

Quantitative First Principles Kinetic Modeling of the Aza-Michael Addition to Acrylates in Polar Aprotic Solvents

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S1 Determination of the experimental concentration profiles using GC

Samples were taken at fixed time intervals and subject to gas chromatography (GC) analysis in a gas chromatograph, equipped with a flame ionization detector and a 5ms capillary column. Samples were taken at fixed time intervals and directly injected into the gas chromatograph. The injector and detector temperature were set at 280 °C. Helium (flow rate: 1.3 mL min⁻¹) was used as a carrier gas and a stepwise temperature program was set as follows: 40 °C during 4 min, followed by a heating ramp of 10 °C min⁻¹ until a temperature of 300 °C was reached, which was maintained for 5 minutes. Decane was used as internal standard and THF was used as a solvent to prepare the samples. Data acquisition and processing was performed with Chrom-Card Trace-Focus GC software.

S1.1 Aza-Michael addition of n-octylamine to ethyl acrylate

Examples of chromatograms for the Aza-Michael addition of n-octylamine to ethyl acrylate can be found in Figure S1. Peak assignment was as follows:

time (min)	molecule
3.8	ethyl acrylate (EAc)
10.7	n-decane (internal standard)
11.5	n-octylamine (OA)
20.5	product P1 (OA-EAc)
25.7	double product P2 (OA-EAc-EAc)

In order to relate the peaks to a concentration, response factors were determined as follows: Firstly, in every chromatogram, all peak areas were standardized using the internal standard. Then, for the reactant molecules EAc and OA, response factors were determined by dividing the starting concentrations by their respective peak areas at time = 0.

Because both P1 and P2 are formed from 1 equivalent of OA, and P1 is formed from 1 equivalent of EAc, while P2 is formed from 2 equivalents of EAc, the following equations are valid:

$$c_{P1} + c_{P2} = c_{OA,0} - c_{OA}$$

$$c_{P1} + 2c_{P2} = c_{EAc,0} - c_{EAc}$$

These expected concentrations for P1 and P2 were then divided by their respective peak areas, at every interval point. The response factors for P1 and P2 were then taken as the respective averages of these values, to account for possible experimental deviations.

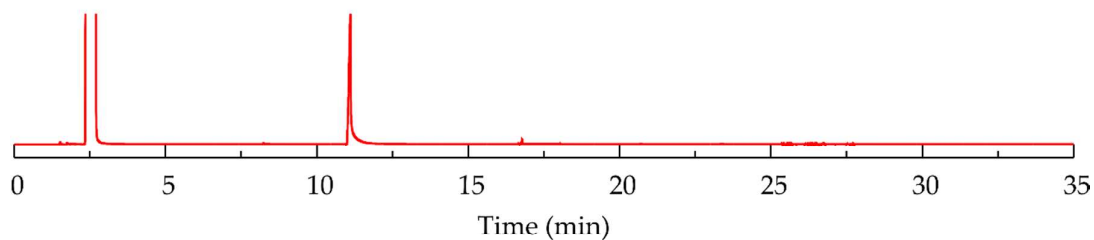
S1.2 Aza-Michael addition of diethylamine to ethyl acrylate

Examples of chromatograms for the Aza-Michael addition of diethylamine to ethyl acrylate can be found in can be found in Figure S2. Peak assignment was as follows:

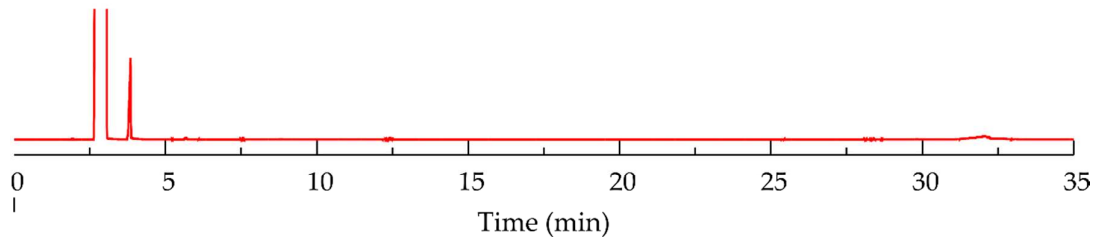
time	molecule
2.0	diethylamine (DEA)
3.8	ethyl acrylate (EAc)
10.7	n-decane (internal standard)
12.8	product P1 (DEA-EAc)

A similar procedure as for octylamine was followed, but now without the double product P2.

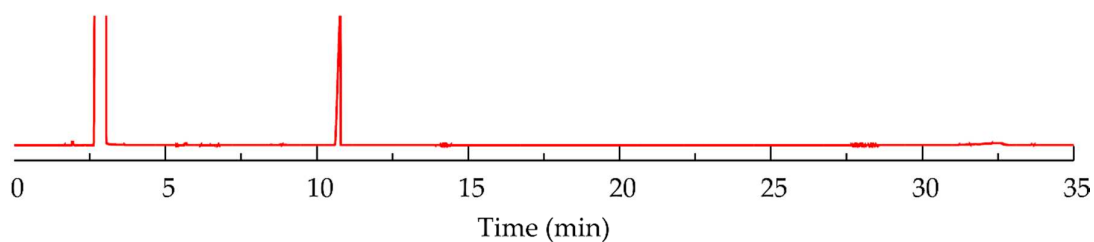
a) Pure octylamine (OA) in THF



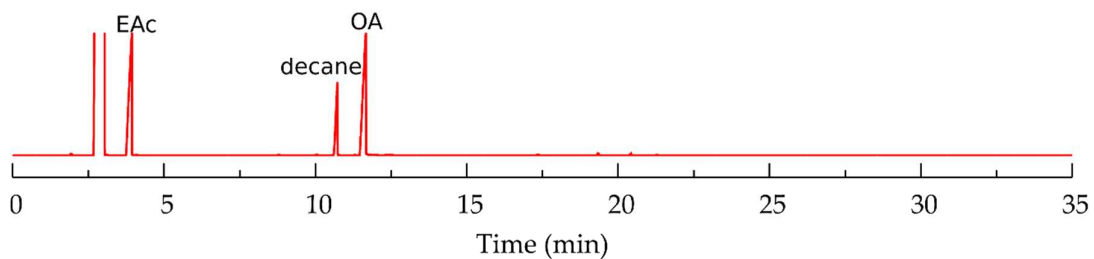
b) Pure ethyl acrylate (EAc) in THF



c) Pure decane in THF



d) Aza-Michael addition of OA to EAc in THF, time = 0



e) Aza-Michael addition of OA to EAc in THF, time = 312 hours

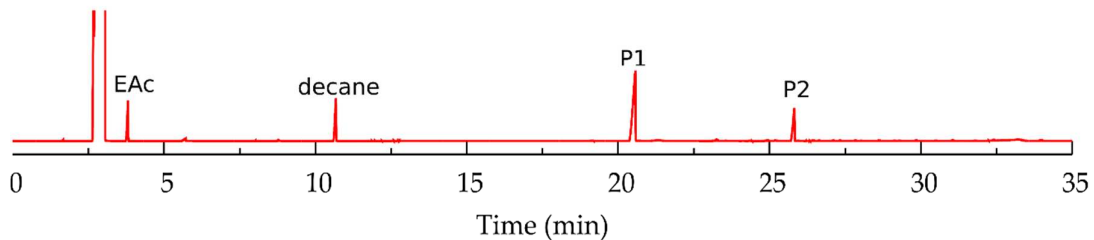
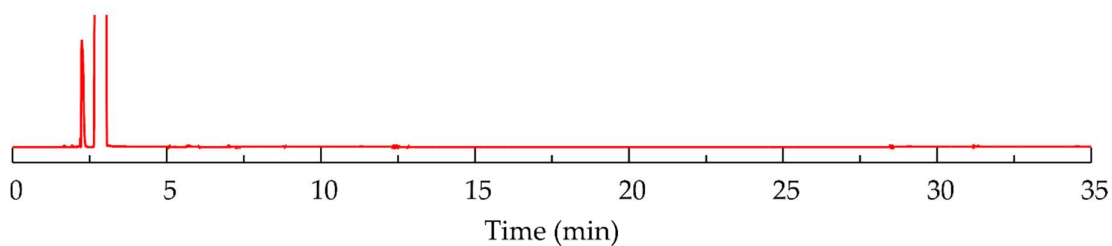
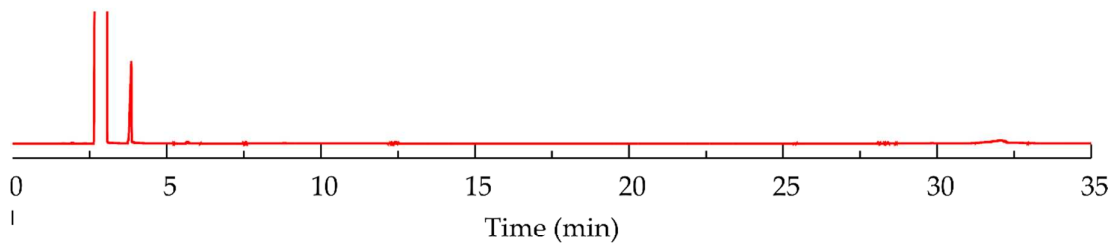


Figure S1. GC chromatograms of a) OA, b) EAc, c) decane, d) the Aza-Michael addition of 1 mol L⁻¹ OA to 2 mol L⁻¹ EAc in THF at the start of the reaction (time=0 hours) and e) the Aza-Michael addition of 1 mol L⁻¹ OA to 2 mol L⁻¹ EAc in THF after 312 hours.

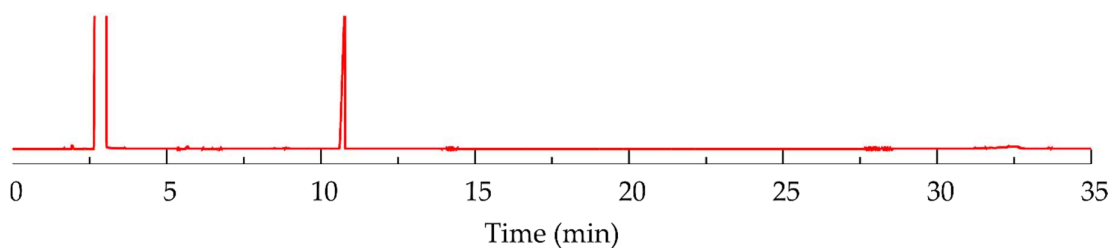
a) Pure diethylamine (DEA) in THF



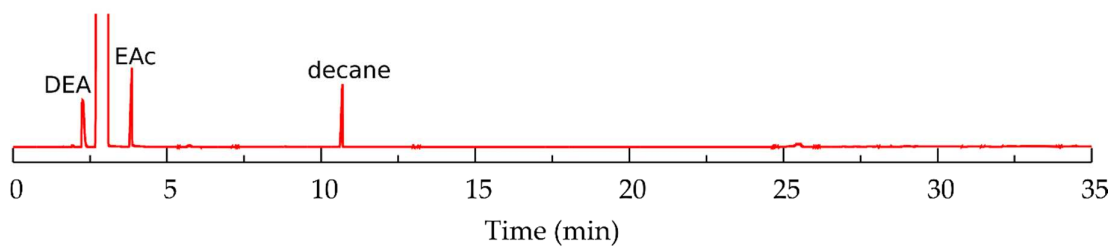
b) Pure ethyl acrylate (EAc) in THF



c) Pure decane in THF



d) Aza-Michael addition of DEA to EAc in THF, time = 0



e) Aza-Michael addition of DEA to EAc in THF, time = 144 hours

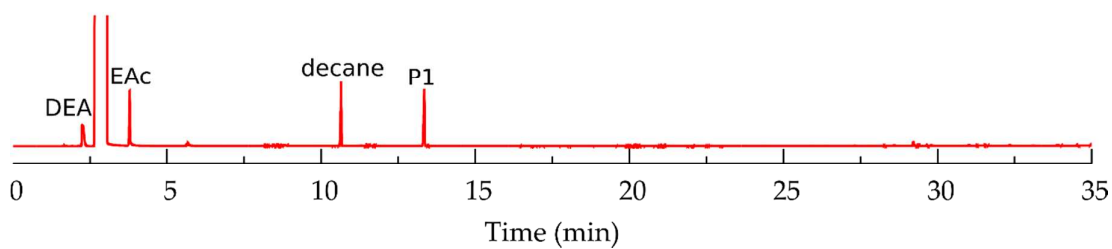


Figure S2. GC chromatograms of a) DEA, b) EAc, c) decane, d) the Aza-Michael addition of 0.5 mol L^{-1} DEA to 1 mol L^{-1} EAc in THF at the start of the reaction (time=0 hours) and e) the Aza-Michael addition of 0.5 mol L^{-1} DEA to 1 mol L^{-1} EAc in THF after 144 hours.

S2 Details on the ONIOM-type calculations

ONIOM-type energy calculations were performed on the B3LYP/6-31G(d,p)//SMD(THF) optimized geometries as follows:

A core was defined including the reaction core and principal substituents, as large as computationally feasible, in which hydrogen atoms were used as so-called link atoms. Energy calculations were done at the CBS-QB3 level of theory, resulting in $E^{\text{core,high}}$ and at the M06-2X/6-311+G(2d,d,p) level of theory, resulting in $E^{\text{core,low}}$. The full molecule/transition structure was then calculated at the M06-2X/6-311+G(2d,d,p) level of theory, resulting in $E^{\text{full,low}}$. This results in the following expression for the electronic energy:

$$E^{\text{ONIOM}} = E^{\text{core,high}} - E^{\text{core,low}} + E^{\text{full,low}}$$

For every molecule the partitioning in the high and the low level is indicated below.

S2.1 *Aza Michael addition with a secondary amine*

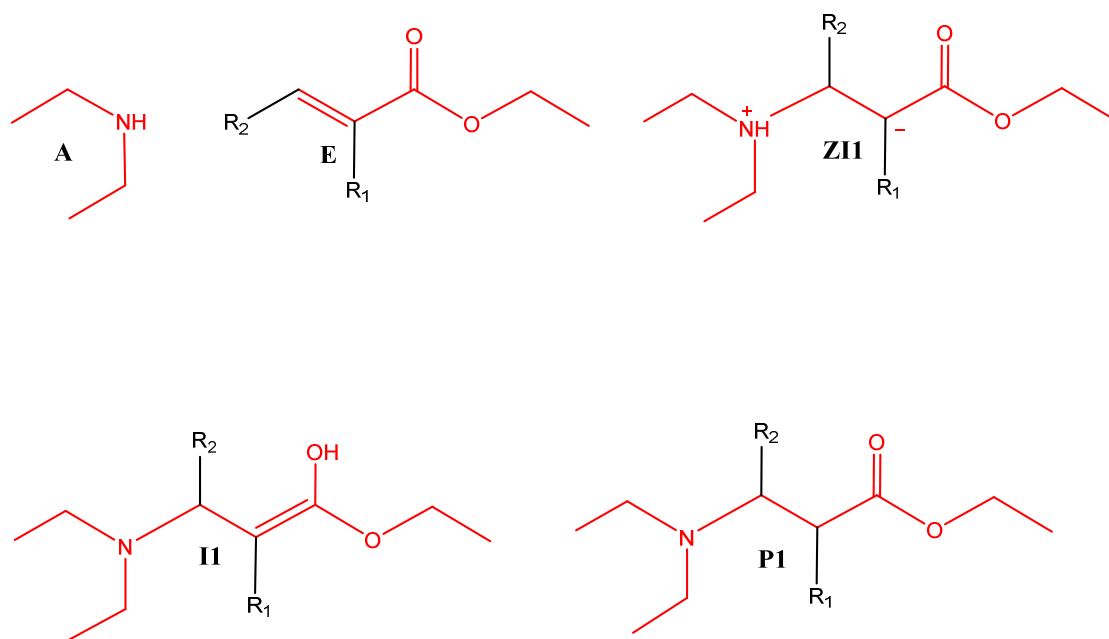


Figure S3. Indication of the ONIOM high level (red) and low level (black) in the reactants, intermediates and products of the aza Michael addition with a secondary amine to an ene.

The transition state structures were partitioned similarly. Assisting diethylamine molecules were calculated at the high level of theory.

S2.2 *Aza Michael addition with a primary amine*

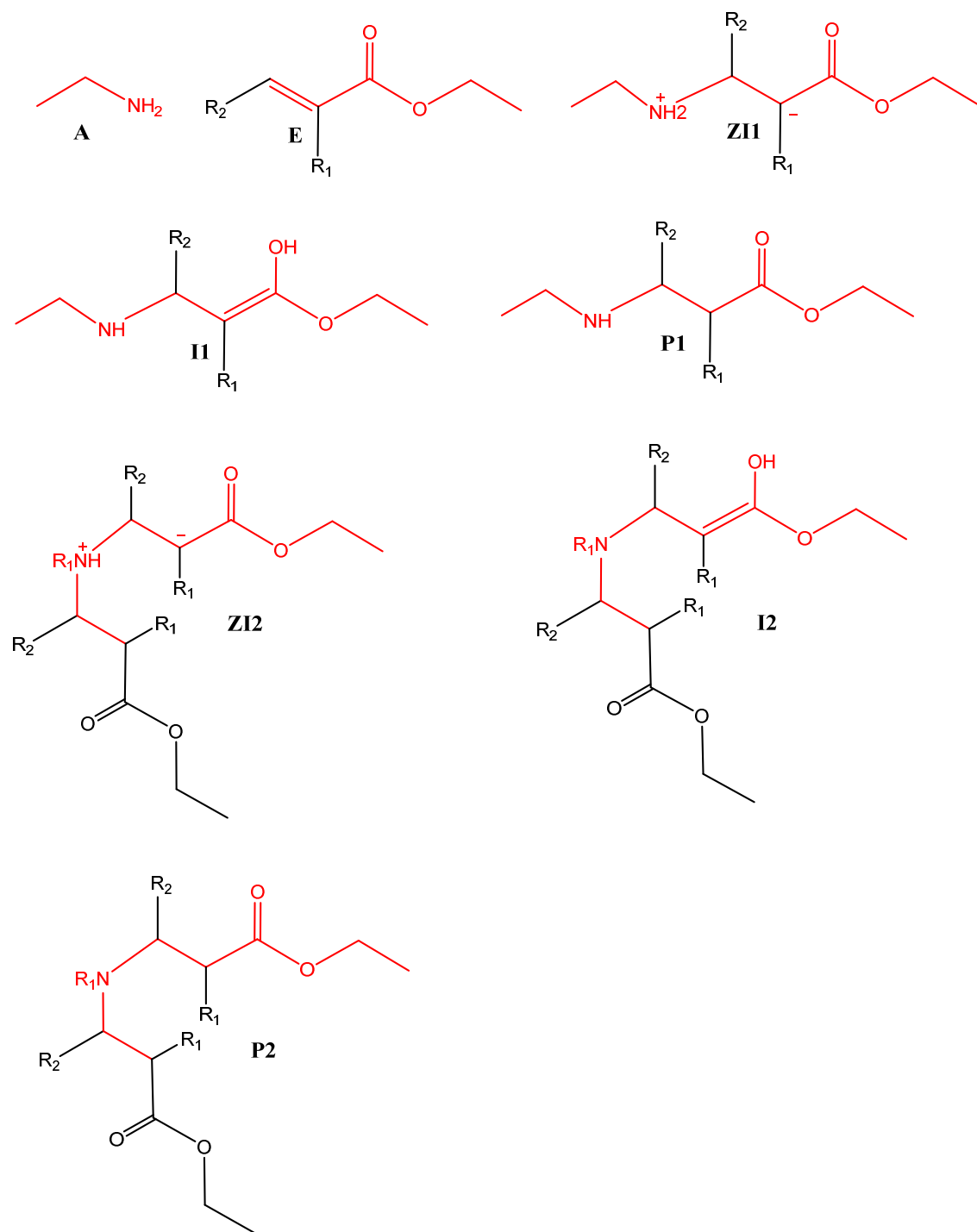


Figure S4. Indication of the ONIOM high level (red) and low level (black) in the reactants, intermediates and products of the aza Michael addition with a primary amine to an ene.

The transition state structures were partitioned similarly. Assisting ethylamine molecules were calculated at the high level of theory, assisting **P1** molecules were partitioned as shown in Figure S5.

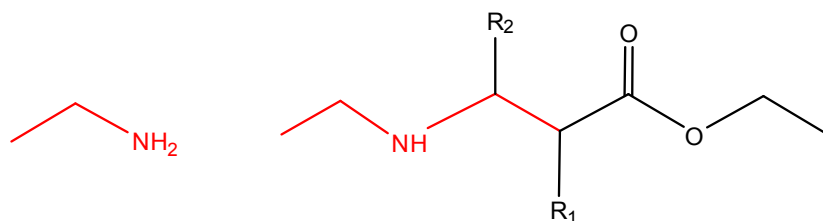


Figure S5. Indication of the ONIOM high level (red) and low level (black) for the assisting primary or secondary amine in the assisted transition states TS5 to TS10 and TS15 to TS20.

S3 Competition with aminolysis side reaction

A possible competition reaction with the Aza-Michael addition is the aminolysis of the ester group. In order for this reaction to occur, the first step is the nucleophilic attack of the amine on the carbonyl carbon of the ester group. This has been simulated by scanning this reaction coordinate at steps of 0.1 Å, both for diethylamine and for ethylamine with ethyl acrylate (cf. Figure S6 and Figure S7, respectively). Upon comparison with a similar scan of the reaction coordinate corresponding to the nucleophilic attack of the amine to the acrylate group, i.e. the first step of the aza-Michael addition, it is clear that the Aza-Michael addition is much more favored.

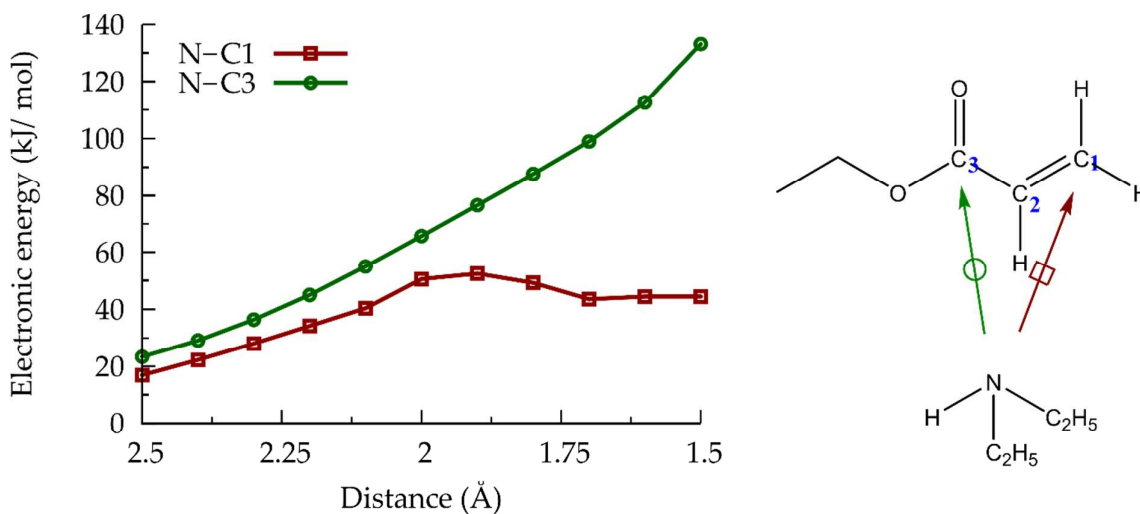


Figure S6. Electronic energy calculated at the B3LYP/6-31G(d)/SMD(THF) level of theory as a function of the distance between the amine nitrogen (N) of diethylamine and either the secondary carbon of the acrylate group (C1, dark red line) or the carbonyl carbon (C3, dark green line) of ethyl acrylate.

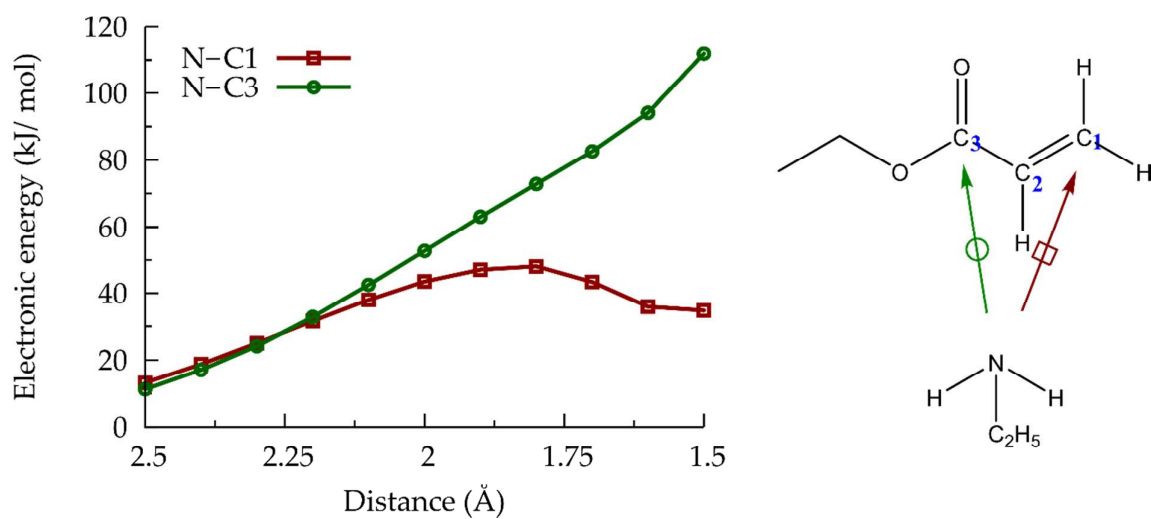


Figure S7. Electronic energy calculated at the B3LYP/6-31G(d)/SMD(THF) level of theory as a function of the distance between the amine nitrogen (N) of ethylamine and either the secondary carbon of the acrylate group (C1, dark red line) or the carbonyl carbon (C3, dark green line) of ethyl acrylate.

S4 Aza-Michael addition of secondary amines to ethyl acrylate

S4.1 Full reaction mechanism

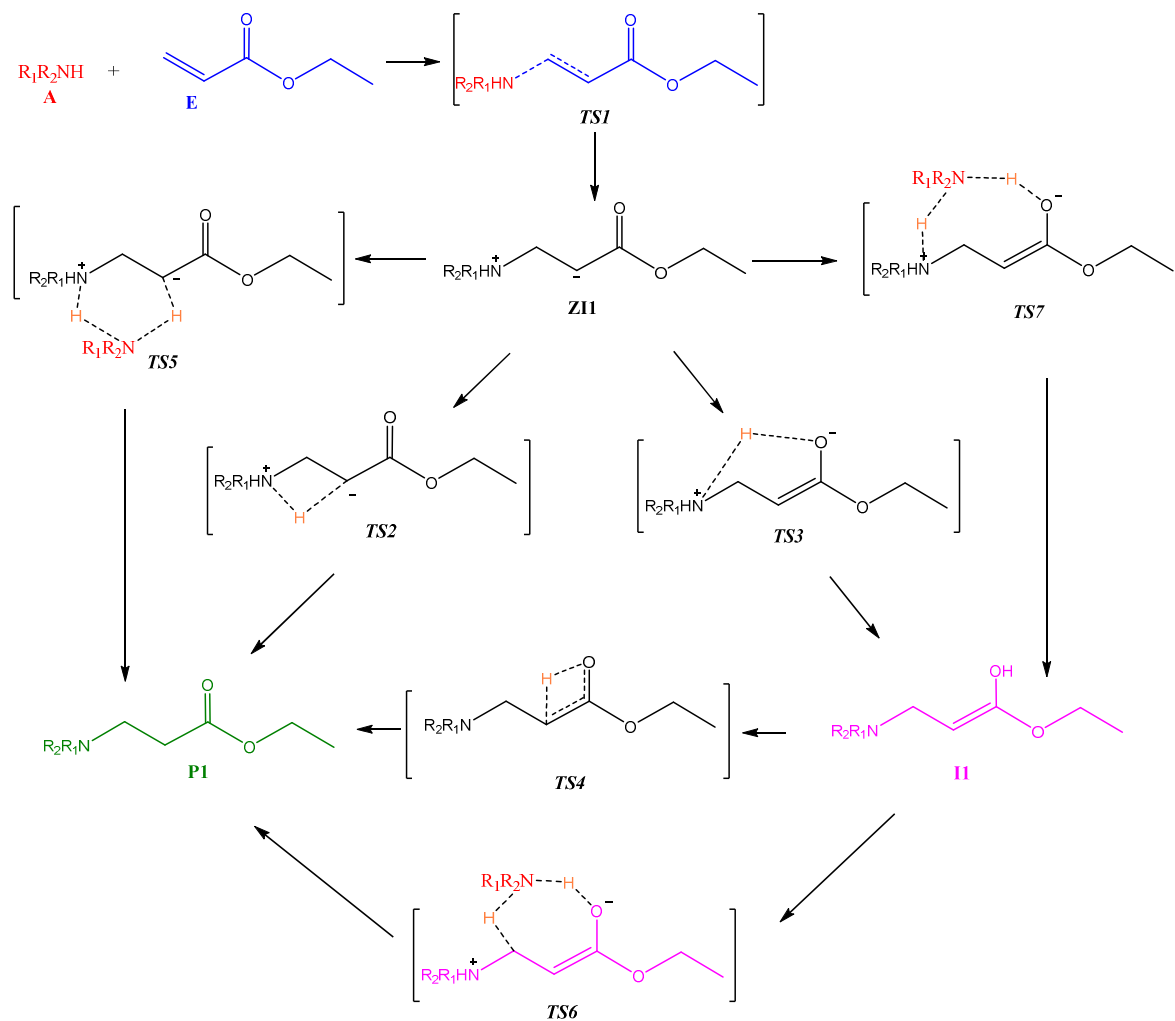


Figure S8. Reaction network for the aza Michael addition of a secondary amine to ethyl acrylate in an aprotic solvent with representation of the transition states.

