

## **Supporting information**

# **One-pot Synthesis of Diblock Polyesters by Catalytic Terpolymerization of Lactide, Epoxides and Anhydrides**

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## Table of Contents

1. Materials and Measurements .....	3
2. Experimental section .....	5
3. NMR spectra of <b>Cat.1</b> .....	7
4. NMR spectra of ECH/PA ROCOP and LA ROP .....	8
5. Structure analysis of ECH/PA/LA terpolymer .....	10
6. Effect of the content of LA incorporation into the first block .....	17
7. Representative DOSY spectra of expanded terpolymers .....	19
8. Characterization of the tetrapolymerization of epoxides, anhydride and LA .....	20
9. Representative NMR spectra of expanded polymers .....	21
10. Thermal analysis of expanded polymers .....	33
11. <sup>1</sup> H NMR spectra of the modified polymers .....	40
12. Cytotoxicity assay .....	43
13. Cartesian coordinates, the Gibbs free energies with solvation corrections (au), and the imaginary frequencies of TSs. ....	44
14. References .....	146

# 1. Materials and Measurements

## 1.1 Materials

All manipulations of air or water sensitive compounds were carried out in an argon-filled glovebox. Propylene oxide (PO), epichlorohydrin (ECH), cyclohexene oxide (CHO), allyl glycidyl ether (AGE), glycidyl propargyl ether (GPE) and 1,2-cyclohexanedicarboxylic anhydride (CHA) were distilled from  $\text{CaH}_2$  under argon atmosphere. Phthalic anhydride (PA) (Aldrich) was recrystallized from  $\text{CHCl}_3$  and dried under vacuum over 24 h. Succinic anhydride (SA) and norbornene anhydride (NA) were recrystallized from tetrahydrofuran and dried under vacuum over 24 h. Lactide acid (L-LA was chosen) was recrystallized from ethyl acetate. Bis(triphenylphosphine)iminium chloride (PPNCl) was dissolved in  $\text{CHCl}_3$  and precipitated by ether, and then the precipitate was dried under vacuum. Toluene was distilled from Na under argon atmosphere.  $\text{AlMe}_3$  was dissolved in toluene with a concentration of 0.3 mmol/g.

## 1.2 Measurements

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on Bruker AV-300 MHz or Bruker AV-500 MHz at 25 °C. 2D NMR spectra were recorded on Bruker AV-500 MHz and Bruker AV-600 MHz at 25 °C.

Gel permeation chromatography (GPC) measurements were conducted with a Waters 515 GPC and  $\text{CH}_2\text{Cl}_2$  as the eluent (flow rate: 1 mL/min, at 30 °C). Molecular weights were calculated using a calibration curve determined from linear polystyrene standards.

*in situ* ATR-IR reaction monitoring was using a Mettler-Toledo ReactIR 15 spectrometer equipped with a MCT detector and a silver halide DiComp probe.

IR spectra were recorded on a FT-IR spectrophotometer (PerkinElmer) instrument by making KBr pellets of the samples.

Differential scanning calorimetry (DSC) measurements were carried out under nitrogen flow on a TA Q100 thermal analyzer from 0 to 200 °C (except for ECH/SA/LA polymer and ECH/PA/LA polymer, a range from -40 to 200 °C) at a heating rate of 10 °C/min, and glass transition temperatures ( $T_g$ ) of the samples were determined from the second run.

## 1.3 Computational Details

The B3LYP<sup>1,2</sup> functional was used for geometrical optimization and subsequent frequency calculations without any symmetry or geometrical constraints. In these calculations, the 6-31G\* basis set<sup>3,4</sup> was used for C, H, O, N and Al atoms. To obtain more accurate energies, single-point energy calculations were also performed for all the stationary points by using the M06 functional<sup>5</sup> together with the Grimme's empirical D3 dispersion correction<sup>6</sup>. All elements were represented by using the 6-311+G\*\* basis set. In the single-point calculations, the solvation effect was considered on the basis of gas-phase optimized geometries by using

the Minnesota solvation model (SMD) developed by Cramer and Truhlar<sup>7</sup>. The energy profiles were described by the relative free energy in solution ( $\Delta G$ , kcal/mol), including the Gibbs free energy correction from gas phase calculations (298 K, 1 atm). All calculations were carried out by using Gaussian 16 program package<sup>8</sup>.

## 2. Experimental section

### 2.1 Synthesis of half salen ligand

The half salen ligand was synthesized according to the literature<sup>9</sup>. In a 50 mL round-bottom flask equipped with a magnetic stir bar, 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (4.68 g, 20 mmol) was dissolved in 30 mL methanol. Then cyclohexylamine (2 g, 20 mmol) was added to the aforementioned solution under argon. After 24 h, the solid was filtered and dried under reduced pressure.

### 2.2 Synthesis of half salen-Al(III) (**Cat.1**) complex

In a glovebox under argon, the half salen ligand (0.0472 g, 0.15 mmol) was dissolved in toluene (4.5 g). Then AlMe<sub>3</sub> (0.5 g, 0.3 mmol/g in toluene) was added to the solution in 10 min. The reaction mixture was stirred 2 h at room temperature and used without further processing.

<sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>): 8.20 (s, 1H, N=CH), 7.53 (d, 1H, Ar-H), 7.02 (d, 1H, Ar-H), 3.37 (m, 1H, N-CH), 2.05-1.20 (m, 10H, Cy), 1.43 (s, 9H, C(CH<sub>3</sub>)<sub>3</sub>), 1.32 (s, 9H, C(CH<sub>3</sub>)<sub>3</sub>), -0.73 (s, 6H, Al(CH<sub>3</sub>)<sub>2</sub>).

<sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>): δ 169.94, 161.35, 140.20, 138.60, 131.39, 128.46, 118.26, 67.73, 35.21, 34.01, 33.79, 31.35, 29.25, 25.48, 25.08, -8.28.

### 2.3 Polymerization process

In a glovebox, the monomers in desired ratios were mixed in toluene into a dry reaction vial equipped with a magnetic stir bar. Then the desired PPNCl and **Cat.1** were added, after which the vial was sealed and heated in a pre-set oil bath for desired time. The vial was then cooled down. A small amount of mixture was extracted for <sup>1</sup>H NMR analysis. The polymer was isolated by precipitation in cold ethanol and dried under vacuum at 45 °C for 16 h.

### 2.4 Modification of functioned polyesters

#### Thiol-ene reaction

To a quartz bottle were added polyester with pendent vinyl (0.175 mmol vinyl group), DMPA (0.005 g, 0.0175 mmol), thiol compound (0.5 mmol) and dry THF (5 ml). The reaction mixture was irradiated for 1 h with 365 nm light at room temperature. After stirring 24 h, the product was collected by precipitating three times into diethyl ether and dried under vacuum at 45 °C for 16 h.

#### Azide–alkyne cycloaddition

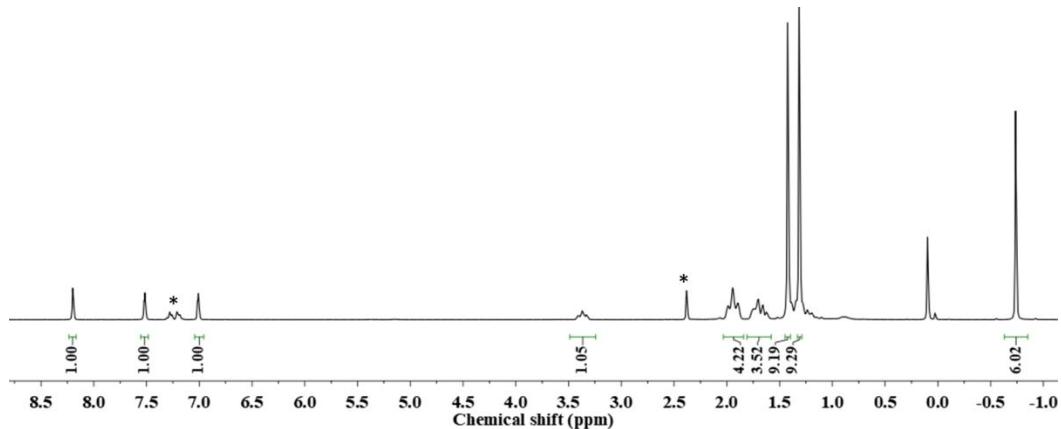
In an inert gas, the ECH/AGE/GPE/PA/LA polymer (0.5 g, 0.41 mmol alkyne), 6-azido-1-hexanol (0.076 g, 0.53 mmol), CuSO<sub>4</sub> (0.131 g, 0.82 mmol), sodium (*L*)-ascorbate (0.244 g, 1.23 mmol) and dry THF (10 mL) were put into a round bottom flask. The mixture was stirred for 12 h at room temperature. After removal of THF, the product was dissolved by 10

mL dichloromethane and washed with dilute hydrochloric acid (0.1 M, 2×10 mL) and brine (2×10 mL), then dried over  $\text{Na}_2\text{SO}_4$ . The modified polymer was obtained by remove of dichloromethane and dried under vacuum at 45 °C for 16 h.

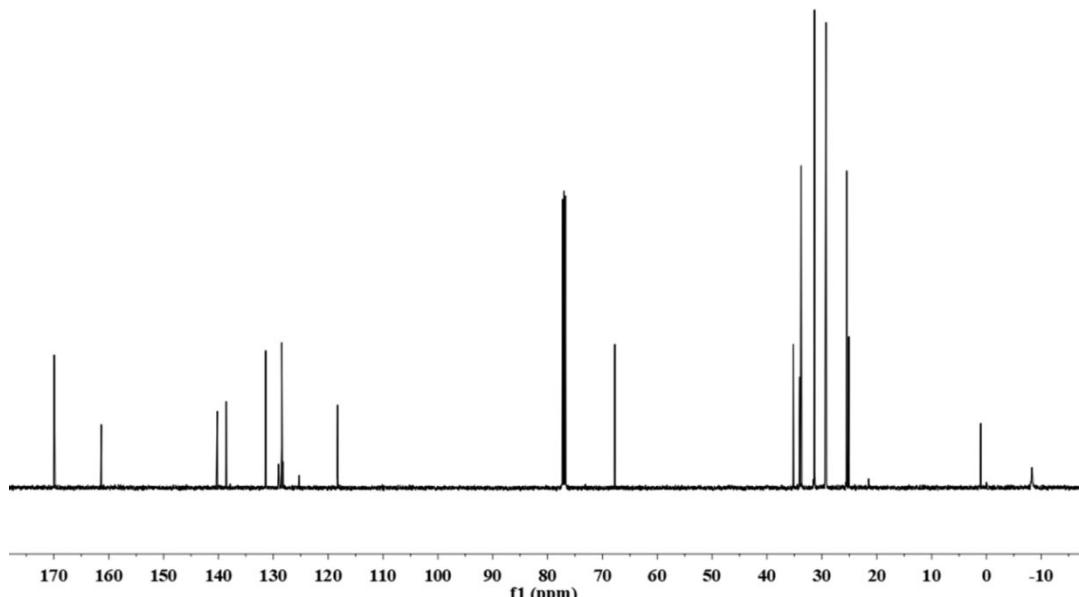
## 2.5 Cell viability assay

The L929 cells were seeded with a density of 7000 cells per well in 200  $\mu\text{L}$  of complete DMEM in 96 well plates. After incubation for 24 h, the medium was replaced by fresh medium containing samples with pre-determined concentrations. The wells without addition of polymer solution were used as control. The cells were incubated for further 48 h and subsequently subjected to CCK-8 treatment for 2 h. The cell viabilities were then calculated based on the absorbance ratio of samples with and without polymer pretreatments at 450 nm (Bio-Rad 680 microplate reader).

### 3. NMR spectra of Cat.1

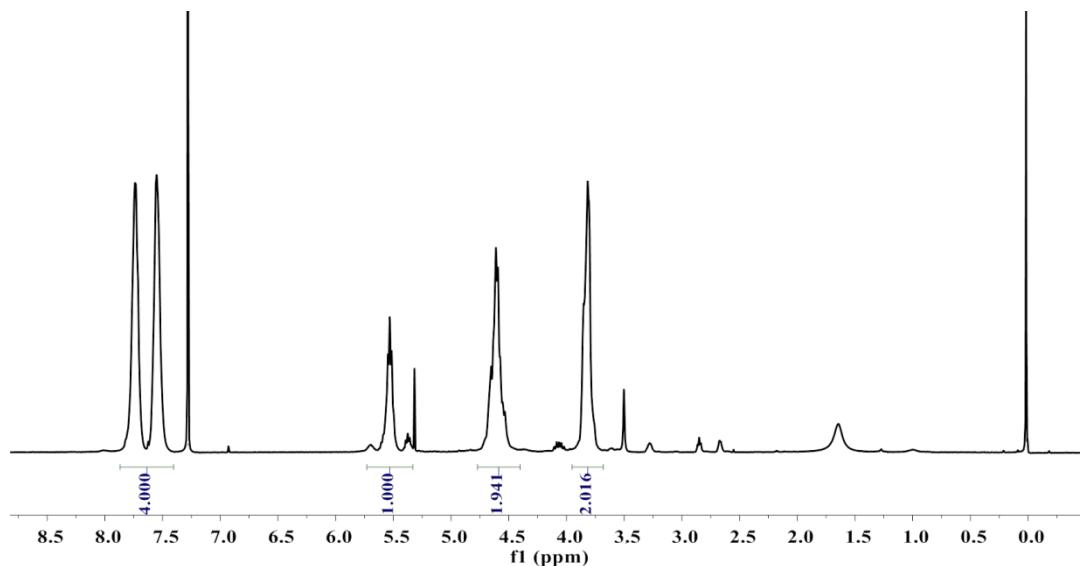


**Figure S1.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of **Cat.1**.

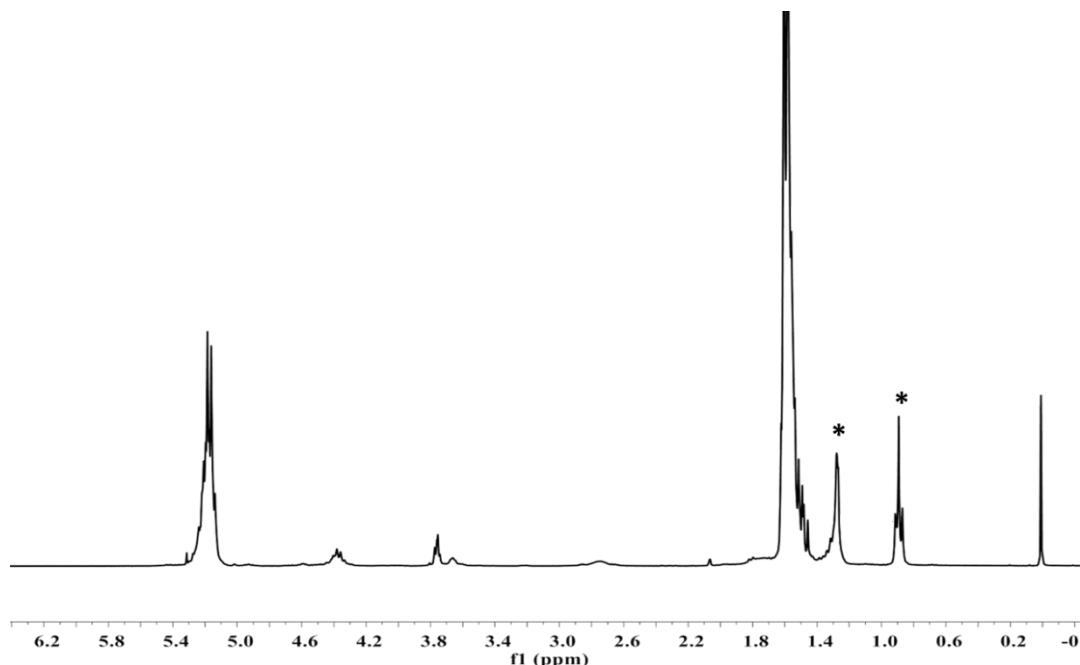


**Figure S2.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of **Cat.1**.

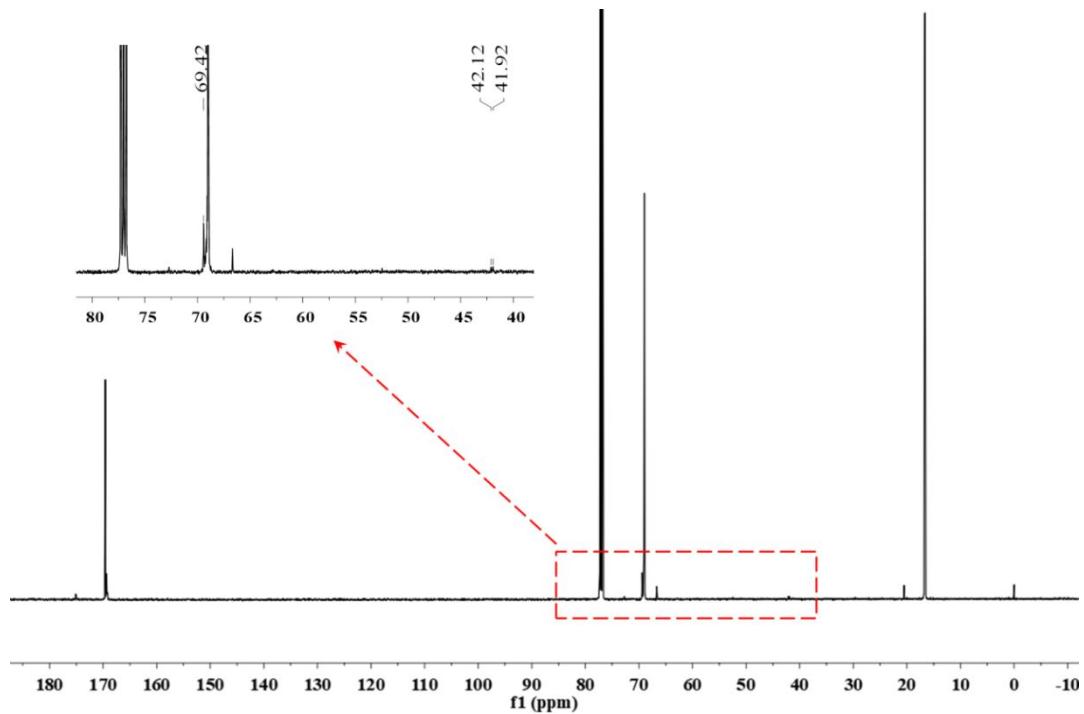
#### 4. NMR spectra of ECH/PA ROCOP and LA ROP



**Figure S3.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA copolymer (entry 1 in **Table 1**). There was no signal of ether linkage (ether linkage was located between 3.7-3.5 ppm<sup>10</sup>).

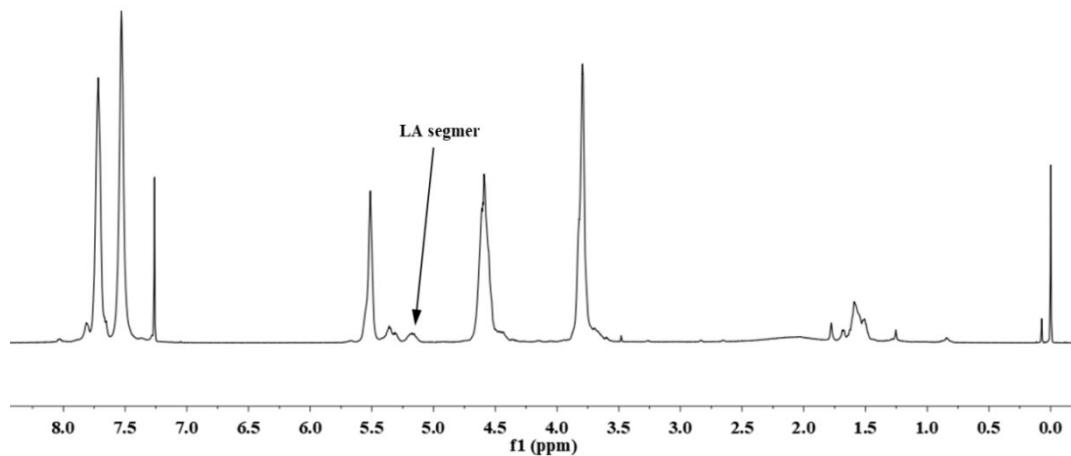


**Figure S4.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PLA (entry 2 in **Table 1**).

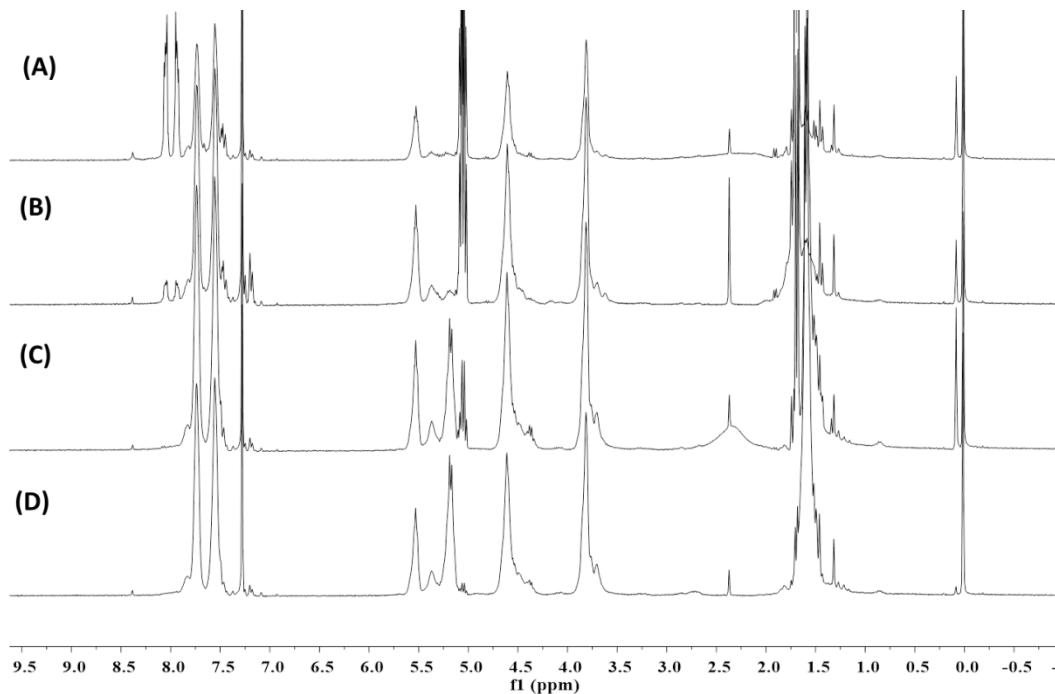


**Figure S5.**  $^{13}\text{C}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of PLA (entry 2 in **Table 1**). There was no signal of ether linkage (the signal of polyepichlorohydrin was recorded at 79.23, 69.82 and 43.74 ppm)<sup>11</sup>.

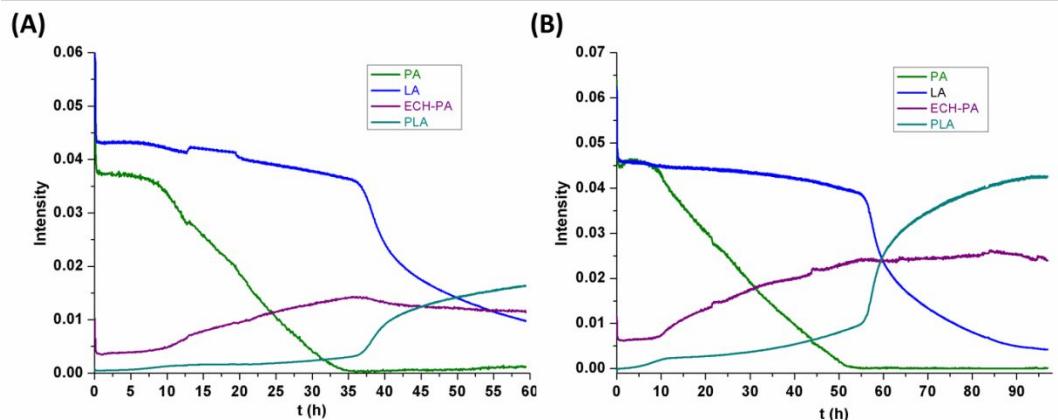
## 5. Structure analysis of ECH/PA/LA terpolymer



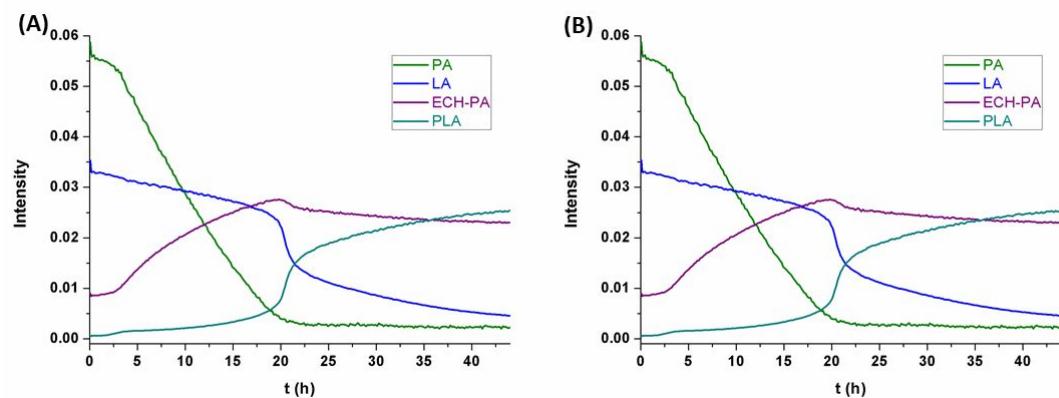
**Figure S6.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of the isolated polymer precipitated from entry 3 in **Table 1**.



