 H  3.388526 -0.047949  1.453450
 H  4.539873  0.685176  0.317795
 H  3.020097  0.168331 -1.601855
 H  2.191850  1.174371 -0.417946
 H  0.294749 -0.157495  1.811196
 H -1.774216 -1.883905  1.396455
 H -2.287151  1.572885 -1.032007

Imaginary Frequency:  164i

TS7
 C  0.379948 -0.504409 -0.718012
 C -0.846507 -0.039642  0.020930
 C -1.261799 -1.271468  0.838928
 N -0.528818 -2.315683  0.358496
 C  0.434589 -1.922075 -0.640802
 S -2.225529  0.417004 -1.165670
 C -3.460984  1.253938 -0.078691
 C -3.091777  2.681005  0.321088
 O -2.087994 -1.316058  1.751780
 O  1.146872 -2.776862 -1.199054
 H -0.706849  0.821828  0.684241
 H  0.720706 -0.000767 -1.618581
 H -0.598675 -3.263068  0.714480
 H -3.621037  0.621159  0.799565
 H -4.390547  1.246332 -0.660240
 H -3.886254  3.112579  0.945963
 H -2.965540  3.320842 -0.560153
 H -2.161413  2.712921  0.900034
 C  3.956108  1.933207 -0.861391
 H  3.017350  2.045472 -1.416519
 H  4.088681  2.827014 -0.239478
 H  4.778554  1.900808 -1.591506
 H  4.903675  0.565104  0.521597
 C  3.951351  0.664388 -0.011021
 H  3.845429 -0.221981 -0.646778
 S  2.617096  0.611414  1.269047
 H  1.575993  0.040547  0.355895

Imaginary Frequency:  441i
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S8 Cartesian coordinates for the intermediate structures in the proton transfer between ethylamine and ethanethiol

The Cartesian coordinates for the structures of Figure 4 in the main manuscript are given below.

[A-T]

C	-2.981414	-0.210444	-0.157983
H	-4.002643	-0.435284	0.190957
H	-2.852640	-0.717594	-1.122197
C	-2.827893	1.296211	-0.341928
H	-3.583417	1.679402	-1.038836
H	-2.955029	1.825423	0.612247
H	-1.836659	1.545800	-0.739559
H	-2.089731	-1.734022	0.909117
N	-1.951071	-0.734248	0.758959
H	-2.047093	-0.295576	1.676004
S	1.248794	-0.865857	-0.485852
H	-0.022974	-0.746747	0.022300
C	2.003273	0.557919	0.427610
H	1.853890	0.402469	1.500693
H	1.481512	1.475892	0.139143
C	3.491014	0.669153	0.108177
H	3.926269	1.514595	0.656245
H	4.034130	-0.237421	0.401382
H	3.661305	0.839475	-0.961835

[AC-TA]

C	-2.738434	-0.257633	0.125729
H	-3.639616	-0.369781	0.734483
H	-2.716249	-1.059854	-0.616898
C	-2.676983	1.112930	-0.530516
H	-3.546379	1.241333	-1.184583
H	-2.697034	1.913981	0.218700
H	-1.773446	1.223363	-1.139543
H	-1.658005	-1.334082	1.568082
N	-1.553734	-0.476906	1.016035
H	-1.435535	0.295487	1.679505
S	1.062658	-0.928319	-0.561259
H	-0.613908	-0.591617	0.441252
C	1.942801	0.681018	-0.277033
H	1.229597	1.423188	0.108499
H	2.292975	1.061464	-1.244968
C	3.130453	0.577162	0.681111
H	3.627209	1.552858	0.800077
H	2.810378	0.236350	1.674148
H	3.874687	-0.137864	0.308720

TS

C	-2.649977	-0.162946	-0.048340
H	-3.624222	-0.302648	0.435367
H	-2.647683	-0.746580	-0.974936
C	-2.405094	1.312352	-0.339449
H	-3.208828	1.704873	-0.972861
H	-2.389667	1.901664	0.586578
H	-1.455016	1.464714	-0.863520
H	-1.809968	-1.673516	1.110579
N	-1.578570	-0.722174	0.815157
H	-1.467346	-0.169015	1.668146
S	1.077649	-1.037361	-0.487778
H	-0.383567	-0.841812	0.207850
C	1.692941	0.690793	-0.215826
H	0.928398	1.247355	0.341073
H	1.795395	1.180487	-1.191159
C	3.023704	0.754108	0.533143
H	3.353520	1.797663	0.645399
H	2.937789	0.313904	1.534218
H	3.809364	0.210061	-0.005557

Imaginary Frequency: 1030i