S4.2 Data in gas phase

Table S1. Standard reaction enthalpy, entropy and Gibbs free energy ($\Delta_r H^\circ$, $\Delta_r S^\circ$, $\Delta_r G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}); standard activation enthalpy, entropy and Gibbs free energy ($\Delta^\ddagger H^\circ$, $\Delta^\ddagger S^\circ$, $\Delta^\ddagger G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}) at 298.15 K in gas phase (reference = 1 mol L^{-1}) for all elementary reactions in the reaction network of the aza Michael addition of diethylamine to ethyl acrylate, as shown in Scheme 1 in the main manuscript.

Reaction	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r G^\circ$	$\Delta^\ddagger H^\circ$	$\Delta^\ddagger S^\circ$	$\Delta^\ddagger G^\circ$	k_+	k_-
R1	42.0	-153.2	87.7	67.1	-219.2	110.7	5.0E-07	1.2E+09
R2	-117.6	6.4	-118.9	78.5	-12.5	81.0	8.0E-02	1.2E-22
R3	-31.5	-14.2	-28.6	-19.8	-25.1	-14.8	4.9E+15	4.7E+10
R4	-86.1	20.6	-90.2	221.7	15.9	218.6	6.2E-26	9.8E-42
R5	-117.6	6.4	-118.9	7.2	-231.0	53.1	6.2E+03	9.1E-18
R6	-86.1	20.6	-90.2	48.2	-198.7	87.7	5.4E-03	8.4E-19
R7	-31.5	-14.2	-28.6	-20.6	-243.2	27.7	1.7E+08	1.7E+03

S4.3 Transition states

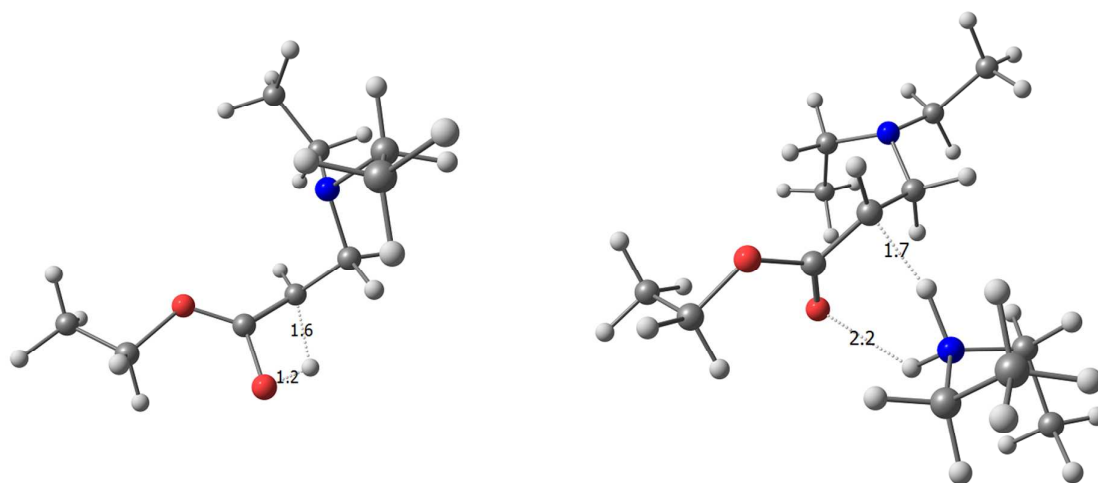


Figure S9. Transition states for the keto-enol tautomerization between the enolic intermediate (I1) and the keto-product (P1). Left: unassisted (reaction 4), Right: amine assisted (reaction 6).

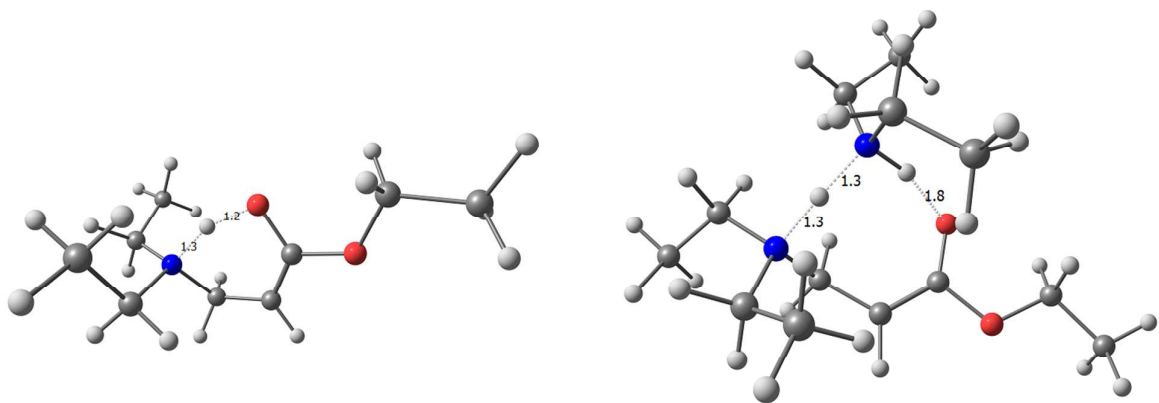


Figure S10. Transition states for the proton transfer from the zwitterionic intermediate (ZI) to the enolic intermediate (II). Left: unassisted (reaction 3), Right: amine assisted (reaction 7).

S4.4 H-bond stabilization in zwitterionic intermediate

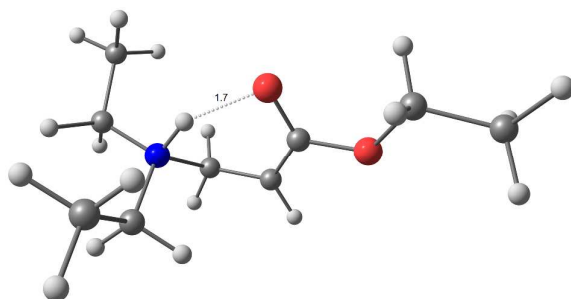


Figure S11. Hydrogen bond in the zwitterionic intermediate (ZI) of the aza-Michael addition of diethylamine to ethyl acrylate.

S4.5 Aza Michael addition of diethylamine to ethyl crotonate and ethyl methacrylate

Table S2. Standard reaction enthalpy, entropy and Gibbs free energy ($\Delta_r H^\circ$, $\Delta_r S^\circ$, $\Delta_r G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}); standard activation enthalpy, entropy and Gibbs free energy ($\Delta^\ddagger H^\circ$, $\Delta^\ddagger S^\circ$, $\Delta^\ddagger G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}) and forward and reverse rate coefficients (in $\text{L mol}^{-1} \text{s}^{-1}$ or s^{-1}) at 298.15 K in THF for the contributing elementary reactions in the aza-Michael addition of diethylamine to ethyl crotonate (ECR) and ethyl methacrylate (EmAc).

Reaction	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r G^\circ$	$\Delta^\ddagger H^\circ$	$\Delta^\ddagger S^\circ$	$\Delta^\ddagger G^\circ$	k_+	k_-
ECR-R1	34.6	-128.2	72.8	49.5	-131.3	88.7	1.8E-03	1.0E+10
ECR-R3	-4.6	-11.9	-1.0	2.4	-27.5	10.7	8.4E+10	5.6E+10
ECR-R5	-97.1	7.2	-99.3	20.8	-136.4	43.1	1.8E+05	7.1E-13
ECR-R6	-92.5	19.1	-98.3	35.1	-104.9	51.2	6.6E+03	4.0E-14
EmAc-R1	39.5	-101.1	69.6	60.6	-94.5	88.8	1.7E-03	2.7E+09
EmAc-R3	-16.2	-4.4	-14.9	-9.8	-16.9	-4.7	4.2E+13	1.0E+11
EmAc-R5	-100.4	6.6	-102.4	11.0	-103.8	41.9	2.8E+05	3.2E-13
EmAc-R6	-84.2	11.1	-87.5	18.8	-81.2	43.0	1.8E+05	8.4E-11

S5 Aza-Michael addition of primary amines

S5.1 Validation of the use of ethylamine as a model compound for larger primary amines

The influence of the length of the alkyl chain of the amine was checked via comparison of the same model reactions, as shown in Figure S12, for different primary amines with an increasing chain length.

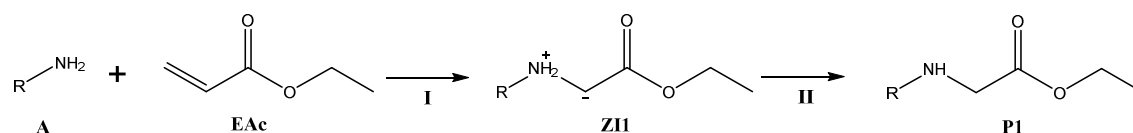


Figure S12. Reaction of a primary amine (A) with ethyl acrylate (EAc) towards the zwitterionic intermediate ZI1 (I) followed by reaction of the latter towards the product P1 (II). R = ethyl, butyl or octyl.

Standard reaction energies at 0 K were calculated using a M06-2X/6-311+G(d,p) single point energy calculation on B3LYP/6-31G(d)/SMD(THF) optimized geometries and are shown in Table S3. Corrections according to an ONIOM-based scheme such as in the main manuscript were not taken into account here, as only a relative comparison is desired. As is immediately apparent, effects of the length of the alkyl chain on the reaction energies is found not to be significant. Note that standard reaction energies were calculated, since these give the best reflection of possible electronic effects.

Table S3. Standard reaction energies, $\Delta_r E$, at 0 K in kJ mol^{-1} in gas phase and in THF for the reaction of a primary amine (ethyl-, butyl- or octylamine) and ethyl acrylate towards the zwitterionic intermediate ZI1 (I) and for the reaction of the zwitterionic intermediate towards the product P1, according to Figure S12.

R =	in gas phase		in THF	
	$\Delta_r E(\text{I})$	$\Delta_r E(\text{II})$	$\Delta_r E(\text{I})$	$\Delta_r E(\text{II})$
ethyl	54.7	-135.8	11.3	-98.7
butyl	53.4	-135.4	11.1	-99.2
octyl	54.0	-135.2	12.0	-99.3

S5.2 Data in gas phase

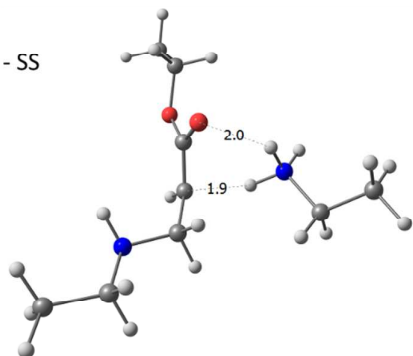
Table S4. Standard reaction enthalpy, entropy and Gibbs free energy ($\Delta_r H^\circ$, $\Delta_r S^\circ$, $\Delta_r G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}); standard activation enthalpy, entropy and Gibbs free energy ($\Delta^\ddagger H^\circ$, $\Delta^\ddagger S^\circ$, $\Delta^\ddagger G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}) and forward and reverse rate coefficients (in $\text{L mol}^{-1} \text{s}^{-1}$ or s^{-1}) at 298.15 K in gas phase (reference = 1 mol L^{-1}) for all elementary reactions in the reaction network of the aza-Michael addition of ethylamine to ethyl acrylate, as shown in Scheme 1 in the main manuscript ($R_1 = \text{C}_3\text{H}_5$, $R_2 = \text{H}$). Values for different diastereomeric transition states are shown if applicable.

Reaction	diastereomer	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r G^\circ$	$\Delta^\ddagger H^\circ$	$\Delta^\ddagger S^\circ$	$\Delta^\ddagger G^\circ$
R1	-	59.7	-154.9	105.9	80.2	-140.5	126.9
R2	-	-137.2	6.9	-139.3	58.8	5.7	64.2
R3	-	-41.5	-1.6	-41.1	-22.7	-10.2	-19.2
R4	-	-95.7	8.5	-98.2	210.7	2.7	213.0
R5	RRS	-137.2	6.9	-139.3	-14.7	-131.9	31.8
	RSS				-21.5	-131.8	24.9
R6	RR	-95.7	8.5	-98.2	49.9	-127.0	88.9
	RS				47.4	-123.1	85.3
R7		-41.5	-1.6	-41.1	-41.8	-133.8	0.2
R8	RRS	-137.2	6.9	-139.3	-24.0	-141.1	24.0
	RSS				-24.0	-137.5	23.0
R9	-	-95.7	8.5	-98.2	46.2	-132.5	86.9
R10	-	-41.5	-1.6	-41.1	-40.5	-141.0	2.0
R11	-	52.8	-158.3	100.0	67.7	-148.0	118.1
R12	-	-127.6	1.3	-128.0	67.4	-5.9	77.9
R13	-	-38.6	-16.9	-33.5	-26.8	-24.5	-19.2
R14	-	-89.0	18.3	-94.5	215.8	-15.0	223.7
R15	RRR	-127.6	1.3	-128.0	-2.8	-139.0	51.9
	RRS				4.2	-129.3	55.9
	RSR				-1.9	-138.1	52.4
	RSS				6.9	-131.4	59.2
TS16	RR	-89.0	18.3	-94.5	50.3	-118.0	90.4
	RS				48.1	-117.2	87.9
R17	-	-38.6	-16.9	-33.5	-29.5	-135.6	13.9
R18	RRR	-127.6	1.3	-128.0	-7.2	-154.7	51.5
	RRS				-2.1	-158.7	57.7
	RSR				1.5	-153.2	59.7
	RSS				0.5	-196.0	71.5
R19	-	-89.0	18.3	-94.5	9.0	-138.0	66.2
R20	-	-38.6	-16.9	-33.5	-8.4	-179.1	42.0

S5.3 Representations of the different diastereomers of the transition states

TS6

a: RR - SS



b: RS - SR

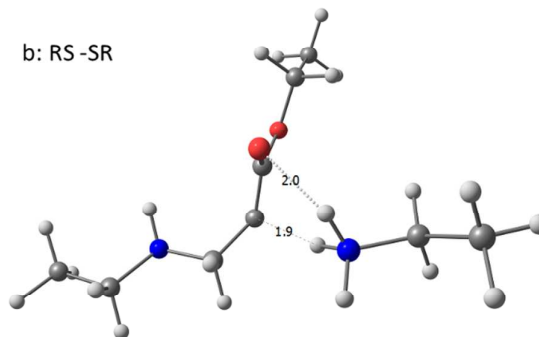
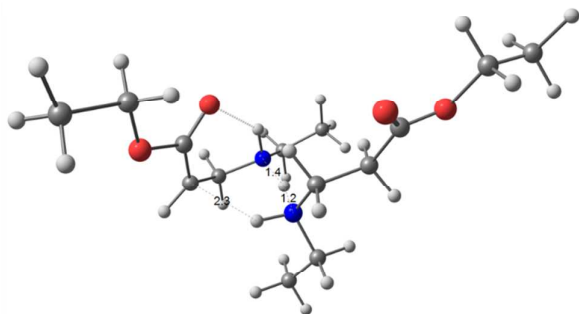


Figure S13. RR – SS and RS – SR diastereomers of TS6.

TS8

a: RRS - SSR



b: RSS - SRR

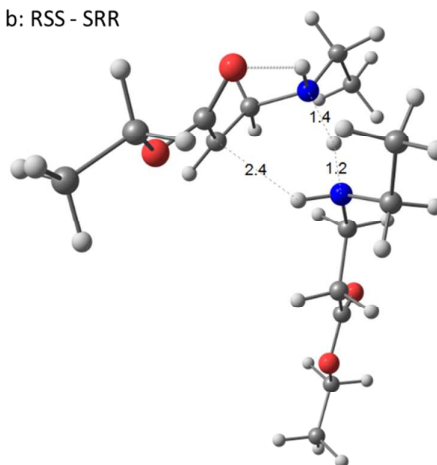
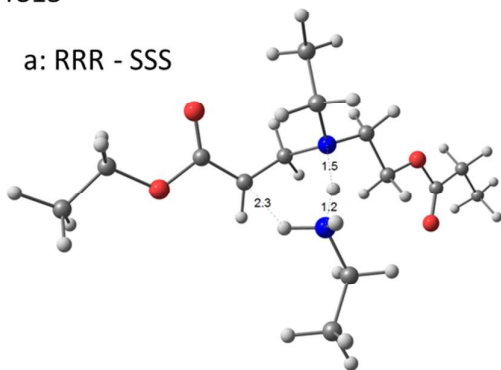


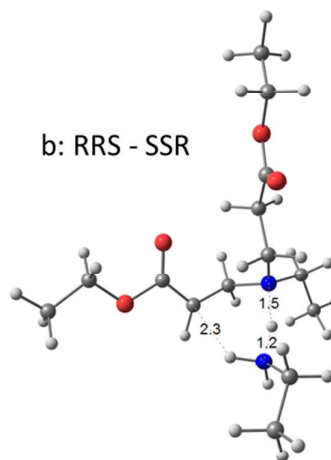
Figure S14. RRS – SSR and RSS – SSR diastereomers of TS8. Diastereomers RRR – SSS and RSR – SRS are not included as they do not have a stabilizing H-bridge and will thus be significantly higher in energy.

TS15

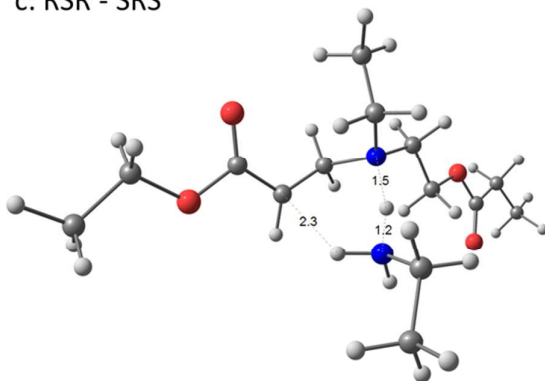
a: RRR - SSS



b: RRS - SSR



c: RSR - SRS



d: RSS - SRR

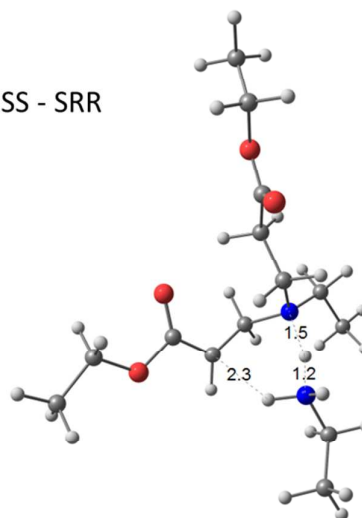
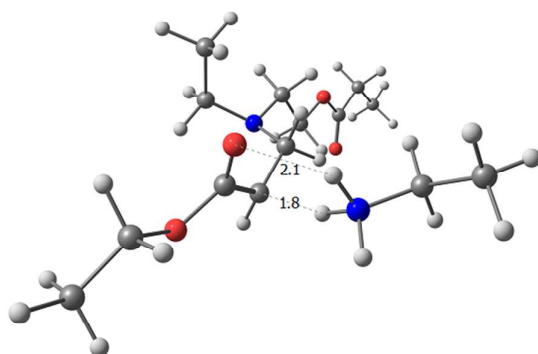


Figure S15. RRR – SSS, RRS – SSR, RSR -SRS and RSS – SSR diastereomers of TS15.

TS16

a: RR - SS



b: RS - SR

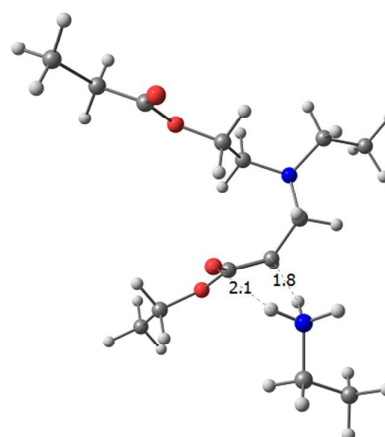
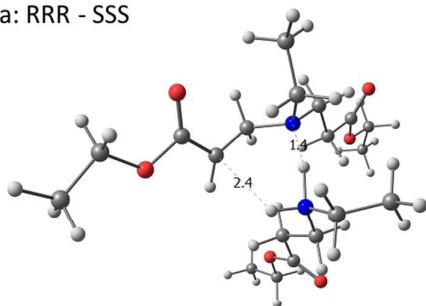


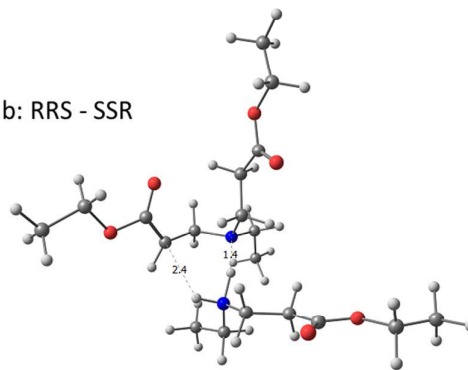
Figure S16. RR – SS and RS – SR diastereomers of TS16.

TS18

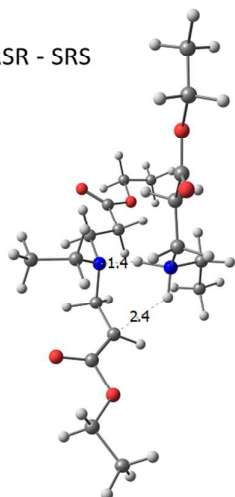
a: RRR - SSS



b: RRS - SSR



c: RSR - SRS



d: RSS - SRR

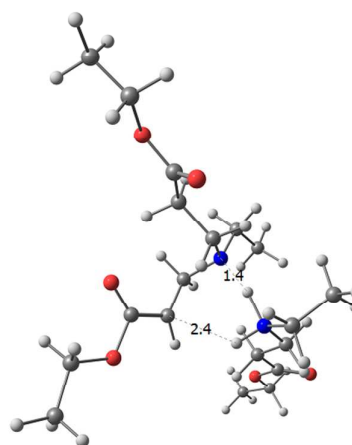


Figure S17. RRR – SSS, RRS – SSR, RSR -SRS and RSS – SSR diastereomers of TS18.

S5.4 *Thermodynamic affinities*

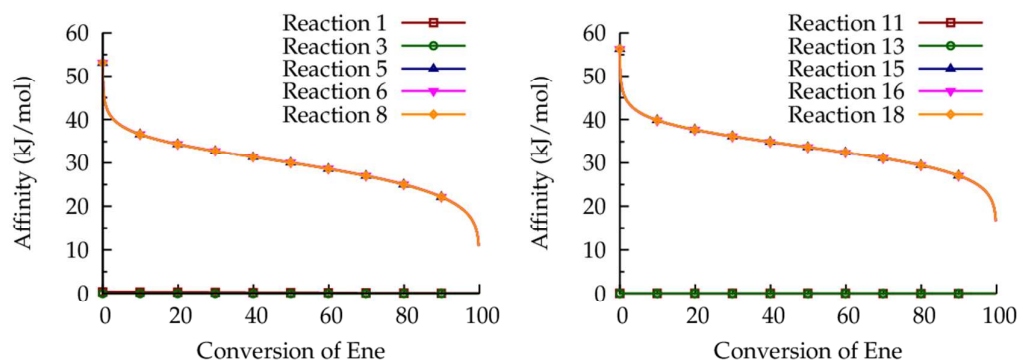


Figure S18. Thermodynamic affinities as a function of the conversion for the contribution elementary steps in the aza Michael addition of n-octylamine to ethyl acrylate. Left: The elementary reactions leading to the single substituted product P1. Right: The elementary reactions leading to the double substituted product P2. $c_{0, \text{amine}} = 1.0 \text{ mol L}^{-1}$, $c_{0, \text{ene}} = 1 \text{ mol L}^{-1}$

S5.5 *Aza Michael addition of ethylamine to ethyl crotonate and ethyl methacrylate*

Table S5. Standard reaction enthalpy, entropy and Gibbs free energy ($\Delta_r H^\circ$, $\Delta_r S^\circ$, $\Delta_r G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}); standard activation enthalpy, entropy and Gibbs free energy ($\Delta^\ddagger H^\circ$, $\Delta^\ddagger S^\circ$, $\Delta^\ddagger G^\circ$, in respectively kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$, kJ mol^{-1}) and forward and reverse rate coefficients (in $\text{L mol}^{-1} \text{s}^{-1}$ or s^{-1}) at 298.15 K in THF for the contributing elementary reactions in the aza-Michael addition of ethylamine to ethyl crotonate (ECR) and ethyl methacrylate (EmAc).

Reaction	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r G^\circ$	$\Delta^\ddagger H^\circ$	$\Delta^\ddagger S^\circ$	$\Delta^\ddagger G^\circ$	k+	k-
ECR-R1	21.4	-186.0	69.4	45.9	-181.2	90.5	8.6E-04	1.3E+09
ECR-R3	4.5	-2.0	-4.3	-2.6	-9.7	-3.7	2.7E+13	4.7E+12
ECR-R5	-85.7	7.7	-96.0	-1.3	-165.2	32.1	1.5E+07	2.3E-10
ECR-R6	-90.2	9.7	-91.6	-6.0	-158.5	40.8	4.4E+05	3.9E-11
ECR-R8	-85.7	7.7	-96.0	11.9	-183.1	50.0	1.1E+04	1.7E-13
ECR-R11	53.0	-199.0	95.0	60.6	-204.2	104.1	3.6E-06	1.6E+11
ECR-R13	-15.7	-9.4	-3.4	-7.8	-16.7	-3.0	2.1E+13	5.3E+12
ECR-R15	-96.3	-1.4	-97.5	-10.9	-173.9	34.0	6.7E+06	5.6E-11
ECR-R16	-80.6	8.0	-94.1	3.4	-153.6	48.4	2.0E+04	6.6E-13
ECR-R18	-96.3	-1.4	-97.5	38.7	-210.2	86.1	5.0E-03	4.1E-20
EmAc-R1	30.1	-177.7	77.6	49.8	-170.8	95.5	1.2E-04	4.6E+09
EmAc-R3	-5.8	-6.0	-13.2	-7.1	-11.3	-6.8	9.5E+13	4.7E+11
EmAc-R5	-93.4	1.2	-104.7	-5.3	-166.7	28.4	6.6E+07	2.9E-11
EmAc-R6	-87.6	7.2	-91.6	1.4	-156.6	47.0	3.7E+04	3.3E-12
EmAc-R8	-93.4	1.2	-104.7	-63.8	-177.7	50.1	1.0E+04	4.6E-15
EmAc-R11	39.1	-199.6	83.4	64.1	-183.4	104.5	3.0E-06	1.3E+09
EmAc-R13	184.5	-0.2	-18.3	-11.0	-9.0	-9.0	2.4E+14	1.5E+11
EmAc-R15	-99.2	12.2	-104.6	0.1	-157.1	40.4	5.3E+05	2.4E-13
EmAc-R16	-283.8	12.4	-86.4	-14.5	-156.0	30.5	2.8E+07	2.1E-08
EmAc-R18	-99.2	12.2	-104.6	18.5	-171.8	54.7	1.6E+03	7.6E-16

S5.6 *Relative contributions*

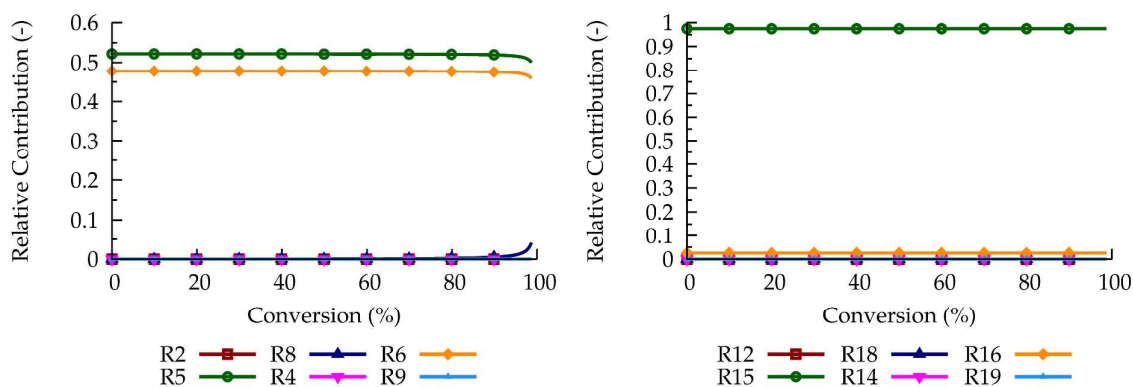


Figure S19. Relative contributions to the formation of the single substituted product P1 (left) and of the double substituted product P2 (right) as a function of the conversion for the aza-Michael addition of n-octylamine to ethyl crotonate in THF at 298.15 K. The numbers of the reactions correspond to Scheme 1. $c_{0, \text{amine}} = 1.0 \text{ mol L}^{-1}$, $c_{0, \text{enc}} = 1 \text{ mol L}^{-1}$

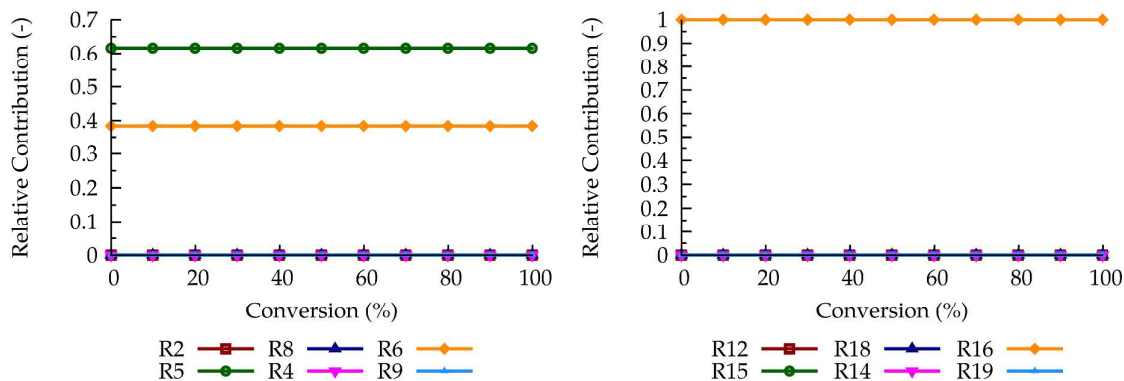


Figure S20. Relative contributions to the formation of the single substituted product P1 (left) and of the double substituted product P2 (right) as a function of the conversion for the aza-Michael addition of n-octylamine to ethyl methacrylate in THF at 298.15 K. The numbers of the reactions correspond to Scheme 1. $c_{0, \text{amine}} = 1.0 \text{ mol L}^{-1}$, $c_{0, \text{enc}} = 1 \text{ mol L}^{-1}$