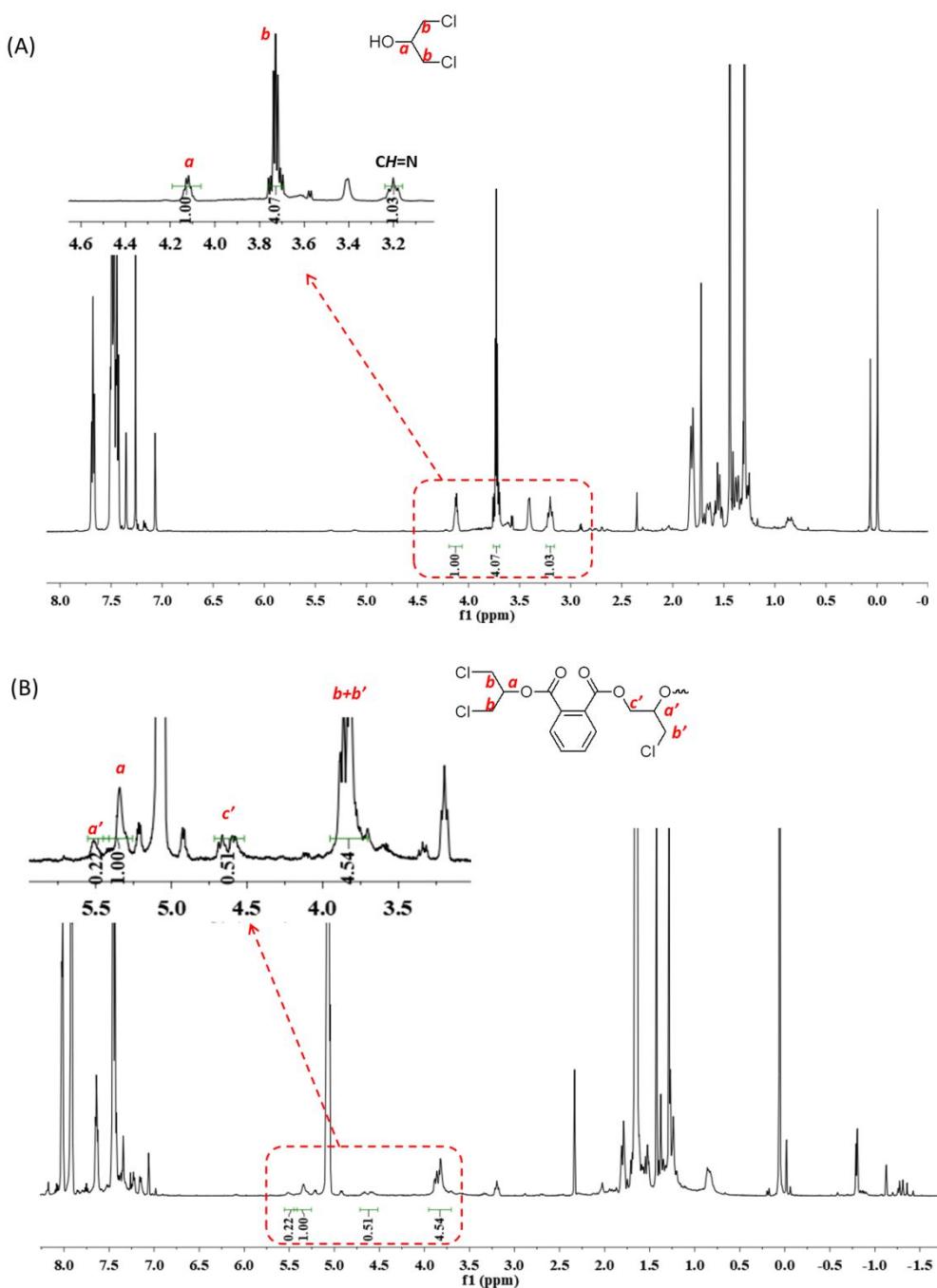
**Figure S7.** <sup>1</sup>H NMR spectrum (300 MHz, CDCl<sub>3</sub>) of the samples extracted from the mixture of ECH/PA/LA terpolymerization (entry 5 in **Table 1**): (A) conv. of PA = 66.5 %, conv. of LA = 4.0 %; (B) conv. of PA= 89.9 %, conv. of LA = 6 %; (C) conv. of PA = 100 %, conv. of LA = 70 %; (D) conv. of PA = 100 %, conv. of LA = 97 %.



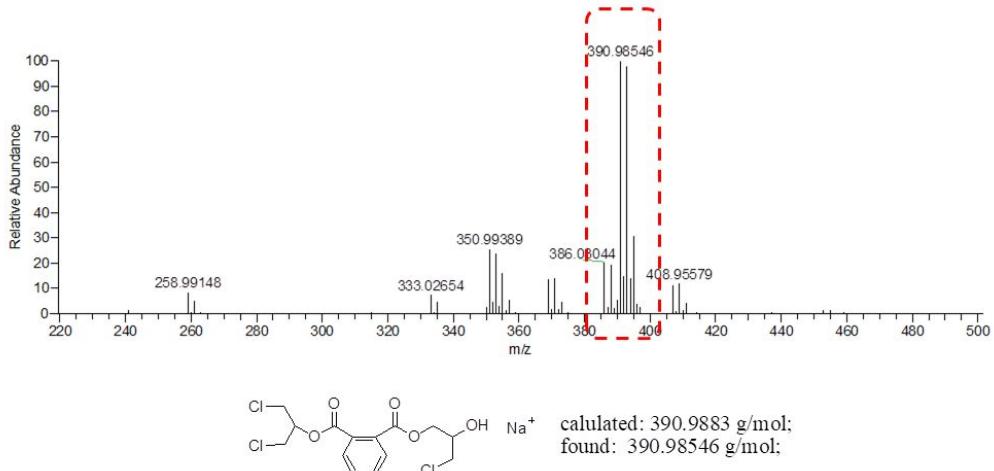
**Figure S8.** *in-situ* ATR-IR spectroscopy for various monomer ratios of ECH/PA/LA terpolymerization (concentrations of **Cat.1** is 0.01 mmol per 1 g toluene; reaction temperature is 80 °C): **(A)** **Cat.1:PPNCl:LA:PA:ECH** = 1:1:100:50:75; **(B)** **Cat.1:PPNCl:LA:PA:ECH** = 1:1:150:100:150.



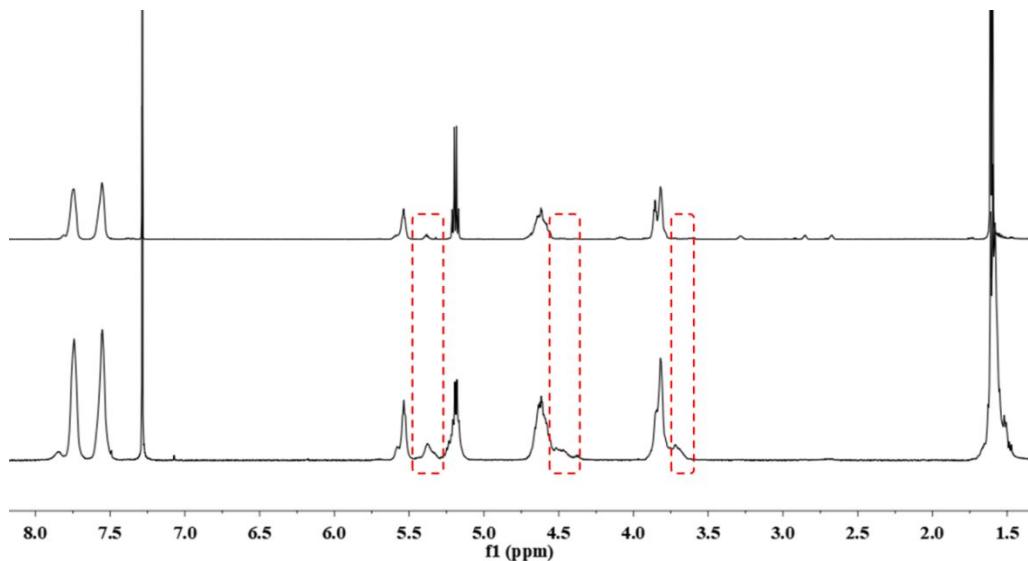
**Figure S9.** *in-situ* ATR-IR spectroscopy for different reaction temperatures (**Cat.1:PPNCl:LA:PA:ECH** = 1:1:100:100:150, concentrations of **Cat.1** is 0.01 mmol per 1 g toluene). the reaction temperature was 90 °C for **(A)** and 100 °C for **(B)**.



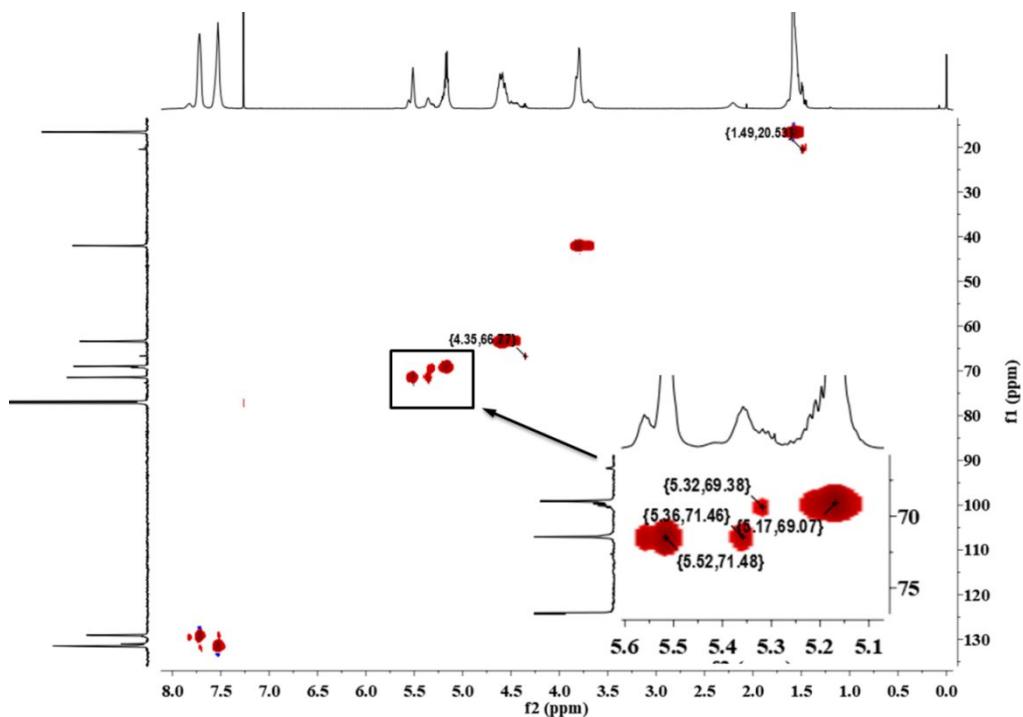
**Figure S10.** Initiation group analysis. **(A)** The binary catalyst catalyzed ring-opening reaction of ECH (reaction condition: **Cat.1**:PPNCl:ECH=1:1:150, the concentration of **Cat.1** is 0.01 mmol per 1 g toluene). After 2 h at 80 °C, a small amount of reaction mixture was extracted for <sup>1</sup>H NMR analysis. The result indicated the ring-opening reaction occurred at the methylene C-O bond. **(B)** Terpolymerization of ECH/PA/LA (reaction condition: **Cat.1**:PPNCl:PA:LA:ECH = 1:1:20:20:30 concentration of **Cat.1** was 0.01 mmol per 1 g toluene; T = 80 °C; t = 2 h). <sup>1</sup>H NMR spectrum for the extracted mixture also demonstrated the end-capped group was 1,3-dichloropropan-2-oxy<sup>12</sup>.



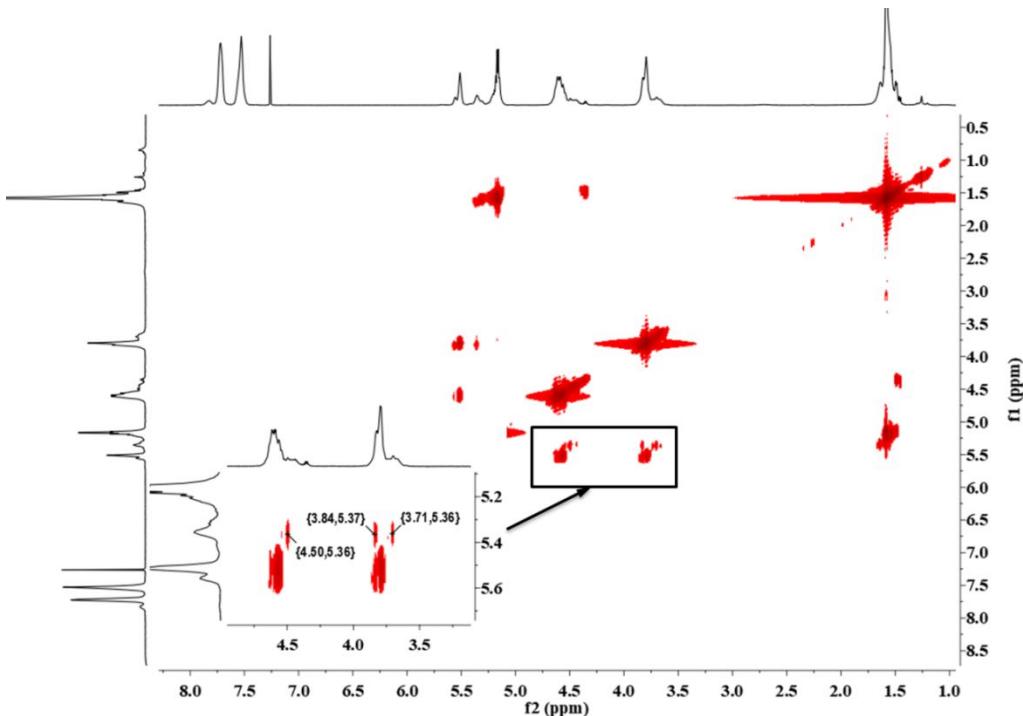
**Figure S11.** Liquid chromatography–mass spectrometry (LC-MS) in methanol for the end-group analysis of oligomer (reaction conduction: the reaction mixture with **Cat.1** 0.03 mmol, PPNCl 0.03 mmol, PA 0.15 mmol, ECH 0.24 mmol and toluene 3 g was heated at 80 °C for 10 h. Then the oligomer was obtained by removing solvent under vacuum). The strongest signal of LC-MS, 390.98546, was corresponding to the calculated molecular weight (390.9883), indicating the polymerization was initiated by chlorine.



**Figure S12.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of the blend of PLA/Poly(ECH-PA) (top) and ECH/PA/LA terpolymer (bottom).

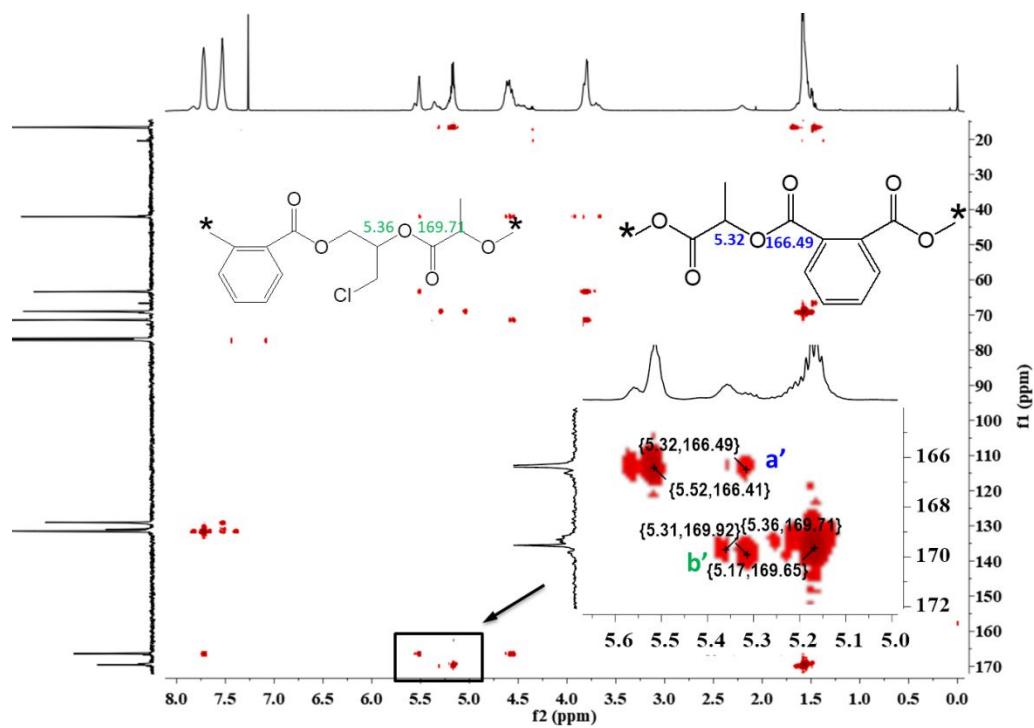


**Figure S13.**  $^1\text{H}$ - $^{13}\text{C}$  HMQC spectrum (600 MHz,  $\text{CDCl}_3$ ) of ECH/PA/LA terpolymer. The peak from 5.40 to 5.30 ppm was assigned to two kinds of protons, namely, 5.36 ppm belonging to methine proton of ECH unit and 5.32 ppm belonging to methine proton of LA unit. In addition, the signals recorded at 1.49/20.53 ppm and 4.35/66.77 ppm belonged to chain end group of PLA segment.

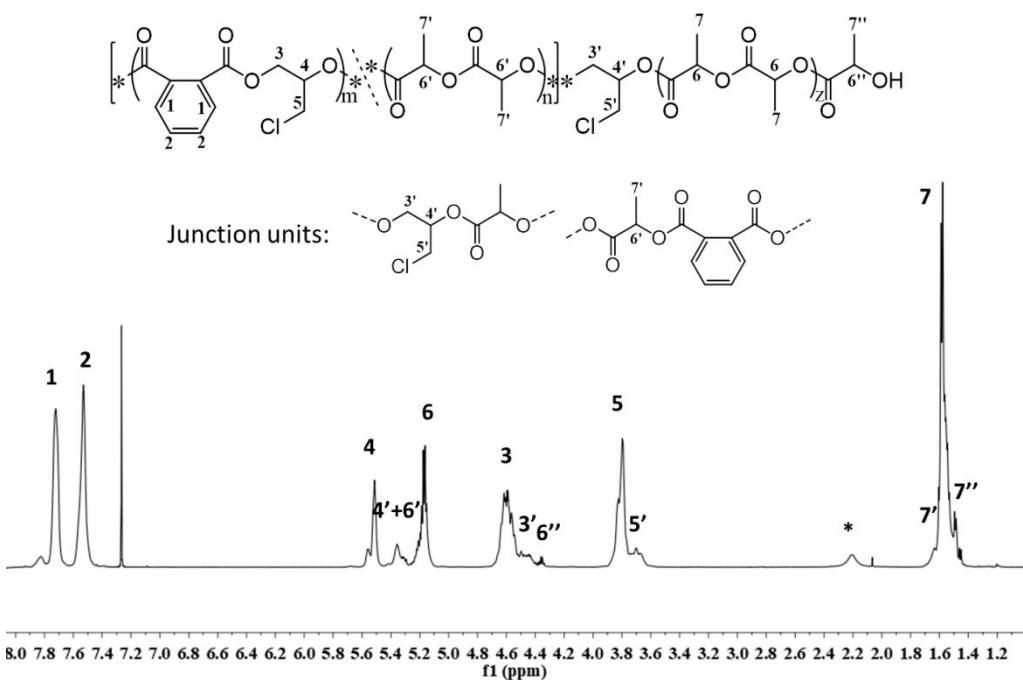


**Figure S14.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz,  $\text{CDCl}_3$ ) of ECH/PA/LA terpolymer. It established that the correlation between peak at 5.36 ppm and the small upfield shoulders at 4.50 and 3.71 ppm, which were assigned to methylene of epoxy group and methyl chloride,

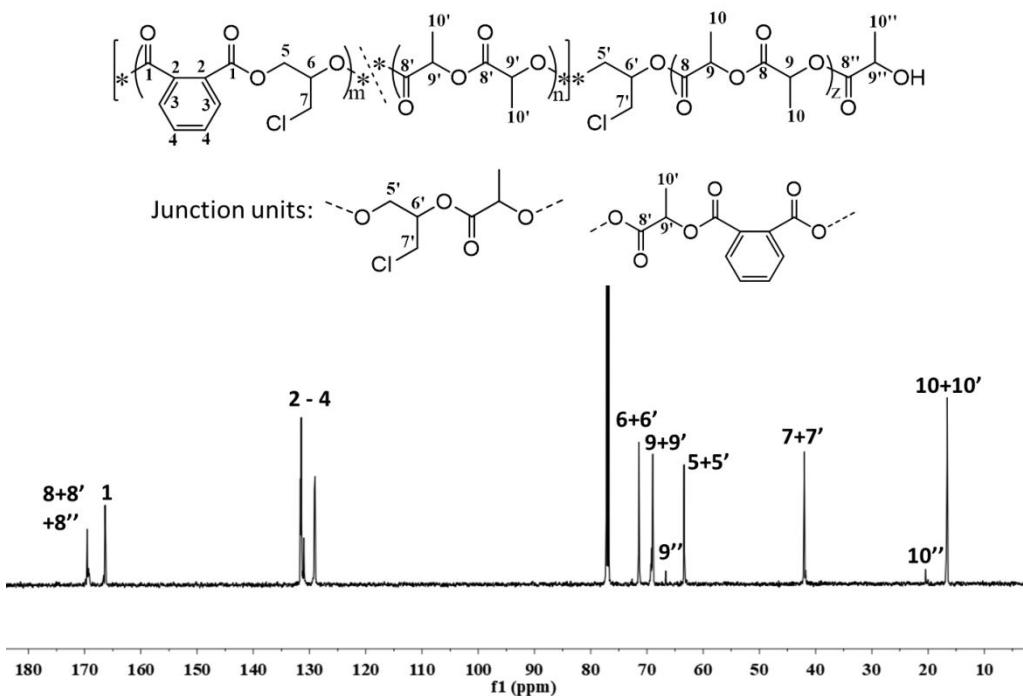
respectively.



**Figure S15.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum (600 MHz,  $\text{CDCl}_3$ ) of ECH/PA/LA terpolymer. It clearly disclosed that the signal recorded at 5.36/169.71 ppm was the direct proof of correlation between methane proton of ECH unit and carboxyl carbon of LA unit, and signal at 5.32/166.49 ppm suggested the formation of ester bond between methoxyl of LA unit and carboxyl of PA unit.