S6 Ordinary differential equations

S6.1 Aza-Michael addition of a secondary amine to an acrylate

$y(1)=c_{\text{amine}}$, $y(2)=c_{\text{ene}}$, $y(3)=c_{\text{ZII}}$, $y(4)=c_{\text{PI}}$, $y(5)=c_{\text{II}}$

$$\begin{aligned}
 dy(1)/dt &= \\
 &\quad - k(1) * y(1) * y(2) \\
 &\quad + kr(1) * y(3) \\
 dy(2)/dt &= \\
 &\quad - k(1) * y(1) * y(2) \\
 &\quad + kr(1) * y(3) \\
 dy(3)/dt &= \\
 &\quad - k(2) * y(3) \\
 &\quad - k(3) * y(3) \\
 &\quad - k(5) * y(1) * y(3) \\
 &\quad - k(7) * y(1) * y(3) \\
 &\quad + kr(2) * y(4) \\
 &\quad + kr(3) * y(5) \\
 &\quad + kr(5) * y(1) * y(4) \\
 &\quad + kr(7) * y(1) * y(5) \\
 &\quad + k(1) * y(1) * y(2) \\
 &\quad - kr(1) * y(3) \\
 dy(4)/dt &= \\
 &\quad + k(2) * y(3) \\
 &\quad + k(4) * y(5) \\
 &\quad + k(5) * y(1) * y(3) \\
 &\quad + k(6) * y(1) * y(5) \\
 &\quad - kr(2) * y(4) \\
 &\quad - kr(4) * y(4) \\
 &\quad - kr(5) * y(1) * y(4) \\
 &\quad - kr(6) * y(1) * y(4) \\
 dy(5)/dt &= \\
 &\quad - k(4) * y(5) \\
 &\quad - k(6) * y(1) * y(5) \\
 &\quad + kr(4) * y(4) \\
 &\quad + kr(6) * y(1) * y(4) \\
 &\quad + k(3) * y(3) \\
 &\quad + k(7) * y(1) * y(3) \\
 &\quad - kr(3) * y(5) \\
 &\quad - kr(7) * y(1) * y(5)
 \end{aligned}$$

S6.2 Aza-Michael addition of a primary amine to an acrylate

$y(1)=c_{\text{amine}}$, $y(2)=c_{\text{ene}}$, $y(3)=c_{\text{ZII}}$, $y(4)=c_{\text{PI}}$, $y(5)=c_{\text{II}}$, $y(6)=c_{\text{ZI2}}$, $y(7)=c_{\text{P2}}$, $y(8)=c_{\text{I2}}$

$$\begin{aligned}
 dy(1)/dt &= \\
 &\quad - k(1) * y(1) * y(2) \\
 &\quad + kr(1) * y(3) \\
 dy(2)/dt &= \\
 &\quad - k(1) * y(1) * y(2) \\
 &\quad - k(11) * y(2) * y(4) \\
 &\quad + kr(1) * y(3) \\
 &\quad + kr(11) * y(6) \\
 dy(3)/dt &= \\
 &\quad - k(2) * y(3) \\
 &\quad - k(3) * y(3) \\
 &\quad - k(5) * y(1) * y(3)
 \end{aligned}$$

```

-      k( 7)*y( 1)*y( 3)
-      k( 8)*y( 3)*y( 4)
-      k(10)*y( 3)*y( 4)
+      kr( 2)*y( 4)
+      kr( 3)*y( 5)
+      kr( 5)*y( 1)*y( 4)
+      kr( 7)*y( 1)*y( 5)
+      kr( 8)*y( 4)*y( 4)
+      kr(10)*y( 4)*y( 5)
+      k( 1)*y( 1)*y( 2)
-      kr( 1)*y( 3)
dy(4)/dt=
-      k(11)*y( 2)*y( 4)
+      kr(11)*y( 6)
+      k( 2)*y( 3)
+      k( 4)*y( 5)
+      k( 5)*y( 1)*y( 3)
+      k( 6)*y( 1)*y( 5)
-      kr( 2)*y( 4)
-      kr( 4)*y( 4)
-      kr( 5)*y( 1)*y( 4)
-      kr( 6)*y( 1)*y( 4)
+      k( 8)*y( 3)*y( 4)
-      kr( 8)*y( 4)*y( 4)
+      k( 9)*y( 4)*y( 5)
-      kr( 9)*y( 4)*y( 4)
dy(5)/dt=
-      k( 4)*y( 5)
-      k( 6)*y( 1)*y( 5)
-      k( 9)*y( 4)*y( 5)
+      kr( 4)*y( 4)
+      kr( 6)*y( 1)*y( 4)
+      kr( 9)*y( 4)*y( 4)
+      k( 3)*y( 3)
+      k( 7)*y( 1)*y( 3)
+      k(10)*y( 3)*y( 4)
-      kr( 3)*y( 5)
-      kr( 7)*y( 1)*y( 5)
-      kr(10)*y( 4)*y( 5)
dy(6)/dt=
-      k(12)*y( 6)
-      k(13)*y( 6)
-      k(15)*y( 1)*y( 6)
-      k(17)*y( 1)*y( 6)
-      k(18)*y( 4)*y( 6)
-      k(20)*y( 4)*y( 6)
+      kr(12)*y( 7)
+      kr(13)*y( 8)
+      kr(15)*y( 1)*y( 7)
+      kr(17)*y( 1)*y( 8)
+      kr(18)*y( 4)*y( 7)
+      kr(20)*y( 4)*y( 8)
+      k(11)*y( 2)*y( 4)
-      kr(11)*y( 6)
dy(7)/dt=
+      k(12)*y( 6)
+      k(14)*y( 8)
+      k(15)*y( 1)*y( 6)
+      k(16)*y( 1)*y( 8)
+      k(18)*y( 4)*y( 6)
+      k(19)*y( 4)*y( 8)

```

```

-      kr(12)*y( 7)
-      kr(14)*y( 7)
-      kr(15)*y( 1)*y( 7)
-      kr(16)*y( 1)*y( 7)
-      kr(18)*y( 4)*y( 7)
-      kr(19)*y( 4)*y( 7)
dy(8)/dt=
-      k(14)*y( 8)
-      k(16)*y( 1)*y( 8)
-      k(19)*y( 4)*y( 8)
+      kr(14)*y( 7)
+      kr(16)*y( 1)*y( 7)
+      kr(19)*y( 4)*y( 7)
+      k(13)*y( 6)
+      k(17)*y( 1)*y( 6)
+      k(20)*y( 4)*y( 6)
-      kr(13)*y( 8)
-      kr(17)*y( 1)*y( 8)
-      kr(20)*y( 4)*y( 8)

```

S7 Cartesian coordinates of the optimized geometries

S7.1 *Diethylamine to ethyl acrylate*

DEA

C	-0.010049	0.518041	1.222687
H	-0.896593	1.166851	1.232358
H	0.867804	1.192925	1.249949
C	-0.010049	-0.369669	2.463751
H	-0.005095	0.236283	3.377330
H	-0.896092	-1.014726	2.482121
H	0.877942	-1.014836	2.488515
N	-0.057805	-0.286009	-0.000000
H	0.749895	-0.911396	0.000000
C	-0.010049	0.518041	-1.222687
H	-0.896593	1.166851	-1.232358
H	0.867804	1.192925	-1.249949
C	-0.010049	-0.369669	-2.463751
H	-0.896092	-1.014726	-2.482121
H	0.877942	-1.014836	-2.488515
H	-0.005095	0.236283	-3.377330

EAc

O	0.202989	-0.686927	0.000000
O	-1.103668	1.163326	0.000000
C	0.000000	0.646507	0.000000
C	1.295050	1.372823	0.000000
H	2.196994	0.767468	0.000000
C	1.338894	2.707248	0.000000
H	0.425539	3.296426	0.000000
H	2.282814	3.244931	0.000000
C	-0.982635	-1.519689	0.000000
H	-1.581320	-1.280547	0.884959
H	-1.581320	-1.280547	-0.884959
C	-0.529430	-2.965475	0.000000
H	0.068895	-3.192416	0.889047
H	0.068895	-3.192416	-0.889047
H	-1.406338	-3.622574	0.000000

ZI1-DEA-EAc

C	4.686363	0.206126	-0.319002
C	3.231724	0.022119	-0.715311
O	2.481082	-0.192835	0.482476
C	1.122097	-0.415750	0.325404
C	0.382240	-0.445239	1.496176
C	-1.069829	-0.742537	1.396252
N	-1.716002	0.070604	0.246195
C	-3.017274	-0.511420	-0.227244
C	-2.828548	-1.685360	-1.180665
O	0.649703	-0.544804	-0.851744
H	4.807103	1.065913	0.350127
H	5.301401	0.376744	-1.210548
H	5.067336	-0.683491	0.195605
H	2.856064	0.908649	-1.244157
H	3.115045	-0.830070	-1.395021
H	0.823712	-0.197103	2.453531
H	-1.622864	-0.495146	2.307601
H	-1.314685	-1.779544	1.128212
H	-0.969707	-0.060738	-0.493682
H	-3.580932	-0.800909	0.665454
H	-3.570751	0.286274	-0.727184

H	-2.284279	-1.379851	-2.080717
H	-2.289405	-2.518003	-0.719253
H	-3.813172	-2.052927	-1.489653
C	-1.812843	1.531393	0.573733
H	-2.728496	1.673788	1.156840
H	-0.952165	1.751040	1.209657
H	-0.859219	2.255446	-1.234357
C	-1.786602	2.408454	-0.671385
H	-2.634503	2.219232	-1.338991
H	-1.828714	3.460867	-0.370430

P1-DEA-EAc

C	3.880242	1.227113	-0.680184
C	3.026969	-0.024230	-0.660586
O	2.041392	0.132640	0.392038
C	1.179232	-0.887862	0.559584
C	0.198521	-0.623386	1.684708
C	-1.248477	-0.813914	1.208797
N	-1.615251	0.132088	0.148633
C	-2.683495	-0.396560	-0.714502
C	-2.172606	-1.388179	-1.759535
O	1.204548	-1.904868	-0.107461
C	-1.945788	1.463630	0.680577
C	-1.681043	2.582442	-0.326786
H	0.407016	-1.346804	2.483896
H	-1.929109	-0.745517	2.077112
H	3.621620	-0.920358	-0.456200
H	2.504267	-0.175423	-1.610324
H	4.398119	1.367501	0.274920
H	3.271891	2.115893	-0.880150
H	4.635081	1.143955	-1.470359
H	-2.995627	1.504054	1.028268
H	-1.324879	1.642370	1.564480
H	-2.282775	2.471444	-1.236251
H	-1.923430	3.557932	0.112321
H	-0.625098	2.586981	-0.620471
H	-1.338458	-1.829071	0.814136
H	0.363786	0.375902	2.094923
H	-3.488107	-0.860212	-0.112001
H	-3.142216	0.449341	-1.236426
H	-1.704108	-2.267605	-1.304679
H	-1.427902	-0.911836	-2.407262
H	-3.002158	-1.739658	-2.385421

I1-DEA-EAc

C	4.701873	0.246413	-0.213377
C	3.248931	0.243287	-0.648129
O	2.506199	-0.499390	0.341167
C	1.155020	-0.484100	0.260211
C	0.389429	-0.720530	1.348405
C	-1.110807	-0.861938	1.252336
N	-1.703379	0.041896	0.224932
C	-3.022860	-0.443098	-0.231275
C	-2.928810	-1.581773	-1.245560
O	0.663604	-0.233515	-0.969161
C	-1.762170	1.431956	0.729584
C	-1.868761	2.478371	-0.377321
H	-1.573611	-0.671837	2.235020
H	3.131825	-0.229179	-1.629257

H	2.855540	1.264731	-0.715944
H	5.089973	-0.775143	-0.134650
H	4.820732	0.737696	0.758594
H	5.306715	0.787149	-0.950171
H	-2.597631	1.539562	1.442769
H	-0.838085	1.602196	1.290860
H	-2.793909	2.386665	-0.957157
H	-1.855709	3.483361	0.060749
H	-1.023336	2.400453	-1.070501
H	-1.397035	-1.885149	0.975154
H	0.875912	-0.865678	2.306085
H	-3.633175	-0.749617	0.635604
H	-3.544107	0.396568	-0.699269
H	-2.416929	-2.461723	-0.840916
H	-2.389263	-1.259476	-2.143753
H	-3.934960	-1.895430	-1.548270
H	-0.328785	-0.086710	-0.814770

TS1-DEA-EAc

C	4.829343	0.620818	-0.424954
C	3.587635	-0.237199	-0.592421
O	2.632895	0.179128	0.389082
C	1.389766	-0.430757	0.325279
C	0.494568	0.041567	1.319227
C	-0.810833	-0.513272	1.381659
N	-1.913963	0.114542	0.132634
C	-3.164556	-0.691051	0.028570
C	-2.991201	-1.913380	-0.865463
O	1.153970	-1.289698	-0.541144
C	-2.124381	1.570058	0.330178
C	-2.566511	2.306340	-0.930332
H	0.776317	0.887567	1.937113
H	-1.407339	-0.274306	2.263393
H	3.824478	-1.300501	-0.458225
H	3.163953	-0.126996	-1.597962
H	5.255844	0.506602	0.578233
H	4.598134	1.681013	-0.579637
H	5.591539	0.325968	-1.155919
H	-2.855925	1.682330	1.137363
H	-1.165825	1.966639	0.681015
H	-3.532143	1.952069	-1.307732
H	-2.668200	3.375281	-0.710702
H	-1.822454	2.198101	-1.728678
H	-0.895912	-1.563064	1.102470
H	-3.438377	-0.982895	1.049115
H	-3.968344	-0.057291	-0.358166
H	-2.190205	-2.571526	-0.514136
H	-2.763134	-1.617264	-1.896319
H	-3.921457	-2.491293	-0.879653
H	-1.341113	-0.026408	-0.703965

Imaginary Frequency: 167i

TS2-DEA-EAc

C	-4.728140	-0.842942	-0.706154
C	-3.649652	0.148243	-0.309460
O	-2.472550	-0.598814	0.035905
C	-1.392394	0.139600	0.462324
C	-0.223364	-0.680478	0.656987
C	0.968849	-0.055956	1.347525
N	1.970540	-0.081027	0.178677

C	2.556664	1.240802	-0.175649
C	1.550384	2.155240	-0.870580
O	-1.474694	1.366077	0.584143
C	2.967828	-1.178296	0.303695
C	3.591843	-1.586001	-1.027306
H	-0.415129	-1.735863	0.843244
H	1.385271	-0.602839	2.197441
H	-3.965266	0.756808	0.545423
H	-3.420409	0.836923	-1.131804
H	-4.964798	-1.519693	0.122685
H	-4.413369	-1.447893	-1.564035
H	-5.643586	-0.306888	-0.982752
H	3.736812	-0.878850	1.027987
H	2.433046	-2.033996	0.727592
H	4.212383	-0.798536	-1.466396
H	4.234567	-2.458926	-0.867678
H	2.818829	-1.862347	-1.753107
H	0.787413	0.981118	1.632656
H	2.940176	1.699941	0.744628
H	3.410879	1.068110	-0.834036
H	0.632532	2.281593	-0.288106
H	1.274057	1.750874	-1.851416
H	2.002701	3.141269	-1.026475
H	0.885948	-0.482988	-0.375266

Imaginary Frequency: 1632i

TS3-DEA-EAc

C	4.637405	0.169003	-0.331009
C	3.164254	0.148714	-0.696527
O	2.443208	-0.319481	0.453119
C	1.082159	-0.395204	0.353027
C	0.354974	-0.649904	1.480670
C	-1.135394	-0.822950	1.363569
N	-1.667802	0.036262	0.238870
C	-2.914288	-0.511899	-0.362972
C	-2.657867	-1.675803	-1.316411
O	0.547872	-0.191287	-0.829608
C	-1.820085	1.454224	0.676983
C	-1.772416	2.445120	-0.481858
H	-1.658349	-0.553496	2.290792
H	2.980782	-0.513808	-1.549966
H	2.815288	1.150461	-0.976342
H	4.987198	-0.832158	-0.055087
H	4.825510	0.843371	0.512019
H	5.228311	0.515208	-1.186918
H	-2.756630	1.545895	1.243199
H	-0.992103	1.652991	1.362511
H	-2.597419	2.307026	-1.189368
H	-1.841689	3.466195	-0.090164
H	-0.828344	2.354592	-1.029551
H	-1.434704	-1.852165	1.121585
H	0.838478	-0.753216	2.444145
H	-3.591293	-0.809492	0.449315
H	-3.400309	0.300221	-0.909117
H	-2.179042	-2.525680	-0.819327
H	-2.021615	-1.368332	-2.153398
H	-3.612483	-2.025042	-1.725782
H	-0.648072	-0.038065	-0.511549

Imaginary Frequency: 1031i

TS4-DEA-EAc

C	-3.930844	1.459437	0.825345
C	-3.258398	0.124250	0.598584
O	-1.997158	0.379282	-0.110200
C	-1.363147	-0.630592	-0.637406
C	-0.261506	-0.592056	-1.561467
C	1.097852	-0.976845	-0.974419
N	1.710184	0.037898	-0.083830
C	2.737174	-0.570303	0.777714
C	2.149974	-1.304287	1.984424
O	-1.748787	-1.858732	-0.452099
C	2.247179	1.171641	-0.849231
C	2.386657	2.448208	-0.018811
H	1.781812	-1.219703	-1.809420
H	-3.860767	-0.549336	-0.016684
H	-3.014649	-0.378077	1.538071
H	-4.160038	1.953502	-0.124566
H	-3.299877	2.122894	1.425820
H	-4.870491	1.298638	1.365432
H	3.218641	0.916450	-1.317277
H	1.555169	1.376287	-1.672474
H	3.096237	2.335328	0.808941
H	2.746817	3.271720	-0.647811
H	1.417791	2.736809	0.404641
H	0.995418	-1.895413	-0.389042
H	-0.222430	0.299105	-2.192421
H	3.389680	-1.254082	0.199967
H	3.387442	0.228579	1.148052
H	1.508431	-2.143917	1.693099
H	1.549112	-0.619401	2.593993
H	2.954129	-1.708668	2.611515
H	-1.005798	-1.977116	-1.403026

Imaginary Frequency: 1952i

TS5-DEA-EAc

C	-5.333817	-1.450071	0.152033
C	-4.425137	-0.236000	0.263869
O	-3.193827	-0.555753	-0.373476
C	-2.212357	0.459799	-0.356626
C	-1.019411	0.049481	-0.963701
C	0.070283	1.022259	-1.249995
N	1.197332	1.098624	-0.205573
C	0.712160	1.674766	1.081976
C	0.322249	3.154159	1.073913
O	-2.490265	1.555633	0.175758
C	2.380200	1.837791	-0.717458
C	3.259996	1.024221	-1.664845
H	-1.020211	-0.900737	-1.491531
H	0.583413	0.767915	-2.183236
H	-4.888714	0.640352	-0.208904
H	-4.256918	0.028128	1.317192
H	-5.519866	-1.705719	-0.897755
H	-4.884880	-2.323578	0.639706
H	-6.299937	-1.249939	0.631300
H	2.979404	2.144661	0.147362
H	2.049288	2.758376	-1.218512
H	3.664452	0.132956	-1.172161
H	4.108745	1.638335	-1.988270
H	2.724959	0.708002	-2.565947

H	-0.313751	2.045600	-1.358588
H	1.504392	1.504915	1.821934
H	-0.159705	1.084113	1.373134
H	1.141855	3.807727	0.755248
H	-0.551204	3.324616	0.440488
H	0.047844	3.447359	2.094818
H	1.452351	-0.259179	0.106098
H	0.374185	-1.586708	0.202475
N	1.370421	-1.451029	0.429161
C	2.196168	-2.387607	-0.384006
H	3.227806	-2.025635	-0.366294
H	2.181100	-3.369613	0.104465
C	1.692100	-2.510261	-1.816560
H	0.672444	-2.910265	-1.846169
H	1.701041	-1.549111	-2.339260
H	2.339427	-3.199736	-2.369450
C	1.537814	-1.618256	1.902643
H	1.303072	-2.658038	2.160310
H	0.785274	-0.981075	2.374385
C	2.934268	-1.249963	2.389705
H	3.201952	-0.225559	2.107016
H	2.963542	-1.314536	3.482818
H	3.700016	-1.927749	1.998261

Imaginary Frequency: 948i

TS6-DEA-EAc

C	0.337066	4.433849	0.211020
C	-0.784259	3.553774	-0.323645
O	-0.281615	2.366299	-0.951588
C	-0.076845	1.259803	-0.134798
C	0.234597	0.077447	-0.859850
C	1.090956	-0.988018	-0.213751
N	2.549654	-0.856693	-0.459853
C	3.288411	-2.059781	-0.059049
C	3.221597	-3.176709	-1.105562
O	-0.297632	1.345411	1.093538
C	3.143622	0.382570	0.053206
C	3.146651	0.588131	1.578020
H	0.412577	0.222393	-1.926254
H	0.873991	-1.015848	0.870515
H	-1.473913	3.282556	0.481214
H	-1.343980	4.077621	-1.106797
H	0.880599	3.919388	1.009611
H	1.045630	4.690046	-0.585350
H	-0.072641	5.367449	0.617369
H	2.614655	1.220460	-0.414400
H	4.177683	0.421038	-0.315590
H	2.127805	0.672079	1.969902
H	3.674510	1.517900	1.827793
H	3.657812	-0.229927	2.100960
H	0.821532	-1.978725	-0.602349
H	2.946269	-2.454204	0.917561
H	4.340216	-1.780284	0.077403
H	2.198432	-3.536060	-1.264542
H	3.606260	-2.823051	-2.069334
H	3.825176	-4.036291	-0.787238
H	-1.314148	-0.548631	-0.371583
H	-2.015882	-0.090726	1.051447
N	-2.230208	-0.731341	0.275939
C	-3.436806	-0.227640	-0.449451

H	-4.286321	-0.229707	0.238852
H	-3.212172	0.812589	-0.701325
C	-3.735653	-1.025103	-1.711552
H	-2.863379	-1.057881	-2.373784
H	-4.046748	-2.051611	-1.492614
H	-4.553727	-0.539394	-2.253844
C	-2.266979	-2.130777	0.794155
H	-1.275545	-2.315742	1.215992
H	-2.393515	-2.797548	-0.061990
C	-3.346655	-2.356750	1.844900
H	-4.355745	-2.249868	1.433728
H	-3.255487	-3.373301	2.242756
H	-3.236299	-1.656936	2.681835

Imaginary Frequency: 189i

TS7-DEA-EAc

C	-4.719927	-0.871728	-1.036865
C	-3.945706	-0.676123	0.261367
O	-2.766070	-1.476256	0.315859
C	-1.606791	-0.940129	-0.266017
C	-0.517922	-1.794352	-0.192592
C	0.764088	-1.496807	-0.874218
N	1.844372	-0.745716	-0.064570
C	3.040240	-0.456097	-0.916624
C	3.874633	-1.657191	-1.368183
O	-1.667657	0.219532	-0.778482
C	2.244838	-1.477079	1.177527
C	1.446760	-1.127131	2.430399
H	-0.649385	-2.760293	0.285068
H	1.243660	-2.420863	-1.220125
H	-3.690019	0.379676	0.392394
H	-4.551953	-0.996402	1.117567
H	-4.127066	-0.524294	-1.888859
H	-4.964760	-1.929443	-1.191312
H	-5.659060	-0.303458	-1.014208
H	3.300156	-1.253675	1.364136
H	2.177134	-2.554715	0.981831
H	1.591277	-0.080637	2.718011
H	1.802334	-1.749464	3.261352
H	0.379739	-1.312456	2.292433
H	0.603137	-0.850769	-1.746279
H	3.671636	0.237823	-0.349336
H	2.677493	0.079795	-1.798640
H	4.278494	-2.225083	-0.523786
H	3.305929	-2.342737	-2.003627
H	4.725053	-1.292316	-1.956014
H	1.274180	0.441074	0.129270
H	-0.344715	1.194463	-0.164862
N	0.599422	1.568512	0.087546
C	0.567696	2.277464	1.397004
H	1.475808	2.010997	1.951213
H	0.609038	3.358205	1.225414
C	-0.677460	1.941473	2.211010
H	-1.583121	2.282342	1.697497
H	-0.771695	0.864976	2.383908
H	-0.630607	2.439886	3.186006
C	1.062616	2.414568	-1.045139
H	1.254561	1.747274	-1.890452
H	2.019781	2.866548	-0.761419
C	0.056488	3.483041	-1.471513

H	-0.156997	4.198824	-0.669948
H	0.453764	4.047721	-2.323086
H	-0.887850	3.021771	-1.780935

Imaginary Frequency: 1170i

S7.2 Diethylamine to ethyl crotonate

ECR

O	1.099311	-0.399075	0.000026
O	0.053124	1.609624	-0.000008
C	0.002155	0.390482	-0.000003
C	-1.230567	-0.425611	-0.000023
C	-2.442222	0.147261	0.000058
C	2.378307	0.279673	-0.000050
H	2.437585	0.921884	-0.884845
H	2.437605	0.922036	0.884629
C	3.462392	-0.779413	0.000034
H	3.393420	-1.415729	-0.888883
H	3.393617	-1.415413	0.889193
H	4.445761	-0.296112	-0.000165
H	-2.489162	1.236131	0.000162
H	-1.109163	-1.505637	-0.000125
C	-3.743377	-0.585898	-0.000015
H	-4.342071	-0.309420	0.878876
H	-4.342029	-0.309288	-0.878901
H	-3.605169	-1.671809	-0.000099

ZI1-DEA-ECR

C	4.802857	-0.242322	-0.198959
C	3.433470	-0.530015	0.392169
O	2.568009	0.547672	0.026323
C	1.222761	0.385894	0.319149
C	0.390392	1.393629	-0.139911
C	-1.063258	1.327091	0.166381
N	-1.571369	-0.143851	-0.107304
C	-2.841209	-0.496546	0.614983
C	-2.603540	-0.891432	2.068229
O	0.846434	-0.661641	0.939928
C	-1.600557	-0.504837	-1.562171
C	-1.348403	-1.991181	-1.787386
H	0.769556	2.195164	-0.763185
H	3.492182	-0.614259	1.485725
H	3.034673	-1.480366	0.018055
H	5.201699	0.708360	0.173288
H	4.754434	-0.187707	-1.292694
H	5.505650	-1.038652	0.073726
H	-2.567356	-0.191226	-1.966187
H	-0.811217	0.084233	-2.034779
H	-2.119773	-2.622002	-1.331658
H	-1.342782	-2.197651	-2.863242
H	-0.374481	-2.285085	-1.380703
H	-1.286395	1.413734	1.239317
H	-3.515632	0.360727	0.538578
H	-3.303059	-1.327397	0.076883
H	-2.138939	-0.088753	2.648679
H	-1.966233	-1.779335	2.139235
H	-3.566318	-1.128212	2.534207
H	-0.765081	-0.664735	0.338672
C	-1.896985	2.356738	-0.588468

H	-2.969477	2.264404	-0.386808	H	2.283946	2.888577	0.253018
H	-1.586156	3.354569	-0.260329	H	1.251741	3.542712	-1.023925
H	-1.734429	2.300790	-1.669757	H	0.523045	2.705618	0.359583
P1-DEA-ECR				H	-0.937998	-1.376137	-1.934123
C	-4.077436	1.064835	-0.169775	H	3.554108	-0.600810	-0.379480
C	-3.187228	0.008073	0.452107	H	3.447065	1.063788	0.145922
O	-2.089762	-0.239258	-0.462951	H	2.658716	-1.309685	1.926041
C	-1.157571	-1.120935	-0.051490	H	2.561539	0.404034	2.364092
C	-0.057764	-1.309774	-1.075332	H	4.136628	-0.341138	2.033263
C	1.327390	-1.018269	-0.462428	H	0.227788	0.284508	0.839174
N	1.380443	0.368478	0.046098	C	1.446550	-2.344130	-0.269212
C	2.318561	0.530779	1.166327	H	1.026241	-2.410872	0.739916
C	1.740214	0.065671	2.503807	H	1.024565	-3.167403	-0.855924
O	-1.214387	-1.707859	1.012776	H	2.528771	-2.503554	-0.215276
C	1.537402	1.402773	-0.986794	TS1-DEA-ECR			
C	0.858747	2.717858	-0.597779	C	-4.905925	-0.528683	0.304657
H	-0.089412	-2.356734	-1.402561	C	-3.531238	-0.733575	-0.306078
H	-3.725725	-0.930842	0.617741	O	-2.699495	0.351662	0.123436
H	-2.776983	0.335164	1.412531	C	-1.400458	0.345991	-0.340683
H	-4.473049	0.731132	-1.135247	C	-0.593416	1.375207	0.186827
H	-3.530616	2.001721	-0.322572	C	0.743193	1.498884	-0.301281
H	-4.924153	1.267365	0.495936	N	1.641735	-0.034056	0.027104
H	2.600652	1.588895	-1.223883	C	2.883557	-0.172032	-0.782234
H	1.077477	1.041100	-1.911873	C	2.984836	-1.503048	-1.525369
H	1.283695	3.146274	0.317592	O	-1.019548	-0.539441	-1.140803
H	0.976848	3.461267	-1.396060	C	1.767435	-0.302365	1.477212
H	-0.211931	2.557690	-0.428072	C	2.000780	-1.767655	1.836184
H	1.410292	-1.661199	0.419104	H	-0.931753	1.956254	1.038626
H	-0.247910	-0.684932	-1.952130	H	-3.584313	-0.753192	-1.400981
H	3.275801	0.012668	0.973203	H	-3.095047	-1.688271	0.014231
H	2.563237	1.594813	1.247207	H	-5.345399	0.418921	-0.026986
H	1.474365	-0.996807	2.492963	H	-4.852875	-0.517350	1.399427
H	0.835253	0.632445	2.750144	H	-5.576518	-1.341895	0.002923
H	2.472823	0.216269	3.306851	H	2.580114	0.324378	1.857747
C	2.455036	-1.408978	-1.434861	H	0.829165	0.047518	1.922235
H	3.439216	-1.181525	-1.009240	H	2.969326	-2.134111	1.480345
H	2.425052	-2.485350	-1.642327	H	1.983519	-1.880081	2.926678
H	2.371048	-0.884023	-2.393291	H	1.213015	-2.407529	1.421539
I1-DEA-ECR				H	0.853424	1.375688	-1.382866
C	-4.821285	0.188482	0.228926	H	2.888470	0.646560	-1.512020
C	-3.359621	0.484068	0.503097	H	3.739251	-0.021671	-0.117948
O	-2.583775	-0.557314	-0.127522	H	2.130440	-1.639111	-2.198570
C	-1.234420	-0.448367	-0.076099	H	3.022836	-2.356856	-0.841979
C	-0.457758	-0.935448	-1.067551	H	3.895924	-1.515386	-2.134684
C	1.054054	-1.020758	-0.949393	H	0.903459	-0.633900	-0.370771
N	1.580366	0.198096	-0.237167	C	1.591531	2.629294	0.241848
C	2.975394	0.083303	0.257933	H	2.641978	2.545175	-0.055685
C	3.082783	-0.321432	1.728171	H	1.213110	3.579790	-0.153162
O	-0.759880	0.156035	1.032682	H	1.540303	2.683583	1.334627
C	1.434118	1.391185	-1.110410	Imaginary Frequency: 218i			
C	1.374648	2.702584	-0.329989	TS3-DEA-ECR			
H	1.485406	-1.036180	-1.965336	C	-3.673950	-1.565965	0.244579
H	-3.155996	0.499880	1.578223	C	-3.633568	-0.218860	-0.463608
H	-3.068983	1.457852	0.087602	O	-2.772981	0.725557	0.194772
H	-5.106286	-0.786069	0.640582	C	-1.423920	0.601656	0.001248
H	-5.028917	0.184177	-0.846778	C	-0.580178	1.290727	0.822271
H	-5.447868	0.955694	0.697874	C	0.908296	1.306843	0.543758
H	2.253457	1.419852	-1.848422	N	1.277056	-0.048673	-0.063989
H	0.502932	1.271799	-1.669976				

C	2.445385	-0.065941	-0.984015
C	2.641295	-1.415958	-1.671415
O	-1.016974	-0.192043	-0.965725
H	-2.697953	-2.059187	0.197452
H	-4.411886	-2.220207	-0.236446
H	-3.957508	-1.446692	1.296619
H	-3.329123	-0.336118	-1.507214
H	-4.619582	0.256066	-0.442212
H	-0.972287	1.905674	1.623719
H	1.465442	1.404441	1.484261
H	0.177802	-0.251384	-0.693239
H	2.261368	0.689186	-1.749449
H	3.355420	0.226472	-0.445477
H	2.949183	-2.205582	-0.979224
H	1.726250	-1.740368	-2.180462
H	3.427242	-1.317391	-2.428659
C	1.312849	2.490087	-0.349827
H	0.972340	3.407702	0.141803
H	2.395844	2.577471	-0.496166
H	0.821011	2.442467	-1.327862
C	1.328552	-1.106950	0.991572
H	0.442023	-0.948812	1.610752
H	1.206056	-2.072860	0.493202
C	2.585442	-1.119894	1.859699
H	2.750911	-0.161924	2.364316
H	3.485984	-1.366474	1.287400
H	2.470495	-1.884353	2.636860

Imaginary Frequency: 978i

TS5-DEA-ECR

C	-5.331951	1.544851	-0.032436
C	-4.532651	0.262055	-0.202385
O	-3.249761	0.461177	0.461182
C	-2.265159	-0.580099	0.275128
C	-1.083685	-0.321403	0.962529
C	0.005255	-1.344231	1.069866
N	1.134441	-1.125155	-0.007230
C	0.591531	-1.393928	-1.389570
C	0.280140	-2.857501	-1.722957
O	-2.573531	-1.571624	-0.471708
C	2.407548	-1.869125	0.271669
C	3.484198	-1.681589	-0.802523
H	-1.063042	0.525136	1.644559
H	-5.058763	-0.592906	0.242905
H	-4.373469	0.025135	-1.260531
H	-5.488734	1.772182	1.028158
H	-4.809248	2.393039	-0.489280
H	-6.314513	1.448346	-0.510955
H	2.198245	-2.940119	0.405542
H	2.795487	-1.496598	1.222420
H	3.226173	-2.170005	-1.747247
H	4.424000	-2.123633	-0.450466
H	3.672452	-0.620698	-1.006298
H	-0.404418	-2.338177	0.845833
H	1.313044	-0.990408	-2.106901
H	-0.327843	-0.810678	-1.470261
H	1.142489	-3.518808	-1.581891
H	-0.560102	-3.222276	-1.127173
H	-0.016329	-2.923766	-2.777548
H	1.340666	0.275963	0.004629

H	0.217443	1.564372	0.108064
N	1.239131	1.509192	-0.015996
C	1.904532	2.151128	1.169958
H	1.664988	3.219590	1.180034
H	1.441947	1.705183	2.055384
C	3.416148	1.937600	1.196924
H	3.672066	0.872206	1.188507
H	3.919750	2.421083	0.352999
H	3.825567	2.372483	2.115690
C	1.608247	2.061054	-1.364541
H	1.071023	1.453642	-2.098319
H	2.677903	1.892068	-1.516012
C	1.253738	3.537430	-1.545655
H	1.836373	4.189833	-0.886791
H	1.461645	3.840042	-2.578383
H	0.188491	3.713346	-1.352794
C	0.608641	-1.378203	2.486204
H	1.114414	-0.437493	2.738287
H	-0.210352	-1.511056	3.200556
H	1.314793	-2.199942	2.640820

Imaginary Frequency: 946i

TS6-DEA-ECR

C	1.551708	4.375620	0.509045
C	1.381350	3.155830	-0.381347
O	0.604403	2.198697	0.340367
C	0.269101	1.019612	-0.349135
C	-0.408241	0.096205	0.467935
C	-1.405121	-0.944600	-0.018971
N	-2.811418	-0.444169	0.153042
C	-3.807845	-1.511621	0.289589
C	-3.875465	-2.092134	1.705526
O	0.710183	0.874635	-1.519394
C	-3.202662	0.594486	-0.803321
C	-4.207101	1.587489	-0.211826
H	-0.665740	0.484465	1.453876
H	0.877207	3.422602	-1.318081
H	2.358662	2.734993	-0.655090
H	0.578731	4.804107	0.775068
H	2.074969	4.117874	1.437334
H	2.135007	5.145553	-0.010210
H	-3.613626	0.171327	-1.740064
H	-2.298091	1.144385	-1.080346
H	-5.142864	1.099976	0.088386
H	-4.461023	2.363304	-0.945841
H	-3.783820	2.074620	0.674375
H	-1.359298	-1.802646	0.666557
H	-3.645809	-2.331042	-0.436021
H	-4.790406	-1.091767	0.047236
H	-2.927426	-2.550738	2.009723
H	-4.114660	-1.306234	2.431303
H	-4.650410	-2.867219	1.766155
H	1.363305	-0.858215	0.353933
H	2.155320	-0.478706	-0.989462
N	2.326239	-0.989110	-0.104786
C	3.321787	-0.217383	0.712047
H	4.259430	-0.174365	0.153299
H	2.915299	0.794317	0.777864
C	3.514926	-0.804058	2.102232
H	2.558213	-0.892897	2.629071

H	3.995989	-1.786757	2.078582
H	4.157431	-0.133799	2.682764
C	2.622854	-2.430125	-0.375735
H	1.754998	-2.816504	-0.914824
H	2.672082	-2.941937	0.587895
C	3.893992	-2.632754	-1.187947
H	4.791555	-2.329196	-0.639694
H	3.996085	-3.695979	-1.429675
H	3.855841	-2.075447	-2.131235
C	-1.142678	-1.500311	-1.433136
H	-0.178107	-2.018230	-1.481077
H	-1.914628	-2.228218	-1.712759
H	-1.114273	-0.708872	-2.184353

Imaginary Frequency: 84i

S7.3 Diethylamine to ethyl methacrylate

EmAc

O	-0.739798	0.229893	0.006758
O	0.287444	-1.781833	0.026205
C	0.349386	-0.564669	0.011797
C	1.617190	0.236072	-0.004040
C	2.771188	-0.441828	-0.049655
H	3.728906	0.071374	-0.065538
C	-2.025880	-0.438587	0.023574
H	-2.077669	-1.123623	-0.828375
H	-2.098539	-1.034252	0.939326
C	-3.100153	0.627737	-0.042321
H	-3.021258	1.210772	-0.966271
H	-3.031024	1.313417	0.809009
H	-4.087189	0.152563	-0.020046
H	2.781642	-1.527215	-0.072727
C	1.536489	1.739969	0.030648
H	1.009880	2.091140	0.925943
H	2.539449	2.177477	0.027297
H	0.985316	2.131704	-0.832344

ZI1-DEA-EmAc

C	-4.554895	-0.839524	-0.053350
C	-3.075001	-1.074453	-0.304301
O	-2.410033	0.183365	-0.171249
C	-1.030594	0.172393	-0.333029
C	-0.366978	1.332535	0.027743
C	1.105517	1.385816	-0.247246
N	1.782782	0.058097	0.114108
C	3.109639	-0.131428	-0.561455
C	2.982061	-0.557868	-2.019304
O	-0.483244	-0.904428	-0.766536
C	1.853298	-0.144474	1.600297
C	1.877095	-1.618298	1.984615
H	1.606626	2.167839	0.335322
H	-2.907492	-1.488280	-1.305858
H	-2.667224	-1.797995	0.414298
H	-4.967582	-0.126634	-0.776497
H	-4.725006	-0.441149	0.953544
H	-5.107557	-1.781980	-0.147619
H	2.737674	0.389810	1.962069
H	0.960850	0.335756	2.007110
H	2.762649	-2.139283	1.604619
H	1.884341	-1.704511	3.076506

H	0.983569	-2.129287	1.610345
H	1.374071	1.543762	-1.301739
H	3.657660	0.811422	-0.462491
H	3.653529	-0.894830	-0.000786
H	2.458617	0.183915	-2.629768
H	2.451884	-1.512116	-2.107907
H	3.985690	-0.687907	-2.438791
H	1.052227	-0.620953	-0.276948
C	-1.040569	2.565235	0.572824
H	-0.481030	3.004056	1.415382
H	-1.158348	3.381382	-0.164398
H	-2.045835	2.329201	0.936373

P1-DEA-EmAc

C	3.582833	-1.929656	-0.059677
C	2.861025	-0.804543	0.653063
O	1.914587	-0.223812	-0.280791
C	1.157828	0.786895	0.186851
C	0.216747	1.339024	-0.873654
C	-1.233589	1.209107	-0.371439
N	-1.619021	-0.181754	-0.108857
C	-2.648643	-0.281263	0.937816
C	-2.077889	-0.155580	2.350312
O	1.243701	1.220902	1.320767
C	-2.008898	-0.889079	-1.338577
C	-1.785871	-2.398526	-1.249696
H	-1.910948	1.693537	-1.098964
H	3.553024	-0.023077	0.983442
H	2.314238	-1.163588	1.530413
H	4.117005	-1.560751	-0.942041
H	2.882559	-2.709706	-0.377725
H	4.314214	-2.381648	0.619843
H	-3.061474	-0.673913	-1.604771
H	-1.400765	-0.499535	-2.161651
H	-2.381676	-2.859959	-0.453751
H	-2.066889	-2.881703	-2.193546
H	-0.730297	-2.615644	-1.049671
H	-1.313736	1.775380	0.560853
H	0.348401	0.747664	-1.784749
H	-3.446518	0.470149	0.782978
H	-3.129403	-1.260374	0.844644
H	-1.573652	0.803364	2.510533
H	-1.348413	-0.950854	2.541446
H	-2.881735	-0.237229	3.092497
C	0.571068	2.805605	-1.170713
H	-0.109346	3.217533	-1.924498
H	0.490908	3.416297	-0.264884
H	1.593674	2.897707	-1.553917

I1-DEA-EmAc

C	4.577138	-0.754529	0.263030
C	3.081522	-1.004488	0.279929
O	2.427658	0.278711	0.370795
C	1.069671	0.279650	0.309858
C	0.390049	1.248129	-0.346988
C	-1.123217	1.324631	-0.249579
N	-1.785603	-0.002376	-0.135668
C	-3.124117	0.105199	0.481713
C	-3.073585	0.234615	2.002943
O	0.493627	-0.740203	0.985209
C	-1.825623	-0.681818	-1.449928

C	-1.976205	-2.197901	-1.342803
H	-1.518635	1.866572	-1.126469
H	2.796449	-1.628037	1.132859
H	2.755092	-1.513625	-0.637121
H	4.896450	-0.239332	1.175885
H	4.866112	-0.142420	-0.598431
H	5.112024	-1.709311	0.202467
H	-2.631416	-0.255745	-2.071993
H	-0.879597	-0.456455	-1.952260
H	-2.912628	-2.495477	-0.857990
H	-1.969426	-2.643116	-2.344655
H	-1.145577	-2.630634	-0.773645
H	-1.424073	1.913634	0.627267
H	-3.676648	0.953127	0.041912
H	-3.684083	-0.798891	0.226516
H	-2.522160	1.123755	2.327862
H	-2.595614	-0.643071	2.453188
H	-4.090667	0.312265	2.405149
H	-0.487394	-0.687687	0.737260
C	1.080667	2.351269	-1.104393
H	0.696598	2.435756	-2.132334
H	0.927253	3.337347	-0.637028
H	2.159079	2.181377	-1.159479

TS1-DEA-EmAc

C	-4.693376	-0.735746	0.668930
C	-3.295528	-1.137871	0.234048
O	-2.565685	0.060836	-0.056003
C	-1.267051	-0.107080	-0.493552
C	-0.566132	1.109354	-0.701260
C	0.738205	0.957989	-1.247894
N	1.866774	0.112572	-0.129933
C	3.134046	-0.286987	-0.800613
C	3.488519	-1.759050	-0.604629
O	-0.797294	-1.255913	-0.647406
C	2.003058	0.844818	1.148565
C	2.571151	0.018520	2.298989
H	1.293808	1.872718	-1.460411
H	-3.327353	-1.778347	-0.655101
H	-2.783534	-1.704246	1.022098
H	-5.205329	-0.176556	-0.122484
H	-4.663152	-0.108911	1.567441
H	-5.286718	-1.629545	0.895281
H	2.627197	1.723065	0.950791
H	0.996547	1.195916	1.397210
H	3.602539	-0.297806	2.111321
H	2.568815	0.620735	3.215192
H	1.962189	-0.874346	2.483414
H	0.863768	0.211982	-2.035212
H	3.013307	-0.081642	-1.871373
H	3.930169	0.366108	-0.431879
H	2.685615	-2.405932	-0.977691
H	3.666149	-2.003320	0.447517
H	4.398195	-1.998673	-1.167158
H	1.266802	-0.710462	0.005343
C	-1.112509	2.445020	-0.245576
H	-0.360549	3.233163	-0.381229
H	-2.002852	2.760350	-0.812004
H	-1.411498	2.464553	0.813689

Imaginary Frequency: 223i

TS3-DEA-EmAc

C	-3.227711	-1.433361	1.325873
C	-3.342817	-1.056394	-0.144591
O	-2.678475	0.179745	-0.449857
C	-1.306709	0.155337	-0.532091
C	-0.617878	1.330127	-0.399359
C	0.873044	1.295968	-0.645137
N	1.457961	-0.028833	-0.215108
C	2.652380	-0.418699	-1.010782
C	3.148931	-1.828285	-0.706706
O	-0.739382	-1.013080	-0.734542
H	-2.185963	-1.639381	1.592542
H	-3.817051	-2.336326	1.529206
H	-3.602708	-0.628295	1.968287
H	-2.953570	-1.855662	-0.781245
H	-4.388189	-0.875675	-0.414717
H	1.381733	2.112183	-0.116684
H	0.465004	-0.724001	-0.501091
H	2.350032	-0.358185	-2.060841
H	3.451052	0.317857	-0.858331
H	3.556731	-1.921849	0.304803
H	2.348233	-2.567128	-0.826809
H	3.949208	-2.082986	-1.410332
H	1.135900	1.403358	-1.708531
C	1.623563	-0.126307	1.265545
H	0.682177	0.235316	1.688615
H	1.702745	-1.188531	1.514330
C	2.803573	0.644966	1.852048
H	2.764046	1.711659	1.606794
H	3.767788	0.250277	1.514697
H	2.775319	0.557537	2.944119
C	-1.261775	2.664139	-0.139379
H	-1.251313	3.334217	-1.017056
H	-2.308951	2.542902	0.153692
H	-0.752691	3.216281	0.666977

Imaginary Frequency: 948i

TS5-DEA-EmAc

C	5.269625	-0.131065	0.013033
C	3.934661	-0.336733	0.709936
O	2.975963	-0.692927	-0.281481
C	1.684068	-0.994739	0.194481
C	0.752410	-1.278921	-0.809465
C	-0.559363	-1.862488	-0.368935
N	-1.648188	-0.883733	0.137257
C	-1.820148	-1.034594	1.609909
C	-2.764743	-0.016468	2.242815
O	1.483550	-0.961100	1.436949
C	-2.915786	-1.001982	-0.633616
C	-3.710852	-2.295737	-0.441523
H	-1.011985	-2.406569	-1.204689
H	4.008351	-1.124199	1.470286
H	3.626256	0.578650	1.234431
H	5.594246	-1.048584	-0.491439
H	5.205047	0.664639	-0.738638
H	6.039183	0.149349	0.742494
H	-2.645911	-0.888976	-1.689424
H	-3.547947	-0.144192	-0.377582
H	-3.113334	-3.183492	-0.675361

H	-4.576613	-2.291081	-1.114202
H	-4.089351	-2.399918	0.580783
H	-0.426071	-2.581985	0.449117
H	-0.812685	-0.939100	2.023794
H	-2.166846	-2.052442	1.837275
H	-2.452559	1.014134	2.039529
H	-3.800527	-0.132104	1.904909
H	-2.759673	-0.153610	3.330524
H	-1.158299	0.395494	-0.092681
H	0.247755	0.901632	-0.855966
N	-0.528015	1.420596	-0.409432
C	-1.227769	2.251235	-1.426442
H	-0.526608	2.981703	-1.844496
H	-1.504678	1.569405	-2.237080
C	-2.467160	2.954113	-0.884022
H	-3.180820	2.240275	-0.457076
H	-2.219522	3.694419	-0.116085
H	-2.969662	3.482494	-1.701713
C	0.032628	2.123408	0.779611
H	0.488114	1.337507	1.388585
H	-0.798091	2.556113	1.344566
C	1.069762	3.189330	0.436232
H	0.639837	4.032462	-0.115209
H	1.504044	3.586189	1.360911
H	1.885447	2.765794	-0.162062
C	1.122502	-1.382727	-2.274762
H	0.345283	-0.971665	-2.940495
H	2.045147	-0.833985	-2.488235
H	1.290779	-2.419967	-2.626813

Imaginary Frequency: 958i

TS6-DEA-EmAc

C	2.097419	4.335708	0.360871
C	1.589642	3.188537	-0.494536
O	0.837678	2.311057	0.352199
C	0.321771	1.170378	-0.246900
C	-0.241889	0.233350	0.669685
C	-1.341382	-0.665534	0.134197
N	-2.722573	-0.150595	0.324563
C	-3.736379	-1.179439	0.068944
C	-3.935858	-2.130660	1.252949
O	0.492435	0.998988	-1.476008
C	-2.998955	1.115670	-0.362407
C	-2.964403	1.111037	-1.900745
H	-1.149959	-0.886659	-0.930770
H	0.954310	3.555911	-1.309103
H	2.421836	2.643893	-0.957827
H	1.265333	4.885118	0.815623
H	2.746848	3.971501	1.165358
H	2.674648	5.035853	-0.254687
H	-2.277539	1.855798	0.002468
H	-3.988810	1.454170	-0.026714
H	-1.958061	0.895039	-2.273202
H	-3.254534	2.099107	-2.281790
H	-3.663235	0.378758	-2.324340
H	-1.319911	-1.629215	0.660862
H	-3.510089	-1.771685	-0.839289
H	-4.689146	-0.672850	-0.127675
H	-3.029469	-2.701522	1.484542
H	-4.219179	-1.571263	2.152020

H	-4.731658	-2.853352	1.031551
H	1.053548	-0.817302	0.238181
H	1.784283	-0.808198	-1.250918
N	1.868234	-1.344699	-0.377836
C	3.198394	-1.060268	0.239569
H	3.983729	-1.391331	-0.445815
H	3.259547	0.029104	0.315690
C	3.354308	-1.695917	1.614557
H	2.536385	-1.402866	2.282283
H	3.389826	-2.789088	1.566980
H	4.293747	-1.353278	2.060962
C	1.521803	-2.771751	-0.641224
H	0.504020	-2.760191	-1.039443
H	1.494737	-3.289240	0.320762
C	2.470590	-3.456671	-1.616879
H	3.482243	-3.558199	-1.210902
H	2.097928	-4.463326	-1.835644
H	2.529730	-2.907126	-2.563904
C	-0.361598	0.597665	2.139605
H	-1.184665	1.296944	2.365554
H	-0.552917	-0.300939	2.744600
H	0.555167	1.060490	2.521846

Imaginary Frequency: 238i

S7.4 Ethylamine to ethyl acrylate

EA

C	0.000000	0.574349	0.000000
H	0.040985	1.231867	0.874631
H	0.040985	1.231867	-0.874631
C	1.217239	-0.359183	0.000000
H	2.155838	0.204841	0.000000
H	1.214130	-1.004964	0.884312
H	1.214130	-1.004964	-0.884312
H	-1.397016	-0.686120	0.812973
N	-1.310781	-0.082486	0.000000
H	-1.397016	-0.686120	-0.812973

EAc

O	0.202989	-0.686927	0.000000
O	-1.103668	1.163326	0.000000
C	0.000000	0.646507	0.000000
C	1.295050	1.372823	0.000000
H	2.196994	0.767468	0.000000
C	1.338894	2.707248	0.000000
H	0.425539	3.296426	0.000000
H	2.282814	3.244931	0.000000
C	-0.982635	-1.519689	0.000000
H	-1.581320	-1.280547	0.884959
H	-1.581320	-1.280547	-0.884959
C	-0.529430	-2.965475	0.000000
H	0.068895	-3.192416	0.889047
H	0.068895	-3.192416	-0.889047
H	-1.406338	-3.622574	0.000000

ZI1-EA-EAc

C	3.757655	-0.827325	0.735784
C	3.047607	-0.596040	-0.591705
O	2.226561	0.575698	-0.565930

O	1.189039	2.327782	0.178742	H	-0.705025	4.653933	-1.297486
C	1.335323	1.605594	-0.947114	H	-0.276076	3.315974	-2.388077
O	0.528120	1.607850	-1.857890	H	0.955509	4.500366	-1.906922
C	2.624490	0.809477	-0.953652	H	-2.974771	0.290015	-0.971515
C	2.342758	-0.682648	-1.178271	H	-2.473566	-1.033268	-2.006986
N	1.575369	-1.281231	-0.079068	H	-4.419374	-1.290707	0.376157
C	0.795767	-2.441343	-0.536257	H	-4.825579	-1.328152	-1.342143
C	-0.552745	-2.031381	-1.134259	H	-3.876383	-2.643242	-0.635937
C	-1.554290	-1.620054	-0.071879	H	-0.855036	-0.996280	1.811659
O	-2.415128	-0.695105	-0.536632	H	-2.708747	1.301749	0.957573
C	-3.472329	-0.284540	0.367820	H	-1.604757	-3.099559	0.412006
C	-4.369281	0.680422	-0.380554	H	-1.268965	-2.736586	-1.278194
C	2.423605	-1.600157	1.080968	H	0.818686	-3.330650	0.612541
C	1.646189	-1.610178	2.396103	H	2.931601	0.160385	0.663335
O	-1.620797	-2.093008	1.047219	H	3.388396	0.091019	-1.050640
H	3.237953	1.180481	-1.784809	H	5.423380	0.015820	0.393422
H	3.297243	-1.213205	-1.348703	H	5.247562	-1.512733	-0.493247
H	-0.008510	3.880567	-0.511769	H	4.802552	-1.426018	1.225548
H	-0.881901	2.471974	0.111125	H	-0.106374	-0.368068	-0.843806
H	0.825240	4.398186	1.815220				
H	-0.052082	2.982980	2.439512				
H	-0.949083	4.359724	1.766195	TS1-EA-EAc			
H	2.945648	-2.565261	0.937551	C	-3.449324	1.610849	-0.359115
H	3.206217	-0.837315	1.147058	C	-3.462890	0.166952	0.124743
H	0.833799	-2.343700	2.389404	O	-2.402495	-0.605498	-0.452644
H	2.315530	-1.852235	3.230971	C	-1.178274	-0.568612	0.200921
H	1.202350	-0.625415	2.581601	C	-0.193179	-1.348323	-0.463836
H	1.760006	-0.775994	-2.099057	C	1.109177	-1.428284	0.074947
H	3.179299	0.984267	-0.028859	N	2.130858	0.013523	-0.332974
H	1.359403	-3.037941	-1.274608	C	3.517749	0.029988	0.184304
H	0.603322	-3.094286	0.318248	C	4.259210	1.328881	-0.117085
H	-0.993322	-2.887102	-1.666090	O	-1.034218	0.083195	1.246387
H	-0.446711	-1.223784	-1.863513	H	-2.542191	2.121161	-0.019929
H	-3.019037	0.181126	1.248959	H	-4.317705	2.151946	0.037570
H	-4.018184	-1.172900	0.700675	H	-3.488405	1.657406	-1.453796
H	-5.173065	1.021511	0.281755	H	-3.395456	0.126716	1.215649
H	-4.825480	0.200517	-1.253219	H	-4.384505	-0.334959	-0.189557
H	-3.810254	1.558811	-0.720786	H	-0.420914	-1.773764	-1.436020
				H	1.772263	-2.196909	-0.321686
				H	1.198265	-1.312208	1.154995
I2-EA-EAc				H	2.106519	0.097969	-1.351363
C	0.081299	3.937851	-1.560093	H	1.583416	0.791048	0.042135
C	0.469166	3.089568	-0.366573	H	3.455257	-0.140901	1.263871
O	-0.714226	2.364661	0.061434	H	4.033579	-0.827383	-0.259521
C	-0.585231	1.609508	1.167943	H	4.331269	1.505302	-1.196735
C	-1.867490	0.876690	1.510180	H	3.754165	2.188147	0.339531
C	-1.740722	-0.638398	1.278595	H	5.277324	1.281479	0.286459
N	-1.575329	-1.020682	-0.135837				
C	-2.766143	-0.784733	-0.980104	Imaginary Frequency: 187i			
C	-4.038072	-1.559561	-0.615003				
O	0.441631	1.525160	1.814857	TS2-EA-EAc			
C	-1.052419	-2.414947	-0.249220	O	-2.154971	0.261390	-0.371147
C	0.424458	-2.490032	0.053700	O	-0.714275	-0.345487	1.280513
C	1.278467	-1.548017	-0.401173	C	-0.925308	0.281423	0.235029
O	0.880905	-0.432203	-1.049460	C	0.062309	1.022435	-0.509254
O	2.616347	-1.679500	-0.262400	H	1.794375	-0.581155	0.810655
C	3.390282	-0.467793	-0.108939	C	1.316406	1.368607	0.267791
C	4.798205	-0.876876	0.277687	H	1.205486	1.580863	1.335235
H	-2.054145	1.033123	2.578464	C	-3.149621	-0.578116	0.240114
H	-2.612610	-1.138279	1.727087	H	-2.793004	-1.614791	0.262067
H	0.827310	3.699799	0.468213	H	-3.306837	-0.265088	1.278459
H	1.245651	2.361629	-0.617647	C	-4.424861	-0.450112	-0.571855

H -4.269177 -0.775393 -1.606633
H -4.778878 0.586835 -0.587082
H -5.211054 -1.074068 -0.131021
C 3.529358 0.075092 -0.137933
H 3.729598 0.727037 -0.994633
H 4.011416 0.520974 0.741309
C 4.056667 -1.331849 -0.389988
H 3.587746 -1.776336 -1.274967
H 5.139172 -1.303080 -0.554355
H 3.862954 -1.987611 0.467338
H 1.892098 2.162695 -0.212904
H -0.305241 1.733798 -1.245487
N 2.065744 0.063967 0.063842
H 1.145406 -0.034551 -0.813227

Imaginary Frequency: 1593i

TS3-EA-EAc

C -3.172162 -1.351161 0.775618
C -3.054490 -0.470985 -0.460943
O -2.298606 0.725038 -0.208869
C -0.932572 0.627488 -0.219592
C -0.201397 1.645083 0.326129
C 1.295816 1.591663 0.198211
N 1.737891 0.159057 0.321414
C 3.093011 -0.145734 -0.188836
C 3.452332 -1.606826 0.049270
O -0.397903 -0.446107 -0.750217
H -2.190508 -1.728649 1.080401
H -3.818226 -2.212433 0.564101
H -3.607841 -0.794054 1.612999
H -2.610195 -1.023523 -1.292720
H -4.040404 -0.110380 -0.771479
H -0.681765 2.488442 0.806038
H 1.803139 2.201043 0.954656
H 1.670682 1.919997 -0.784556
H 1.660242 -0.122804 1.301760
H 0.772695 -0.363566 -0.287621
H 3.091781 0.083996 -1.259286
H 3.821368 0.518579 0.294041
H 3.459775 -1.845504 1.119824
H 2.741320 -2.277071 -0.447011
H 4.451537 -1.816082 -0.347497