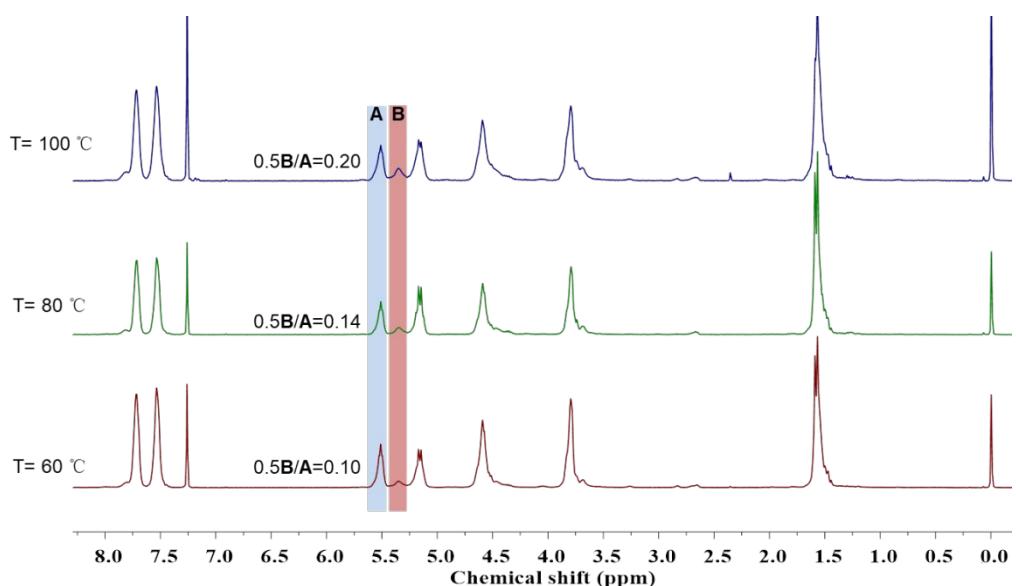


**Figure S16.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of ECH/PA/LA terpolymer.

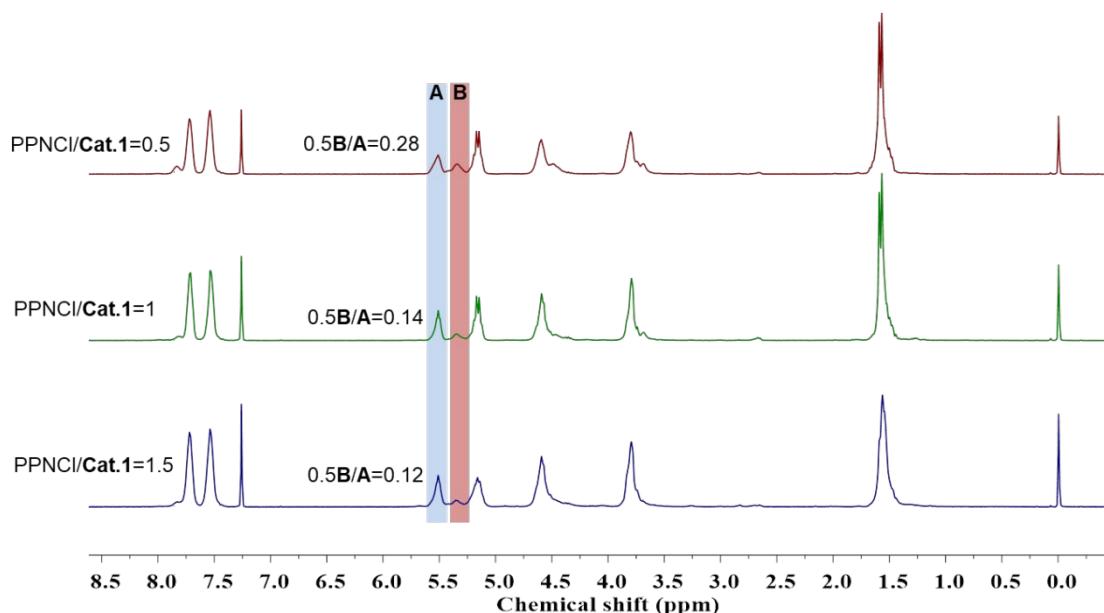


**Figure S17.**  $^{13}\text{C}$  NMR spectrum (500 MHz,  $\text{CDCl}_3$ ) of ECH/PA/LA terpolymer.

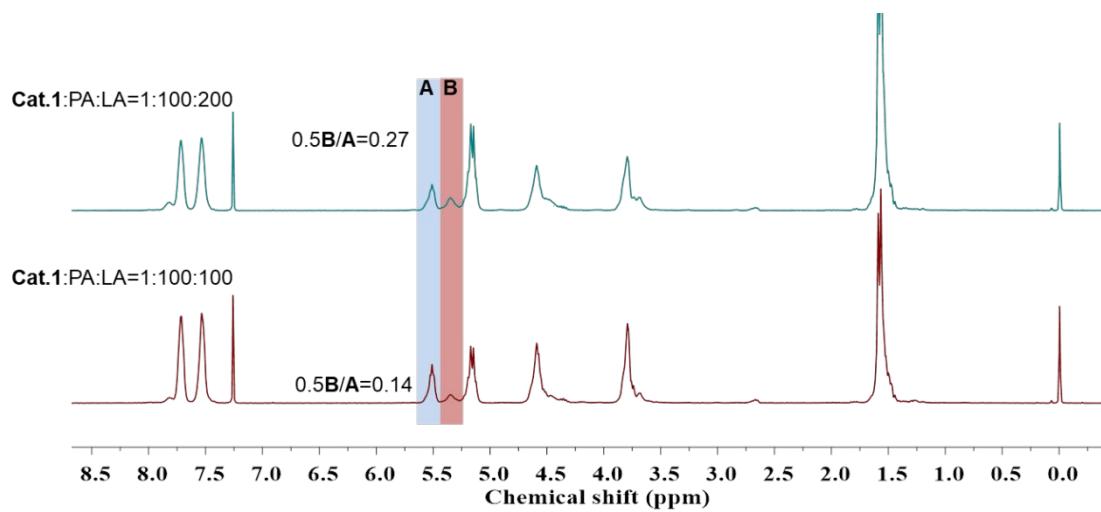
## 6. Effect of the content of LA incorporation into the first block



**Figure S18.** Effect of reaction temperature for LA content in the first block of ECH/PA/LA terpolymer (reaction condition: **Cat.1**:PPNCl:PA:LA:ECH=1:1:100:100:150, the concentration of **Cat.1** is 0.01 mmol per 1 g toluene). In the  $^1\text{H}$  NMR spectra of result polymers, “**A**” represented the content of ECH-PA block, and “**B**” represented to the total content of “ECH-LA” unit and “LA-PA” unit. Thus the content of LA insertion into ECH-PA block could be calculated by the formula:  $0.5*\mathbf{B}/\mathbf{A}$ .

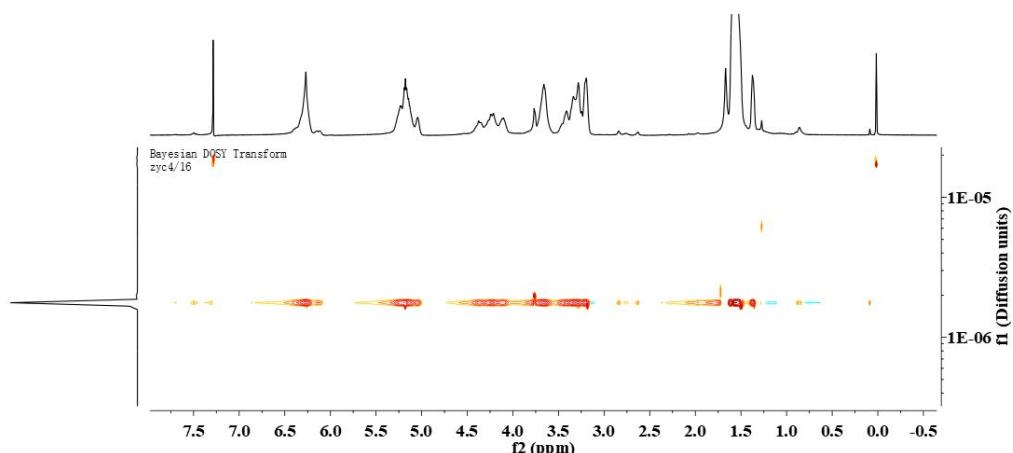


**Figure S19.** Effect of cocatalyst ratio for LA content in the first block of ECH/PA/LA terpolymer (reaction condition: **Cat.1**:PA:LA:ECH=1:100:100:150,  $T=80$  °C, the concentration of **Cat.1** is 0.01 mmol per 1 g toluene). The calculation method referred to **Figure S18**.

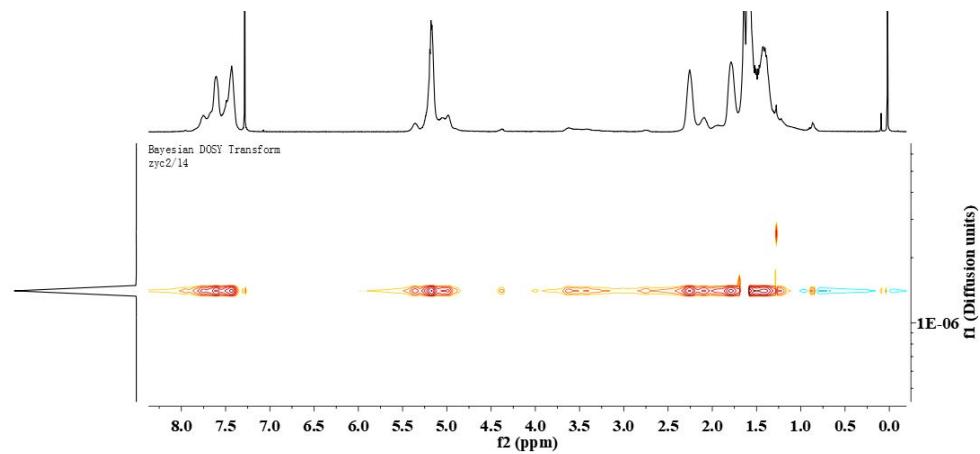


**Figure S20.** Effect of monomer ratio for LA content in the first block of ECH/PA/LA terpolymer (reaction condition: the concentration of **Cat.1** is 0.01 mmol per 1 g toluene, and T=80 °C). The calculation method referred to **Figure S18**.

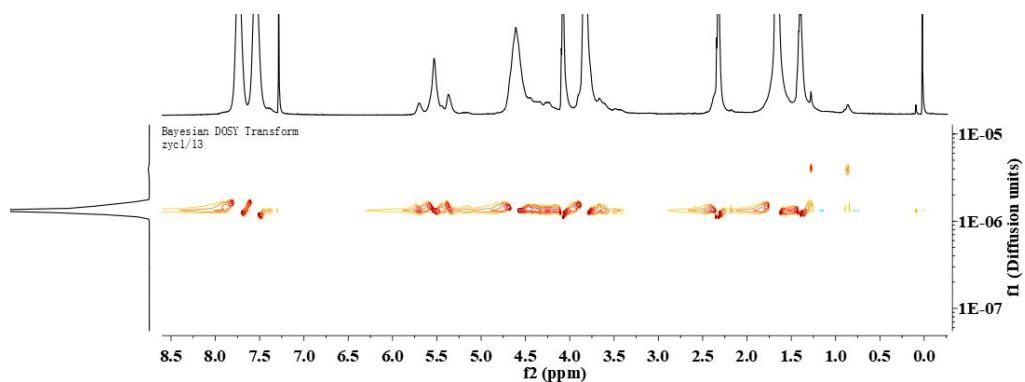
## 7. Representative DOSY spectra of expanded terpolymers



**Figure S21.** DOSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of ECH/NA/LA polymer (entry 3 in **Table 2**).

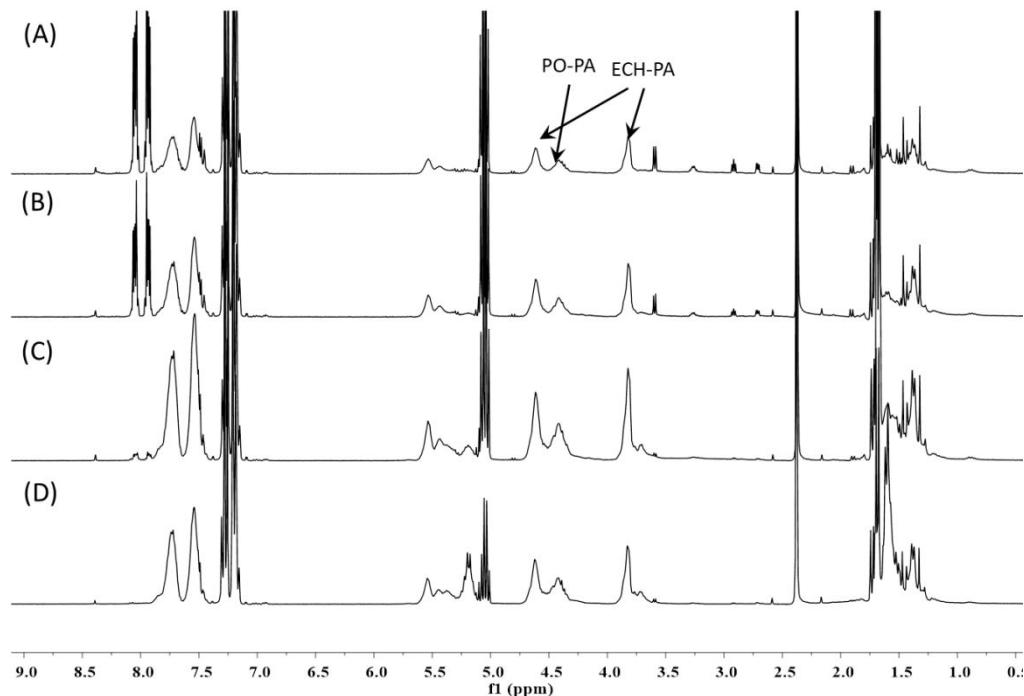


**Figure S22.** DOSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of CHO/PA/LA polymer (entry 5 in **Table 2**).

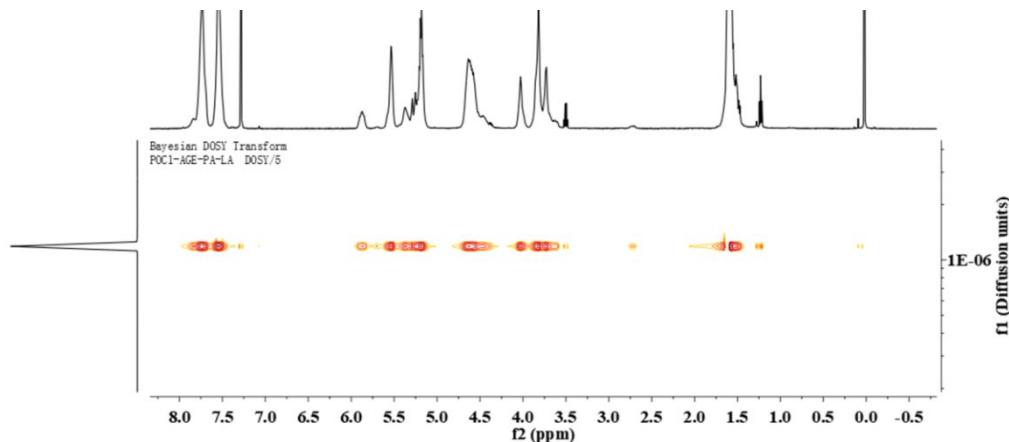


**Figure S23.** DOSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of ECH/PA/ε-CL polymer (entry 7 in **Table 2**).

## 8. Characterization of the tetrapolymerization of epoxides, anhydride and LA

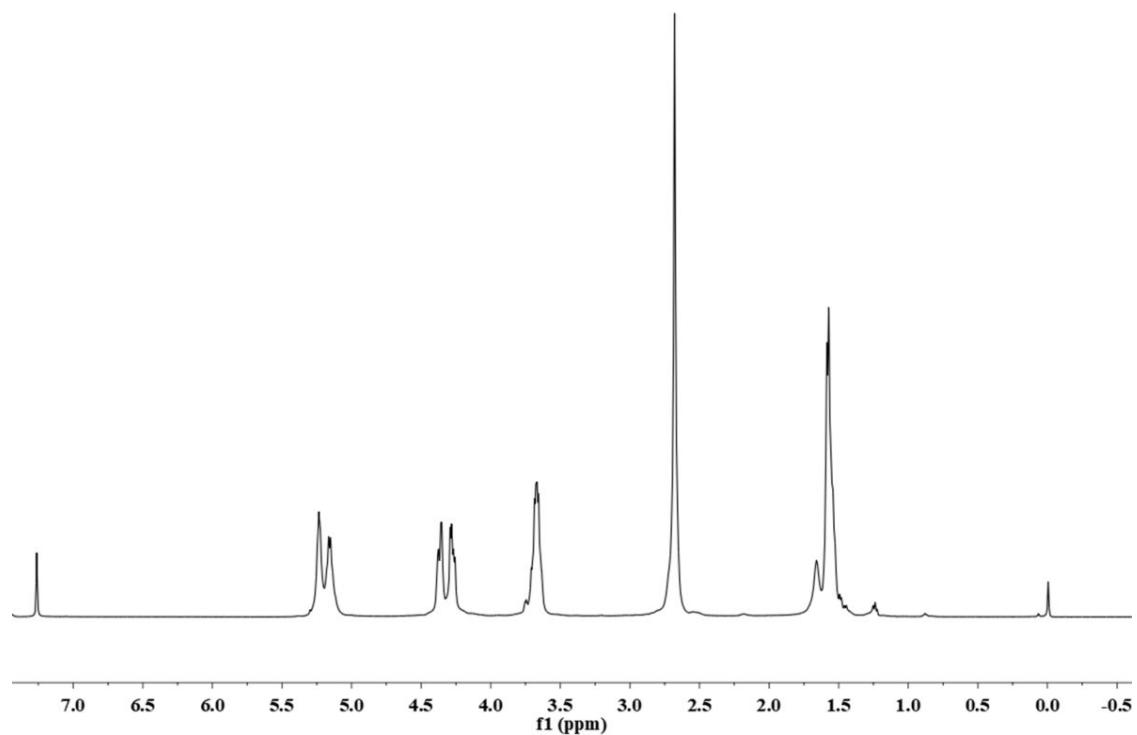


**Figure S24.** The  $^1\text{H}$  NMR spectrum recorded for conversions of ECH and PO during the polymerization of ECH, PA, PA and LA (entry 11 in **Table 2**). During the first stage of epoxides and anhydride polymerization, ECH and PO were consumed simultaneously.

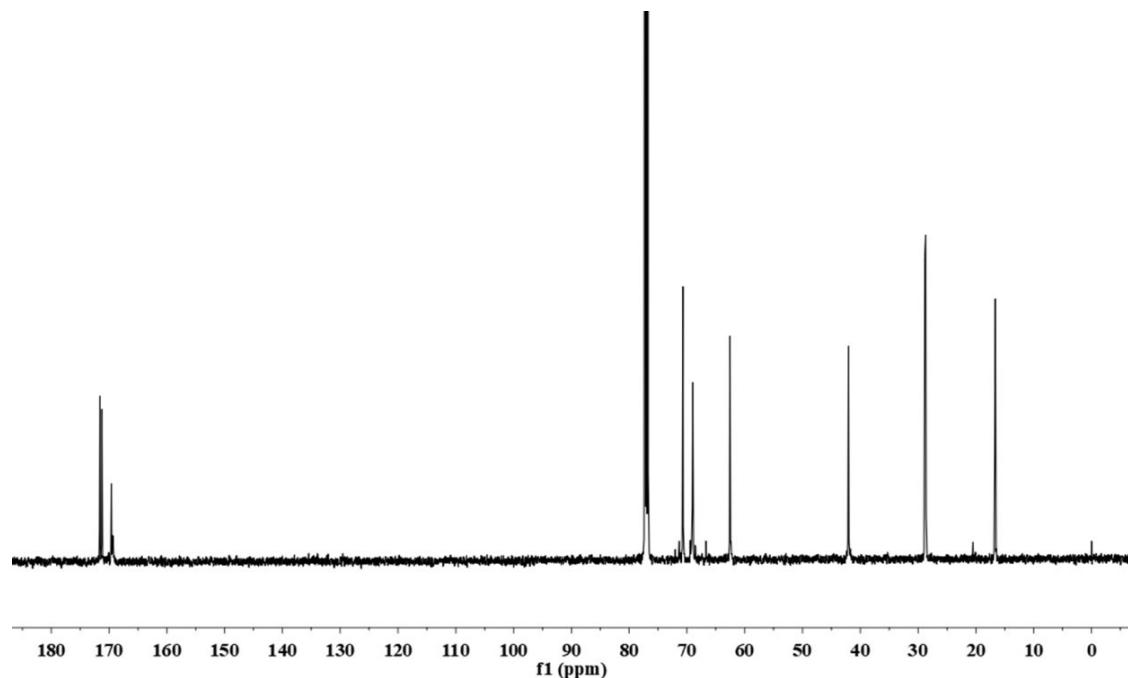


**Figure S25.** DOSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of ECH/AGE/PA/LA polymer (entry 12 in **Table 2**).

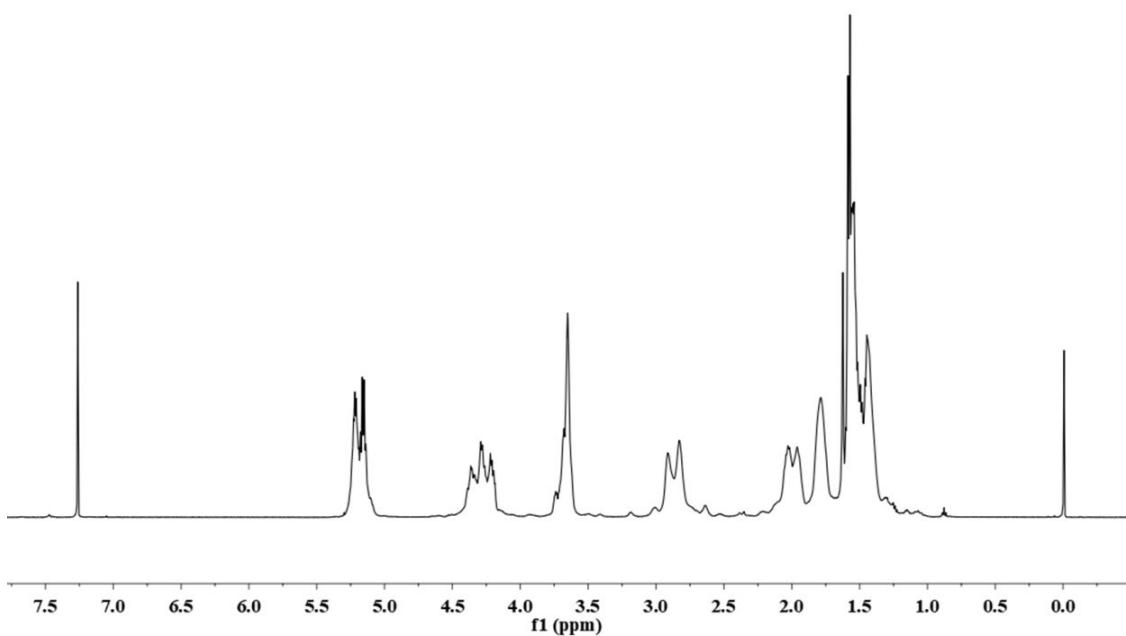
## 9. Representative NMR spectra of expanded polymers



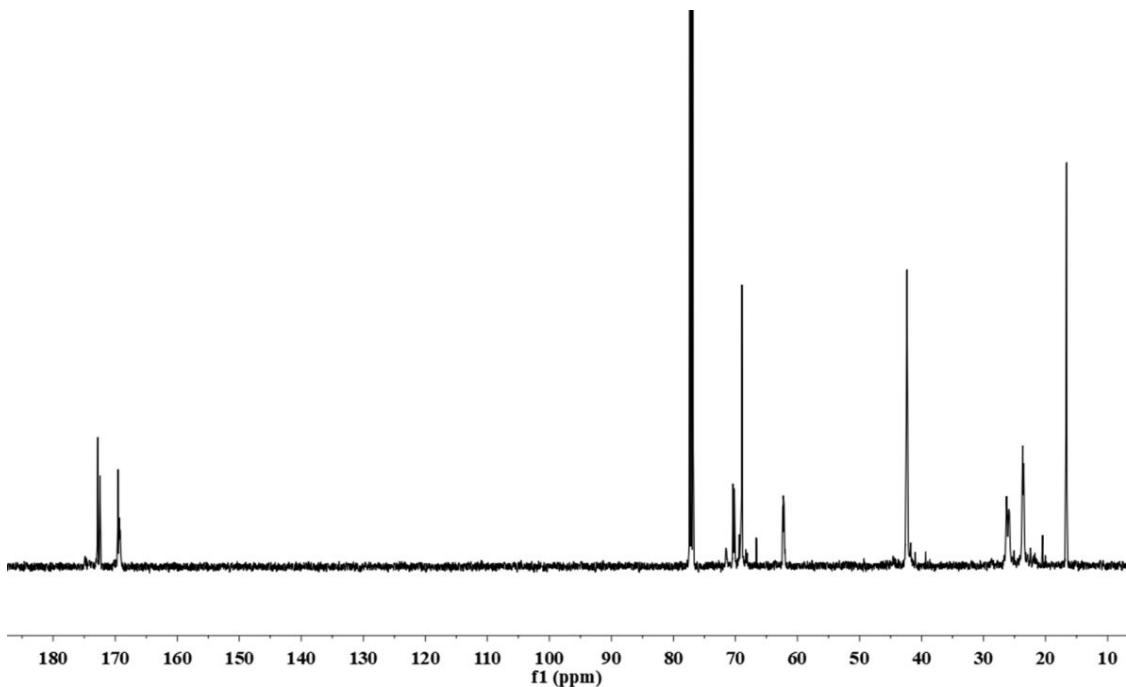
**Figure S26.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/SA/LA polymer.



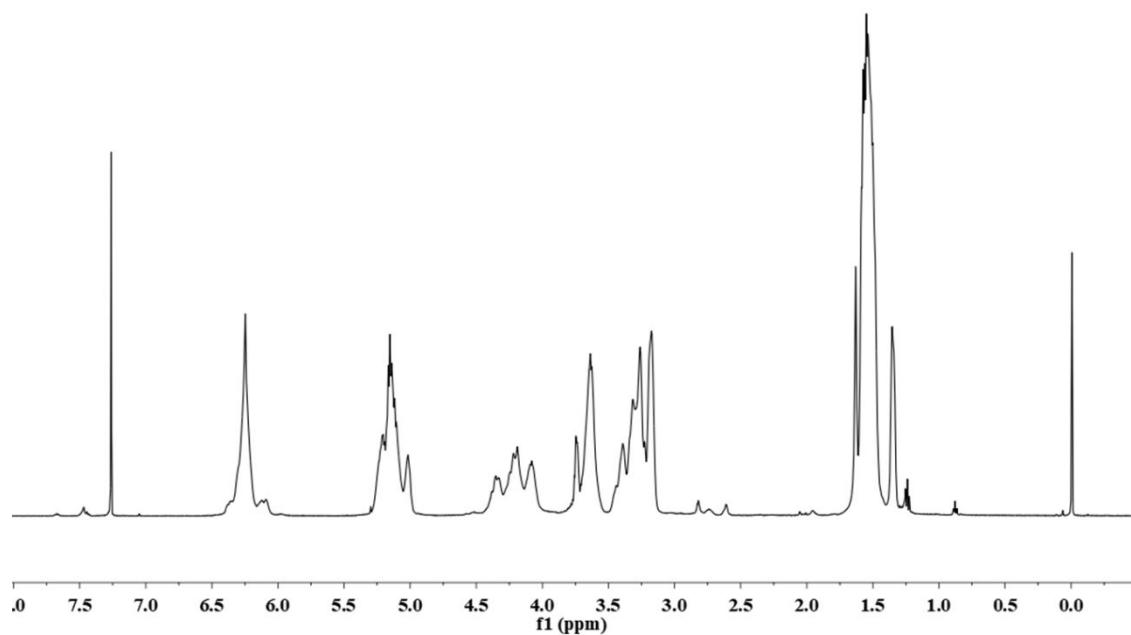
**Figure S27.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/SA/LA polymer.



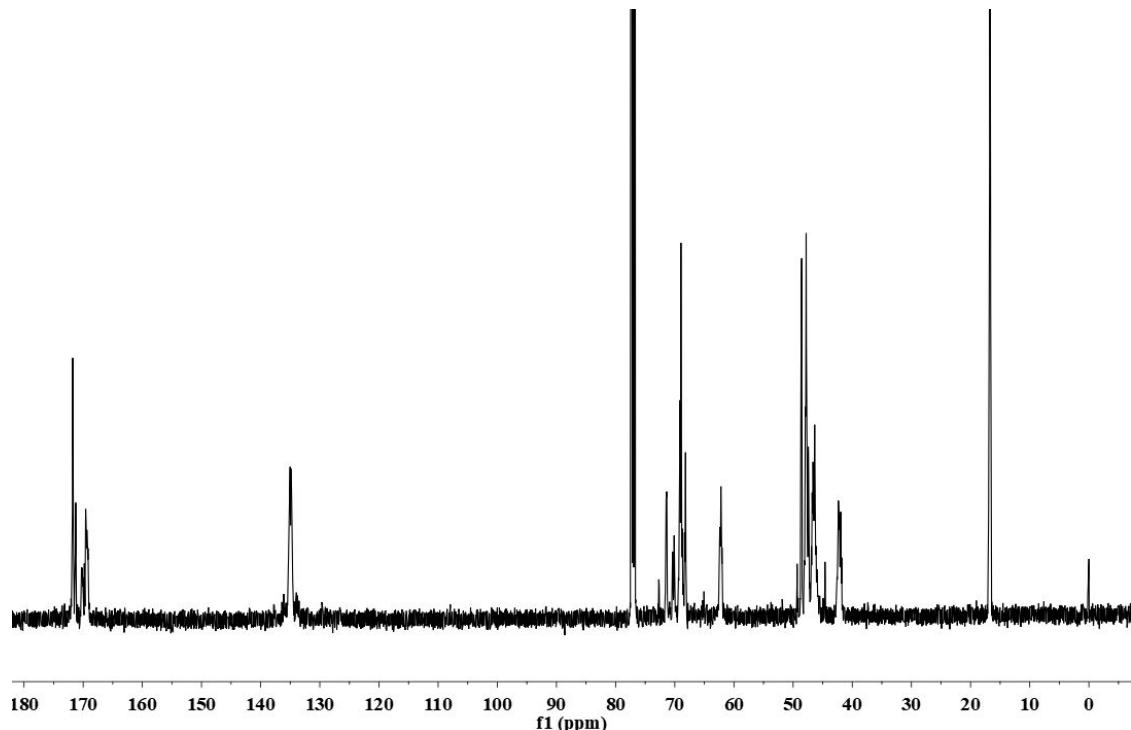
**Figure S28.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/CHA/LA polymer.



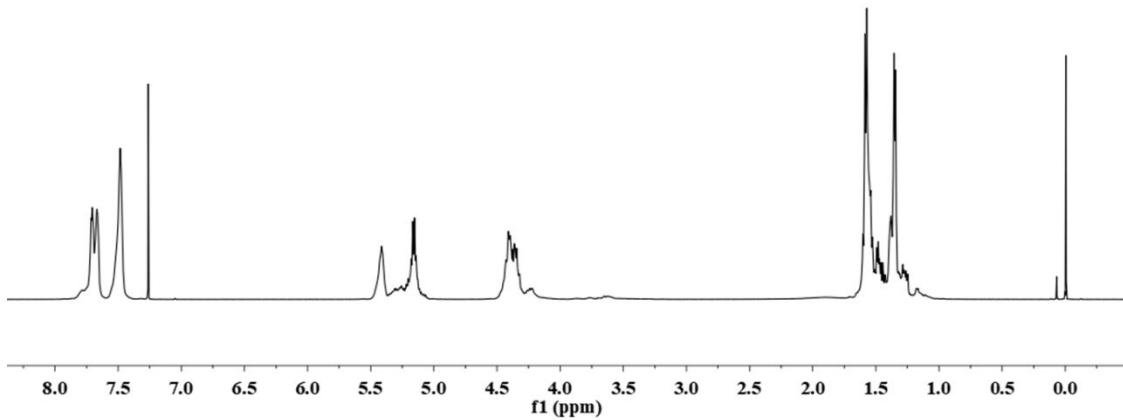
**Figure S29.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/CHA/LA polymer.



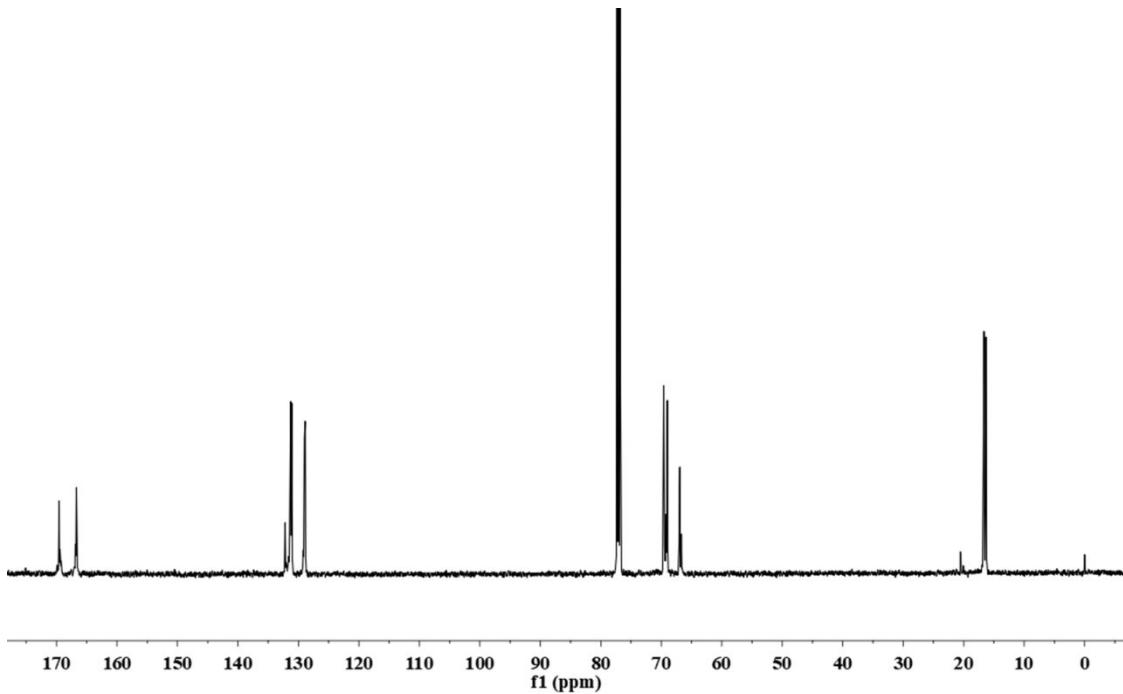
**Figure S30.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/NA/LA polymer.



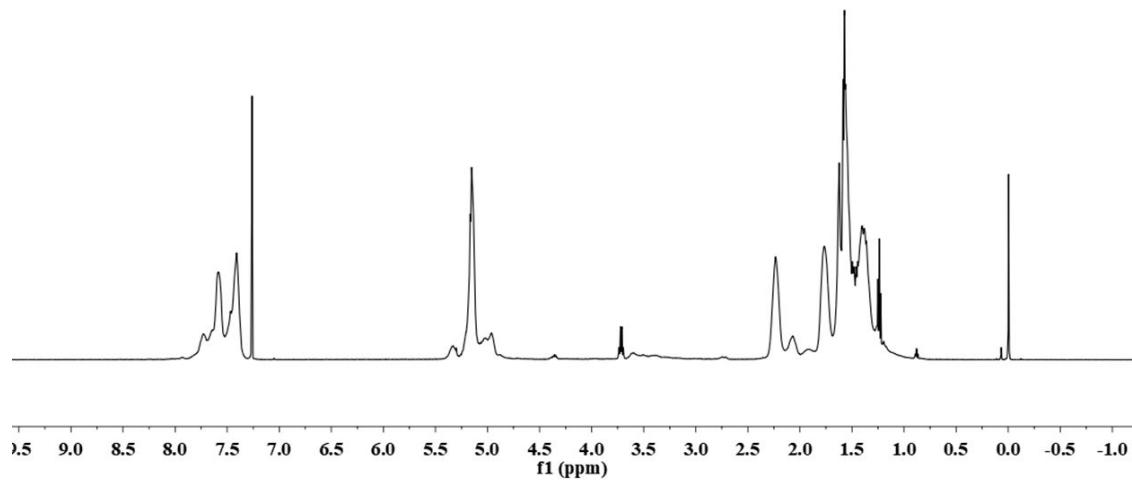
**Figure S31.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/NA/LA polymer.



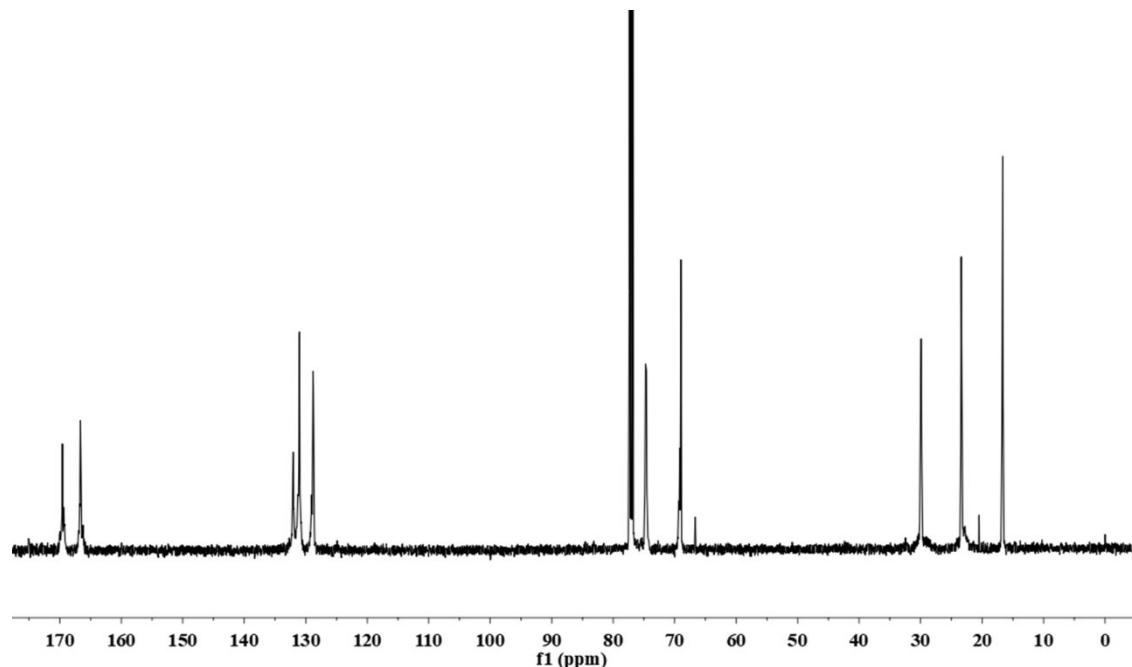
**Figure S32.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PO/PA/LA polymer.



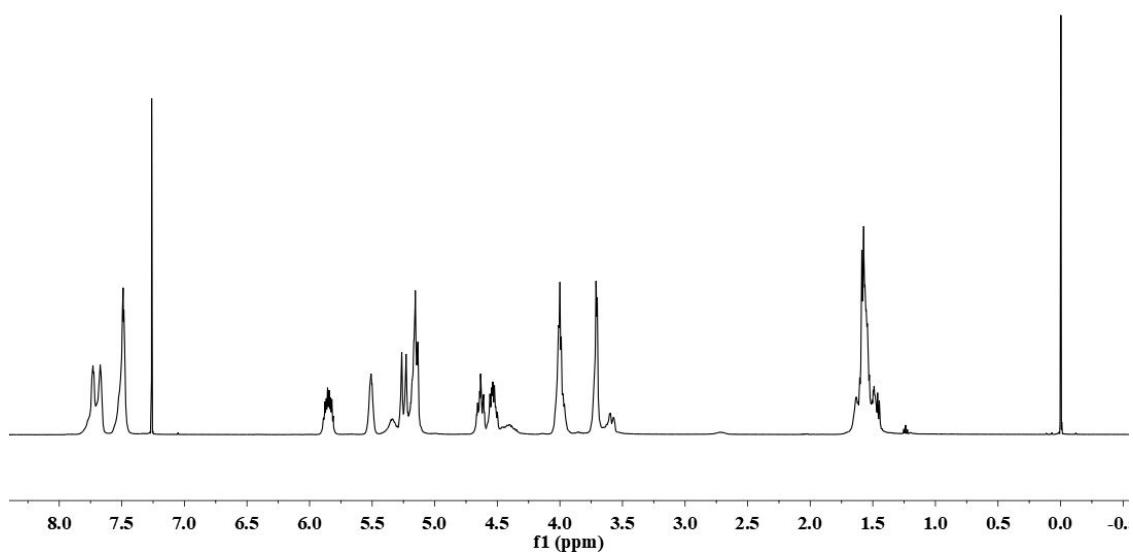
**Figure S33.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PO/PA/LA polymer.



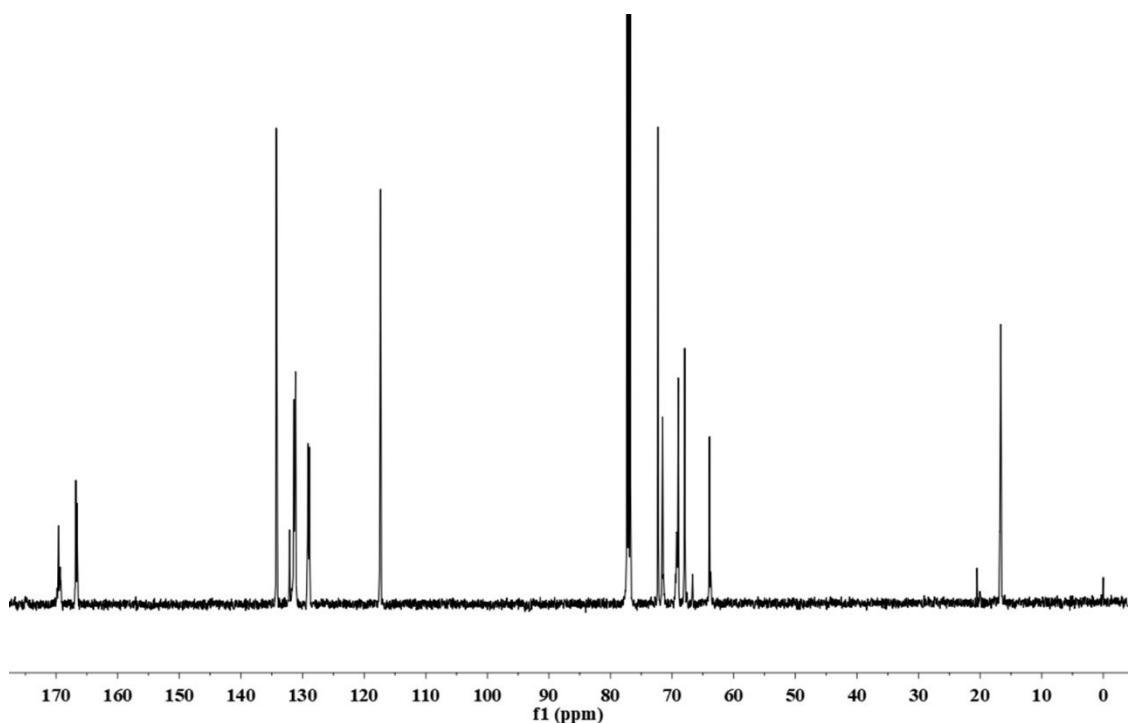
**Figure S34.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of CHO/PA/LA polymer.



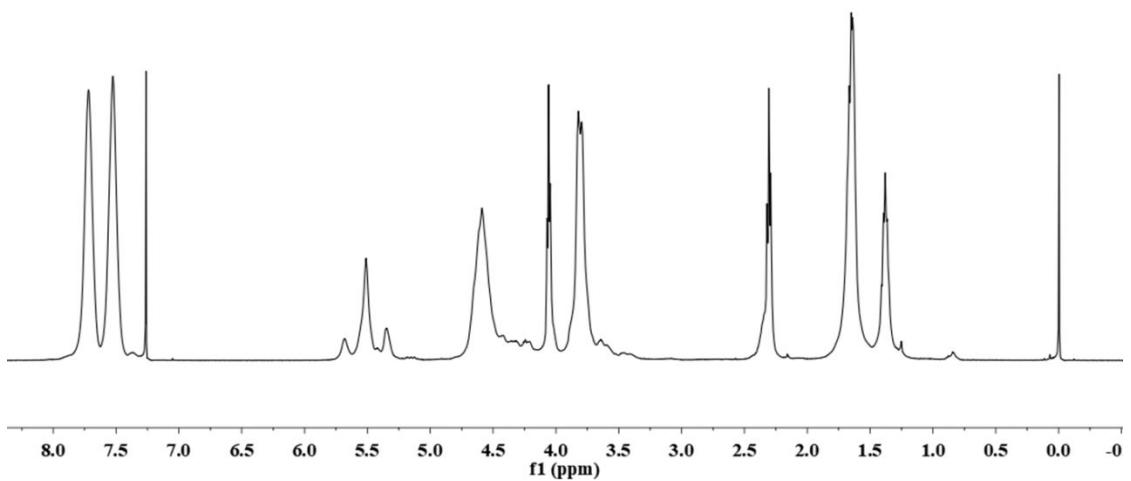
**Figure S35.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of CHO/PA/LA polymer.



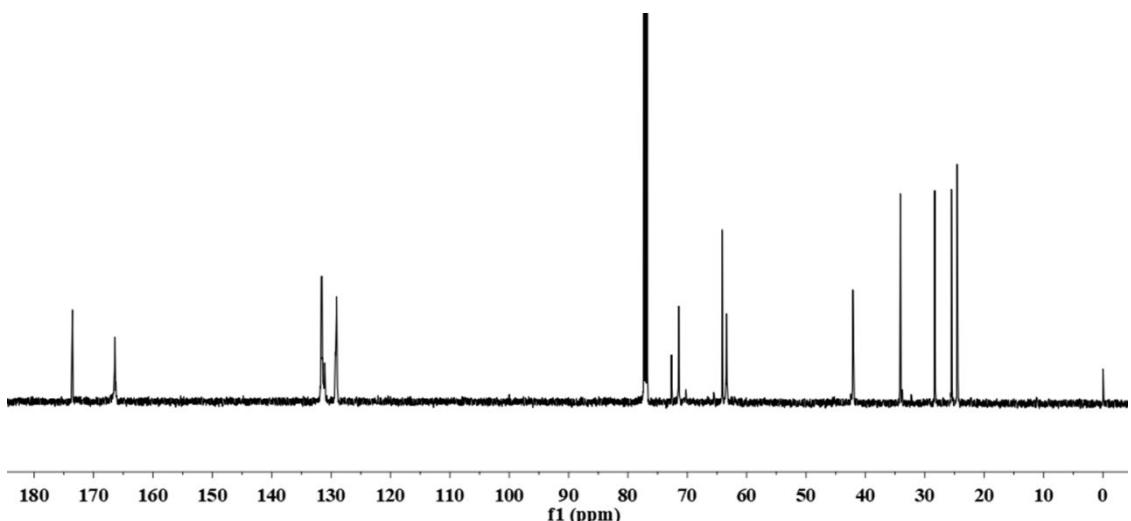
**Figure S36.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of AGE/PA/LA polymer.



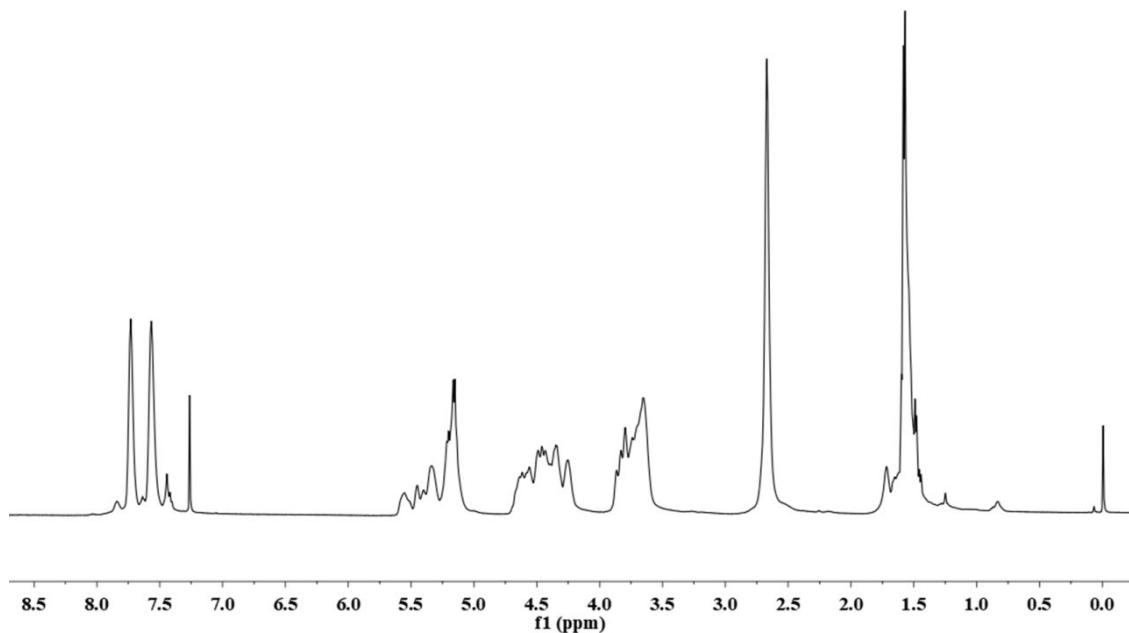
**Figure S37.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of AGE/PA/LA polymer.