Imaginary Frequency: 990i

TS4-EA-EAc

C -2.836090 1.840259 0.557635
C -3.040484 0.682514 -0.398456
O -1.751414 0.149357 -0.856046
C -1.176927 -0.795509 -0.163906
C -0.043502 -1.591278 -0.547794
C 1.255945 -1.290632 0.195113
N 1.853401 -0.001631 -0.197413
C 3.188277 0.203805 0.370140
C 3.795343 1.517666 -0.114373
O -1.661786 -1.226589 0.963796
H -2.342729 1.510870 1.477477
H -3.812942 2.260688 0.823255
H -2.236291 2.631155 0.095442
H -3.605564 -0.133507 0.057324

H -3.532484 0.999298 -1.320072
H 0.111477 -1.691855 -1.626406
H 1.950017 -2.134287 0.022010
H 1.087177 -1.252396 1.279673
H 1.933418 0.008119 -1.215760
H -0.898020 -2.126001 0.656709
H 3.088146 0.224390 1.464256
H 3.879284 -0.630645 0.138960
H 3.936550 1.509632 -1.203185
H 3.143058 2.362856 0.134252
H 4.775314 1.690017 0.345806

Imaginary Frequency: 1966i

TS5-RRS-EA-EAc

C 4.673744 -0.495648 -0.141298
C 3.318849 -0.607294 0.538193
O 2.349766 -0.884210 -0.469131
C 1.020524 -0.991300 -0.033218
O 0.779190 -0.865510 1.203668
C 0.104394 -1.189440 -1.059900
C -1.324028 -1.534309 -0.731776
C -3.214644 -0.956269 0.822263
C -4.330523 -0.614009 -0.162673
H 4.673190 0.307667 -0.887436
H 5.452899 -0.276389 0.598735
H 4.937860 -1.430542 -0.649222
H 3.072232 0.324120 1.065617
H 3.326695 -1.403957 1.293987
H 0.461527 -1.371971 -2.068979
H -1.952412 -1.454707 -1.627411
H -1.464305 -2.566499 -0.348071
H -1.177481 -0.674005 1.068944
H -3.361746 -0.398107 1.754204
H -3.257281 -2.026859 1.076826
H -4.235201 -1.174958 -1.098840
H -4.330284 0.455889 -0.404776
H -5.305830 -0.860540 0.272462
N -1.874885 -0.611779 0.313025
H -1.613129 0.729104 -0.177935
N -1.087813 1.698224 -0.619992
H -1.724606 2.274777 -1.176058
H -0.394874 1.263583 -1.246541
C -0.412083 2.485402 0.448546
H -1.195671 2.865380 1.111088
H 0.193123 1.769207 1.011441
C 0.436290 3.620334 -0.107686
H -0.173039 4.331136 -0.678813
H 1.226633 3.237899 -0.764123
H 0.913796 4.167613 0.712664

Imaginary Frequency: 382i

TS5-RSS-EA-EAc

C -3.851382 1.109382 -0.946773
C -3.888015 -0.116547 -0.041612
O -2.794623 -0.142713 0.874674
C -1.606861 -0.740645 0.417681
O -1.608363 -1.343580 -0.690556
C -0.524481 -0.564706 1.276621
C 0.724994 -1.367389 1.037602

C	2.305197	-2.089928	-0.783385
C	3.646825	-1.749632	-0.139572
H	-2.965549	1.083002	-1.590967
H	-4.740592	1.139892	-1.589991
H	-3.825500	2.033387	-0.356382
H	-3.892216	-1.030958	-0.642174
H	-4.791295	-0.102300	0.580375
H	-0.682250	-0.124597	2.256733
H	1.521327	-1.055515	1.723833
H	0.596112	-2.459064	1.183641
H	0.374398	-1.380597	-0.929272
H	2.390685	-2.020013	-1.874033
H	2.033844	-3.130327	-0.545771
H	3.611978	-1.842524	0.951400
H	3.960070	-0.727753	-0.386079
H	4.420793	-2.434809	-0.504334
N	1.217373	-1.182615	-0.370442
H	1.360630	0.247947	-0.516375
N	1.170195	1.425419	-0.429969
H	0.769666	1.777009	-1.303839
H	0.411566	1.408617	0.273592
C	2.328682	2.248423	0.003469
H	2.716834	1.794087	0.919709
H	3.098560	2.157329	-0.768581
C	1.955478	3.706962	0.235660
H	1.191257	3.799394	1.015908
H	1.570636	4.169659	-0.680897
H	2.837342	4.273336	0.555295

Imaginary Frequency: 526i

TS6-RR-EA-EAc

C	-3.442422	-3.241994	-0.143321
C	-2.649834	-2.116382	0.498247
O	-1.571946	-1.789107	-0.384341
C	-0.718163	-0.776211	0.031379
O	-0.875975	-0.274811	1.173598
C	0.172577	-0.338721	-0.975373
C	1.497205	0.258554	-0.574093
H	0.182238	-0.934885	-1.887694
H	1.358220	0.878559	0.332754
H	-2.257650	-2.417810	1.476678
H	-3.284021	-1.235012	0.664460
H	-2.812224	-4.125038	-0.298956
H	-3.845727	-2.934802	-1.115110
H	-4.281636	-3.529195	0.501302
H	1.885538	0.933141	-1.353230
H	-0.792702	1.280057	-0.888219
N	-1.316213	2.050535	-0.314666
H	-1.309823	1.607327	0.620991
H	-2.286784	2.094405	-0.638873
H	0.356888	3.251793	0.013020
C	-0.666171	3.391760	-0.343454
H	-0.624167	3.703380	-1.390333
H	-1.458414	4.082575	1.558840
C	-1.421066	4.399346	0.510381
H	-2.447724	4.535983	0.150969
H	-0.915723	5.369919	0.466972
N	2.545622	-0.764370	-0.354830
H	2.172374	-1.433835	0.320115
C	3.791148	-0.212739	0.178656

H	3.633893	0.374797	1.105853
H	4.192599	0.492343	-0.563419
C	4.816358	-1.312812	0.443591
H	5.024698	-1.879515	-0.471390
H	4.450203	-2.019250	1.200140
H	5.759647	-0.891550	0.811474

Imaginary Frequency: 156i

TS6-RS-EA-EAc

C	2.484196	3.651017	-0.221113
C	1.871888	2.454576	0.486528
O	0.935485	1.849982	-0.411080
C	0.287091	0.712091	0.049339
O	0.507355	0.316880	1.223167
C	-0.471289	0.050513	-0.942648
C	-1.653516	-0.787370	-0.526625
H	-0.576748	0.578984	-1.889861
H	-1.413679	-1.316738	0.415882
H	1.363852	2.761848	1.408671
H	2.645091	1.729828	0.773182
H	1.713992	4.379867	-0.497739
H	3.007614	3.344129	-1.133927
H	3.206217	4.148394	0.437405
H	-1.872071	-1.569129	-1.271361
H	0.763594	-1.356252	-0.726161
N	1.366699	-1.995536	-0.077052
H	1.264162	-1.479822	0.815690
H	0.922268	-2.913047	0.009520
H	2.780648	-2.553583	-1.512453
C	2.787333	-2.103401	-0.516431
H	3.162128	-1.080825	-0.607076
H	3.240286	-3.944657	0.546742
C	3.618048	-2.918978	0.462181
H	3.616687	-2.464601	1.459498
H	4.654873	-2.968648	0.113163
N	-2.897694	0.002477	-0.379267
H	-2.683642	0.781386	0.245647
C	-4.002353	-0.763638	0.198162
H	-3.735854	-1.226267	1.170075
H	-4.226929	-1.597065	-0.482834
C	-5.247859	0.102302	0.371984
H	-5.565891	0.524926	-0.588138
H	-5.054478	0.936947	1.058552
H	-6.079110	-0.481836	0.784797

Imaginary Frequency: 174i

TS7-EA-EAc

C	-4.740862	-0.155170	0.982807
C	-3.496389	0.378127	0.292047
O	-2.636446	-0.728831	0.032947
C	-1.398533	-0.428023	-0.547524
C	-0.568298	-1.530941	-0.676742
C	0.729316	-1.450157	-1.392458
N	1.939220	-1.110645	-0.519934
H	2.761600	-1.041172	-1.126833
O	-1.171205	0.775880	-0.880796
C	2.220409	-2.102453	0.538840
C	3.455573	-1.723876	1.348833
H	-0.926140	-2.495427	-0.330057

H	0.972600	-2.393686	-1.901964
H	-3.759555	0.888304	-0.643694
H	-2.987951	1.118384	0.924423
H	-5.262253	-0.880818	0.347831
H	-4.484375	-0.651407	1.926153
H	-5.433061	0.666118	1.204338
H	2.346569	-3.097634	0.088655
H	1.332787	-2.143710	1.177272
H	4.352837	-1.683248	0.718528
H	3.633997	-2.466903	2.134354
H	3.334873	-0.747054	1.832066
H	0.716569	-0.651515	-2.144550
H	1.682940	0.102682	-0.027314
H	0.297747	1.257636	-0.090161
H	1.180530	1.316807	1.335360
N	1.264060	1.258410	0.318286
C	2.079498	2.376457	-0.206835
H	3.103403	2.252745	0.163246
H	2.108723	2.265813	-1.296002
C	1.532524	3.747898	0.175452
H	0.513989	3.885879	-0.205326
H	1.510430	3.874958	1.264852
H	2.162559	4.541327	-0.243359

Imaginary Frequency: 932i

TS8-RRS-EA-EAc

C	-3.672962	4.202645	0.345221
C	-2.886098	3.144744	-0.411024
O	-3.344633	1.867750	0.028314
C	-2.741037	0.755283	-0.567840
C	-3.143282	-0.464595	-0.028450
C	-2.770438	-1.736049	-0.739834
N	-1.298379	-1.790406	-1.035965
H	-1.127136	-0.916596	-1.556280
O	-1.887333	0.941709	-1.481909
C	-0.892926	-2.963249	-1.831494
C	0.574639	-2.897828	-2.240875
H	-3.966154	-0.493200	0.679328
H	-3.015817	-2.613345	-0.127521
H	-3.030260	3.251355	-1.493642
H	-1.809626	3.253635	-0.221580
H	-4.747362	4.108069	0.148919
H	-3.514810	4.113052	1.426415
H	-3.355261	5.205468	0.035123
H	-1.528304	-3.039640	-2.726214
H	-1.081580	-3.860375	-1.228890
H	0.780699	-1.996499	-2.831070
H	0.834334	-3.766140	-2.857065
H	1.237857	-2.896313	-1.368180
H	-3.286624	-1.880555	-1.710004
H	-0.668635	-1.540692	0.178094
H	-1.330076	-0.639075	1.446739
N	-0.387688	-1.035217	1.277400
C	0.539339	0.113897	1.093854
H	0.593476	0.683490	2.027584
H	0.086904	0.753501	0.331543
C	1.935040	-0.323338	0.655484
H	1.891943	-0.910447	-0.269308
H	2.415919	-0.962338	1.405405
C	-0.033166	-1.986200	2.360939

H	0.863811	-2.533146	2.055880
H	0.216253	-1.412844	3.262684
C	-1.175674	-2.954724	2.644299
H	-1.410142	-3.570647	1.769095
H	-2.084904	-2.421013	2.943774
H	-0.894162	-3.626854	3.462105
C	2.843483	0.867777	0.420336
O	2.540512	2.028934	0.612943
O	4.046373	0.468697	-0.028478
C	5.019478	1.514049	-0.294683
H	4.600177	2.202244	-1.035095
H	5.193463	2.075006	0.628923
C	6.282774	0.845274	-0.795966
H	6.692153	0.159506	-0.046286
H	6.093153	0.282298	-1.716285
H	7.038807	1.608628	-1.011001

Imaginary Frequency: 921i

TS8-RSS-EA-EAc

C	-3.991234	-4.261917	-0.281720
C	-3.986977	-2.778838	0.049739
O	-3.018434	-2.148432	-0.785829
C	-2.929829	-0.755306	-0.684376
O	-3.725386	-0.147431	0.086802
C	-1.910178	-0.192457	-1.448975
C	-1.880705	1.301017	-1.629985
C	-2.020435	3.476409	-0.364089
C	-0.746808	4.174968	-0.833418
H	-3.006049	-4.708928	-0.103736
H	-4.723577	-4.787582	0.342823
H	-4.254739	-4.428430	-1.332639
H	-3.742470	-2.621194	1.109738
H	-4.977838	-2.338147	-0.114911
H	-1.369158	-0.810778	-2.158968
H	-0.983299	1.606299	-2.179268
H	-2.745847	1.703390	-2.193823
H	-2.708643	1.601375	0.164759
H	-2.281962	3.821621	0.642820
H	-2.858901	3.742539	-1.025274
H	-0.468554	3.879736	-1.850958
H	0.097541	3.953205	-0.169761
H	-0.896171	5.260782	-0.834410
N	-1.884222	2.007063	-0.301346
H	-0.826448	1.448267	0.438064
N	-0.033670	0.633896	0.900059
H	-0.423337	-0.174847	0.381194
C	1.338202	0.908491	0.409906
H	1.253159	1.164546	-0.649639
H	1.710936	1.791658	0.935383
C	2.295674	-0.271349	0.582391
H	2.439425	-0.522417	1.640434
H	1.893026	-1.171481	0.101905
C	3.657986	0.028669	-0.012022
O	4.007461	1.112498	-0.438985
O	4.442108	-1.062171	-0.000435
C	5.781257	-0.901223	-0.541690
H	5.699686	-0.577751	-1.584107
H	6.293656	-0.112855	0.018325
C	6.490702	-2.233482	-0.417623
H	6.563622	-2.546875	0.629385

H 5.967587 -3.014661 -0.979587
H 7.505961 -2.143426 -0.819954
C -0.167861 0.428976 2.369609
H 0.220083 -0.561946 2.628050
H 0.468183 1.173150 2.859977
C -1.615866 0.576365 2.828436
H -2.299971 -0.032898 2.227325
H -1.949168 1.618116 2.761123
H -1.701043 0.265164 3.875218

Imaginary Frequency: 830i

TS9-EA-EAc

C 4.629212 -2.537673 -0.372813
C 4.874085 -1.035562 -0.429361
O 3.793695 -0.325012 -1.047087
C 2.762216 0.108083 -0.218480
O 2.807374 -0.137059 1.009741
C 1.689048 0.708091 -0.926013
C 0.881118 1.775081 -0.228626
H 1.874808 0.886840 -1.985473
H 0.719047 1.479542 0.825436
H 5.749553 -0.817280 -1.051082
H 5.048753 -0.637839 0.574056
H 4.414829 -2.938471 -1.370528
H 3.787631 -2.768471 0.288368
H 5.516987 -3.052532 0.016141
H -0.119211 1.878129 -0.678213
H 0.647585 -0.702319 -0.365757
N 0.308353 -1.472769 0.347357
H 1.025222 -1.342062 1.077223
H -1.328725 -1.919880 1.610209
C -1.033501 -1.137594 0.908172
H -0.908251 -0.212191 1.472925
H -2.254880 -1.875166 -0.749497
C -2.078423 -0.950452 -0.188412
H -1.746902 -0.202229 -0.918396
N 1.506015 3.115646 -0.307107
H 2.462296 3.020046 0.038602
C 0.818893 4.119645 0.505841
H 0.717053 3.811049 1.565983
H -0.205488 4.222020 0.119897
C 1.526962 5.470325 0.436577
H 1.595898 5.822113 -0.599426
H 2.547122 5.401735 0.836552
H 0.990889 6.226297 1.022909
C 0.483123 -2.824441 -0.272295
H -0.276780 -2.934792 -1.049015
H 1.457292 -2.795065 -0.766941
C 0.421573 -3.959984 0.739414
H -0.569091 -4.059143 1.194838
H 1.159077 -3.821299 1.538796
H 0.648764 -4.903784 0.232295
C -3.402642 -0.499202 0.397324
O -3.616547 -0.331032 1.582446
O -4.316057 -0.311118 -0.567801
C -5.631393 0.131713 -0.134167
H -6.045739 -0.618688 0.546185
H -5.517889 1.067551 0.421331
C -6.489118 0.307667 -1.369570
H -6.592470 -0.635206 -1.917377

H -7.489073 0.642365 -1.071479
H -6.063518 1.058175 -2.044239

Imaginary Frequency: 107i

TS10-EA-EAc

C 4.893616 -3.438356 0.217827
C 3.483727 -2.873080 0.266612
O 3.439760 -1.747894 -0.608019
C 2.207588 -1.094763 -0.720786
C 2.216228 -0.060870 -1.644645
C 0.976626 0.662158 -2.016116
N 0.649499 1.899629 -1.170925
H -0.257331 2.259735 -1.485358
O 1.249274 -1.496020 0.010223
C 1.641539 2.989355 -1.303687
C 1.238395 4.223446 -0.505059
H 3.132793 0.140970 -2.189846
H 1.008600 1.010713 -3.057730
H 2.751251 -3.628994 -0.045817
H 3.217614 -2.578601 1.290390
H 5.157586 -3.745806 -0.800652
H 5.627279 -2.694431 0.549682
H 4.974292 -4.314891 0.871956
H 1.754696 3.243602 -2.366963
H 2.601452 2.592769 -0.961188
H 0.275566 4.623935 -0.846663
H 1.989108 5.012398 -0.627414
H 1.154711 4.003105 0.565487
H 0.091643 0.025403 -1.901477
H 0.476944 1.462455 0.061944
H 0.665333 -0.099912 0.958446
N 0.271964 0.839227 1.193096
C -1.172422 0.697029 1.477158
H -1.312223 0.134162 2.408951
H -1.602133 1.694753 1.622337
C -1.890572 -0.025109 0.342798
H -1.905795 0.564682 -0.577885
H -1.419594 -0.988248 0.125561
C 1.003627 1.442207 2.334122
H 0.663409 2.479585 2.437373
H 0.720615 0.914398 3.254753
C 2.515147 1.385082 2.148016
H 2.839644 1.924616 1.252925
H 2.864592 0.350426 2.066028
H 3.007104 1.839773 3.015137
O -3.244772 -0.231225 0.798416
C -4.122151 -0.700443 -0.118254
O -3.822446 -0.926242 -1.272953
C -5.490699 -0.900352 0.498767
H -5.777864 0.036043 0.993110
H -5.382326 -1.638917 1.304056
C -6.547328 -1.342466 -0.509799
H -6.675140 -0.600372 -1.304755
H -6.273626 -2.292070 -0.980441
H -7.512895 -1.475242 -0.010211

Imaginary Frequency: 1075i

TS11-EA-EAc

C -6.097225 -1.862765 0.585022
 C -4.579069 -1.843208 0.557701
 O -4.170590 -0.794611 -0.328148
 C -2.806201 -0.599719 -0.448078
 C -2.467775 0.478317 -1.304959
 C -1.092662 0.740088 -1.538951
 N -0.274356 1.480134 -0.131665
 C 1.206400 1.471494 -0.261592
 C 1.804243 0.119908 0.123251
 O -2.008067 -1.325987 0.171144
 C -0.856682 2.816490 0.144531
 C -0.661613 3.289283 1.581251
 H -3.239137 1.155275 -1.655666
 H -0.853014 1.488402 -2.295444
 H -4.178756 -2.803474 0.210162
 H -4.167545 -1.667673 1.559353
 H -6.506593 -2.048549 -0.414483
 H -6.496889 -0.908167 0.946113
 H -6.450833 -2.656971 1.253130
 H -0.410925 3.515138 -0.571349
 H -1.924242 2.729758 -0.082882
 H 0.395644 3.403829 1.844528
 H -1.143781 4.264635 1.712769
 H -1.121035 2.590082 2.290011
 H -0.441918 -0.131453 -1.605166
 H 1.441878 1.720172 -1.301467
 H 1.637426 2.254845 0.367082
 H 1.383919 -0.699626 -0.468577
 H 1.580146 -0.115581 1.172469
 H -0.571972 0.827468 0.599482
 C 3.311202 0.113986 -0.045846
 O 3.983252 1.084839 -0.336791
 O 3.814100 -1.110527 0.177893
 H 5.568649 -0.932499 -0.926032
 C 5.256781 -1.250503 0.073553
 H 5.725768 -0.583173 0.803504
 H 5.120405 -3.358704 -0.402726
 C 5.594930 -2.703457 0.335577
 H 5.269860 -3.011815 1.335145
 H 6.679900 -2.842057 0.270151

Imaginary Frequency: 184i

TS12-EA-EAc

C 4.043990 2.995184 1.367259
 C 3.310667 2.486842 0.143248
 O 3.306388 1.034205 0.205814
 C 2.637436 0.394900 -0.768199
 C 2.747509 -1.112901 -0.624679
 C 1.475648 -1.838507 -1.061893
 N 0.294407 -1.520743 -0.223863
 C 0.420050 -1.803105 1.234434
 C 0.732957 -3.255842 1.583847
 O 2.043170 0.957143 -1.667741
 C -1.050163 -1.974483 -0.830171
 C -1.702639 -0.620095 -1.003729
 C -2.703126 -0.238306 -0.038403
 O -2.910576 -0.758864 1.062855
 O -3.414215 0.868595 -0.438649
 C -4.340055 1.403550 0.520511

C -5.006343 2.615890 -0.103497
 H 3.558287 -1.437461 -1.290708
 H 1.648809 -2.920088 -1.067031
 H 3.802305 2.795221 -0.784942
 H 2.275025 2.837500 0.111580
 H 5.077763 2.633635 1.388473
 H 3.543148 2.675774 2.287544
 H 4.064208 4.090656 1.350555
 H 1.189775 -1.136811 1.633987
 H -0.535822 -1.499175 1.669535
 H 1.721560 -3.565315 1.227926
 H 0.721975 -3.373680 2.673502
 H -0.012998 -3.942210 1.167702
 H 1.221737 -1.532590 -2.080459
 H 3.054901 -1.375935 0.390139
 H -0.853982 -2.504434 -1.764311
 H -1.557868 -2.638449 -0.128569
 H -1.860510 -0.265913 -2.020237
 H -3.804738 1.673140 1.438800
 H -5.078586 0.638862 0.787099
 H -5.722221 3.052102 0.603073
 H -5.549592 2.342280 -1.015134
 H -4.267696 3.383293 -0.360969
 H -0.290033 -0.412582 -0.461112

Imaginary Frequency: 1627i

TS13-EA-EAc

C -0.506693 3.529969 -1.798986
 C -0.037923 2.999936 -0.459427
 O -1.076339 2.122816 0.052394
 C -0.858615 1.572797 1.261069
 C -1.956714 0.589934 1.625273
 C -1.580558 -0.868966 1.319716
 N -1.329318 -1.165117 -0.116848
 C -2.485008 -0.929411 -1.026353
 C -3.705873 -1.813391 -0.782235
 O 0.098712 1.826045 1.964755
 C -0.708456 -2.541065 -0.278859
 C 0.756567 -2.480676 0.050863
 C 1.451418 -1.355771 -0.292034
 O 0.880166 -0.284719 -0.793964
 O 2.801489 -1.326708 -0.094877
 C 3.453017 -0.048825 -0.172677
 C 4.927502 -0.273494 0.109665
 H -2.111224 0.656719 2.706462
 H -2.374387 -1.525208 1.693532
 H 0.127856 3.805797 0.262159
 H 0.881164 2.415776 -0.550162
 H -1.440286 4.094382 -1.697579
 H -0.667446 2.713277 -2.511166
 H 0.255068 4.199953 -2.213517
 H -2.751453 0.127574 -0.949095
 H -2.104024 -1.085634 -2.040822
 H -4.144734 -1.653450 0.208413
 H -4.474448 -1.572409 -1.525222
 H -3.466808 -2.877248 -0.884940
 H -0.658525 -1.127958 1.846986
 H -2.891679 0.870486 1.133789
 H -1.242665 -3.260724 0.352092
 H -0.909716 -2.818924 -1.324192

H	1.244518	-3.320198	0.529764
H	3.012927	0.638138	0.560312
H	3.305873	0.386383	-1.167257
H	5.466605	0.679246	0.050970
H	5.366332	-0.961916	-0.621417
H	5.078471	-0.692628	1.110742
H	-0.320397	-0.521315	-0.514477

Imaginary Frequency: 1043i

TS14-EA-EAc

C	3.772266	2.575829	0.246329
C	2.462229	1.925871	0.658187
O	2.534468	0.478780	0.573520
C	2.261799	-0.077441	-0.624676
O	1.988267	0.560677	-1.623307
C	2.340100	-1.589677	-0.578485
C	0.977320	-2.222890	-0.905909
N	-0.060794	-1.879234	0.069897
C	-1.418141	-2.036483	-0.507900
C	-1.876769	-0.892608	-1.412965
C	-2.340277	0.292240	-0.746856
O	-1.760961	1.461295	-0.710842
C	-2.520969	2.614474	-0.214827
C	-2.390538	2.743613	1.289252
C	0.075904	-2.641333	1.322407
C	-0.510145	-1.903338	2.526662
O	-3.531167	0.094252	-0.257015
H	3.062166	-1.907191	-1.340748
H	1.105866	-3.317055	-1.008407
H	1.629563	2.272704	0.041477
H	2.235978	2.123302	1.709092
H	3.991962	2.383473	-0.808203
H	4.603550	2.200929	0.853578
H	3.706027	3.660809	0.390879
H	-0.380498	-3.645626	1.230594
H	1.141433	-2.809069	1.508728
H	-0.372117	-2.493228	3.441176
H	-0.010026	-0.937165	2.658553
H	-1.584206	-1.713290	2.416630
H	0.664211	-1.847532	-1.884476
H	2.716165	-1.916781	0.393639
H	-1.481166	-2.983540	-1.074083
H	-2.114278	-2.137064	0.329711
H	-1.216928	-0.719317	-2.265680
H	-3.560854	2.499684	-0.528986
H	-2.073168	3.463010	-0.735537
H	-2.906013	3.654078	1.616277
H	-1.339535	2.818038	1.587877
H	-2.845809	1.888875	1.799038
H	-3.388305	-0.872966	-0.986557

Imaginary Frequency: 1978i

TS15-RRR-EA-EAc

C	6.617220	0.750224	-1.310054
C	5.627922	-0.276308	-0.782440
O	4.316158	0.238896	-0.985686
C	3.258574	-0.608626	-0.600071
C	2.002512	-0.020278	-0.806111
C	0.759155	-0.833798	-0.690428

N	0.031864	-0.771066	0.663543
C	0.792954	-1.462580	1.741824
C	0.916320	-2.982746	1.630508
O	3.526682	-1.733739	-0.128962
C	-1.359208	-1.260656	0.567795
C	-2.300110	-0.178474	0.047952
H	1.962222	0.907543	-1.372572
H	0.010659	-0.499599	-1.416954
H	5.749021	-1.235162	-1.302655
H	5.803739	-0.472450	0.284800
H	6.454734	0.937296	-2.378009
H	6.517052	1.704228	-0.779030
H	7.645125	0.391235	-1.177757
H	-1.697106	-1.566860	1.563195
H	-1.421111	-2.142554	-0.084950
H	-2.350477	0.671505	0.735868
H	-2.003440	0.195381	-0.936084
H	0.950845	-1.897638	-0.885941
H	0.308696	-1.195474	2.690281
H	1.795605	-1.026542	1.737545
H	-0.058040	-3.480892	1.567497
H	1.525459	-3.262995	0.767907
H	1.421790	-3.361656	2.527278
H	0.189313	0.620164	1.073348
H	1.526585	1.605804	0.778990
N	0.645247	1.691220	1.315708
C	-0.169066	2.849928	0.863500
H	-0.409062	2.676945	-0.189435
H	-1.105466	2.831620	1.428456
C	0.556407	4.176491	1.045842
H	0.792711	4.359333	2.100816
H	1.491202	4.197699	0.474003
H	-0.075280	4.999481	0.693717
H	0.882240	1.766637	2.308325
O	-3.605829	-0.787643	-0.052570
C	-4.600352	0.002227	-0.515171
O	-4.435374	1.163530	-0.831147
C	-5.910602	-0.754897	-0.572223
H	-6.154955	-1.067668	0.451699
H	-5.737704	-1.682818	-1.131618
C	-7.048596	0.057746	-1.183605
H	-6.823548	0.340702	-2.217232
H	-7.973151	-0.529475	-1.185560
H	-7.229297	0.977264	-0.617674

Imaginary Frequency: 498i

TS15-RRS-EA-EAc

C	-2.962626	4.906595	0.194460
C	-1.776271	3.982666	-0.027783
O	-2.280579	2.722206	-0.459699
C	-1.312276	1.759026	-0.799663
C	-1.881654	0.528683	-1.154291
C	-1.044650	-0.534491	-1.783063
N	-0.509175	-1.618583	-0.839220
C	0.474286	-1.090628	0.136856
C	1.764901	-0.515313	-0.459575
O	-0.103502	2.075961	-0.747349
C	0.001396	-2.797122	-1.580611
C	-1.109841	-3.739473	-2.043703
H	-2.958228	0.495348	-1.307085

H	-1.623832	-1.088979	-2.529289
H	-1.092786	4.399514	-0.777962
H	-1.195388	3.866943	0.898434
H	-3.532173	5.041692	-0.732506
H	-3.641963	4.502424	0.954364
H	-2.619536	5.892105	0.532251
H	0.677166	-3.344843	-0.914488
H	0.598571	-2.470392	-2.444722
H	-1.669785	-4.141370	-1.190894
H	-0.673970	-4.586422	-2.586421
H	-1.819072	-3.247701	-2.718017
H	-0.171341	-0.111960	-2.299747
H	0.712404	-1.903349	0.831209
H	-0.028702	-0.303313	0.703874
H	2.217415	-1.184168	-1.200735
H	1.536288	0.434142	-0.958554
H	-1.678426	-1.892184	-0.010820
H	-2.814496	-0.762025	0.533036
N	-2.669277	-1.781924	0.637125
C	-2.570639	-2.214348	2.056739
H	-2.289112	-3.271596	2.053894
H	-1.748998	-1.649161	2.504775
C	-3.868004	-1.994492	2.823593
H	-4.144232	-0.933876	2.837692
H	-4.694179	-2.560415	2.376643
H	-3.752036	-2.329042	3.860385
H	-3.444666	-2.250865	0.160566
C	2.797396	-0.230991	0.607849
O	2.621935	-0.320733	1.808891
O	3.966335	0.153499	0.055910
C	5.040977	0.477504	0.973145
H	4.717982	1.298364	1.621488
H	5.240792	-0.393375	1.605950
C	6.250447	0.858975	0.144101
H	6.040782	1.733751	-0.480909
H	7.087296	1.104336	0.807807
H	6.559229	0.032951	-0.505904

Imaginary Frequency: 498i

TS15-RSR-EA-EAc

C	6.573890	0.142167	-1.598122
C	5.565571	-0.652764	-0.784537
O	4.261558	-0.245267	-1.186683
C	3.193377	-0.876416	-0.518916
C	1.943750	-0.396924	-0.937898
C	0.692848	-1.093754	-0.524800
N	-0.038288	-0.504989	0.694307
C	0.716220	-0.712147	1.961184
C	0.842049	-2.154721	2.453969
O	3.448498	-1.744206	0.341969
C	-1.431895	-0.989853	0.786489
C	-2.370537	-0.141199	-0.065774
H	1.913707	0.242453	-1.817642
H	-0.053273	-1.061618	-1.326865
H	5.699362	-1.730399	-0.947575
H	5.708171	-0.477092	0.290403
H	6.446462	-0.043386	-2.671088
H	6.460404	1.218629	-1.423138
H	7.595994	-0.143180	-1.320910
H	-1.762397	-0.934371	1.828578

H	-1.503359	-2.041265	0.475781
H	-2.419634	0.888463	0.302618
H	-2.069259	-0.114430	-1.117507
H	0.874950	-2.151162	-0.291226
H	0.224629	-0.097660	2.726174
H	1.717376	-0.306654	1.791786
H	-0.132202	-2.640090	2.583769
H	1.458022	-2.746619	1.772842
H	1.340698	-2.152568	3.430992
H	0.086173	0.929855	0.461964
H	1.386653	1.746846	-0.247185
N	0.471915	2.012863	0.158534
C	0.595255	2.997760	1.266217
H	-0.401204	3.125306	1.699615
H	1.236936	2.542145	2.025206
C	1.164004	4.330722	0.798185
H	2.167055	4.206710	0.374116
H	0.521956	4.791049	0.037821
H	1.235964	5.024095	1.643463
H	-0.104371	2.381839	-0.603240
O	-3.677583	-0.746315	0.036410
C	-4.683998	-0.107934	-0.601057
O	-4.529180	0.924860	-1.221744
C	-5.990543	-0.855647	-0.436894
H	-6.143908	-1.036322	0.634348
H	-5.860243	-1.848032	-0.888576
C	-7.180652	-0.125480	-1.052528
H	-7.036631	0.033298	-2.125990
H	-8.095685	-0.710989	-0.913716
H	-7.330124	0.854583	-0.587431

Imaginary Frequency: 499i

TS15-RSS-EA-EAc

C	-2.484862	5.143555	0.156089
C	-1.375129	4.132793	-0.083702
O	-1.985903	2.889868	-0.417777
C	-1.106925	1.840787	-0.745085
C	-1.778423	0.630446	-0.963481
C	-1.060822	-0.536770	-1.552205
N	-0.542498	-1.585318	-0.558376
C	0.524295	-1.058188	0.327077
C	1.820773	-0.622683	-0.366270
O	0.119774	2.077791	-0.800385
C	-0.143900	-2.840765	-1.240812
C	-1.327108	-3.753080	-1.562286
H	-2.863687	0.660511	-1.034938
H	-1.723600	-1.102362	-2.216081
H	-0.711495	4.464612	-0.892000
H	-0.749824	4.024407	0.814168
H	-3.098279	5.271924	-0.743356
H	-3.142019	4.821733	0.972789
H	-2.060433	6.118852	0.423544
H	0.550149	-3.375898	-0.583325
H	0.406772	-2.607041	-2.164076
H	-1.844883	-4.071222	-0.649854
H	-0.968883	-4.653809	-2.074571
H	-2.057174	-3.270264	-2.220770
H	-0.194491	-0.220391	-2.150571
H	0.737569	-1.832618	1.072251
H	0.106593	-0.196610	0.853790

H	2.194221	-1.373104	-1.071590
H	1.629703	0.301552	-0.925584
H	-1.646607	-1.704038	0.387722
H	-2.635491	-0.437496	0.909519
N	-2.519441	-1.437899	1.150025
C	-3.783186	-2.201774	0.979401
H	-4.074225	-2.102751	-0.070292
H	-3.555037	-3.255073	1.166702
C	-4.888551	-1.707239	1.903069
H	-4.602197	-1.810511	2.956504
H	-5.122028	-0.653749	1.710752
H	-5.801032	-2.291899	1.742130
H	-2.177649	-1.494305	2.112959
C	2.913983	-0.327363	0.635204
O	2.764273	-0.227017	1.838929
O	4.104200	-0.171991	0.020287
C	5.235898	0.144491	0.869199
H	5.048613	1.101838	1.366529
H	5.324428	-0.625252	1.642376
C	6.468219	0.201449	-0.010300
H	6.371477	0.976146	-0.778618
H	7.344911	0.436022	0.604110
H	6.643843	-0.759836	-0.505575

Imaginary Frequency: 505i

TS16-RR-EA-EAc

C	5.937884	-1.986675	-1.519567
C	5.141077	-1.200481	-0.493094
O	3.792340	-1.109992	-0.966123
C	2.903789	-0.405207	-0.169108
C	1.661510	-0.146394	-0.797904
C	0.417490	0.025550	0.035937
N	-0.363600	-1.221522	0.261749
C	-1.684569	-0.944312	0.828332
C	-2.696252	-0.703590	-0.289341
O	3.293457	0.035822	0.940660
C	0.362885	-2.288333	0.959211
C	0.801888	-2.006326	2.405373
H	1.513372	-0.633037	-1.762117
H	0.686995	0.496181	0.999424
H	5.163376	-1.693827	0.485534
H	5.561605	-0.195471	-0.356052
H	5.524032	-2.992937	-1.650743
H	5.930169	-1.484014	-2.493559
H	6.979696	-2.084576	-1.191934
H	1.248576	-2.527713	0.360584
H	-0.277954	-3.179844	0.941260
H	1.537667	-1.196606	2.444603
H	1.271061	-2.901885	2.833580
H	-0.048334	-1.742102	3.047210
H	-0.283372	0.714985	-0.454711
H	-1.684639	-0.077250	1.512590
H	-2.020871	-1.806358	1.414908
H	-2.401617	0.124468	-0.940924
H	-2.811019	-1.598409	-0.908320
H	2.164734	1.599086	-0.751564
H	3.072770	2.038868	0.540453
N	2.640520	2.485022	-0.284422
C	1.700603	3.585682	0.069735
H	1.217837	3.904849	-0.857780

H	0.937935	3.149739	0.719423
C	2.417816	4.740896	0.752362
H	2.901914	4.414554	1.679917
H	3.180369	5.178877	0.097717
H	1.697331	5.526574	1.003568
H	3.391843	2.814380	-0.897336
O	-3.963585	-0.382932	0.336117
C	-4.994853	-0.115813	-0.489960
O	-4.904608	-0.128509	-1.702155
C	-6.252895	0.195159	0.296412
H	-6.020629	1.015236	0.987892
H	-6.471664	-0.674143	0.930229
C	-7.446168	0.542390	-0.588992
H	-7.696268	-0.284662	-1.261324
H	-8.325091	0.757345	0.028449
H	-7.240335	1.422800	-1.206620

Imaginary Frequency: 172i

TS16-RS-EA-EAc

C	1.550533	-4.042858	-2.154747
C	1.250808	-3.147463	-0.965226
O	1.517916	-1.796046	-1.358408
C	1.292821	-0.820104	-0.400888
C	1.779194	0.457344	-0.766751
C	1.157822	1.701659	-0.183167
N	0.022043	2.270753	-0.957716
C	-1.106438	1.363019	-1.148491
C	-1.852044	0.941333	0.123747
O	0.806130	-1.152082	0.709575
C	-0.370344	3.602326	-0.477789
C	0.544227	4.715618	-0.997447
H	2.145389	0.549291	-1.789088
H	0.855025	1.504305	0.862701
H	0.205464	-3.246895	-0.651010
H	1.873219	-3.419092	-0.102310
H	0.921991	-3.778579	-3.012778
H	2.599699	-3.957299	-2.460221
H	1.352860	-5.089947	-1.896254
H	-0.411473	3.650046	0.627442
H	-1.389221	3.801981	-0.831024
H	1.575671	4.606099	-0.643669
H	0.183380	5.694700	-0.657713
H	0.562514	4.715913	-2.093463
H	1.902299	2.506837	-0.134430
H	-0.745394	0.461261	-1.653964
H	-1.821976	1.847329	-1.825115
H	-1.223937	0.329131	0.774967
H	-2.222729	1.802218	0.689393
H	2.945181	0.279165	0.615569
H	2.364899	-0.548098	1.903938
N	3.208839	-0.008319	1.653506
C	4.456603	-0.821032	1.729137
H	4.537991	-1.222450	2.742899
H	4.323935	-1.657179	1.037550
C	5.670184	0.017294	1.358857
H	5.581670	0.414860	0.341763
H	5.799498	0.857274	2.051700
H	6.573152	-0.600075	1.405923
H	3.258593	0.825656	2.244267
O	-2.986897	0.146583	-0.311018

C -3.812192 -0.305421 0.651998
O -3.656436 -0.075938 1.836054
C -4.947412 -1.116783 0.057616
H -4.508076 -1.888662 -0.586559
H -5.510720 -0.455739 -0.614397
C -5.862798 -1.732335 1.112080
H -6.320215 -0.961258 1.740441
H -6.665961 -2.301036 0.630856
H -5.310387 -2.412513 1.768873

Imaginary Frequency: 175i

TS17-EA-EAc

C -6.525326 -1.817534 -0.529320
C -5.350535 -0.907251 -0.847618
O -4.161432 -1.570662 -0.424424
C -2.962651 -0.875701 -0.618000
C -1.855342 -1.530566 -0.100070
C -0.473700 -1.053980 -0.358844
N 0.141764 -0.125886 0.701650
C 1.452145 0.424705 0.269732
C 2.581784 -0.595873 0.082646
O -3.008455 0.238903 -1.224943
C 0.191333 -0.746894 2.060361
C -0.921053 -0.267257 2.992069
H -2.001318 -2.489777 0.387125
H 0.218116 -1.899920 -0.464657
H -5.307461 -0.689335 -1.922355
H -5.455391 0.057197 -0.332186
H -6.432968 -2.775360 -1.054224
H -6.584061 -2.023086 0.545903
H -7.465335 -1.346122 -0.840490
H 1.159963 -0.510242 2.511727
H 0.144501 -1.836915 1.954645
H -0.844290 0.808662 3.189443
H -0.840512 -0.786657 3.954669
H -1.907672 -0.478746 2.569995
H -0.431313 -0.460997 -1.281274
H 1.756266 1.171643 1.010413
H 1.287283 0.956380 -0.672296
H 2.757067 -1.181904 0.991632
H 2.342248 -1.317739 -0.706925
H -0.691595 0.931804 0.668111
H -2.205668 1.373845 -0.209701
N -1.552670 1.846021 0.464939
H -2.068418 2.018976 1.330322
C -1.029637 3.117698 -0.089249
H -0.497027 2.870565 -1.013106
H -0.295256 3.520732 0.616360
C -2.126990 4.140955 -0.364825
H -2.663919 4.402725 0.555300
H -1.695443 5.060915 -0.776218
H -2.854965 3.754393 -1.087375
C 3.879291 0.084712 -0.305044
O 3.990806 1.257698 -0.607270
O 4.907042 -0.783245 -0.285891
C 6.203773 -0.256633 -0.673711
H 6.131653 0.139860 -1.691348
H 6.459822 0.571560 -0.005708
C 7.208016 -1.386594 -0.580396
H 7.275474 -1.774048 0.441967

H 6.938796 -2.211825 -1.248423
H 8.197435 -1.017798 -0.873615

Imaginary Frequency: 1004i

TS18-RRR-EA-EAc

C 6.615003 2.213804 -1.007343
C 5.933094 0.866883 -1.189221
O 4.532514 1.062353 -1.023964
C 3.737346 -0.099601 -1.103167
C 2.378067 0.173937 -0.898592
C 1.347957 -0.865529 -1.167806
N 0.855014 -1.657544 0.057668
C 1.931977 -2.526626 0.618480
C 2.374188 -3.714464 -0.237555
O 4.292611 -1.195893 -1.325989
C -0.362658 -2.447553 -0.243737
C -1.643521 -1.609795 -0.260893
H 2.070436 1.216265 -0.872758
H 0.439369 -0.417327 -1.584753
H 6.150128 0.455104 -2.184400
H 6.308719 0.137670 -0.459029
H 6.248170 2.941521 -1.740761
H 6.427939 2.617900 -0.005390
H 7.699280 2.113352 -1.138522
H -0.465113 -3.226055 0.517108
H -0.247796 -2.959849 -1.207892
H -1.792130 -1.108179 0.704993
H -1.616311 -0.822580 -1.020396
H 1.702212 -1.613443 -1.889676
H 1.573488 -2.882816 1.592265
H 2.792119 -1.874666 0.788347
H 1.549363 -4.393941 -0.478952
H 2.852872 -3.374264 -1.158592
H 3.119181 -4.290614 0.324817
H 0.685173 -0.660541 1.049102
H 1.599448 0.757095 1.344813
N 0.829371 0.281867 1.838192
C -0.336133 1.198108 1.950575
H -1.217883 0.603447 2.199490
H -0.161503 1.890696 2.780321
C -0.569703 1.981736 0.661804
H 0.313421 2.579929 0.403285
H -0.751272 1.317750 -0.189843
C 1.345581 -0.193319 3.157099
H 1.583724 0.685443 3.767997
H 2.281492 -0.718680 2.950675
C 0.368635 -1.105574 3.889123
H 0.100778 -1.978702 3.283375
H 0.838625 -1.468148 4.809735
H -0.551555 -0.583968 4.172266
C -2.866503 -2.472369 -0.510231
O -2.895923 -3.685018 -0.425899
O -3.936799 -1.717915 -0.817633
C -5.183703 -2.428994 -1.041442
H -5.032435 -3.155617 -1.845508
H -5.440845 -2.980607 -0.131546
C -6.240958 -1.404870 -1.398396
H -6.382782 -0.682212 -0.587485
H -5.971489 -0.858637 -2.308760
H -7.195297 -1.913925 -1.573916

C	-1.748449	2.926300	0.800051
O	-2.370553	3.117595	1.827369
O	-2.011556	3.540384	-0.364434
C	-3.101435	4.502332	-0.356268
H	-4.016078	3.991824	-0.039479
H	-2.874379	5.279723	0.379835
C	-3.227238	5.068657	-1.755073
H	-3.456577	4.282255	-2.482070
H	-4.040437	5.802861	-1.776033
H	-2.304366	5.571248	-2.063731

Imaginary Frequency: 951i

TS18-RRS-EA-EAc

C	4.854097	-2.578010	-3.356311
C	4.461938	-1.541022	-2.316154
O	3.547872	-2.156790	-1.414036
C	3.067645	-1.340417	-0.373048
C	2.137830	-2.003632	0.437178
C	1.675064	-1.394888	1.712444
N	0.329075	-0.647031	1.654601
C	0.388892	0.544915	0.768502
C	1.345732	1.661567	1.200608
O	3.492377	-0.166877	-0.284090
C	-0.164807	-0.297331	3.012553
C	-0.830123	-1.458948	3.748447
H	2.009953	-3.073012	0.291248
H	1.520910	-2.159505	2.481076
H	5.346870	-1.175412	-1.778609
H	4.000011	-0.666390	-2.794275
H	5.338260	-3.442356	-2.886656
H	3.974744	-2.937010	-3.903981
H	5.555039	-2.145481	-4.080616
H	-0.890274	0.516671	2.904563
H	0.667269	0.093618	3.615090
H	-1.714479	-1.820031	3.211402
H	-1.158459	-1.119868	4.738022
H	-0.149649	-2.302636	3.901344
H	2.404937	-0.675762	2.108772
H	-0.628805	0.938719	0.682648
H	0.696051	0.189321	-0.217655
H	1.202922	1.954233	2.248288
H	2.379710	1.321621	1.081099
H	-0.497746	-1.543774	0.934863
H	-0.097481	-2.598770	-0.355529
N	-0.978668	-2.323350	0.102659
C	-1.632979	-3.531656	0.683390
H	-2.371274	-3.192892	1.415482
H	-2.173073	-4.046941	-0.119801
C	-0.629096	-4.477612	1.329969
H	0.088598	-4.859176	0.595308
H	-0.072855	-3.994384	2.138789
H	-1.163591	-5.334874	1.753438
C	-1.808043	-1.605431	-0.905882
H	-2.119202	-2.315711	-1.678542
H	-1.164061	-0.861104	-1.379012
C	-3.025893	-0.930346	-0.279523
H	-2.729163	-0.247171	0.524225
H	-3.705599	-1.664126	0.170810
C	1.161024	2.899572	0.350196
O	0.304352	3.054999	-0.500429

O	2.080262	3.837028	0.654660
C	2.013854	5.073291	-0.100558
H	2.109707	4.840855	-1.165870
H	1.031956	5.531772	0.056825
C	3.135879	5.969121	0.382248
H	3.030479	6.196366	1.448762
H	4.112452	5.499744	0.221698
H	3.113550	6.913273	-0.173760
C	-3.817254	-0.147193	-1.309289
O	-3.612720	-0.165984	-2.507265
O	-4.791784	0.566590	-0.721442
C	-5.644026	1.350361	-1.600323
H	-5.016701	2.038727	-2.174697
H	-6.137644	0.672729	-2.304068
C	-6.641769	2.086788	-0.730769
H	-7.260448	1.387461	-0.158028
H	-6.134275	2.758426	-0.030010
H	-7.302157	2.689001	-1.364701

Imaginary Frequency: 947i

TS18-RSR-EA-EAc

C	-7.182529	-0.223810	1.042549
C	-6.182207	-0.454378	-0.078879
O	-4.953472	-0.861767	0.513569
C	-3.889628	-1.099811	-0.380960
C	-2.703682	-1.433670	0.285841
C	-1.526752	-1.941029	-0.468163
N	-0.448065	-0.895900	-0.815757
C	-0.952290	0.098621	-1.808676
C	-1.198557	-0.410707	-3.229717
O	-4.095653	-0.987646	-1.607681
C	0.808503	-1.529875	-1.283414
C	1.666259	-2.078158	-0.141284
H	-2.757332	-1.618138	1.355603
H	-0.990587	-2.703839	0.106715
H	-6.548276	-1.221605	-0.774362
H	-6.041101	0.462214	-0.668134
H	-7.348538	-1.143207	1.616271
H	-6.825817	0.548325	1.734599
H	-8.146347	0.102615	0.633235
H	1.389349	-0.780612	-1.829861
H	0.582135	-2.335116	-1.993495
H	1.926436	-1.283643	0.568892
H	1.140967	-2.846766	0.436170
H	-1.821847	-2.398319	-1.421777
H	-0.224484	0.919601	-1.831510
H	-1.890762	0.484207	-1.403584
H	-0.295170	-0.820105	-3.695234
H	-1.992131	-1.161343	-3.245541
H	-1.533143	0.431514	-3.847613
H	-0.320509	-0.140380	0.375344
H	-1.511977	0.311033	1.516709
N	-0.517674	0.548108	1.384651
C	0.249742	0.140875	2.597034
H	1.311038	0.119971	2.332625
H	0.114336	0.914708	3.362308
C	-0.196787	-1.211455	3.137479
H	-1.245841	-1.187459	3.451887
H	-0.076405	-2.009873	2.398938
H	0.410363	-1.468548	4.012181

C	-0.438461	2.002753	1.074198
H	-0.746068	2.569474	1.959151
H	-1.164795	2.202136	0.283920
C	0.959581	2.426029	0.631088
H	1.280792	1.855465	-0.249109
H	1.707221	2.240918	1.410249
C	2.958998	-2.686241	-0.649060
O	3.311640	-2.714457	-1.805615
O	3.680038	-3.195802	0.364746
C	4.948587	-3.810022	0.013733
H	4.754616	-4.659145	-0.649340
H	5.552453	-3.082169	-0.536736
C	5.620515	-4.243355	1.300321
H	5.824221	-3.385030	1.949643
H	4.998377	-4.957011	1.851109
H	6.574254	-4.729785	1.066822
C	1.008659	3.899819	0.277578
O	0.056321	4.644194	0.273042
O	2.257874	4.275226	-0.036693
C	2.444334	5.671582	-0.394952
H	1.808885	5.900791	-1.255794
H	2.116513	6.293220	0.443897
C	3.912717	5.872012	-0.706923
H	4.087631	6.919410	-0.976901
H	4.537771	5.633340	0.160346
H	4.227936	5.244631	-1.547582

Imaginary Frequency: 960i

TS18-RSS-EA-EAc

C	1.086971	5.731571	1.096561
C	1.695963	4.499050	0.447623
O	0.644012	3.566660	0.217785
C	1.020137	2.350325	-0.382329
C	-0.060383	1.470857	-0.524594
C	0.074749	0.228961	-1.331923
N	0.369440	-1.060247	-0.543239
C	1.691845	-1.011398	0.134208
C	2.914331	-0.915385	-0.785320
O	2.217320	2.183968	-0.705803
C	0.232594	-2.270581	-1.395816
C	-1.213832	-2.707492	-1.618361
H	-1.056622	1.858290	-0.327358
H	-0.853392	0.007086	-1.869109
H	2.191566	4.760866	-0.496437
H	2.465228	4.058159	1.096348
H	0.332186	6.185838	0.443915
H	0.604899	5.477019	2.047908
H	1.862738	6.480664	1.296173
H	0.778574	-3.085644	-0.907965
H	0.719067	-2.094104	-2.365485
H	-1.704284	-2.965354	-0.673053
H	-1.229322	-3.600973	-2.253489
H	-1.810611	-1.939936	-2.121392
H	0.871743	0.314981	-2.083341
H	1.767115	-1.902165	0.766238
H	1.680511	-0.136220	0.787385
H	2.907629	-1.671633	-1.578678
H	2.931412	0.073140	-1.258710
H	-0.552774	-0.992042	0.529455
H	-1.114121	0.378216	1.392425

N	-1.237146	-0.639576	1.498471
C	-2.681388	-0.983428	1.410197
H	-2.768633	-2.053989	1.212818
H	-3.150631	-0.785951	2.379881
C	-3.383843	-0.179713	0.319523
H	-3.305506	0.897098	0.514023
H	-2.927246	-0.348091	-0.662158
C	-0.599735	-1.047062	2.786919
H	-1.158304	-0.580535	3.606774
H	0.405598	-0.618588	2.782100
C	-0.538871	-2.557822	2.971771
H	-0.007891	-3.044453	2.145924
H	0.002316	-2.784589	3.896702
H	-1.535082	-3.004534	3.053887
C	4.201363	-1.066502	-0.006093
O	4.289690	-1.191810	1.201325
O	5.269640	-1.033598	-0.828119
C	6.571991	-1.135599	-0.199220
H	6.673596	-0.328785	0.533401
H	6.632272	-2.087870	0.338000
C	7.619594	-1.039560	-1.289633
H	7.509231	-1.849907	-2.018530
H	7.550337	-0.083559	-1.819742
H	8.618083	-1.113942	-0.844094
C	-4.854928	-0.536348	0.229434
O	-5.419813	-1.352657	0.931869
O	-5.460794	0.174663	-0.734885
C	-6.881334	-0.065773	-0.924695
H	-7.029636	-1.126224	-1.151204
H	-7.401887	0.157137	0.011972
C	-7.348305	0.824404	-2.057416
H	-6.814997	0.593895	-2.986002
H	-8.418823	0.664486	-2.227933
H	-7.192354	1.882139	-1.819689

Imaginary Frequency: 944i

TS19-EA-EAc

C	-1.414693	-6.117738	-0.814080
C	-2.045810	-5.155319	0.182390
O	-1.074589	-4.254472	0.734076
C	-0.860259	-3.064098	0.053115
C	0.011187	-2.173992	0.740980
C	0.846403	-1.197104	-0.052758
N	2.196101	-1.691653	-0.435782
C	3.052158	-0.615321	-0.936944
C	3.788024	0.053746	0.220902
O	-1.509602	-2.814055	-0.985944
C	2.199863	-2.887188	-1.286507
C	1.590156	-2.748143	-2.691014
H	0.506083	-2.595816	1.616412
H	0.277780	-0.877107	-0.945176
H	-2.851197	-4.586031	-0.290350
H	-2.453610	-5.701327	1.040321
H	-1.022836	-5.571580	-1.678198
H	-0.592292	-6.674902	-0.350573
H	-2.159558	-6.840094	-1.171445
H	1.669345	-3.677950	-0.744980
H	3.243668	-3.216289	-1.375218
H	0.518726	-2.530263	-2.638210
H	1.711092	-3.688706	-3.244328

H	2.081443	-1.958072	-3.273155
H	1.032971	-0.286959	0.533297
H	2.492901	0.149778	-1.504270
H	3.798765	-1.030521	-1.622781
H	3.099901	0.477924	0.957740
H	4.435179	-0.663893	0.734331
H	-1.369324	-1.152021	1.009945
H	-2.578777	-1.052778	-0.108273
N	-2.356130	-0.626747	0.800935
C	-3.365536	-1.075876	1.812476
H	-4.349232	-0.699213	1.518436
H	-3.387362	-2.166182	1.734227
C	-2.998176	-0.653036	3.227628
H	-1.996114	-1.004954	3.496059
H	-3.035885	0.432508	3.363314
H	-3.712634	-1.098621	3.927690
C	-2.146003	0.834489	0.633470
H	-1.332308	0.953072	-0.086021
H	-1.820021	1.249579	1.589323
C	-3.392070	1.547062	0.122852
H	-4.205295	1.544484	0.853767
H	-3.758739	1.089612	-0.802839
O	4.596901	1.118448	-0.337429
C	5.270779	1.888948	0.540017
O	5.217752	1.737886	1.745046
C	6.089213	2.942828	-0.179700
H	5.419970	3.481122	-0.862482
H	6.809172	2.419354	-0.822704
O	-2.982672	2.904071	-0.132724
C	-3.946032	3.741564	-0.588625
O	-5.092548	3.390116	-0.774705
C	-3.387868	5.128882	-0.820500
H	-2.537189	5.033852	-1.507337
H	-2.964576	5.479843	0.129511
C	6.801337	3.903195	0.768668
H	7.480169	3.367454	1.439864
H	7.388866	4.631340	0.199060
H	6.086058	4.454127	1.388380
C	-4.424066	6.111181	-1.358544
H	-5.259765	6.230034	-0.661409
H	-3.966202	7.094257	-1.511119
H	-4.832545	5.773295	-2.316404

Imaginary Frequency: 203i

TS20-EA-EAc

C	-4.013002	-3.347996	-2.836555
C	-3.620774	-3.711088	-1.409364
O	-2.209010	-3.858469	-1.254965
C	-1.472044	-2.690109	-1.028675
C	-0.105281	-2.909936	-0.955301
C	0.863262	-1.793769	-0.877744
N	1.302001	-1.324478	0.534421
C	2.185597	-0.128049	0.446976
C	3.563801	-0.355017	-0.176622
O	-2.097351	-1.590578	-0.914099
C	1.953706	-2.413348	1.330772
C	1.007072	-3.270165	2.166158
H	0.264227	-3.923096	-1.078148
H	1.792677	-2.046456	-1.403043
H	-3.998814	-2.959112	-0.710052

H	-4.042433	-4.685339	-1.134762
H	-3.617206	-2.362178	-3.100186
H	-3.621766	-4.084033	-3.549087
H	-5.105700	-3.320763	-2.938864
H	2.678666	-1.940231	2.000714
H	2.522097	-3.050464	0.641245
H	0.515252	-2.681428	2.947195
H	1.590788	-4.054963	2.663283
H	0.244204	-3.745970	1.547137
H	0.450233	-0.883410	-1.329328
H	2.317693	0.264240	1.461313
H	1.661708	0.631681	-0.139225
H	4.142788	-1.119979	0.347382
H	3.506038	-0.630502	-1.232247
H	0.166364	-0.855881	1.046191
H	-1.576338	-0.837696	0.582200
N	-1.011502	-0.331800	1.303342
C	-1.499545	-0.618991	2.683982
H	-0.625403	-0.763900	3.329470
H	-2.035050	0.255271	3.068662
C	-2.413222	-1.838486	2.729553
H	-3.330293	-1.662464	2.156400
H	-1.923168	-2.727689	2.321203
H	-2.695838	-2.052962	3.766420
C	-1.026907	1.104882	0.939408
H	-0.419778	1.237615	0.040436
H	-0.564876	1.682708	1.746259
C	-2.437390	1.611126	0.649575
H	-3.098138	1.534453	1.518234
H	-2.885509	1.050420	-0.175909
O	4.241580	0.916612	-0.056947
C	5.499538	0.973757	-0.551067
O	6.053397	0.026935	-1.071610
C	6.092044	2.354413	-0.360425
H	6.039593	2.594686	0.709280
H	5.428017	3.072970	-0.858176
O	-2.298480	2.999466	-0.276531
C	-3.441137	3.653862	-0.032211
O	-4.536792	3.131813	0.002506
C	-3.155998	5.091882	-0.412632
H	-2.415495	5.084033	-1.222633
H	-2.656658	5.568804	0.440961
C	7.521047	2.472017	-0.882406
H	8.189458	1.770141	-0.373207
H	7.570938	2.261464	-1.955571
H	7.900482	3.485874	-0.716384
C	-4.408583	5.863437	-0.817820
H	-4.148985	6.895468	-1.076925
H	-4.893584	5.405930	-1.686263
H	-5.139550	5.889930	-0.003260