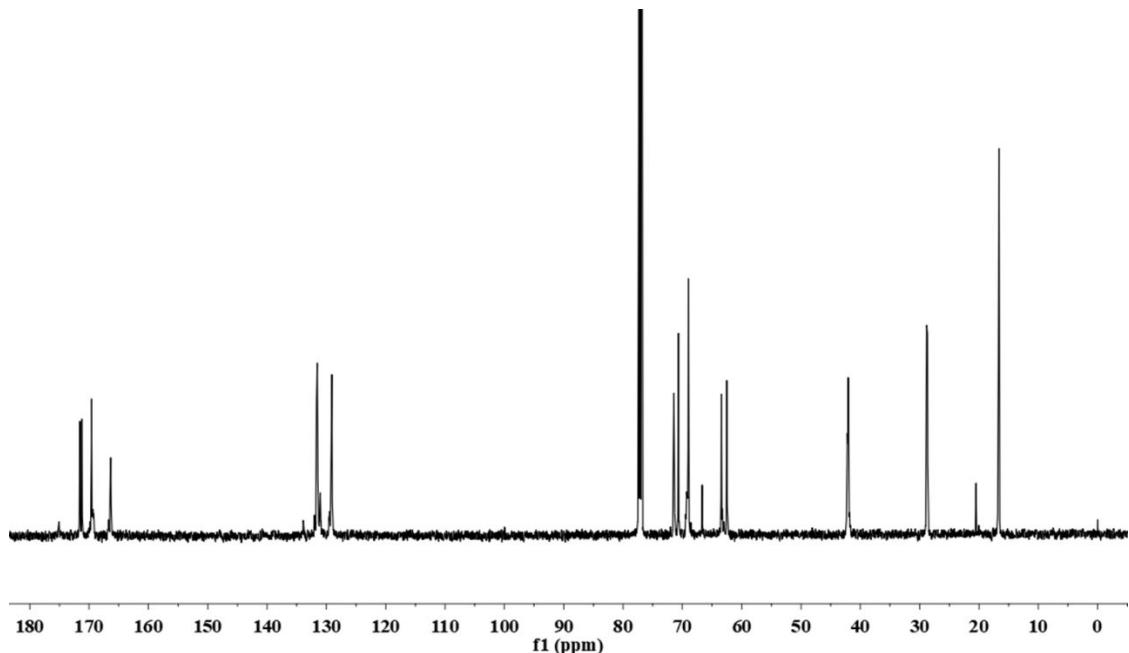
**Figure S38.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA/ε-CL polymer.



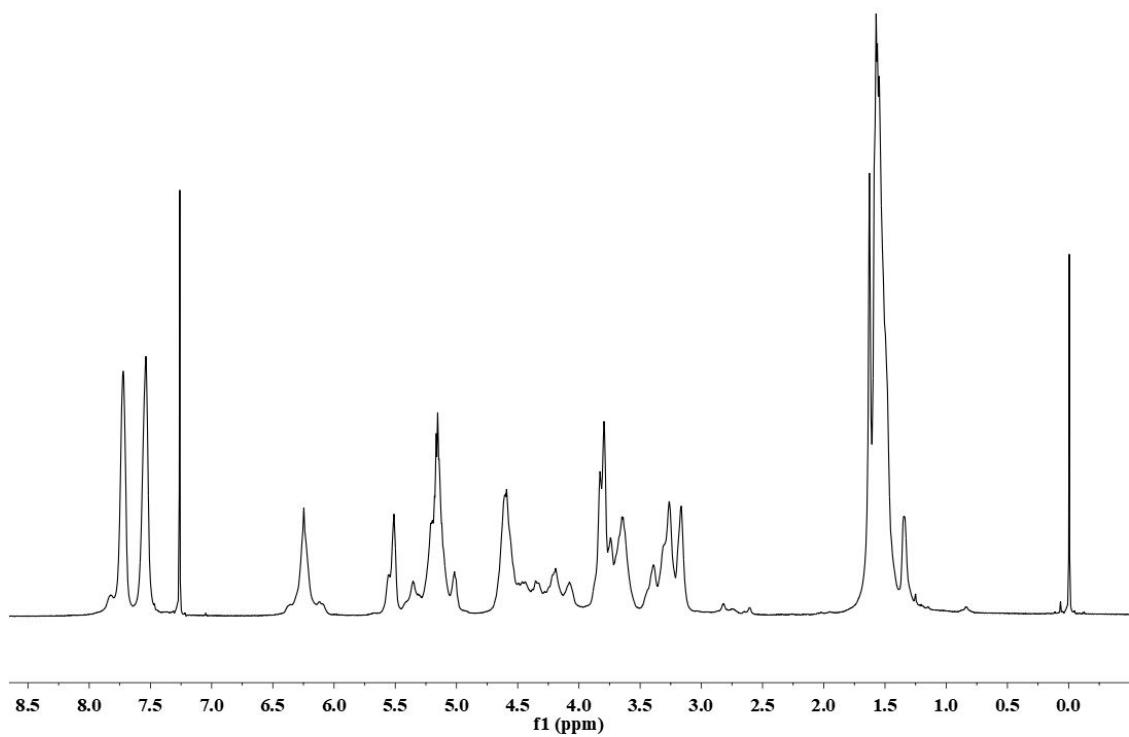
**Figure S39.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA/ε-CL polymer.



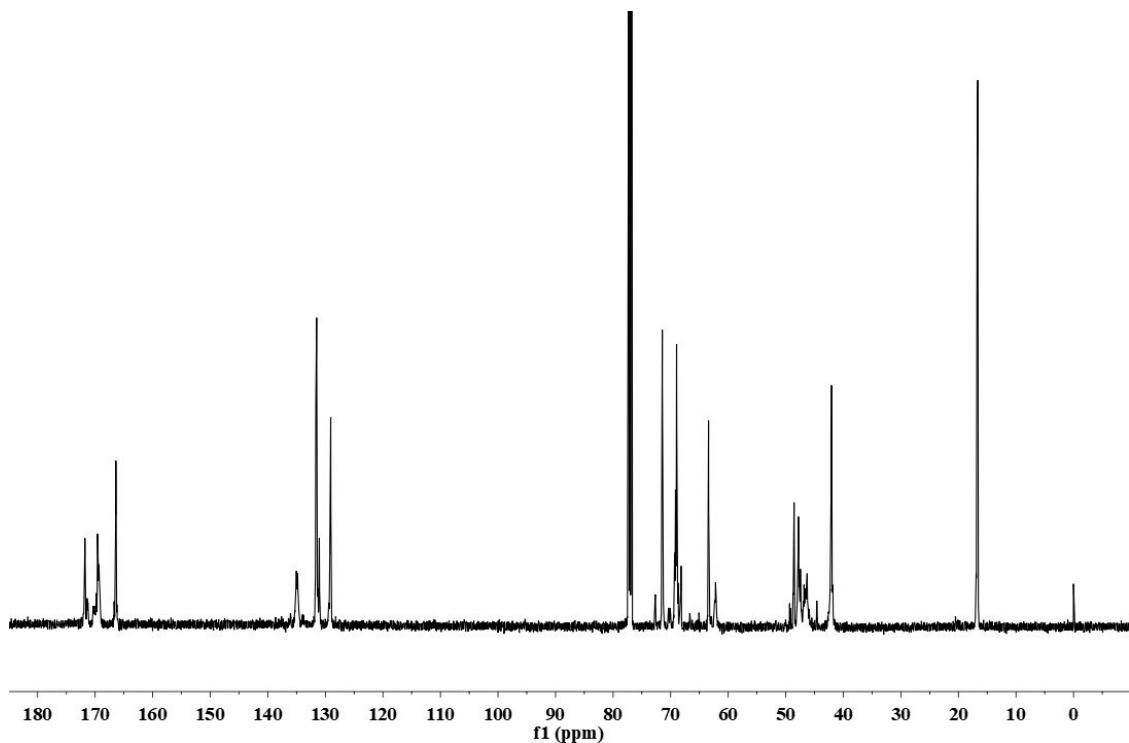
**Figure S40.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA/SA/LA polymer.



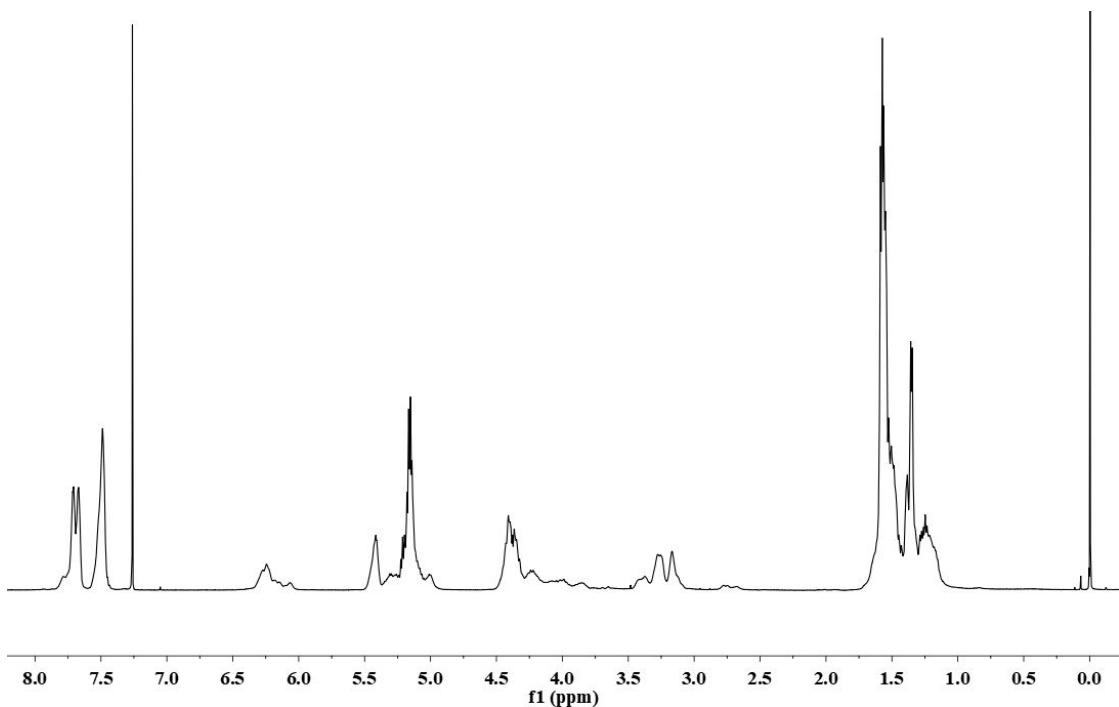
**Figure S41.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA/SA/LA polymer.



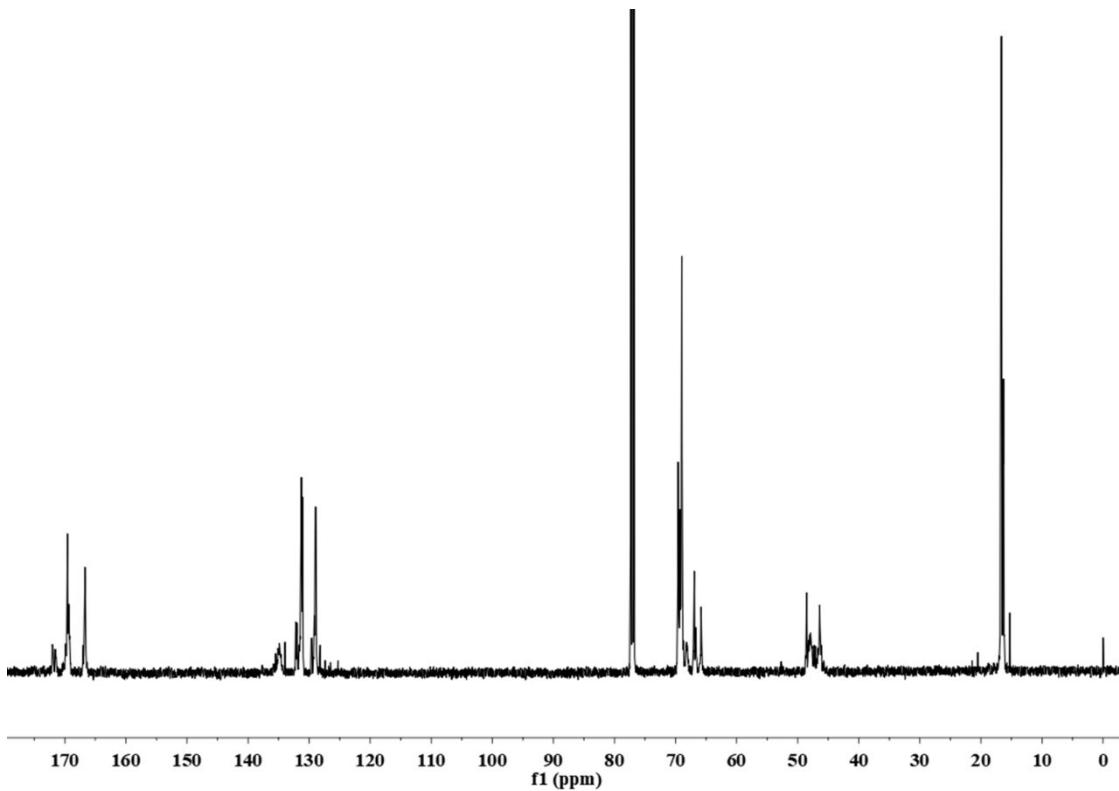
**Figure S42.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA/NA/LA polymer.



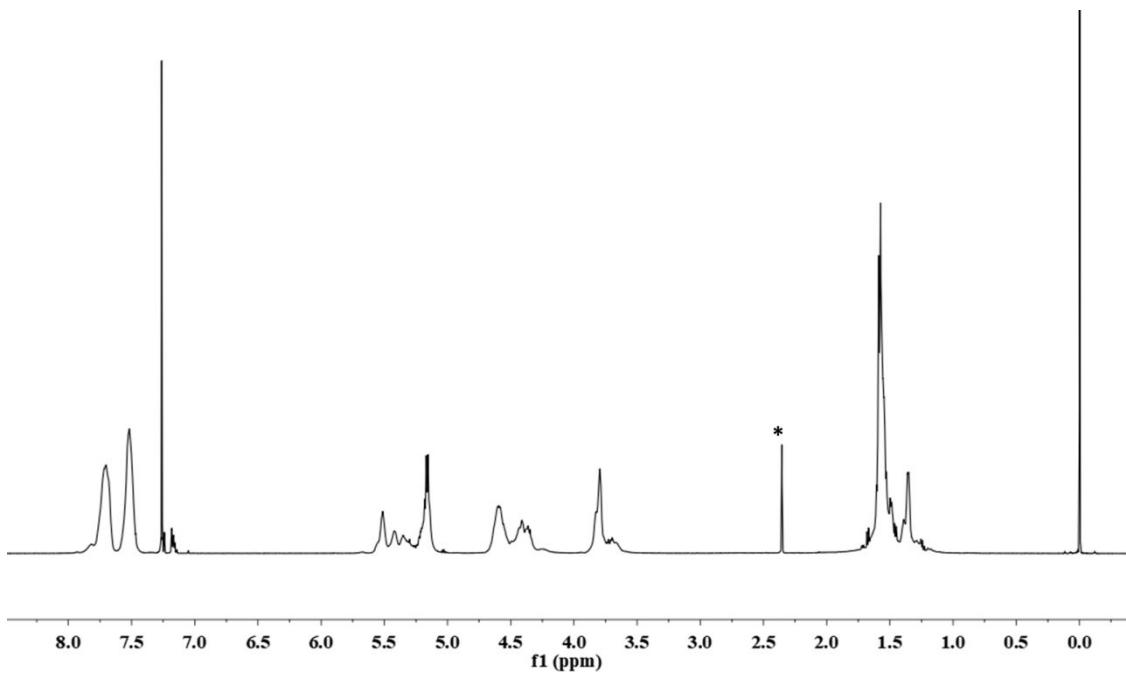
**Figure S43.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PA/NA/LA polymer.



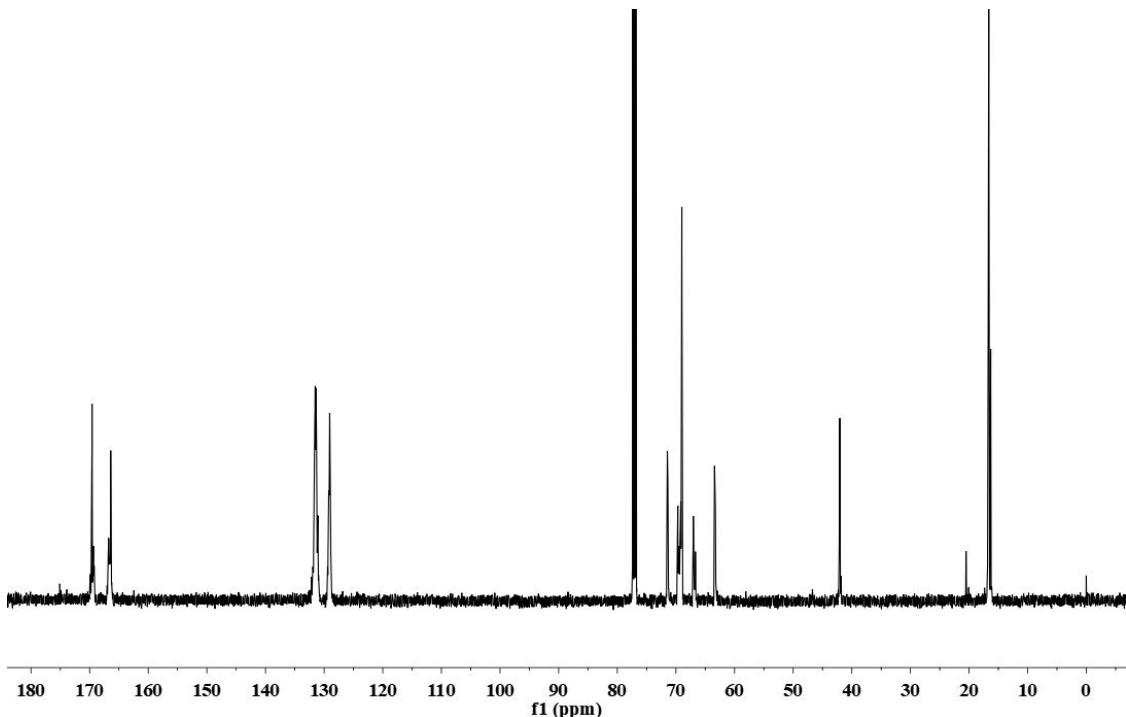
**Figure S44.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PO/PA/NA/LA polymer.



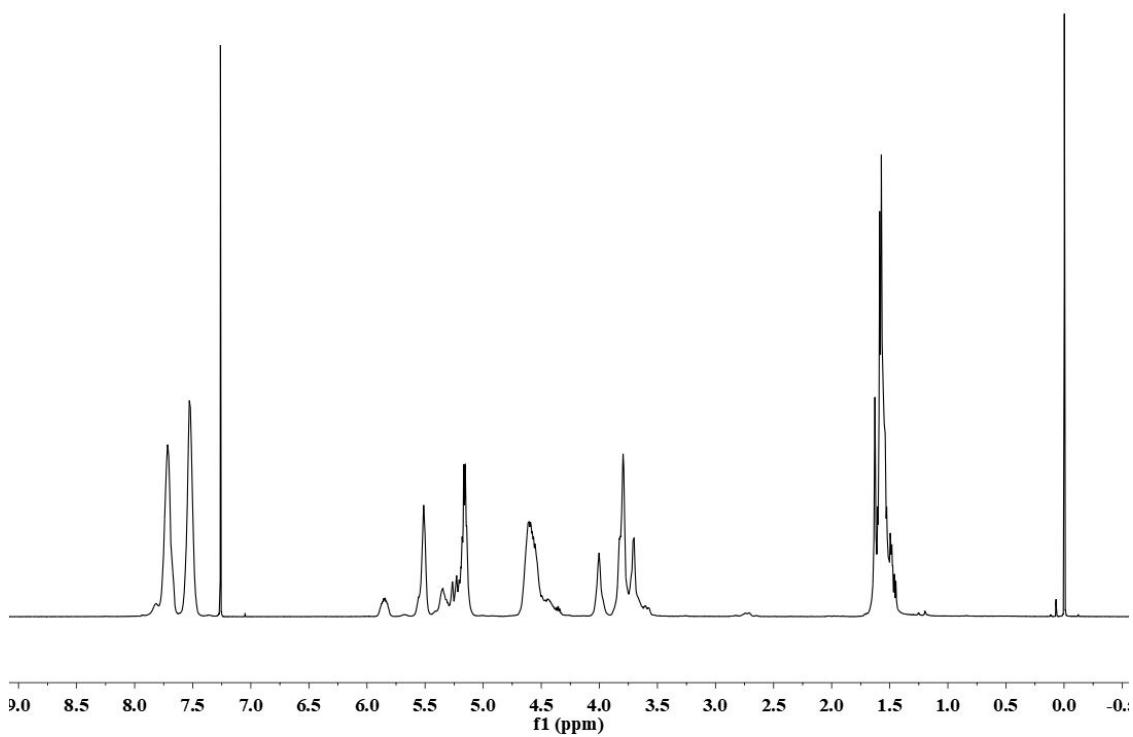
**Figure S45.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of PO/PA/NA/LA polymer.



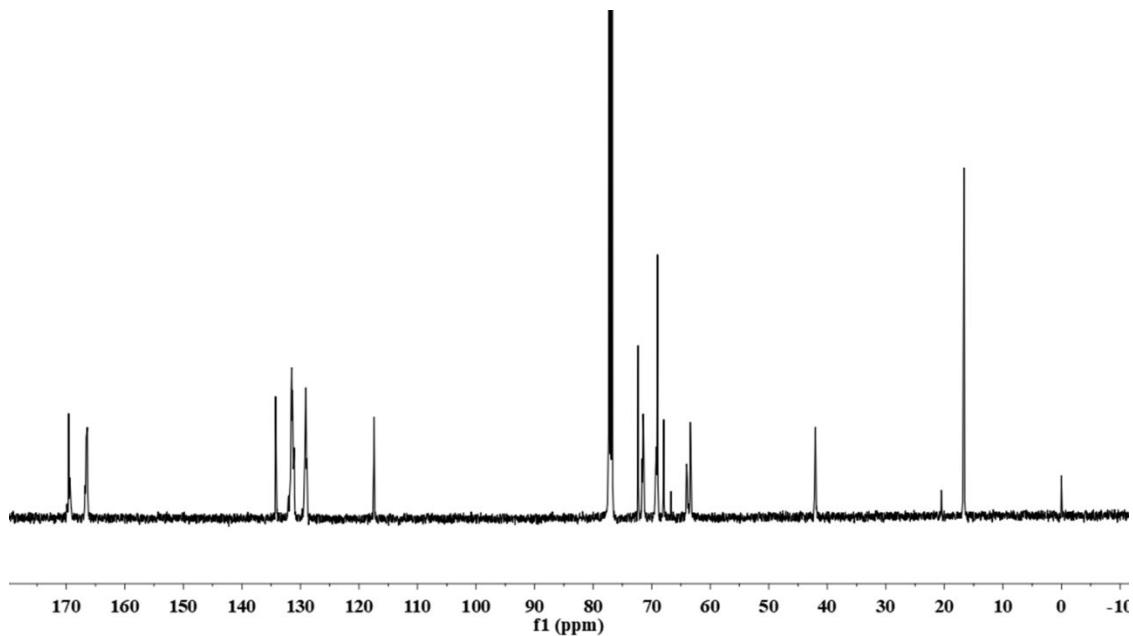
**Figure S46.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PO/PA/LA polymer.