Imaginary Frequency: 1178i

S7.5 Ethylamine to ethyl crotonate

ECR

O	1.099311	-0.399075	0.000026
O	0.053124	1.609624	-0.000008
C	0.002155	0.390482	-0.000003
C	-1.230567	-0.425611	-0.000023
C	-2.442222	0.147261	0.000058

C	2.378307	0.279673	-0.000050
H	2.437585	0.921884	-0.884845
H	2.437605	0.922036	0.884629
C	3.462392	-0.779413	0.000034
H	3.393420	-1.415729	-0.888883
H	3.393617	-1.415413	0.889193
H	4.445761	-0.296112	-0.000165
H	-2.489162	1.236131	0.000162
H	-1.109163	-1.505637	-0.000125
C	-3.743377	-0.585898	-0.000015
H	-4.342071	-0.309420	0.878876
H	-4.342029	-0.309288	-0.878901
H	-3.605169	-1.671809	-0.000099

ZI1-EA-ECR

C	3.991577	-0.691126	0.758540
C	3.297962	-0.475194	-0.580012
O	2.363387	0.608321	-0.535072
C	1.078596	0.309546	-0.103200
C	0.182470	1.363622	-0.134637
C	-1.197868	1.143971	0.384242
N	-1.715580	-0.179492	-0.233996
C	-2.934327	-0.810469	0.351664
C	-3.196416	-2.173262	-0.275411
O	0.801511	-0.885006	0.250225
H	4.485719	0.227966	1.095192
H	4.753777	-1.476448	0.672613
H	3.265466	-0.996021	1.518546
H	4.027103	-0.190912	-1.347490
H	2.791019	-1.390318	-0.900065
H	0.461338	2.335069	-0.525507
H	-1.233455	0.907148	1.459915
H	-1.828225	-0.038254	-1.243331
H	-0.861720	-0.797033	-0.099817
H	-2.756059	-0.897166	1.427067
H	-3.776731	-0.132509	0.195437
H	-3.368255	-2.091002	-1.355036
H	-2.355407	-2.855847	-0.109181
H	-4.089700	-2.619907	0.173909
C	-2.162180	2.285412	0.084967
H	-2.233191	2.467266	-0.994360
H	-3.166826	2.101914	0.479865
H	-1.783854	3.200971	0.552081

P1-EA-ECR

C	3.626776	-1.933383	0.433450
C	3.206837	-0.589131	-0.155527
N	1.887781	-0.197107	0.354448
C	1.303797	0.989376	-0.293340
C	-0.146297	1.156810	0.182932
C	-1.088081	0.049731	-0.249082
O	-0.774345	-0.948951	-0.873382
O	-2.345889	0.306110	0.150644
C	-3.351189	-0.688584	-0.180222
C	-4.646483	-0.271537	0.485302
H	-4.535619	-0.234024	1.574399
H	-0.559371	2.103220	-0.186322
H	1.290035	0.874771	-1.393731
H	-3.449470	-0.736175	-1.269594
H	-3.008207	-1.666135	0.171589
H	-5.430132	-0.998927	0.245278

H	-4.974417	0.712952	0.134334
H	3.226890	-0.648127	-1.261116
H	3.940665	0.173803	0.129439
H	2.929717	-2.728985	0.139819
H	4.625052	-2.218335	0.081624
H	3.646261	-1.889722	1.528698
H	-0.173836	1.215052	1.279077
H	1.254147	-0.971612	0.155507
C	2.103374	2.253138	0.041872
H	3.123571	2.203538	-0.352067
H	1.625513	3.137123	-0.396372
H	2.164207	2.395554	1.127897

I1-EA-ECR

C	3.962235	-0.882739	0.665773
C	3.327246	-0.321352	-0.596836
O	2.385873	0.732079	-0.304625
C	1.089406	0.413477	-0.071391
C	0.150241	1.384377	0.012605
C	-1.289163	1.094029	0.385832
N	-1.693560	-0.223417	-0.190367
C	-2.921865	-0.818022	0.360707
C	-3.198170	-2.177392	-0.274071
O	0.829784	-0.899025	0.056160
H	4.440548	-0.086456	1.247300
H	4.730332	-1.619153	0.398657
H	3.215637	-1.376796	1.295163
H	4.082750	0.158569	-1.226665
H	2.840795	-1.107898	-1.179168
H	0.456822	2.413881	-0.135460
H	-1.389707	0.960620	1.475654
H	-1.797553	-0.108994	-1.201183
H	-0.190486	-0.945898	0.002084
H	-2.775700	-0.931071	1.441649
H	-3.794535	-0.161788	0.221594
H	-3.342168	-2.087442	-1.358293
H	-2.367984	-2.871398	-0.098653
H	-4.109069	-2.618774	0.146144
C	-2.211554	2.247345	-0.031775
H	-2.184209	2.390822	-1.119603
H	-3.249508	2.068998	0.269095
H	-1.886551	3.183926	0.436915

ZI2-EA-ECR

C	-5.651223	-2.656884	0.091407
C	-4.175820	-2.305341	0.011917
O	-4.079761	-0.936044	-0.391379
C	-2.804161	-0.415434	-0.509296
C	-2.737844	0.941358	-0.802546
C	-1.407080	1.544178	-0.998839
N	-0.452140	1.126974	0.241470
C	1.030308	1.226094	-0.079316
C	1.723775	-0.107997	0.243680
O	-1.802142	-1.174216	-0.318690
C	-0.917896	1.677994	1.553368
C	-0.555104	0.796626	2.743774
H	-3.625670	1.563385	-0.799353
H	-3.657582	-2.949294	-0.709022
H	-3.685220	-2.449134	0.983203
H	-6.139494	-2.526806	-0.881304
H	-6.168077	-2.022624	0.820817

H	1.833478	2.137066	1.709302
H	2.780052	2.357465	0.232808
H	1.278576	3.258696	0.451560

TS1-EA-ECR

C	4.183163	-0.561471	0.698424
C	3.333488	-0.694840	-0.557875
O	2.389038	0.377477	-0.686656
C	1.165466	0.208140	-0.065937
C	0.268286	1.278784	-0.285931
C	-1.002602	1.234120	0.345159
N	-1.914674	-0.216644	-0.332124
C	-3.173596	-0.677870	0.290757
C	-3.609086	-2.058735	-0.194716
O	0.917419	-0.826907	0.587286
H	4.699870	0.404994	0.721529
H	4.941029	-1.354607	0.727783
H	3.560831	-0.646431	1.594827
H	3.959079	-0.631585	-1.454941
H	2.804226	-1.652038	-0.565153
H	0.478410	2.013932	-1.056865
H	-1.010436	0.816608	1.354143
H	-2.016819	-0.063116	-1.337172
H	-1.161315	-0.899833	-0.193412
H	-3.007886	-0.685355	1.373624
H	-3.943049	0.069293	0.076045
H	-3.793020	-2.060145	-1.275573
H	-2.845454	-2.813744	0.026008
H	-4.536461	-2.359205	0.306868
C	-1.941732	2.406504	0.172787
H	-2.014462	2.710161	-0.877935
H	-2.948443	2.192254	0.545290
H	-1.555360	3.262971	0.738743

Imaginary Frequency: 249i

TS3-EA-ECR

C	-3.489684	-0.988764	1.024391
C	-3.323418	-0.372457	-0.357426
O	-2.410264	0.737413	-0.355101
C	-1.070341	0.457265	-0.372575
C	-0.191418	1.465412	-0.093790
C	1.291641	1.217572	-0.220984
N	1.548307	-0.220044	0.177843
C	2.789971	-0.842429	-0.335088
C	2.946254	-2.260788	0.200600
O	-0.705650	-0.771815	-0.650176
H	-2.550398	-1.435751	1.365824
H	-4.253545	-1.775923	0.995289
H	-3.804467	-0.233950	1.754223
H	-2.995962	-1.122602	-1.082070
H	-4.269458	0.055309	-0.704388
H	-0.548128	2.453257	0.172301
H	1.634871	1.261377	-1.267870
H	1.519659	-0.282864	1.199212
H	0.477760	-0.728895	-0.260718
H	2.717359	-0.847577	-1.427623
H	3.657636	-0.229917	-0.062147
H	3.023319	-2.265932	1.294869
H	2.096064	-2.890307	-0.085912
H	3.857915	-2.715834	-0.201304

C	2.132256	2.193749	0.601660
H	1.867748	2.134301	1.664812
H	3.206039	2.003460	0.494421
H	1.941187	3.220010	0.267674

Imaginary Frequency: 961i

TS5-EA-ECR

C	-3.943450	1.062503	-0.794360
C	-3.855572	-0.312267	-0.141048
O	-2.764646	-0.405283	0.772967
C	-1.517852	-0.766908	0.228574
O	-1.463331	-1.134799	-0.977928
C	-0.461978	-0.630644	1.128521
C	0.881909	-1.260059	0.814022
C	2.550487	-1.372915	-1.130141
C	3.801394	-0.932764	-0.373563
H	-3.062777	1.244446	-1.420068
H	-4.835314	1.131688	-1.430702
H	-4.002033	1.853129	-0.036630
H	-3.769048	-1.090405	-0.905304
H	-4.754414	-0.506629	0.456560
H	-0.690335	-0.436521	2.173362
H	1.633025	-0.865627	1.511980
H	0.501108	-1.063367	-1.156929
H	2.605973	-1.016964	-2.166153
H	2.512485	-2.469644	-1.176843
H	3.811959	-1.307778	0.655839
H	3.881795	0.160564	-0.337448
H	4.696430	-1.318757	-0.874994
N	1.306406	-0.817261	-0.563329
H	1.196126	0.642074	-0.530151
N	0.814837	1.744610	-0.322831
H	0.347298	2.110021	-1.156637
H	0.084219	1.511311	0.374603
C	1.819753	2.704180	0.201745
H	2.262709	2.245364	1.090432
H	2.605463	2.800303	-0.553689
C	1.211880	4.061239	0.533257
H	0.429962	3.970012	1.296061
H	0.772096	4.526330	-0.357164
H	1.984841	4.735213	0.919047
C	0.877136	-2.796592	0.947524
H	0.164803	-3.235089	0.238789
H	1.861651	-3.255295	0.782696
H	0.554853	-3.069810	1.958965

Imaginary Frequency: 419i

TS6-EA-ECR

C	1.369160	4.334528	0.544894
C	0.762274	3.192327	-0.251625
O	0.836731	2.011242	0.553522
C	0.318254	0.850133	-0.007716
O	-0.105953	0.879028	-1.188482
C	0.200612	-0.221580	0.911884
C	0.303481	-1.659889	0.428562
H	0.644774	-0.038945	1.893607
H	-0.185169	-1.729276	-0.553926
H	1.301122	3.039987	-1.194256
H	-0.282939	3.407298	-0.511570

H	2.416797	4.127222	0.791026
H	0.823963	4.495520	1.482072
H	1.331360	5.262647	-0.037854
H	-1.590410	-0.014195	0.704183
N	-2.513575	0.237123	0.127518
H	-2.086427	0.549603	-0.759106
H	-2.956470	1.048202	0.568900
H	-2.939195	-1.694077	-0.538644
C	-3.484212	-0.876895	-0.060623
H	-3.791576	-1.206536	0.935341
H	-4.367191	-0.109853	-1.892838
C	-4.679935	-0.444406	-0.896980
H	-5.230044	0.371252	-0.413081
H	-5.367519	-1.287669	-1.022728
N	1.683668	-2.189611	0.218269
H	2.171809	-2.118895	1.114522
C	2.481029	-1.473642	-0.777789
H	2.585855	-0.397724	-0.552641
H	1.954104	-1.535264	-1.739474
C	3.868709	-2.098608	-0.908341
H	3.799993	-3.159972	-1.174797
H	4.424290	-2.025632	0.036269
H	4.458219	-1.586736	-1.678697
C	-0.386235	-2.635438	1.393493
H	-0.304656	-3.669115	1.036781
H	0.080743	-2.588506	2.387489
H	-1.447119	-2.393254	1.524034

Imaginary Frequency: 209i

TS8-EA-ECR

C	3.279704	4.737181	-0.244645
C	3.454846	3.288949	0.181527
O	2.618650	2.486961	-0.650295
C	2.703034	1.102372	-0.461039
O	3.511526	0.655667	0.402689
C	1.814537	0.369984	-1.248056
C	2.006009	-1.127063	-1.391050
C	2.308052	-3.191605	0.106610
C	1.318786	-4.076403	-0.645913
H	2.237734	5.058698	-0.131593
H	3.908537	5.391536	0.371173
H	3.566019	4.875059	-1.293690
H	3.183160	3.162383	1.238707
H	4.501995	2.976712	0.084420
H	1.282520	0.881889	-2.045539
H	1.137992	-1.550107	-1.911950
H	2.741939	-1.206799	0.483535
H	2.274020	-3.428818	1.177014
H	3.329598	-3.407600	-0.231736
H	1.377360	-3.928721	-1.729528
H	0.286168	-3.883683	-0.333580
H	1.539653	-5.130581	-0.443084
N	2.015277	-1.745363	-0.011045
H	0.853301	-1.292590	0.638591
N	-0.043828	-0.536426	1.032868
H	0.319841	0.267303	0.483627
C	-1.373850	-0.903263	0.453265
H	-1.165438	-1.121231	-0.598594
C	-2.343662	0.288064	0.496130
H	-2.695000	0.491139	1.512553

H	-1.830816	1.196844	0.150199
C	-3.541626	0.095702	-0.416368
O	-3.575600	-0.647608	-1.378595
O	-4.561571	0.887469	-0.045380
C	-5.753416	0.843676	-0.876270
H	-5.474184	1.090815	-1.905038
H	-6.146114	-0.177882	-0.867631
C	-6.745818	1.835734	-0.306117
H	-7.010629	1.582158	0.726108
H	-6.341635	2.853614	-0.322589
H	-7.661546	1.821679	-0.907742
C	0.001991	-0.215637	2.487634
H	-0.498623	0.744744	2.653786
H	-0.564727	-0.981077	3.022468
C	1.435558	-0.169799	3.010426
H	2.079950	0.467435	2.394967
H	1.880161	-1.171450	3.033240
H	1.435000	0.217477	4.035400
C	3.270333	-1.502710	-2.189712
H	3.216890	-1.038062	-3.180833
H	4.164005	-1.118279	-1.685434
H	3.390394	-2.583916	-2.340130
C	-1.955427	-2.158511	1.104393
H	-2.324546	-1.968096	2.117853
H	-2.798399	-2.516145	0.505684
H	-1.213076	-2.961858	1.154362

Imaginary Frequency: 946i

TS11-EA-ECR

C	-5.747293	-2.600723	0.182582
C	-4.270095	-2.303305	-0.001992
O	-4.147135	-0.919267	-0.353808
C	-2.864952	-0.446546	-0.535111
C	-2.779633	0.934923	-0.783636
C	-1.486261	1.489687	-1.068628
N	-0.394775	1.118652	0.288614
C	1.063356	1.234270	-0.066555
C	1.817468	-0.045550	0.335378
O	-1.886087	-1.230064	-0.445071
C	-0.874063	1.692566	1.570522
C	-0.471006	0.892471	2.807111
H	-3.638253	1.578703	-0.623851
H	-3.837907	-2.929459	-0.791690
H	-3.706949	-2.506802	0.917329
H	-6.306063	-2.399623	-0.738537
H	-6.175205	-1.987160	0.983632
H	-5.887946	-3.655578	0.446295
H	-0.532503	2.726805	1.640161
H	-1.965962	1.702092	1.478908
H	0.609457	0.907334	2.982815
H	-0.958688	1.320582	3.690776
H	-0.792225	-0.152261	2.721462
H	-0.889196	0.911059	-1.780775
H	1.085554	1.283407	-1.160582
H	1.217305	-0.932000	0.087886
H	2.004981	-0.088065	1.413076
H	-0.650079	0.115701	0.277415
C	-1.414281	2.977896	-1.343985
H	-0.389499	3.324359	-1.507746
H	-1.984964	3.194011	-2.254986

H	-1.859737	3.562875	-0.531863
C	3.136078	-0.205106	-0.401239
O	3.474889	0.424473	-1.385273
O	3.879296	-1.172753	0.160816
C	5.141756	-1.483429	-0.488837
H	4.943317	-1.746142	-1.532413
H	5.770539	-0.587762	-0.478031
C	5.776990	-2.629011	0.271271
H	5.138055	-3.518415	0.252086
H	6.736270	-2.885994	-0.191901
H	5.963038	-2.355858	1.315568
C	1.730852	2.496204	0.478773
H	1.817227	2.479049	1.570257
H	2.739857	2.561564	0.061212
H	1.191800	3.401819	0.185967

Imaginary Frequency: 209i

TS13-EA-ECR

C	-5.414152	-2.860666	-0.038785
C	-4.006664	-2.318421	0.129279
O	-3.951500	-1.048312	-0.541515
C	-2.769256	-0.371004	-0.503817
C	-2.735489	0.941579	-0.875828
C	-1.401729	1.638635	-0.948710
N	-0.515709	1.130041	0.204370
C	0.959348	1.226788	-0.091721
C	1.652707	-0.119546	0.195090
O	-1.705782	-1.022368	-0.083064
C	-0.966830	1.621509	1.538151
C	-0.571899	0.708605	2.697499
H	-3.641112	1.469830	-1.148318
H	-3.266679	-3.001575	-0.301170
H	-3.760118	-2.189393	1.190706
H	-5.655470	-3.005481	-1.097794
H	-6.153760	-2.176935	0.392771
H	-5.502507	-3.827936	0.469340
H	-0.606620	2.640394	1.708431
H	-2.057510	1.664110	1.476051
H	0.507864	0.692258	2.876041
H	-1.050767	1.069951	3.615111
H	-0.911883	-0.317554	2.522567
H	-0.838866	1.308703	-1.834650
H	1.030222	1.381258	-1.171245
H	1.034990	-0.943218	-0.187008
H	1.787628	-0.297842	1.265422
H	-0.949640	-0.084811	0.128974
C	-1.522502	3.160816	-1.018083
H	-0.544829	3.644385	-1.114861
H	-2.112872	3.428498	-1.902179
H	-2.035872	3.572530	-0.142735
C	2.994409	-0.238821	-0.505410
O	3.311029	0.355210	-1.519064
O	3.787592	-1.127805	0.117057
C	5.074630	-1.394180	-0.502400
H	4.904227	-1.774750	-1.514374
H	5.626619	-0.452745	-0.583312
C	5.800287	-2.401607	0.364591
H	5.235569	-3.337122	0.440528
H	6.777394	-2.625611	-0.077880
H	5.963060	-2.009121	1.374168

C	1.682160	2.395155	0.586345
H	1.742154	2.276702	1.673131
H	2.705527	2.444849	0.200232
H	1.202387	3.353489	0.366946

Imaginary Frequency: 1051i

TS15-EA-ECR

C	-0.469978	5.544013	-0.347076
C	-0.927201	4.167953	0.108466
O	0.229554	3.347792	0.247878
C	-0.002181	2.034578	0.696329
C	1.177632	1.278447	0.758732
C	1.203197	-0.031935	1.480367
N	1.149402	-1.278310	0.535965
C	-0.026922	-1.241617	-0.399585
C	-1.389537	-1.318256	0.311188
O	-1.171405	1.691699	0.974747
C	1.242185	-2.569118	1.279536
C	2.593370	-3.267839	1.125794
H	2.113678	1.832829	0.695599
H	-1.468546	4.233823	1.061215
H	-1.623071	3.730073	-0.620409
H	0.208882	5.995482	0.385915
H	0.055515	5.486629	-1.307596
H	-1.333574	6.209040	-0.469357
H	0.464201	-3.248224	0.923213
H	1.020344	-2.395297	2.338863
H	2.786397	-3.526420	0.077791
H	2.600774	-4.200497	1.703630
H	3.423066	-2.649278	1.482538
H	0.316352	-0.122705	2.122127
H	0.029692	-0.257185	-0.871476
H	-1.565879	-2.297937	0.770213
H	-1.430809	-0.556033	1.096547
H	2.223912	-0.939834	-0.390919
H	2.624956	0.625141	-0.932906
N	2.900381	-0.345121	-1.167114
C	4.369462	-0.562787	-1.091782
H	4.672010	-0.362465	-0.060712
H	4.549609	-1.622540	-1.294452
C	5.136492	0.320695	-2.066832
H	4.844905	0.115461	-3.103772
H	4.958329	1.382679	-1.862235
H	6.212088	0.132910	-1.975673
H	2.557931	-0.526877	-2.114185
C	-2.555725	-0.992207	-0.597095
O	-2.492671	-0.517090	-1.715409
O	-3.724691	-1.273094	0.017148
C	-4.931206	-0.947943	-0.715942
H	-4.919084	0.118459	-0.962316
H	-4.937299	-1.510033	-1.655697
C	-6.113714	-1.307418	0.160452
H	-6.100190	-0.736473	1.095105
H	-7.044837	-1.076415	-0.369513
H	-6.114724	-2.375348	0.405189
C	0.100824	-2.315072	-1.490596
H	1.075550	-2.284572	-1.990073
H	-0.039069	-3.329459	-1.098962
H	-0.667090	-2.146461	-2.250346
C	2.447589	-0.121626	2.378547

H	2.530583	-1.053019	2.946784
H	3.372695	0.006657	1.802847
H	2.402185	0.698251	3.103139

H	2.370512	-0.129488	2.529929
H	2.160155	1.620854	2.701212

Imaginary Frequency: 530i

Imaginary Frequency: 179i

TS16-EA-ECR

C	-2.671622	-3.617499	2.407800
C	-2.204770	-3.006109	1.098092
O	-2.131377	-1.588063	1.280626
C	-1.698365	-0.844958	0.187044
C	-1.861807	0.552722	0.371055
C	-0.910418	1.602566	-0.196444
N	0.237504	1.860535	0.728123
C	1.210259	0.779338	0.916379
C	2.423130	0.847792	-0.030871
O	-1.358000	-1.452582	-0.857272
C	0.755752	3.230406	0.702420
C	-0.096068	4.204796	1.525510
H	-2.195792	0.815520	1.376119
H	-1.222531	-3.398400	0.809741
H	-2.898233	-3.249704	0.282165
H	-1.974836	-3.383173	3.220597
H	-3.662352	-3.242151	2.689067
H	-2.732071	-4.708253	2.313371
H	0.856209	3.619048	-0.327510
H	1.767415	3.231993	1.121409
H	-1.127768	4.257545	1.158876
H	0.322784	5.218626	1.478723
H	-0.130144	3.891732	2.575557
H	-1.454001	2.556711	-0.184891
H	0.682753	-0.149763	0.678009
H	2.118642	0.973062	-1.071581
H	3.104862	1.664704	0.226640
H	-3.123931	0.421661	-0.929695
H	-2.918746	-0.785082	-2.014673
N	-3.586507	-0.017833	-1.836527
C	-4.974809	-0.504844	-1.596617
H	-5.278165	-1.104567	-2.459222
H	-4.929034	-1.158972	-0.722034
C	-5.922957	0.661402	-1.364066
H	-5.617135	1.253313	-0.494355
H	-5.962658	1.321903	-2.238491
H	-6.934043	0.283388	-1.181045
H	-3.545804	0.645543	-2.614000
O	3.145578	-0.406374	0.090695
C	4.256130	-0.540946	-0.660532
O	4.665861	0.319135	-1.416352
C	4.910595	-1.888108	-0.424759
H	4.140202	-2.661687	-0.531408
H	5.221481	-1.922932	0.628079
C	6.093103	-2.152071	-1.352498
H	6.871112	-1.391539	-1.231513
H	6.534747	-3.130373	-1.134080
H	5.782712	-2.146473	-2.402787
C	-0.477190	-1.378055	-1.661405
H	0.230184	2.154383	-1.977676
H	-0.022659	0.396211	-1.807716
H	-1.337732	1.440889	-2.340400
C	1.664300	0.695191	2.381898
H	0.798806	0.533228	3.032790

TS18-EA-ECR

C	-1.311823	5.968198	1.156602
C	-0.193525	5.123739	0.565720
O	-0.725910	3.836098	0.280872
C	0.175250	2.913937	-0.309413
C	-0.423428	1.659998	-0.473072
C	0.107801	0.534989	-1.316930
N	0.665425	-0.685957	-0.502735
C	2.050443	-0.572132	0.097801
C	3.230282	-0.763341	-0.891385
O	1.332126	3.313451	-0.572622
C	0.581762	-1.961733	-1.282366
C	-0.814983	-2.549585	-1.482097
H	-1.488487	1.636349	-0.263595
H	-0.756633	0.062256	-1.795477
H	0.203194	5.589107	-0.346337
H	0.647391	5.048150	1.269760
H	-2.144969	6.064997	0.450566
H	-1.699153	5.519680	2.079264
H	-0.945654	6.974573	1.393776
H	1.188858	-2.701670	-0.749825
H	1.042015	-1.827580	-2.268324
H	-1.306848	-2.792057	-0.535783
H	-0.711457	-3.486029	-2.043293
H	-1.473805	-1.899189	-2.065016
H	2.102409	-1.424305	0.785350
H	3.011318	-1.527861	-1.644561
H	3.463314	0.157389	-1.428033
H	-0.247281	-0.777377	0.576346
H	-0.962956	0.405860	1.555533
N	-0.961802	-0.624622	1.575202
C	-2.384361	-1.114608	1.514210
H	-2.331981	-2.194809	1.364967
C	-3.111883	-0.503547	0.310909
H	-3.422087	0.526858	0.514579
H	-2.463138	-0.460859	-0.568165
C	-0.211012	-1.093947	2.784552
H	-0.699928	-0.711133	3.684200
H	0.774323	-0.630084	2.735788
C	-0.066704	-2.610154	2.849881
H	0.389815	-3.011782	1.938081
H	0.587166	-2.867496	3.690222
H	-1.023000	-3.118358	3.009125
C	4.475519	-1.249484	-0.171914
O	4.485502	-2.034854	0.758351
O	5.589480	-0.731439	-0.719467
C	6.854806	-1.170931	-0.159123
H	6.861464	-0.945959	0.911810
H	6.933155	-2.256490	-0.277562
C	7.960421	-0.442345	-0.894959
H	7.938015	-0.667826	-1.966733
H	7.873671	0.641847	-0.765113
H	8.931859	-0.758664	-0.498529
C	-4.333649	-1.313163	-0.086987
O	-4.586350	-2.441835	0.290637
O	-5.098205	-0.623229	-0.948431

C	-6.284899	-1.295965	-1.450066
H	-5.987070	-2.251085	-1.892880
H	-6.948739	-1.505209	-0.605077
C	-6.934536	-0.379994	-2.466440
H	-6.259227	-0.180251	-3.305338
H	-7.839230	-0.856878	-2.860021
H	-7.220055	0.575280	-2.013113
C	1.040102	0.966274	-2.460964
H	0.451242	1.559349	-3.170984
H	1.844854	1.609009	-2.104087
H	1.458328	0.117145	-3.013217
C	2.298885	0.707211	0.901852
H	2.304998	1.603826	0.276334
H	1.554515	0.868679	1.684021
H	3.275637	0.614411	1.394374
C	-3.155189	-0.825584	2.807231
H	-3.123719	0.242886	3.053658
H	-4.202749	-1.111630	2.671657
H	-2.773553	-1.391562	3.661409

Imaginary Frequency: 992i

S7.6 Ethylamine to ethyl methacrylate

EmAc

O	-0.739798	0.229893	0.006758
O	0.287444	-1.781833	0.026205
C	0.349386	-0.564669	0.011797
C	1.617190	0.236072	-0.004040
C	2.771188	-0.441828	-0.049655
H	3.728906	0.071374	-0.065538
C	-2.025880	-0.438587	0.023574
H	-2.077669	-1.123623	-0.828375
H	-2.098539	-1.034252	0.939326
C	-3.100153	0.627737	-0.042321
H	-3.021258	1.210772	-0.966271
H	-3.031024	1.313417	0.809009
H	-4.087189	0.152563	-0.020046
H	2.781642	-1.527215	-0.072727
C	1.536489	1.739969	0.030648
H	1.009880	2.091140	0.925943
H	2.539449	2.177477	0.027297
H	0.985316	2.131704	-0.832344

ZI1-EA-EmAc

C	3.568868	-1.460763	0.655388
C	2.927898	-0.931169	-0.620765
O	2.198654	0.279261	-0.395049
C	0.867883	0.150407	-0.012471
C	0.143827	1.327828	0.078366
C	-1.253331	1.187435	0.593768
N	-1.963276	0.062832	-0.157311
C	-3.274415	-0.390522	0.387660
C	-3.865622	-1.510284	-0.457201
O	0.398228	-1.024564	0.191063
H	4.216935	-0.702863	1.111319
H	4.180242	-2.345975	0.437037
H	2.797577	-1.742252	1.378968
H	3.698162	-0.668113	-1.355168
H	2.269155	-1.686294	-1.059220
H	-1.846288	2.097609	0.462085

H	-2.054042	0.335045	-1.140965
H	-1.212916	-0.694614	-0.110491
H	-3.090153	-0.720052	1.413730
H	-3.936940	0.479680	0.420571
H	-4.053560	-1.179033	-1.485164
H	-3.199473	-2.379766	-0.489108
H	-4.820486	-1.829938	-0.026766
H	-1.339285	0.877969	1.647277
C	0.689817	2.700381	-0.217258
H	-0.002446	3.303868	-0.827783
H	1.631424	2.630381	-0.771077
H	0.900425	3.307071	0.682899

Pl-EA-EmAc

C	-4.192513	-1.463418	-0.363443
C	-3.539006	-0.147564	0.049258
N	-2.114300	-0.139902	-0.292714
C	-1.430051	1.070447	0.162123
C	0.025683	1.133813	-0.317780
C	0.848179	-0.022717	0.238384
O	0.463348	-0.829648	1.067081
O	2.082601	-0.048964	-0.294692
C	2.972660	-1.098831	0.167163
C	4.328979	-0.858001	-0.462783
H	4.268309	-0.883562	-1.556212
H	-1.958122	1.935763	-0.257892
H	3.018694	-1.067103	1.259853
H	2.552685	-2.066364	-0.126369
H	5.025888	-1.639506	-0.139870
H	4.736958	0.112082	-0.158904
H	-3.714310	0.028301	1.128367
H	-4.018766	0.686629	-0.480962
H	-3.749102	-2.310294	0.176215
H	-5.265951	-1.452245	-0.141603
H	-4.062967	-1.642725	-1.437089
H	0.035736	1.028812	-1.410550
H	-1.671513	-0.930121	0.176352
H	-1.455196	1.187017	1.261473
C	0.680838	2.479096	0.051488
H	0.715518	2.616266	1.139126
H	1.702428	2.541603	-0.333293
H	0.103607	3.306702	-0.375217

I1-EA-EmAc

C	-3.573515	-1.632428	-0.448503
C	-2.969372	-0.760833	0.640157
O	-2.245379	0.360189	0.086228
C	-0.901819	0.248374	-0.074291
C	-0.097775	1.338601	-0.063543
C	1.368690	1.181843	-0.417416
N	1.949535	-0.052916	0.160187
C	3.314093	-0.349771	-0.298994
C	3.866173	-1.592173	0.391580
O	-0.466369	-1.016241	-0.267651
H	-4.210415	-1.036449	-1.112183
H	-4.192625	-2.417724	0.002924
H	-2.791762	-2.108378	-1.047636
H	-3.757073	-0.307997	1.251434
H	-2.315078	-1.341479	1.296358
H	1.924424	2.075089	-0.088843
H	1.956606	0.045919	1.176975

H	0.539856	-0.962005	-0.153052
H	3.272374	-0.507920	-1.383507
H	3.987305	0.506971	-0.126073
H	3.923296	-1.449336	1.478085
H	3.232791	-2.465231	0.196421
H	4.876975	-1.813958	0.031289
H	1.520385	1.111713	-1.506319
C	-0.616867	2.728167	0.192609
H	-1.656523	2.708562	0.531175
H	-0.021709	3.246083	0.959992
H	-0.579233	3.364280	-0.706556

ZI2-EA-EmAc

C	-1.043814	3.382499	-2.066473
C	-0.594935	2.983791	-0.676457
O	-1.479375	1.922430	-0.216186
C	-1.266406	1.460171	1.029170
C	-2.160024	0.257142	1.323831
C	-1.448149	-1.052816	0.928855
N	-1.067380	-1.172140	-0.513663
C	-2.214442	-1.186004	-1.483071
C	-3.158429	-2.371289	-1.331256
O	-0.459830	1.932434	1.804298
C	-0.060753	-2.328780	-0.733739
C	1.272659	-1.994367	-0.150844
C	1.769253	-0.737237	-0.452667
O	1.123574	0.180616	-1.074660
O	3.056186	-0.465876	-0.017306
C	3.473830	0.900936	-0.060091
C	4.904343	0.958046	0.447968
H	-2.087790	-1.902777	1.178650
H	-0.658454	3.818251	0.028135
H	0.422599	2.587236	-0.674368
H	-2.076411	3.749003	-2.063471
H	-0.973475	2.537977	-2.760483
H	-0.397401	4.184811	-2.440040
H	-2.745500	-0.239316	-1.366319
H	-1.756850	-1.181338	-2.476178
H	-3.675538	-2.372954	-0.366426
H	-3.922700	-2.307299	-2.113436
H	-2.641063	-3.328304	-1.451426
H	-0.511674	-1.149047	1.483950
H	-3.076541	0.367208	0.735986
H	-0.492604	-3.230582	-0.290045
H	-0.072758	-2.452769	-1.827226
H	2.813085	1.515995	0.565328
H	3.405812	1.285902	-1.084025
H	5.268375	1.992193	0.432907
H	5.567154	0.351357	-0.179867
H	4.972100	0.585528	1.476520
H	-0.423047	-0.363251	-0.775213
C	2.012108	-3.038460	0.645482
H	1.358451	-3.539155	1.378017
H	2.452967	-3.847274	0.033960
H	2.838894	-2.586292	1.202871
C	-2.519018	0.201054	2.814217
H	-3.170843	-0.654934	3.019086
H	-1.619700	0.109746	3.430674
H	-3.047195	1.110132	3.119373

P2-EA-EmAc

C	2.149284	3.486835	1.441081
C	1.687373	2.749619	0.200452
O	2.235565	1.408510	0.259610
C	1.951148	0.596243	-0.775659
O	1.289296	0.938885	-1.737406
C	2.586119	-0.776863	-0.614290
C	1.484469	-1.852179	-0.636659
N	0.494008	-1.691884	0.434885
C	-0.782357	-2.331422	0.082215
C	-1.702240	-1.420615	-0.744990
C	-2.276490	-0.312576	0.127847
O	-2.377213	0.849519	-0.543968
C	-3.009865	1.949013	0.159223
C	-3.081846	3.125468	-0.792442
C	0.996939	-2.152177	1.741137
C	0.340909	-1.421231	2.911598
O	-2.663912	-0.456394	1.273090
H	1.959100	-2.851132	-0.610068
H	2.037992	3.234653	-0.716111
H	0.596369	2.678445	0.149083
H	3.242719	3.540132	1.482676
H	1.790235	2.992962	2.350494
H	1.757020	4.510015	1.428203
H	0.868053	-3.245099	1.850762
H	2.075241	-1.967968	1.777041
H	-0.747210	-1.541306	2.913572
H	0.727407	-1.802648	3.864970
H	0.555881	-0.347894	2.855330
H	0.965766	-1.774073	-1.597290
H	3.109149	-0.796720	0.346076
H	-0.615660	-3.274131	-0.468679
H	-1.310792	-2.593625	1.002455
H	-1.136579	-0.949509	-1.554550
H	-2.420343	2.181561	1.051733
H	-4.004746	1.631769	0.487709
H	-3.553747	3.975375	-0.286370
H	-3.677666	2.881060	-1.678571
H	-2.083109	3.432574	-1.121077
C	3.605747	-1.010511	-1.741726
H	4.069955	-1.997730	-1.638945
H	3.121066	-0.956843	-2.722556
H	4.402873	-0.258957	-1.715024
C	-2.874576	-2.216489	-1.353804
H	-2.496991	-2.984955	-2.037421
H	-3.460962	-2.713108	-0.571950
H	-3.546649	-1.562514	-1.920179

I2-EA-EmAc

C	-1.105528	3.704177	-1.922457
C	-0.615586	3.146191	-0.602046
O	-1.501424	2.055964	-0.231110
C	-1.229419	1.430551	0.929046
C	-2.187495	0.276332	1.191746
C	-1.475259	-1.066841	0.922384
N	-1.059674	-1.280374	-0.476033
C	-2.174636	-1.427220	-1.437089
C	-3.106055	-2.629220	-1.238627
O	-0.323473	1.752883	1.674307
C	-0.073239	-2.394072	-0.567809
C	1.319112	-1.998258	-0.110574

C	1.815222	-0.795331	-0.479499
O	1.098192	0.145375	-1.139837
O	3.106907	-0.449491	-0.252128
C	3.365486	0.927365	0.100329
C	4.827835	1.029346	0.487627
H	-2.129299	-1.881629	1.270483
H	-0.636168	3.899541	0.191787
H	0.400852	2.751298	-0.677047
H	-2.130016	4.083041	-1.837660
H	-1.080281	2.939913	-2.706842
H	-0.458598	4.533087	-2.231213
H	-2.758451	-0.501668	-1.417398
H	-1.719709	-1.482657	-2.432931
H	-3.644030	-2.586660	-0.285179
H	-3.856698	-2.641301	-2.037927
H	-2.561509	-3.579230	-1.280963
H	-0.566997	-1.099659	1.532613
H	-3.043792	0.382603	0.519867
H	-0.411722	-3.265553	0.014362
H	-0.064357	-2.712584	-1.620251
H	2.711865	1.218829	0.931800
H	3.141003	1.575298	-0.753055
H	5.069238	2.065370	0.751707
H	5.473699	0.728662	-0.344977
H	5.054190	0.392115	1.349535
H	0.137421	-0.137079	-1.013230
C	2.128720	-3.015047	0.649027
H	1.595293	-3.370269	1.543407
H	2.347897	-3.910098	0.045103
H	3.086824	-2.598629	0.971624
C	-2.681484	0.328174	2.645105
H	-3.369053	-0.500796	2.845087
H	-1.843266	0.261391	3.345939
H	-3.214272	1.264543	2.844749

TS1-EA-EmAc

C	-4.002962	-1.050626	-0.506351
C	-3.140243	-0.777819	0.718451
O	-2.229403	0.307720	0.505195
C	-1.016438	-0.007181	-0.091358
C	-0.173252	1.123015	-0.268142
C	1.071879	0.864609	-0.901200
N	2.228118	0.038958	0.185576
C	3.540805	-0.350546	-0.377589
C	4.385409	-1.175066	0.588543
O	-0.749366	-1.185471	-0.397283
H	-4.549168	-0.149755	-0.809637
H	-4.735662	-1.837507	-0.286495
H	-3.382381	-1.382236	-1.344700
H	-3.761145	-0.467407	1.566191
H	-2.581263	-1.674724	1.001230
H	1.081815	0.082429	-1.660398
H	2.332151	0.624692	1.016673
H	1.680763	-0.781566	0.457914
H	3.336104	-0.912969	-1.294220
H	4.056025	0.572967	-0.659802
H	4.614628	-0.610549	1.499928
H	3.869885	-2.098932	0.875721
H	5.334515	-1.451458	0.114928
H	1.672848	1.729231	-1.185347
C	-0.496413	2.468620	0.343294

H	-1.480862	2.844654	0.030808
H	-0.511244	2.473400	1.446472
H	0.243619	3.218998	0.034518

Imaginary Frequency: 227i

TS3-EA-EmAc

C	-2.934705	-1.682599	0.953259
C	-2.882907	-1.080065	-0.444032
O	-2.241728	0.204465	-0.461332
C	-0.867359	0.223678	-0.394427
C	-0.250127	1.375803	0.017293
C	1.256621	1.410643	-0.072366
N	1.813942	0.056418	0.269191
C	3.201215	-0.205641	-0.179316
C	3.669382	-1.586719	0.261492
O	-0.233630	-0.873636	-0.731668
H	-1.925544	-1.898172	1.319717
H	-3.499864	-2.622972	0.939055
H	-3.424171	-0.999445	1.657080
H	-2.379717	-1.756363	-1.140231
H	-3.893550	-0.885873	-0.817701
H	1.687687	2.161664	0.601129
H	1.740071	-0.084226	1.279818
H	0.937227	-0.621120	-0.250839
H	3.204109	-0.124273	-1.270803
H	3.861024	0.576589	0.216245
H	3.670720	-1.677889	1.354440
H	3.026177	-2.373533	-0.148586
H	4.691069	-1.764134	-0.090864
H	1.635864	1.631642	-1.083155
C	-0.975492	2.626271	0.432389
H	-2.037805	2.422954	0.598601
H	-0.568807	3.048583	1.365636
H	-0.918984	3.436786	-0.315624

Imaginary Frequency: 895i

TS5-EA-EmAc

C	-3.612635	1.096659	-1.262699
C	-3.758451	-0.173785	-0.431914
O	-2.754090	-0.286620	0.574747
C	-1.507083	-0.794166	0.159767
O	-1.417028	-1.289621	-1.002239
C	-0.489470	-0.665528	1.105201
C	0.802683	-1.405149	0.835269
C	2.456646	-1.986138	-0.962870
C	3.768229	-1.584126	-0.291913
H	-2.675391	1.074406	-1.828601
H	-4.441369	1.186769	-1.976965
H	-3.615622	1.987591	-0.622991
H	-3.736505	-1.054217	-1.081103
H	-4.710419	-0.164940	0.112262
H	1.571824	-1.081268	1.548914
H	0.719037	-2.505647	0.957050
H	0.490298	-1.362883	-1.135561
H	2.554534	-1.885814	-2.050172
H	2.243993	-3.046547	-0.754186
H	3.726248	-1.707719	0.795866
H	4.021140	-0.538824	-0.507767
H	4.587159	-2.211112	-0.663244

N	1.313067	-1.152589	-0.549336
H	1.372137	0.306725	-0.661139
N	1.106505	1.455351	-0.558320
H	0.713872	1.801946	-1.437761
H	0.329751	1.381437	0.120510
C	2.206626	2.329663	-0.073372
H	2.599533	1.869637	0.837777
H	2.996152	2.304223	-0.830337
C	1.744998	3.756516	0.191671
H	0.961017	3.781522	0.957352
H	1.352744	4.223324	-0.719591
H	2.585804	4.362514	0.546922
C	-0.742090	-0.227629	2.528950
H	-1.610687	0.435909	2.592217
H	-0.938481	-1.060831	3.233578
H	0.118463	0.316488	2.951949

Imaginary Frequency: 394i

TS6-EA-EmAc

C	3.699251	-2.904099	-0.182339
C	2.794383	-1.834481	-0.768779
O	1.722671	-1.616383	0.153897
C	0.774674	-0.669661	-0.216321
O	0.856459	-0.144727	-1.356155
C	-0.124490	-0.311949	0.821699
C	-1.469161	0.229546	0.387487
H	-1.344817	0.862851	-0.510288
H	2.395703	-2.144790	-1.741517
H	3.347806	-0.899869	-0.932470
H	3.153247	-3.843011	-0.036162
H	4.104281	-2.589840	0.786482
H	4.539821	-3.098552	-0.859210
H	-1.902629	0.872374	1.170418
H	0.712732	1.328819	0.716241
N	1.165804	2.189657	0.187595
H	1.162462	1.829104	-0.779621
H	2.141260	2.279299	0.486287
H	-0.603300	3.280681	0.024895
C	0.422221	3.470586	0.349717
H	0.405195	3.694445	1.419706
H	1.070021	4.372375	-1.518979
C	1.058857	4.599482	-0.446795
H	2.088651	4.786497	-0.120560
H	0.486386	5.521816	-0.301629
N	-2.466668	-0.838333	0.136271
H	-2.055543	-1.475981	-0.547644
C	-3.726988	-0.331800	-0.405843
H	-3.581910	0.273907	-1.323464
H	-4.165432	0.346879	0.339747
C	-4.704024	-1.467957	-0.698307
H	-4.902721	-2.054066	0.206425
H	-4.300135	-2.149636	-1.458386
H	-5.657938	-1.079133	-1.074598
C	-0.107726	-1.063830	2.140356
H	-0.607354	-2.046954	2.104990
H	0.913335	-1.244188	2.494419
H	-0.628103	-0.488445	2.920678

Imaginary Frequency: 142i

TS8-EA-EmAc

C	5.171585	-2.987324	0.065015
C	4.108566	-2.135505	-0.609012
O	3.890964	-0.986560	0.209216
C	3.023273	-0.016297	-0.298069
C	2.730307	1.026514	0.590192
C	2.080729	2.261691	-0.001674
N	0.877697	1.939506	-0.832750
H	1.232412	1.267238	-1.529239
O	2.557794	-0.178302	-1.464654
C	0.264017	3.110401	-1.482627
C	-0.878829	2.707540	-2.408807
H	1.750179	2.934799	0.801559
H	4.427459	-1.831403	-1.612661
H	3.175449	-2.704081	-0.728396
H	6.109896	-2.430686	0.170613
H	4.849399	-3.305503	1.063386
H	5.371208	-3.885198	-0.532226
H	1.028941	3.665070	-2.046135
H	-0.101387	3.781021	-0.695013
H	-0.531731	2.017810	-3.187848
H	-1.293538	3.591635	-2.906052
H	-1.691459	2.220124	-1.857339
H	2.765847	2.858091	-0.637357
H	0.104380	1.130825	-0.005211
H	0.836931	0.209274	1.175704
N	-0.152708	0.238032	0.820206
C	-0.398792	-1.045090	0.107316
H	-0.401962	-1.870535	0.827876
H	0.453872	-1.171518	-0.565040
C	-1.695156	-1.070283	-0.716019
H	-1.830226	-0.108311	-1.221051
C	-1.107139	0.588811	1.899629
H	-2.074002	0.812299	1.437139
H	-1.241793	-0.282943	2.550327
C	-0.629458	1.789374	2.708745
H	-0.525169	2.683635	2.084451
H	0.334136	1.588469	3.190471
H	-1.357979	2.012814	3.495706
C	-2.921900	-1.341976	0.146861
O	-2.973970	-2.177235	1.029739
O	-3.966797	-0.579021	-0.223175
C	-5.220149	-0.810935	0.475632
H	-5.512190	-1.855656	0.331488
H	-5.058888	-0.648633	1.545722
C	-6.245942	0.147410	-0.093053
H	-5.937113	1.188432	0.051371
H	-6.398563	-0.026125	-1.163664
H	-7.204107	0.000668	0.417907
C	3.524216	1.245937	1.859089
H	2.931343	1.764915	2.629281
H	3.857166	0.296079	2.289479
H	4.436057	1.860771	1.721686
C	-1.615853	-2.181033	-1.785608
H	-2.542616	-2.234235	-2.366989
H	-0.790168	-1.979495	-2.475723
H	-1.447479	-3.158880	-1.321079

Imaginary Frequency: 959i

TS11-EA-EmAc

C	6.124144	-1.743901	-0.755487
C	4.614485	-1.660472	-0.891196
O	4.117696	-0.889113	0.209378
C	2.751070	-0.689681	0.246721
C	2.323776	0.145359	1.309708
C	0.911586	0.298976	1.425684
N	0.209273	1.229741	0.063433
C	-1.273949	1.294856	0.062359
C	-1.969749	-0.067764	-0.096646
O	2.019703	-1.205400	-0.628021
C	0.855808	2.560023	-0.065250
C	0.787868	3.147141	-1.471999
H	0.546328	0.877634	2.275621
H	4.161264	-2.658772	-0.881306
H	4.328032	-1.185755	-1.837806
H	6.409412	-2.229914	0.184434
H	6.578219	-0.746575	-0.776750
H	6.542707	-2.328078	-1.583531
H	0.383867	3.222454	0.667879
H	1.899155	2.412084	0.228441
H	-0.239084	3.344508	-1.797349
H	1.331624	4.098414	-1.494688
H	1.258736	2.475970	-2.200145
H	0.312636	-0.592760	1.249339
H	-1.569929	1.762355	1.007787
H	-1.606012	1.952030	-0.746482
H	-1.795478	-0.692209	0.784122
H	0.547951	0.628697	-0.695092
C	-3.473094	0.172782	-0.187169
O	-3.994832	1.176796	-0.634515
O	-4.161438	-0.891658	0.258166
H	-5.962558	0.024357	0.746594
C	-5.608592	-0.819256	0.145725
H	-5.868746	-0.624053	-0.898975
H	-5.904801	-2.324332	1.675973
C	-6.175470	-2.136874	0.631338
H	-5.812990	-2.971709	0.021990
H	-7.268648	-2.109330	0.560441
C	3.301257	0.906807	2.179538
H	2.764443	1.573840	2.866475
H	3.920767	0.245029	2.804947
H	4.009861	1.531396	1.614115
C	-1.514148	-0.850770	-1.347465
H	-0.465593	-1.154209	-1.258711
H	-2.111745	-1.760852	-1.461691
H	-1.633308	-0.246759	-2.254892

Imaginary Frequency: 236i

TS13-EA-EmAc

C	-1.165422	3.442289	-2.049282
C	-0.758146	3.041030	-0.646790
O	-1.587962	1.913883	-0.255347
C	-1.369351	1.404781	0.970196
C	-2.219657	0.161294	1.212998
C	-1.410670	-1.120294	0.924507
N	-0.929625	-1.280823	-0.476416
C	-2.000894	-1.353218	-1.511591
C	-2.931046	-2.558543	-1.404445
O	-0.593834	1.878694	1.776638

C	0.064270	-2.423328	-0.567704
C	1.423910	-1.990923	-0.076031
C	1.802241	-0.705295	-0.355240
O	1.007918	0.187533	-0.900921
O	3.078382	-0.310052	-0.046782
C	3.323313	1.100995	0.046596
C	4.793255	1.287809	0.377269
H	-2.021770	-1.989068	1.193479
H	-0.911918	3.853688	0.069946
H	0.285386	2.722088	-0.599900
H	-2.220666	3.734396	-2.088853
H	-1.002299	2.621238	-2.755707
H	-0.561721	4.297489	-2.373686
H	-2.567752	-0.420722	-1.461050
H	-1.483614	-1.358963	-2.476121
H	-3.497569	-2.564899	-0.467256
H	-3.655374	-2.523488	-2.226013
H	-2.384808	-3.504510	-1.483523
H	-0.515258	-1.132650	1.552580
H	-3.084108	0.207227	0.543977
H	-0.314988	-3.277100	0.007392
H	0.060711	-2.724694	-1.626261
H	2.687643	1.538600	0.827265
H	3.069994	1.588241	-0.900655
H	5.024411	2.356352	0.458568
H	5.428403	0.857821	-0.405578
H	5.047967	0.807470	1.328739
H	-0.126920	-0.387455	-0.749188
C	2.309457	-3.014344	0.579357
H	1.786022	-3.556447	1.383187
H	2.678027	-3.787620	-0.117589
H	3.191817	-2.541341	1.021226
C	-2.713753	0.130620	2.666095
H	-3.331592	-0.756730	2.840907
H	-1.873233	0.114277	3.366620
H	-3.320488	1.014871	2.888082

Imaginary Frequency: 957i

TS15-EA-EmAc

C	-0.580963	5.350842	0.061704
C	0.093837	4.001989	-0.128193
O	-0.899128	3.073819	-0.551354
C	-0.452337	1.749937	-0.748247
C	-1.478344	0.850526	-1.076938
C	-1.068154	-0.517760	-1.540842
N	-0.945891	-1.602970	-0.466168
C	0.254129	-1.430901	0.395664
C	1.658592	-1.498860	-0.243616
O	0.769703	1.509533	-0.603217
C	-1.112142	-2.967418	-1.024513
C	-2.578313	-3.351998	-1.223430
H	-1.813722	-0.910167	-2.241539
H	0.897294	4.070867	-0.873385
H	0.561503	3.664927	0.807048
H	-1.037631	5.696836	-0.872993
H	-1.367459	5.294685	0.823703
H	0.152508	6.100700	0.382381
H	-0.649599	-3.676766	-0.330769
H	-0.574378	-3.052793	-1.979350
H	-3.114346	-3.384986	-0.267953

H -2.641268 -4.348542 -1.676417
H -3.102978 -2.655770 -1.886852
H -0.108803 -0.499113 -2.076025
H 0.183287 -2.171568 1.201468
H 0.157167 -0.439788 0.841669
H 1.677400 -0.868376 -1.134746
H -1.961850 -1.248307 0.518867
H -2.493235 0.299673 0.935462
N -2.620117 -0.656266 1.312558
C -4.049307 -1.050888 1.418130
H -4.457834 -1.041749 0.404370
H -4.074077 -2.082525 1.781100
C -4.840093 -0.127496 2.335280
H -4.439415 -0.141437 3.355801
H -4.817517 0.905500 1.969441
H -5.886487 -0.449369 2.378326
H -2.162950 -0.686347 2.227593
C 2.651422 -0.875070 0.729424
O 2.492572 -0.767549 1.931453
O 3.779221 -0.496205 0.097705
C 4.826352 0.070044 0.922913
H 4.423561 0.934577 1.459688
H 5.134581 -0.674500 1.664696
C 5.968935 0.459093 0.006765
H 5.645652 1.202856 -0.729522
H 6.782953 0.893123 0.598375
H 6.361077 -0.412799 -0.528297
C -2.875489 1.318709 -1.440362
H -3.019784 1.513333 -2.522276
H -3.651368 0.580895 -1.175384
H -3.134885 2.250422 -0.927176
C 2.160617 -2.912974 -0.603504
H 3.197169 -2.871904 -0.954564
H 2.124797 -3.581877 0.265552
H 1.561298 -3.358475 -1.401138

Imaginary Frequency: 499i

TS16-EA-EmAc

C -0.760155 -4.187085 1.932529
C -0.650722 -3.245338 0.745795
O -1.072678 -1.948140 1.180538
C -1.061067 -0.941321 0.224424
C -1.699061 0.256243 0.633825
C -1.280210 1.543661 -0.047288
N -0.246575 2.321217 0.678366
C 1.027362 1.646764 0.882320
C 1.858336 1.225291 -0.352865
O -0.606100 -1.199275 -0.921300
C -0.193667 3.735012 0.298389
C -1.259455 4.575043 1.011478
H -0.958643 1.328880 -1.081879
H 0.378600 -3.199513 0.371443
H -1.279280 -3.587903 -0.086503
H -0.122242 -3.853207 2.758751
H -1.791750 -4.242475 2.298893
H -0.444491 -5.196491 1.642981
H -0.292509 3.878265 -0.793837
H 0.792970 4.126649 0.568316
H -2.274906 4.236344 0.775471
H -1.184587 5.627875 0.709848

H -1.130786 4.516808 2.098446
H -2.141727 2.222116 -0.126786
H 0.837715 0.729734 1.452487
H 1.655452 2.289796 1.512601
H 1.296971 0.513891 -0.963205
H -2.882219 -0.104188 -0.697456
H -2.296334 -0.843247 -2.033691
N -3.184085 -0.422299 -1.715866
C -4.313448 -1.394712 -1.707667
H -4.432241 -1.783922 -2.722579
H -4.008012 -2.219079 -1.058044
C -5.590519 -0.738044 -1.206673
H -5.466798 -0.356060 -0.187300
H -5.892309 0.092785 -1.855451
H -6.402503 -1.472388 -1.199023
H -3.389886 0.398628 -2.290433
O 2.988022 0.498439 0.236517
C 3.637192 -0.403955 -0.522991
O 3.365006 -0.650775 -1.682311
C 4.756517 -1.058389 0.266368
H 4.328759 -1.443409 1.200389
H 5.455351 -0.265793 0.565497
C 5.477179 -2.159496 -0.506231
H 5.925434 -1.771728 -1.426689
H 6.276213 -2.590990 0.106588
H 4.789418 -2.965141 -0.784000
C -2.214400 0.402952 2.053151
H -2.937690 1.229474 2.118242
H -2.722930 -0.504371 2.397231
H -1.431070 0.626501 2.797994
C 2.395587 2.365100 -1.208244
H 2.968280 3.078644 -0.603815
H 3.047057 1.974648 -1.996162
H 1.574497 2.904096 -1.691301

Imaginary Frequency: 156i

TS18-EA-EmAc

C -3.736946 -4.991474 -2.294340
C -3.981722 -3.917901 -1.246596
O -3.015704 -2.890105 -1.438931
C -3.111637 -1.791044 -0.557744
C -2.093119 -0.841156 -0.737637
C -2.261641 0.487087 -0.058225
N -1.622569 0.625930 1.330135
C -2.392254 -0.124692 2.371212
C -3.767812 0.424898 2.752297
O -4.048179 -1.778567 0.274193
C -1.415043 2.032727 1.759531
C -0.403150 2.835427 0.917763
H -1.781348 1.258604 -0.667055
H -4.997382 -3.511596 -1.335886
H -3.900065 -4.339069 -0.234623
H -3.831805 -4.580520 -3.306339
H -2.732574 -5.419920 -2.194185
H -4.467410 -5.802481 -2.184395
H -1.051375 1.990140 2.792390
H -2.364924 2.580601 1.773844
H 0.366620 2.171956 0.515058
H -3.315673 0.773268 0.056872
H -1.754188 -0.165885 3.263069

H	-2.521807	-1.136568	1.984327
H	-3.724841	1.439571	3.162059
H	-4.452751	0.407361	1.901261
H	-4.194922	-0.223583	3.527018
H	-0.420271	-0.120351	1.272286
H	-0.001973	-1.487526	0.352549
N	0.466976	-0.967499	1.108816
C	1.721546	-0.346164	0.608458
H	1.450772	0.269776	-0.252025
H	2.090469	0.325512	1.387629
C	2.824680	-1.338813	0.204843
H	3.122105	-1.941223	1.069798
C	0.596723	-1.875891	2.288075
H	1.230437	-2.727010	2.018490
H	-0.406614	-2.266717	2.474616
C	1.139239	-1.178412	3.528968
H	0.538408	-0.301825	3.795958
H	1.107012	-1.876378	4.372476
H	2.179464	-0.858814	3.406688
C	-1.073275	3.555457	-0.247589
O	-2.104799	4.194176	-0.162467
O	-0.350026	3.450145	-1.377329
C	-0.862760	4.148557	-2.544098
H	-1.882024	3.801709	-2.738313
H	-0.904653	5.219168	-2.319472
C	0.067246	3.848591	-3.701660
H	1.086484	4.188878	-3.489125
H	0.095584	2.774737	-3.915665
H	-0.287978	4.367858	-4.598777
C	4.053476	-0.548846	-0.230177
O	4.035241	0.591603	-0.652993
O	5.170333	-1.286666	-0.112099
C	6.410344	-0.666348	-0.548914
H	6.332254	-0.444447	-1.618001
H	6.534180	0.279775	-0.013755
C	7.536653	-1.635125	-0.253311
H	7.396372	-2.581252	-0.787011
H	8.487442	-1.197478	-0.577279
H	7.604300	-1.846539	0.819319
C	-1.186988	-0.881690	-1.956392
H	-0.236786	-0.352675	-1.785488
H	-0.935807	-1.907970	-2.244543
H	-1.623478	-0.410952	-2.860937
C	0.281014	3.909744	1.790703
H	0.855985	3.435489	2.593292
H	0.968113	4.522681	1.196922
H	-0.462251	4.574143	2.245013
C	2.405145	-2.292299	-0.932023
H	2.134988	-1.733739	-1.834952
H	3.223435	-2.974741	-1.181169
H	1.544384	-2.901461	-0.636458

Imaginary Frequency: 948i