**Figure S47.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/PO/PA/LA polymer.

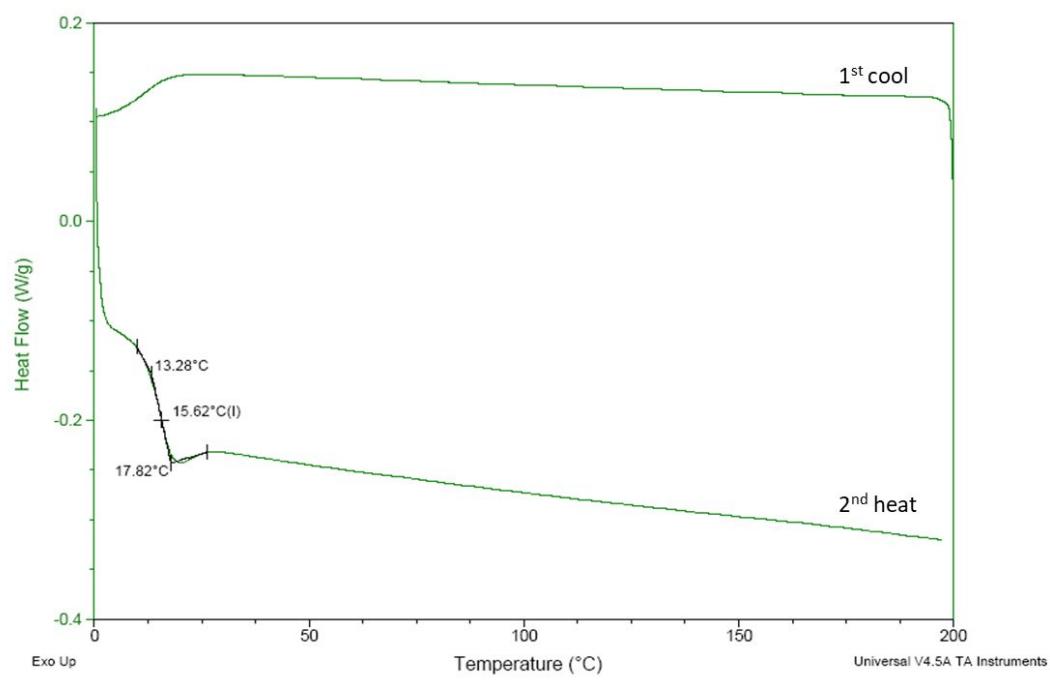


**Figure S48.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/AGE/PA/LA polymer.

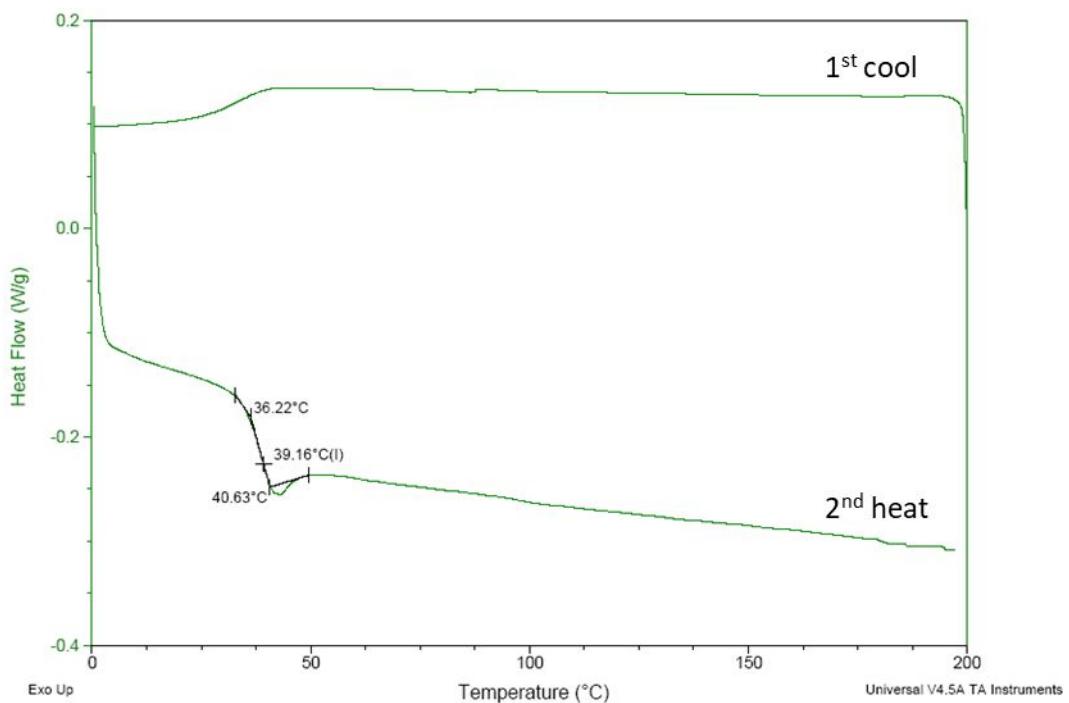


**Figure S49.** <sup>13</sup>C NMR spectrum (500 MHz, CDCl<sub>3</sub>) of ECH/AGE/PA/LA polymer.

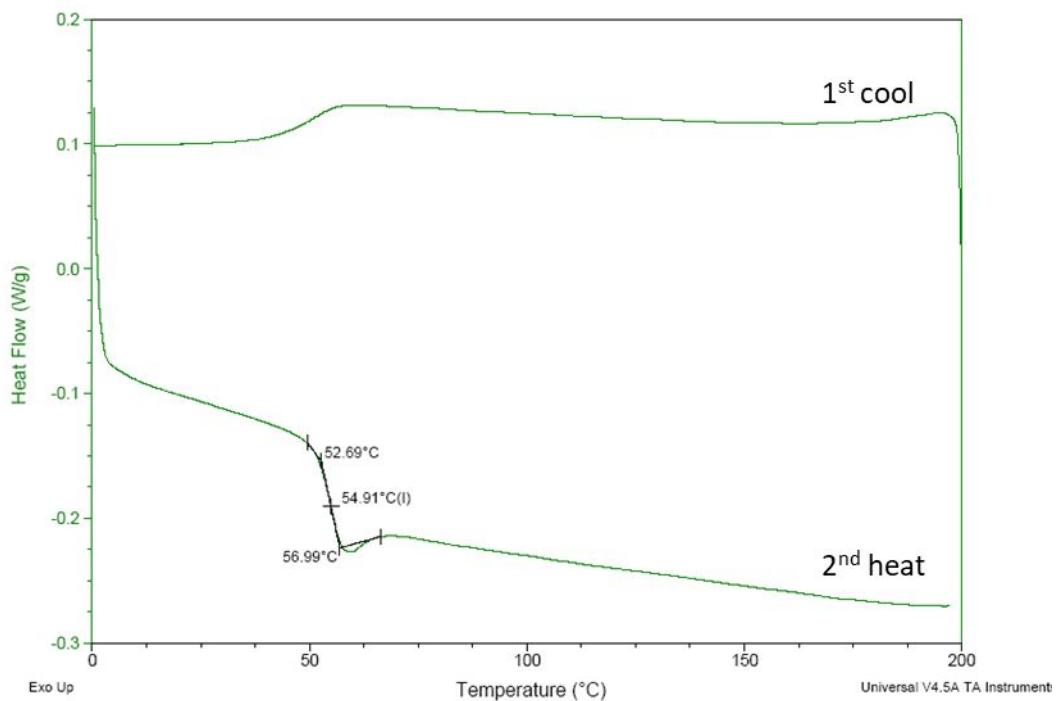
## 10. Thermal analysis of expanded polymers



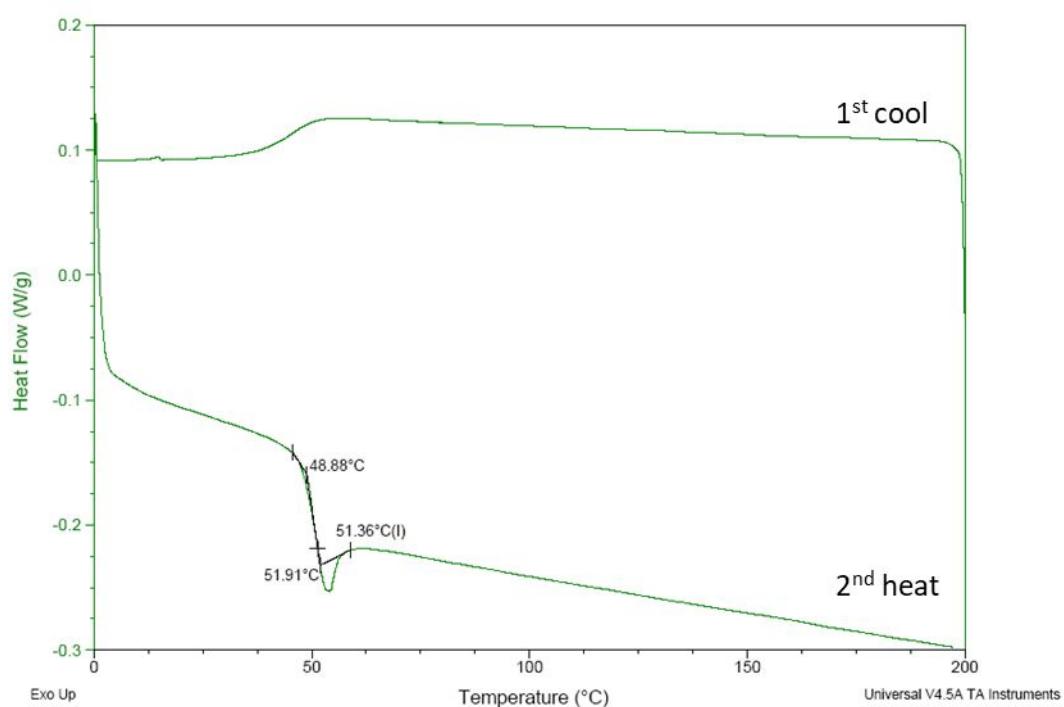
**Figure S50.** DSC trace of ECH/SA/LA polymer.



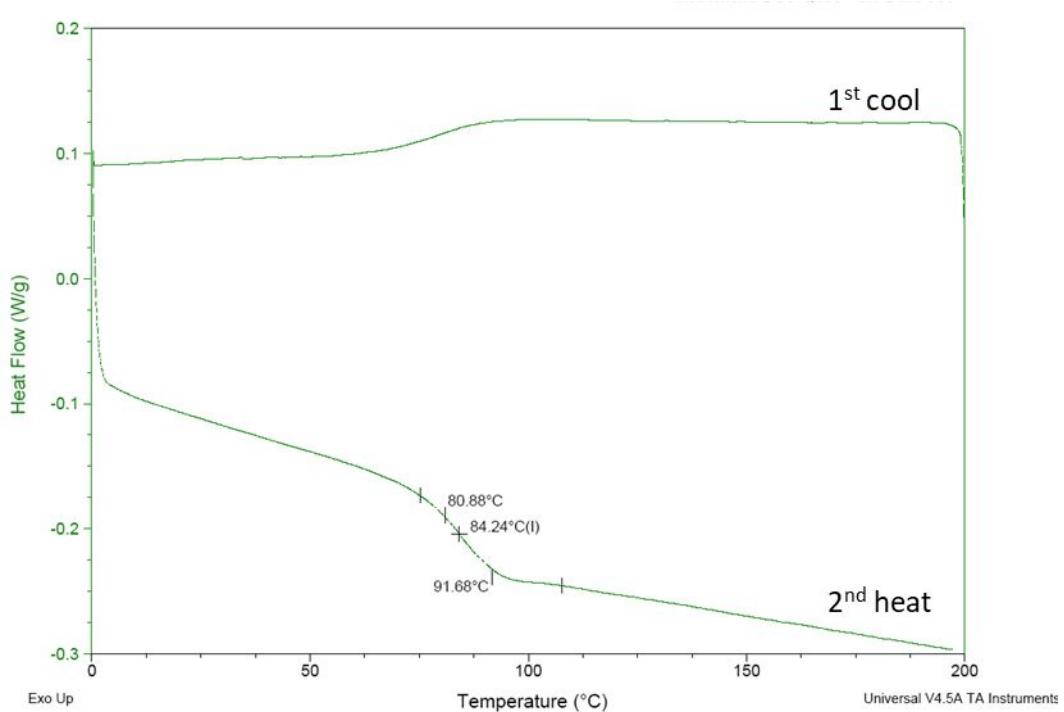
**Figure S51.** DSC trace of ECH/CHA/LA polymer.



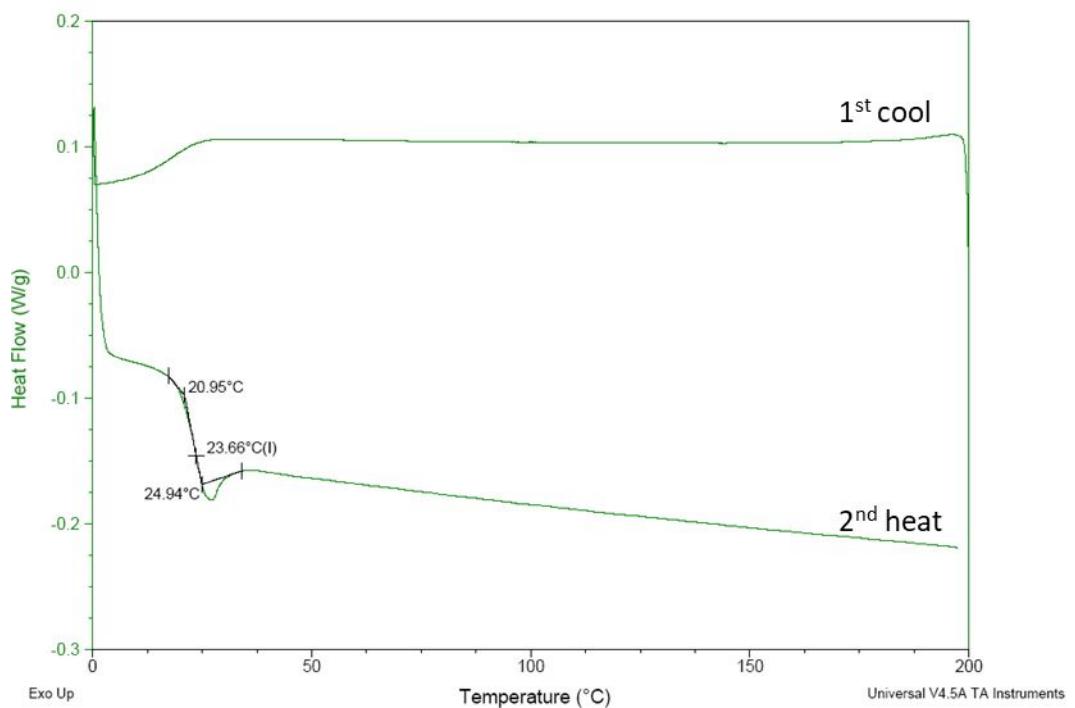
**Figure S52.** DSC trace of ECH/NA/LA polymer.



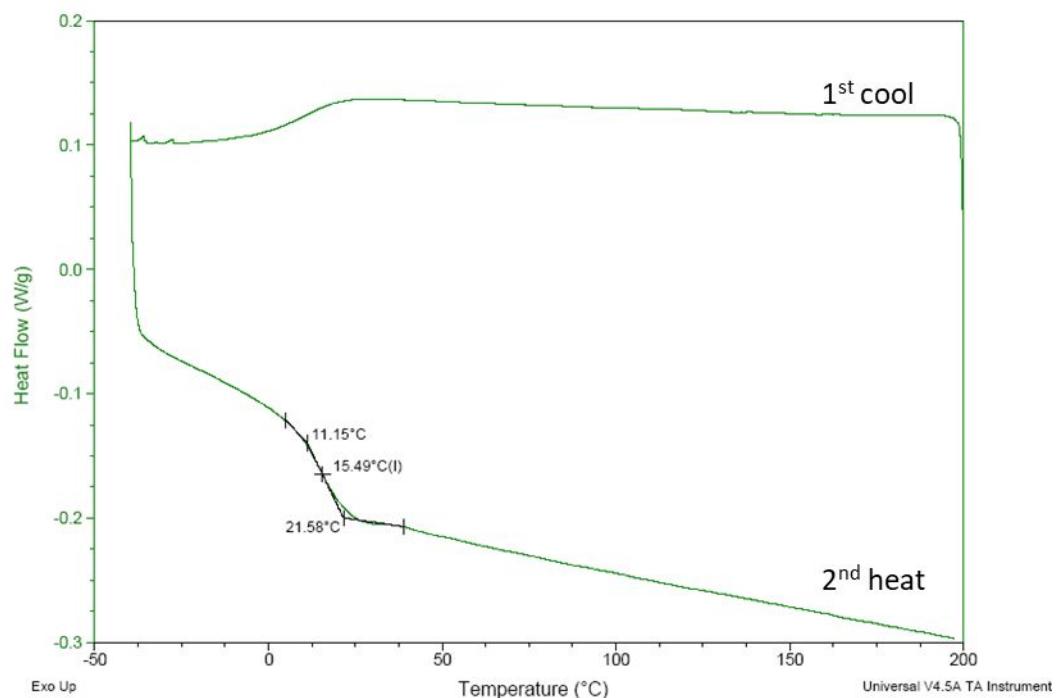
**Figure S53.** DSC trace of PO/PA/LA polymer.



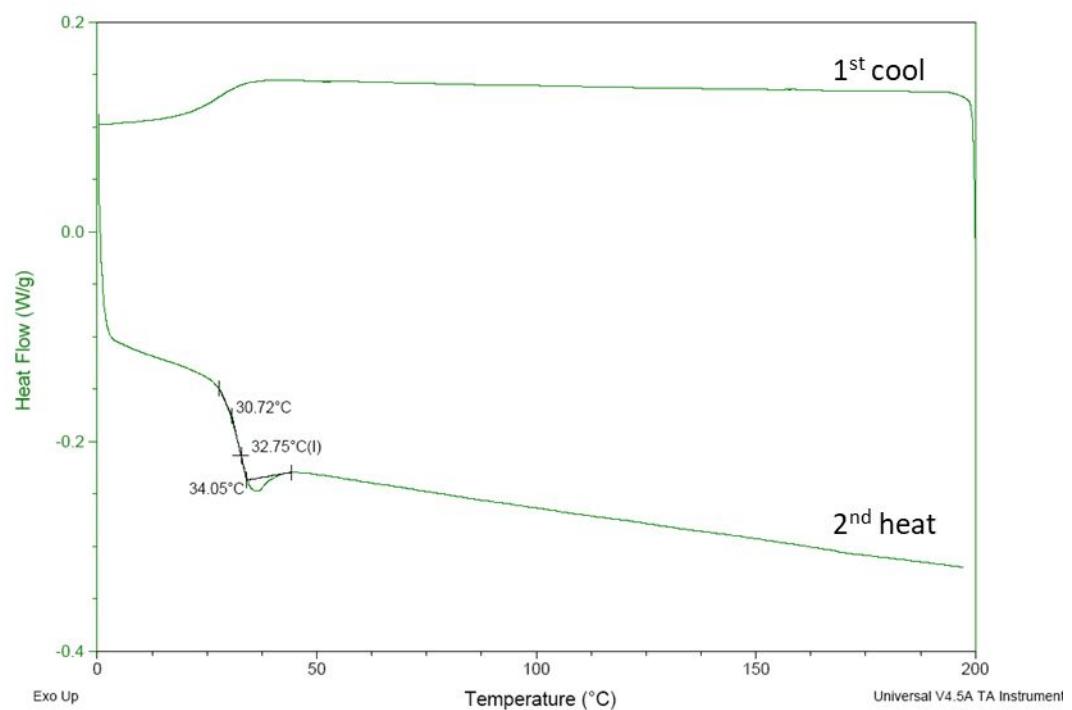
**Figure S54.** DSC trace of CHO/PA/LA polymer.



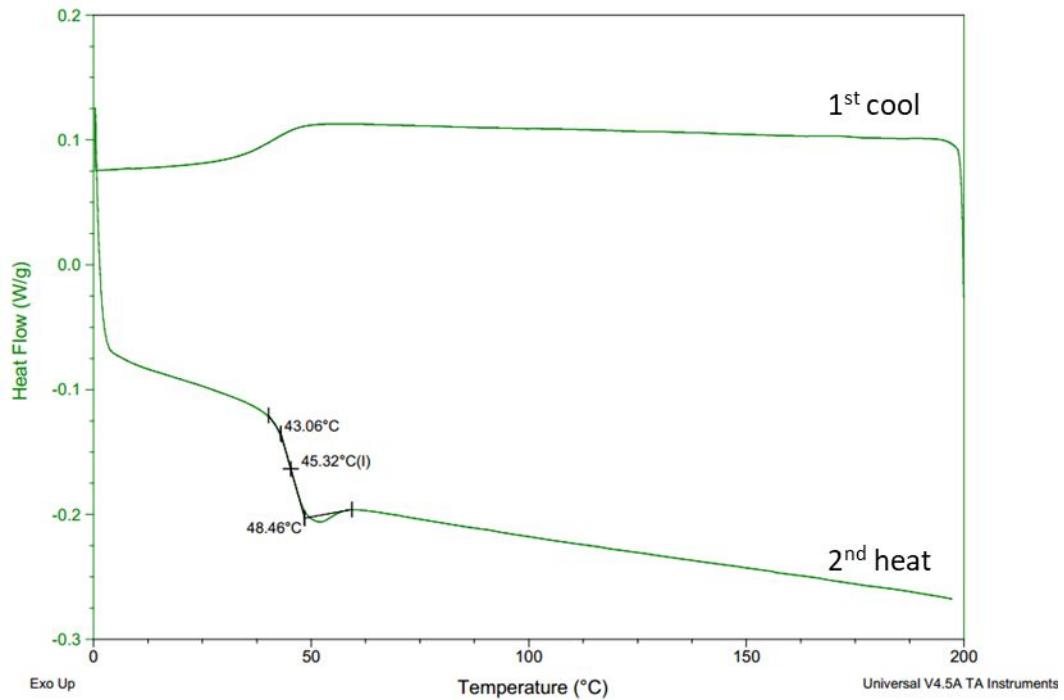
**Figure S55.** DSC trace of AGE/PA/LA polymer.



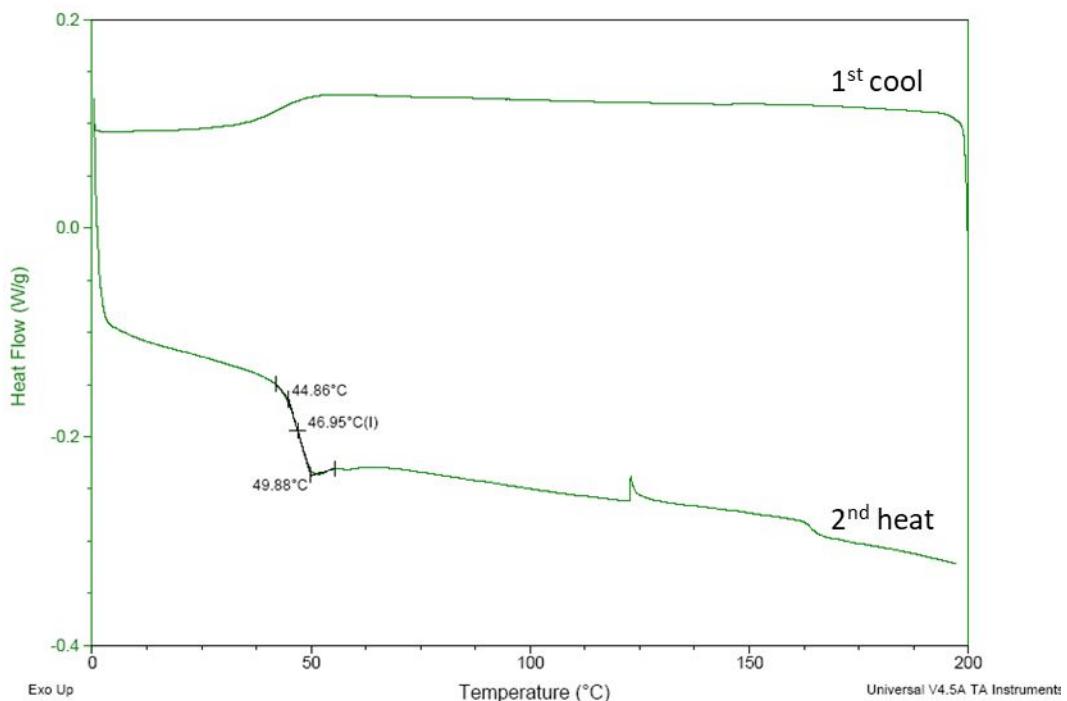
**Figure S56.** DSC trace of ECH/PA/ε-CL polymer.



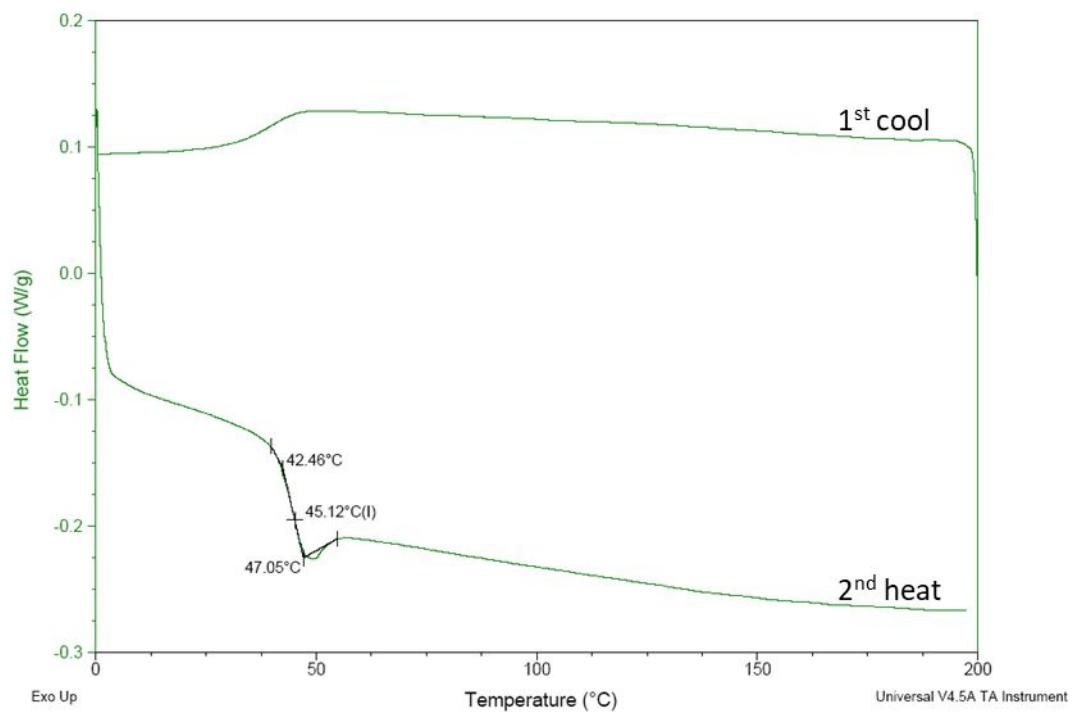
**Figure S57.** DSC trace of ECH/PA/SA/LA polymer.



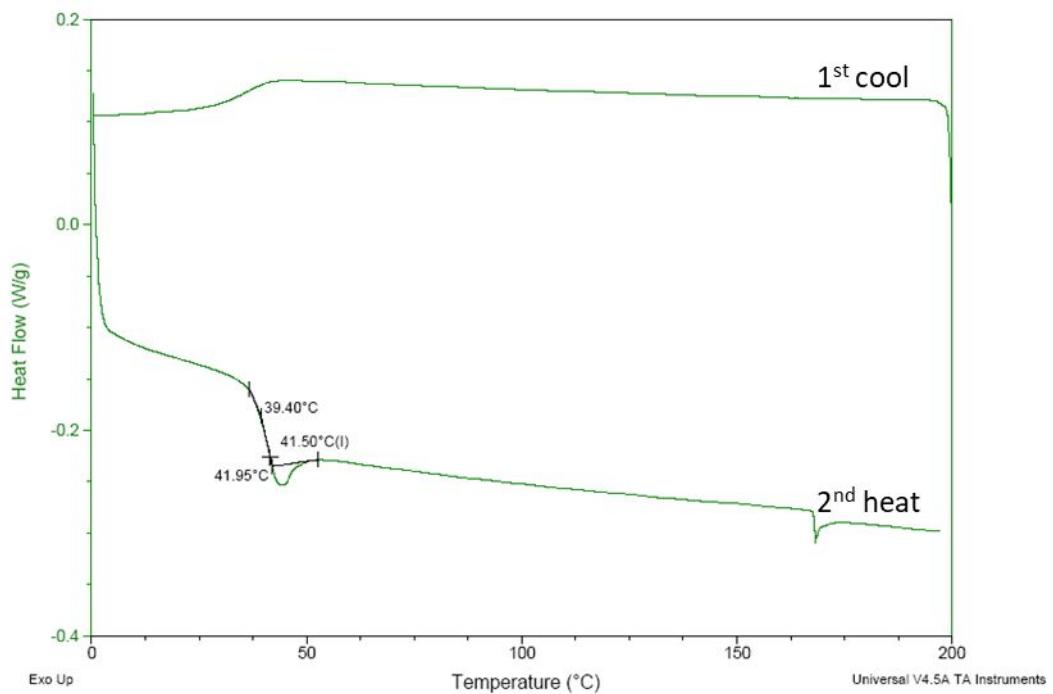
**Figure S58.** DSC trace of ECH/PA/NA/LA polymer.



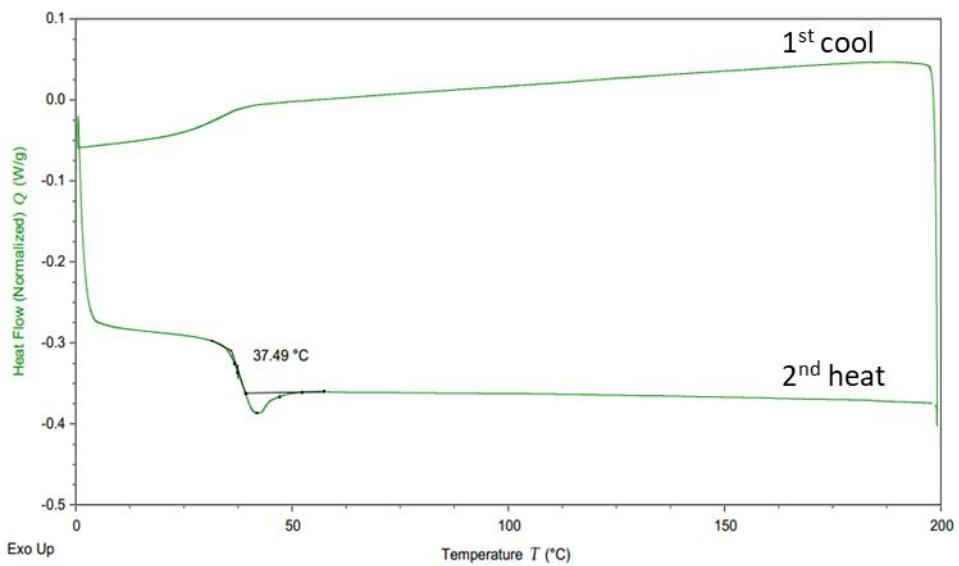
**Figure S59.** DSC thermogram of PO/PA/NA/LA polymer.



**Figure S60.** DSC trace of ECH/PO/PA/LA polymer.

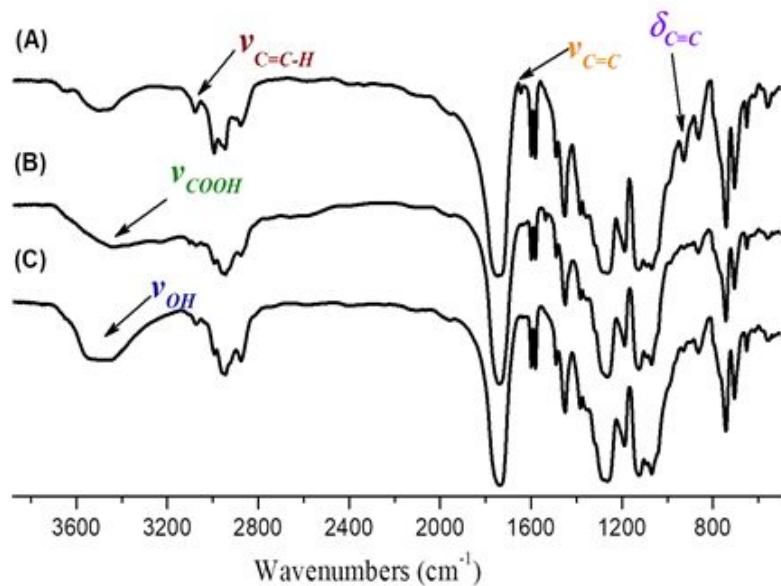


**Figure S61.** DSC trace of ECH/AGE/PA/LA polymer.

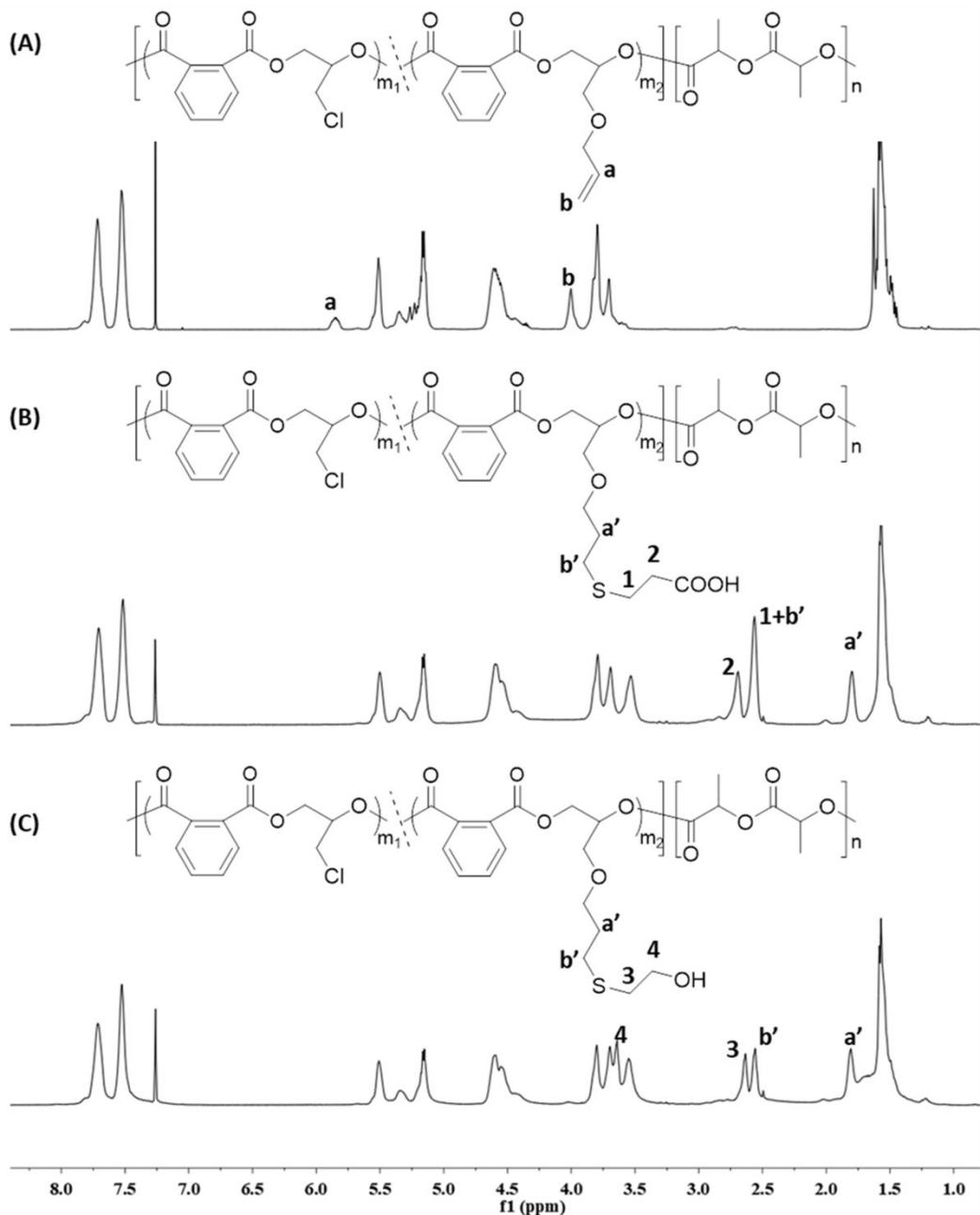


**Figure S62.** DSC trace of ECH/AGE/PA/LA polymer.

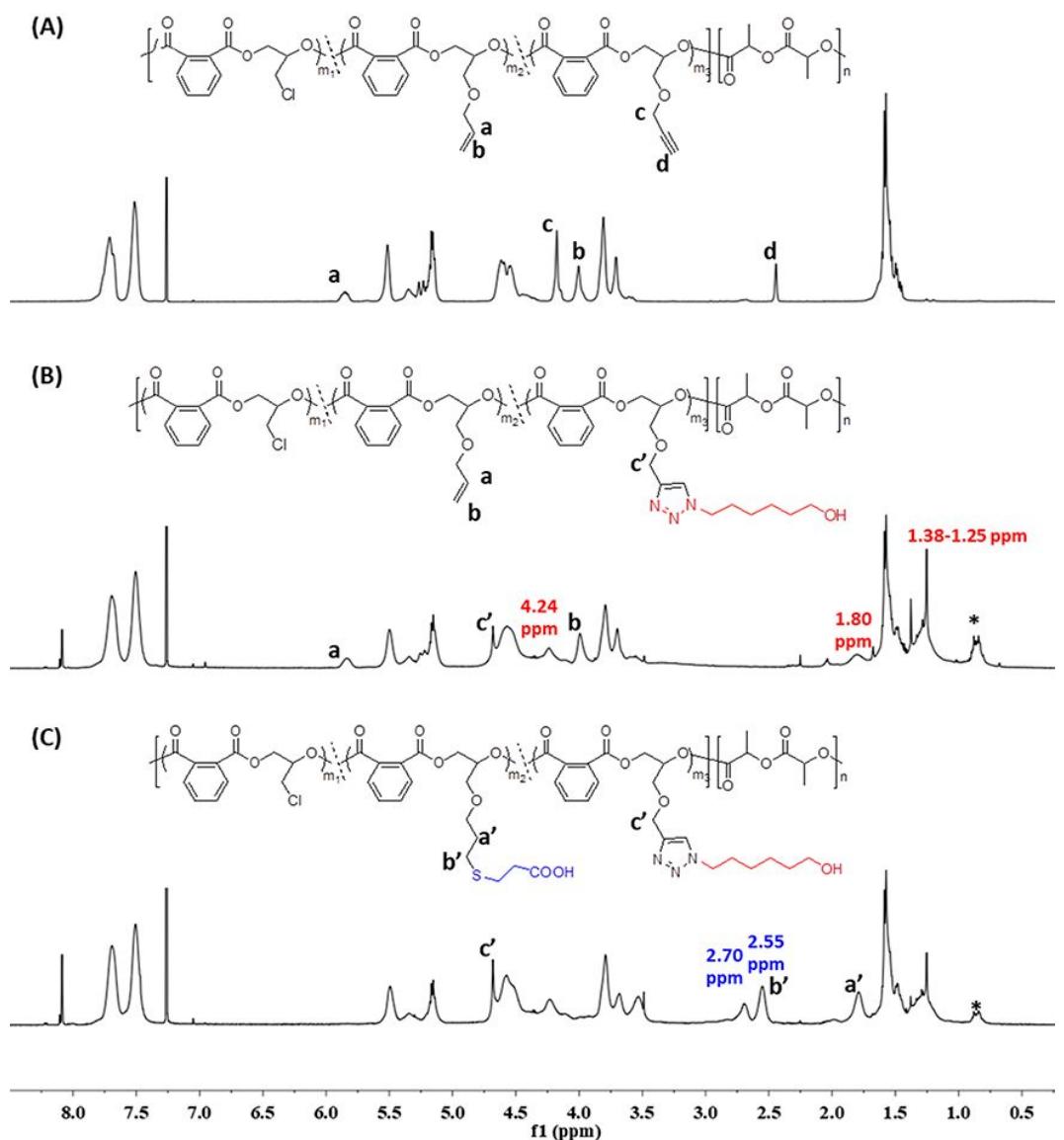
## 11. $^1\text{H}$ NMR spectra of the modified polymers



**Figure S63.** Comparative FT-IR spectra for the ECH/AGE/PA/LA polymer before modification (A); after thiol-ene reaction with thiohydrylic acid (B); after thiol-ene reaction with mercaptoethanol (C).

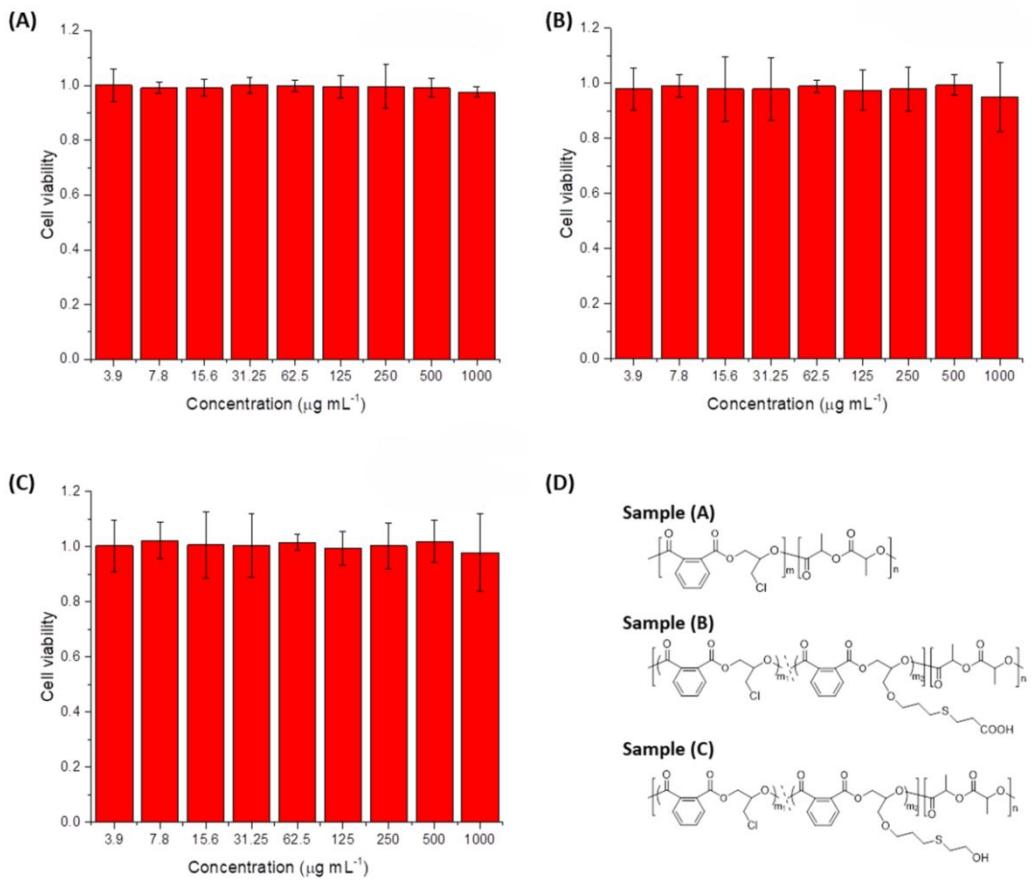


**Figure S64.** Comparative  $^1\text{H}$  NMR spectrum for the modification of ECH/AGE/PA/LA polymer.  
 (A) The precursor polyester (entry 12 in **Table 2**) had the pendent vinyl signed at 5.85 and 4.00 ppm. After performing thiol-ene reaction with thiohydrazic acid (B) or mercaptoethanol (C), the vinyl signals were disappeared with the appearance of propionic acid chain or propyl alcohol, respectively.



**Figure S65.** Comparative  $^1\text{H}$  NMR spectrum for the modification of bifunctional polymer. (A) The precursor polyester (entry 13 in **Table 2**) had two kinds of functional group, *i.e.*, vinyl (5.85 and 4.00 ppm) and alkyne (4.18 and 2.44 ppm). (B) After performing azide-alkyne cycloaddition with 6-azido-1-hexanol, the signals of alkyne disappeared with the generating of 1-hexanol chain (4.24, 1.80 and 1.38-1.25 ppm). While the vinyl was stable. (C) The vinyl was operated thiol-ene reaction with thiohydracrylic acid to introduce carboxylic acid (2.70 and 2.55 ppm).

## **12. Cytotoxicity assay**



**Figure S66.** The cellular viability assayed by CCK-8: (A) ECH/PA/LA polyester; (B) modified ECH/AGE/PA/LA polymer with thiohydracrylic acid; (C) modified ECH/AGE/PA/LA polymer with mercaptoethanol; and (D) the samples' structures. The relative cell viabilities were all greater than 95 % at different polymer concentrations, even up to 1000  $\mu\text{g/mL}^{-1}$ .

### **13. Cartesian coordinates, the Gibbs free energies with solvation corrections (au), and the imaginary frequencies of TSs.**

64

**1 E = -1271.8861128**

Al	6.985580000	0.835983000	15.281393000
O	5.8444889000	1.419965000	13.992324000
N	5.876279000	1.596743000	16.779500000
C	8.703489000	1.815988000	15.176256000
C	7.003228000	-1.141916000	15.332250000
C	4.908136000	2.343431000	14.002726000
C	4.446582000	2.895215000	15.235165000
C	4.929941000	2.452631000	16.513609000
C	4.315935000	2.799051000	12.781551000
C	3.333813000	3.778972000	12.873851000
C	2.863727000	4.353969000	14.080828000
C	3.434511000	3.886601000	15.247161000
C	4.759519000	2.223409000	11.419823000
C	6.262817000	2.511955000	11.186014000
C	4.501652000	0.696783000	11.381699000
C	3.983123000	2.849727000	10.243425000
C	6.090585000	1.259832000	18.204706000
C	5.420834000	-0.084602000	18.550607000
C	5.629056000	-0.443585000	20.030904000
C	7.117708000	-0.446182000	20.409286000
C	7.784098000	0.890440000	20.051034000
C	7.584097000	1.241764000	18.567510000
H	9.153695000	1.689872000	14.180805000
H	8.590158000	2.898126000	15.330402000
H	9.451907000	1.465601000	15.899875000
H	7.411486000	-1.536348000	14.390334000
H	7.632906000	-1.556185000	16.132119000
H	6.003258000	-1.581609000	15.445470000
H	4.412290000	2.898517000	17.370750000
H	2.888252000	4.133655000	11.952310000

H	3.119195000	4.270298000	16.212825000
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H	6.452620000	3.592016000	11.172475000
H	6.883505000	2.063787000	11.963113000
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H	4.332225000	2.403208000	9.305799000
H	2.904722000	2.663963000	10.312559000
H	5.605863000	2.042410000	18.809795000
H	5.845041000	-0.868495000	17.911348000
H	4.350701000	-0.027505000	18.314548000
H	5.096607000	0.284680000	20.660664000
H	5.178543000	-1.421677000	20.239096000
H	7.626832000	-1.259533000	19.872324000
H	7.236479000	-0.654605000	21.479778000
H	8.856275000	0.857837000	20.278935000
H	7.357562000	1.689360000	20.675651000
H	8.099667000	0.495015000	17.948857000
H	8.034969000	2.212912000	18.333254000
C	1.769424000	5.434402000	14.039708000
C	1.393070000	5.930125000	15.448680000
H	0.999299000	5.120382000	16.074035000
H	2.250031000	6.377639000	15.965431000
H	0.614641000	6.697931000	15.375827000
C	2.269104000	6.648700000	13.221030000
H	2.521197000	6.371967000	12.191754000
H	1.495194000	7.424917000	13.175773000
H	3.164324000	7.086646000	13.677151000
C	0.494827000	4.860269000	13.376256000
H	-0.291718000	5.623779000	13.333438000
H	0.683735000	4.522000000	12.351868000
H	0.109129000	4.005611000	13.943811000

**2' E = -1732.1609462**

Al	7.259025000	0.661478000	15.206975000
O	5.708504000	1.186857000	14.054247000
N	6.018709000	1.414118000	16.774387000
C	8.436980000	2.112074000	14.478336000
C	7.024578000	-1.255740000	14.688199000
C	5.088784000	2.316792000	14.052514000
C	4.920278000	3.049945000	15.271098000
C	5.281208000	2.459184000	16.530471000
C	4.492981000	2.869089000	12.853860000
C	3.8633388000	4.100008000	12.946297000
C	3.719564000	4.852832000	14.142996000
C	4.237411000	4.287172000	15.292399000
C	4.577500000	2.095198000	11.523657000
C	6.057588000	1.900688000	11.114791000
C	3.899417000	0.712161000	11.684808000
C	3.867161000	2.829638000	10.368974000
C	5.980085000	0.980254000	18.198731000
C	6.016961000	-0.550378000	18.321381000
C	5.951626000	-0.983332000	19.794748000
C	7.071091000	-0.330333000	20.619598000
C	7.010321000	1.200594000	20.507517000
C	7.076382000	1.659098000	19.041779000
H	9.330125000	1.657440000	14.025349000
H	7.975460000	2.759455000	13.719452000
H	8.814663000	2.755837000	15.284520000
H	6.360691000	-1.382568000	13.821749000
H	7.994709000	-1.710329000	14.447796000
H	6.607492000	-1.856746000	15.509032000
H	4.810238000	2.946600000	17.395278000
H	3.440426000	4.523960000	12.041451000
H	4.134715000	4.785349000	16.253307000
H	6.119039000	1.329917000	10.177866000
H	6.544446000	2.870384000	10.952682000
H	6.607815000	1.365492000	11.889044000

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H	2.835552000	0.829522000	11.928742000
H	4.319596000	3.806913000	10.159992000
H	3.947729000	2.228709000	9.454917000
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H	5.008440000	1.309032000	18.606000000
H	6.942775000	-0.917763000	17.869241000
H	5.177839000	-0.978143000	17.757865000
H	4.976129000	-0.704742000	20.226506000
H	6.018694000	-2.077488000	19.859627000
H	8.041978000	-0.678152000	20.242563000
H	7.001429000	-0.639303000	21.672481000
H	7.832324000	1.657976000	21.074574000
H	6.075537000	1.557327000	20.970963000
H	8.049778000	1.411537000	18.608028000
H	6.950743000	2.749414000	18.979585000
Cl	9.095884000	0.025623000	16.799122000
C	3.000039000	6.211714000	14.108132000
C	2.936164000	6.871351000	15.498726000
H	2.383951000	6.252545000	16.215517000
H	3.937203000	7.051546000	15.906776000
H	2.423893000	7.839196000	15.431056000
C	1.548934000	6.029881000	13.601548000
H	1.026487000	6.995418000	13.558552000
H	1.521906000	5.591452000	12.598299000
H	0.986152000	5.366101000	14.268240000
C	3.749625000	7.177102000	13.158634000
H	3.804622000	6.780076000	12.139386000
H	3.242880000	8.150868000	13.112051000
H	4.776298000	7.341343000	13.505262000

75

**3TS'** E = -2384.8171542, Imaginary frequency =374.89i

Al	7.685263000	0.995717000	15.232493000
O	6.246731000	1.407072000	14.143577000

N	5.727881000	1.461677000	17.025081000
C	8.551466000	2.605153000	15.995623000
C	7.512075000	-0.890275000	15.890815000
C	5.185588000	2.175829000	14.072465000
C	4.464746000	2.602004000	15.230801000
C	4.781262000	2.213640000	16.602512000
C	4.687848000	2.597305000	12.787989000
C	3.559899000	3.411619000	12.742100000
C	2.852178000	3.861640000	13.874614000
C	3.332720000	3.432744000	15.100722000
C	5.403770000	2.181575000	11.484705000
C	6.835452000	2.769371000	11.471886000
C	5.450155000	0.638699000	11.366359000
C	4.687493000	2.705207000	10.221502000
C	5.751393000	1.204845000	18.466004000
C	5.278328000	-0.233870000	18.762596000
C	5.318016000	-0.543495000	20.267391000
C	6.715241000	-0.294987000	20.855586000
C	7.192117000	1.134873000	20.558980000
C	7.152369000	1.447221000	19.054613000
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H	5.954811000	0.193368000	12.223971000
H	4.434179000	0.226959000	11.314502000

H	4.658237000	3.800818000	10.184008000
H	5.231959000	2.362482000	9.333323000
H	3.659556000	2.330648000	10.142163000
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H	4.261729000	-0.366922000	18.369268000
H	4.587876000	0.091995000	20.792915000
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H	7.876007000	0.818556000	18.522524000
H	7.452899000	2.484285000	18.870286000
Cl	11.715845000	0.373441000	15.705287000
C	9.075309000	-0.398698000	12.977981000
C	10.238883000	-0.777166000	13.783611000
O	8.952961000	0.757009000	13.770098000
H	8.223509000	-1.088926000	13.035636000
H	11.243429000	-0.563477000	13.450666000
H	10.126731000	-1.401621000	14.656332000
C	9.357753000	-0.015657000	11.533169000
H	8.488053000	0.451994000	11.075024000
H	10.217706000	0.652820000	11.471956000
Cl	9.754538000	-1.493986000	10.529974000
C	1.624455000	4.773486000	13.707964000
C	0.999551000	5.161983000	15.062199000
H	0.657212000	4.281490000	15.618472000
H	1.709246000	5.708860000	15.694927000
H	0.129619000	5.810720000	14.899552000
C	2.035066000	6.077579000	12.981362000
H	2.440163000	5.874369000	11.983976000
H	1.170478000	6.744193000	12.860812000
H	2.804589000	6.613823000	13.549472000
C	0.539877000	4.049519000	12.873619000

H	-0.340305000	4.691945000	12.738561000
H	0.908988000	3.774704000	11.879531000
H	0.216513000	3.128226000	13.373095000
75			
<b>4'</b> E = -2384.9012151			
Al	7.808613000	1.022401000	15.045531000
O	6.199187000	1.392254000	14.220323000
N	5.572750000	1.408826000	17.114813000
C	8.530852000	2.646293000	15.952594000
C	7.734109000	-0.777398000	15.940137000
C	5.153053000	2.172620000	14.134350000
C	4.419948000	2.612613000	15.283448000
C	4.682697000	2.209313000	16.665463000
C	4.669370000	2.590194000	12.840293000
C	3.565060000	3.435128000	12.778302000
C	2.859921000	3.912924000	13.900776000
C	3.312447000	3.473032000	15.133461000
C	5.366440000	2.127232000	11.540916000
C	6.810261000	2.681812000	11.486864000
C	5.386722000	0.581111000	11.464059000
C	4.640365000	2.627452000	10.273141000
C	5.557721000	1.155733000	18.548451000
C	5.221177000	-0.324955000	18.817841000
C	5.265151000	-0.658345000	20.317244000
C	6.620189000	-0.285316000	20.937663000
C	6.959268000	1.190013000	20.675661000
C	6.915471000	1.523170000	19.176218000
H	8.981569000	3.325470000	15.214695000
H	7.777365000	3.217231000	16.509761000
H	9.331602000	2.392785000	16.664883000
H	8.375223000	-1.550887000	15.491135000
H	8.031008000	-0.709551000	16.997097000
H	6.708488000	-1.169473000	15.930720000
H	3.972139000	2.671674000	17.378727000
H	3.220257000	3.752453000	11.800944000

H	2.805386000	3.781625000	16.043838000
H	7.276822000	2.421303000	10.526217000
H	6.802628000	3.776329000	11.566001000
H	7.431610000	2.275940000	12.285542000
H	5.887015000	0.254750000	10.541950000
H	5.910226000	0.153646000	12.319039000
H	4.364232000	0.181939000	11.447707000
H	4.638648000	3.721753000	10.198355000
H	5.161134000	2.241602000	9.388595000
H	3.601680000	2.277795000	10.223097000
H	4.777549000	1.771707000	19.044558000
H	5.939573000	-0.947637000	18.271270000
H	4.229858000	-0.549190000	18.403025000
H	4.467683000	-0.107531000	20.840144000
H	5.056294000	-1.725918000	20.470659000
H	7.403993000	-0.918283000	20.496432000
H	6.617652000	-0.492933000	22.016912000
H	7.949876000	1.431470000	21.083890000
H	6.238333000	1.824386000	21.214887000
H	7.703369000	0.976105000	18.644881000
H	7.114773000	2.588679000	19.011437000
Cl	12.111110000	0.443903000	13.298554000
C	9.404787000	-0.341450000	13.043911000
C	10.768064000	-0.759123000	13.616220000
O	8.916099000	0.816938000	13.601704000
H	8.765958000	-1.225086000	13.244163000
H	11.111657000	-1.704648000	13.192748000
H	10.691498000	-0.834738000	14.700910000
C	9.425734000	-0.126464000	11.524141000
H	8.426790000	0.130612000	11.178737000
H	10.133321000	0.655566000	11.249592000
Cl	9.916775000	-1.627668000	10.575805000
C	1.659453000	4.857028000	13.716508000
C	1.026170000	5.263906000	15.060618000
H	0.650073000	4.393817000	15.611005000

H	1.743188000	5.787280000	15.703407000
H	0.179261000	5.939343000	14.886165000
C	2.114276000	6.148554000	12.995366000
H	2.548480000	5.931251000	12.013741000
H	1.266464000	6.830821000	12.843698000
H	2.875039000	6.673581000	13.584444000
C	0.567749000	4.162398000	12.867653000
H	-0.292514000	4.828903000	12.716152000
H	0.945296000	3.874787000	11.880681000
H	0.211765000	3.252108000	13.364024000

75

**2 E = -2384.8673269**

Al	7.121323000	0.982420000	15.596994000
O	5.859931000	1.030604000	14.259534000
N	5.604281000	1.890716000	16.904830000
C	8.388674000	2.519356000	15.670589000
C	7.243405000	-0.768876000	16.543372000
C	4.808206000	1.764516000	13.989991000
C	4.168700000	2.534828000	15.003612000
C	4.591667000	2.504020000	16.384569000
C	4.253329000	1.792162000	12.665048000
C	3.141955000	2.598783000	12.445595000
C	2.504165000	3.387914000	13.431636000
C	3.038602000	3.327768000	14.705292000
C	4.882434000	0.966295000	11.523355000
C	6.334001000	1.439051000	11.265008000
C	4.870986000	-0.538250000	11.888992000
C	4.106888000	1.117800000	10.198093000
C	5.698244000	1.969620000	18.378344000
C	5.097662000	0.704064000	19.025565000
C	5.169952000	0.769790000	20.559580000
C	6.604754000	1.019786000	21.046994000
C	7.191937000	2.283551000	20.402012000
C	7.134418000	2.218946000	18.866925000
H	8.715936000	2.782577000	14.656033000

H	7.969467000	3.429679000	16.119269000
H	9.299542000	2.273656000	16.235497000
H	7.983776000	-1.457713000	16.119606000
H	7.527379000	-0.662392000	17.598869000
H	6.277105000	-1.295269000	16.533053000
H	3.936190000	3.072964000	17.059983000
H	2.729722000	2.629129000	11.443725000
H	2.596196000	3.892884000	15.521062000
H	6.772510000	0.867573000	10.436691000
H	6.347431000	2.499032000	10.982011000
H	6.969963000	1.307749000	12.140761000
H	5.328766000	-1.123504000	11.080931000
H	5.424556000	-0.725681000	12.809477000
H	3.842375000	-0.896980000	12.022790000
H	4.108607000	2.151727000	9.832253000
H	4.587294000	0.500026000	9.430708000
H	3.065289000	0.784299000	10.284824000
H	5.084561000	2.824777000	18.712705000
H	5.639362000	-0.175553000	18.662734000
H	4.056273000	0.593726000	18.695670000
H	4.519634000	1.580795000	20.922650000
H	4.775300000	-0.160538000	20.988282000
H	7.232211000	0.156003000	20.785417000
H	6.625674000	1.104315000	22.141657000
H	8.230623000	2.429172000	20.723393000
H	6.630150000	3.162861000	20.754176000
H	7.788395000	1.415455000	18.510690000
H	7.515329000	3.148374000	18.431183000
C	9.683337000	-0.446696000	14.009268000
C	10.867361000	0.154273000	13.307918000
O	8.399311000	0.246401000	13.910325000
H	9.972682000	-0.778342000	15.008587000
H	11.699993000	-0.546673000	13.409259000
C	8.539862000	-1.089034000	13.361013000
H	7.995878000	-1.862213000	13.898105000

H	8.472954000	-1.114842000	12.276940000
Cl	12.242615000	-1.792418000	15.616420000
H	11.141963000	1.101412000	13.774096000
Cl	10.597253000	0.524214000	11.533495000
C	1.281730000	4.243845000	13.057978000
C	0.150137000	3.335727000	12.520062000
H	-0.726264000	3.934378000	12.238681000
H	0.466800000	2.773046000	11.635519000
H	-0.161682000	2.610582000	13.280661000
C	0.729983000	5.025912000	14.264979000
H	0.401369000	4.355256000	15.067404000
H	1.477245000	5.712510000	14.679183000
H	-0.136110000	5.624096000	13.957364000
C	1.674563000	5.266897000	11.965529000
H	2.046479000	4.772864000	11.061732000
H	0.809429000	5.879578000	11.679474000
H	2.463684000	5.936806000	12.325733000

75

**3TS** E = -2384.8602342, Imaginary frequency =374.36i

Al	7.239359000	0.944270000	15.501793000
O	5.881377000	1.022720000	14.276300000
N	5.584809000	1.891119000	16.937435000
C	8.384827000	2.574395000	15.724928000
C	7.321278000	-0.730529000	16.597296000
C	4.828048000	1.751323000	14.003670000
C	4.182181000	2.527181000	15.008364000
C	4.588824000	2.507937000	16.398651000
C	4.276381000	1.763715000	12.676464000
C	3.165517000	2.567733000	12.442937000
C	2.525712000	3.366941000	13.418158000
C	3.055048000	3.317138000	14.695297000
C	4.908037000	0.923708000	11.545715000
C	6.357350000	1.397702000	11.277380000
C	4.907156000	-0.576097000	11.930645000
C	4.128589000	1.052989000	10.220099000

C	5.655391000	1.986850000	18.405591000
C	5.100448000	0.702585000	19.057074000
C	5.157861000	0.777369000	20.591202000
C	6.578559000	1.082993000	21.088420000
C	7.123552000	2.364469000	20.440824000
C	7.077268000	2.291081000	18.905904000
H	8.793826000	2.875957000	14.750976000
H	7.857029000	3.444739000	16.135631000
H	9.249108000	2.393017000	16.383410000
H	8.009795000	-1.489865000	16.203619000
H	7.628766000	-0.560539000	17.638612000
H	6.331430000	-1.207746000	16.641678000
H	3.923317000	3.092657000	17.054496000
H	2.756740000	2.586585000	11.439300000
H	2.607808000	3.888652000	15.504203000
H	6.790500000	0.822850000	10.448433000
H	6.368017000	2.457060000	10.990711000
H	6.998899000	1.266146000	12.148952000
H	5.355916000	-1.169761000	11.123994000
H	5.477170000	-0.749804000	12.843432000
H	3.881830000	-0.936764000	12.084379000
H	4.126656000	2.081144000	9.837705000
H	4.608662000	0.424128000	9.461590000
H	3.087838000	0.718515000	10.314760000
H	5.006693000	2.819779000	18.735953000
H	5.678763000	-0.156808000	18.702045000
H	4.067061000	0.549574000	18.719911000
H	4.475874000	1.565572000	20.946233000
H	4.795214000	-0.164715000	21.023031000
H	7.238869000	0.241135000	20.834656000
H	6.589088000	1.172733000	22.183150000
H	8.153617000	2.551114000	20.771167000
H	6.526691000	3.223272000	20.785634000
H	7.759511000	1.510131000	18.552679000
H	7.426807000	3.231914000	18.467624000

C	9.698078000	-0.263460000	14.143019000
C	10.885068000	0.402319000	13.485413000
O	8.396547000	0.298990000	13.969197000
H	9.947977000	-0.507656000	15.180224000
H	11.663097000	-0.357800000	13.383638000
C	8.875004000	-1.228617000	13.454945000
H	8.331762000	-1.972342000	14.014073000
H	8.815232000	-1.218074000	12.378553000
Cl	10.670327000	-3.156099000	13.150742000
H	11.234431000	1.253052000	14.073613000
Cl	10.552998000	1.047299000	11.820851000
C	1.305681000	4.221039000	13.032268000
C	0.173528000	3.309968000	12.500415000
H	-0.701544000	3.906872000	12.210253000
H	0.492470000	2.737470000	11.623058000
H	-0.140932000	2.592855000	13.267471000
C	0.751392000	5.016824000	14.229116000
H	0.418824000	4.355000000	15.037238000
H	1.499219000	5.705282000	14.639231000
H	-0.112317000	5.614070000	13.912459000
C	1.702587000	5.232311000	11.930269000
H	2.077668000	4.727956000	11.033716000
H	0.838891000	5.842742000	11.634143000
H	2.491048000	5.905521000	12.286541000

75

**4 E= -2384.9019588**

Al	7.484659000	0.793733000	15.176809000
O	5.850407000	0.963669000	14.376314000
N	5.377813000	1.838257000	17.133191000
C	8.357193000	2.557903000	15.550351000
C	7.534539000	-0.679527000	16.538062000
C	4.826211000	1.725239000	14.093752000
C	4.174518000	2.526851000	15.083927000
C	4.487894000	2.516221000	16.512097000
C	4.282177000	1.739219000	12.758290000

C	3.212497000	2.588191000	12.487711000
C	2.595896000	3.429628000	13.436207000
C	3.095252000	3.361199000	14.725993000
C	4.872328000	0.847619000	11.640880000
C	6.318413000	1.287031000	11.307991000
C	4.862671000	-0.639326000	12.072618000
C	4.055334000	0.937863000	10.333034000
C	5.395319000	1.960046000	18.584117000
C	5.017803000	0.606947000	19.221503000
C	5.091249000	0.653842000	20.755512000
C	6.473588000	1.117597000	21.238849000
C	6.851127000	2.468805000	20.612844000
C	6.778762000	2.421881000	19.078491000
H	8.372564000	3.183193000	14.644791000
H	7.866822000	3.144698000	16.336720000
H	9.409591000	2.435977000	15.856665000
H	8.267123000	-1.465815000	16.298547000
H	7.771125000	-0.331480000	17.553465000
H	6.552735000	-1.170788000	16.596595000
H	3.815271000	3.175505000	17.095403000
H	2.821140000	2.607262000	11.477179000
H	2.650252000	3.956282000	15.519207000
H	6.695014000	0.712139000	10.450780000
H	6.342283000	2.349399000	11.032870000
H	7.002489000	1.118213000	12.139804000
H	5.270761000	-1.263856000	11.266605000
H	5.465937000	-0.791132000	12.966850000
H	3.837893000	-0.977814000	12.275554000
H	4.075801000	1.944056000	9.896563000
H	4.491581000	0.255470000	9.593982000
H	3.007066000	0.645851000	10.475183000
H	4.647834000	2.709335000	18.921471000
H	5.700290000	-0.159018000	18.833660000
H	4.009041000	0.325386000	18.893038000
H	4.326134000	1.346497000	21.139689000

H	4.852718000	-0.333905000	21.172945000
H	7.224817000	0.366605000	20.953791000
H	6.494073000	1.183798000	22.335682000
H	7.858957000	2.767874000	20.930922000
H	6.164215000	3.242639000	20.989991000
H	7.536134000	1.732939000	18.685956000
H	7.005061000	3.407390000	18.653667000
C	9.634868000	-0.418948000	13.765564000
C	10.699062000	0.489636000	13.134710000
O	8.369981000	0.118546000	13.716659000
H	10.007731000	-0.564624000	14.801738000
H	11.702347000	0.073536000	13.243016000
C	9.539579000	-1.808293000	13.120998000
H	8.797377000	-2.400256000	13.654322000
H	9.275327000	-1.730164000	12.066685000
Cl	11.108939000	-2.773462000	13.194787000
H	10.640904000	1.475036000	13.597621000
Cl	10.4716444000	0.773346000	11.340800000
C	1.428209000	4.339756000	13.018032000
C	0.259623000	3.482769000	12.475013000
H	-0.578592000	4.119564000	12.160069000
H	0.565917000	2.882478000	11.611829000
H	-0.105363000	2.793100000	13.245032000
C	0.892931000	5.178583000	14.194131000
H	0.510430000	4.544895000	15.002601000
H	1.669021000	5.829731000	14.612385000
H	0.068564000	5.817639000	13.853592000
C	1.895216000	5.316132000	11.911975000
H	2.262092000	4.781051000	11.029758000
H	1.069978000	5.966761000	11.591024000
H	2.710745000	5.951786000	12.275696000

90

**5TS<sup>PA</sup>** E =-2917.8160916, Imaginary frequency =197.02i

Al	6.976042000	0.798142000	14.991648000
O	5.541730000	1.124320000	13.741318000

N	5.785320000	1.731338000	16.599749000
C	7.832165000	2.596359000	14.594498000
C	6.256999000	-1.033163000	15.479693000
C	4.418187000	1.768249000	13.818790000
C	3.935015000	2.324204000	15.051301000
C	4.635493000	2.243595000	16.320261000
C	3.590914000	1.942737000	12.644404000
C	2.387481000	2.621560000	12.772493000
C	1.893454000	3.166950000	13.980926000
C	2.693758000	2.998338000	15.096030000
C	4.049420000	1.383203000	11.281904000
C	5.394797000	2.032468000	10.874432000
C	4.200504000	-0.155329000	11.367546000
C	3.043130000	1.677667000	10.150229000
C	6.219607000	1.816870000	18.001624000
C	6.460924000	0.417961000	18.599837000
C	6.912845000	0.513894000	20.065870000
C	8.163110000	1.393959000	20.213644000
C	7.929980000	2.786056000	19.607680000
C	7.480902000	2.692050000	18.140580000
H	8.277648000	2.596440000	13.586776000
H	7.089966000	3.409366000	14.601155000
H	8.629515000	2.892525000	15.290765000
H	6.092729000	-1.640085000	14.574370000
H	6.910361000	-1.625769000	16.132803000
H	5.273640000	-0.970433000	15.969935000
H	4.072847000	2.701037000	17.148793000
H	1.777252000	2.745500000	11.884435000
H	2.380919000	3.390888000	16.060137000
H	5.758611000	1.598503000	9.934269000
H	5.268747000	3.112557000	10.725789000
H	6.149963000	1.880772000	11.646156000
H	4.576855000	-0.554706000	10.416965000
H	4.891417000	-0.437409000	12.162340000
H	3.229594000	-0.623830000	11.573817000

H	2.896332000	2.753706000	9.995450000
H	3.426820000	1.259772000	9.211805000
H	2.063395000	1.220993000	10.337146000
H	5.413945000	2.298382000	18.587103000
H	7.225144000	-0.093102000	18.006257000
H	5.542766000	-0.175980000	18.518149000
H	6.100247000	0.936404000	20.678413000
H	7.107071000	-0.492601000	20.459122000
H	9.002798000	0.912734000	19.693093000
H	8.449516000	1.479394000	21.271232000
H	8.844176000	3.390675000	19.677435000
H	7.162938000	3.312836000	20.197553000
H	8.280987000	2.256184000	17.534457000
H	7.276174000	3.690475000	17.734523000
C	8.268955000	-0.956283000	12.713689000
C	8.737138000	-2.414662000	12.720484000
O	8.540639000	-0.193205000	13.860862000
H	7.173692000	-1.049014000	12.625361000
H	8.200796000	-2.976267000	11.955736000
C	8.769003000	-0.137150000	11.517820000
H	8.332680000	0.859173000	11.554541000
H	9.856845000	-0.075830000	11.508304000
Cl	8.274350000	-0.848782000	9.899373000
H	8.574706000	-2.854011000	13.703069000
Cl	10.506599000	-2.671808000	12.325257000
C	13.623479000	0.462822000	14.309823000
C	12.727421000	1.538396000	14.193558000
C	11.370278000	1.391566000	14.493124000
C	10.935630000	0.133315000	14.897081000
C	11.822645000	-0.928685000	15.013418000
C	13.178142000	-0.791593000	14.728058000
C	9.586053000	-0.326193000	15.371160000
O	9.748528000	-1.754140000	15.603425000
C	11.066896000	-2.118079000	15.478768000
O	11.472576000	-3.222942000	15.749070000

O	8.873522000	0.300203000	16.164914000
H	14.673334000	0.612937000	14.070508000
H	13.099861000	2.505899000	13.865326000
H	10.671872000	2.217382000	14.408261000
H	13.851860000	-1.637658000	14.826403000
C	0.540131000	3.897241000	13.999892000
C	0.172634000	4.405770000	15.406802000
H	0.092892000	3.582957000	16.126700000
H	0.914182000	5.117945000	15.786222000
H	-0.796754000	4.918509000	15.377991000
C	-0.582102000	2.939169000	13.533138000
H	-1.556093000	3.448331000	13.535362000
H	-0.401690000	2.569137000	12.518164000
H	-0.649458000	2.068468000	14.196111000
C	0.588535000	5.118554000	13.050473000
H	0.815626000	4.821339000	12.020984000
H	-0.375619000	5.645269000	13.041957000
H	1.362482000	5.826574000	13.369088000

90

**6<sup>PA</sup>** E = -2917.8405961

Al	6.470164000	0.313834000	14.211164000
O	4.574365000	0.527317000	13.596111000
N	5.702944000	1.053998000	16.033653000
C	7.101218000	1.774354000	12.966956000
C	6.302139000	-1.664098000	13.953959000
C	3.810007000	1.552232000	13.752567000
C	3.928517000	2.371772000	14.922635000
C	4.765483000	1.957270000	16.014016000
C	2.770342000	1.893026000	12.803330000
C	2.014591000	3.028913000	13.044635000
C	2.148600000	3.870810000	14.182141000
C	3.096782000	3.498507000	15.115146000
C	2.533942000	1.005308000	11.565664000
C	3.804257000	0.971515000	10.682289000
C	2.183412000	-0.433417000	12.019693000

C	1.370778000	1.513658000	10.690609000
C	6.192187000	0.722001000	17.399989000
C	6.504527000	-0.774838000	17.546826000
C	6.909619000	-1.099717000	18.994258000
C	8.098265000	-0.242935000	19.457448000
C	7.808022000	1.255831000	19.275875000
C	7.385984000	1.591462000	17.835144000
H	7.991617000	1.430734000	12.418734000
H	6.375431000	2.121258000	12.220130000
H	7.418767000	2.659835000	13.540310000
H	6.210923000	-1.900326000	12.881658000
H	7.151904000	-2.240015000	14.338619000
H	5.387859000	-2.055667000	14.423986000
H	4.524140000	2.444838000	16.968519000
H	1.255024000	3.297886000	12.317996000
H	3.231269000	4.069120000	16.030772000
H	3.640932000	0.323775000	9.809942000
H	4.047434000	1.976688000	10.315742000
H	4.658492000	0.594419000	11.245072000
H	2.026047000	-1.078212000	11.144289000
H	2.987618000	-0.854496000	12.624946000
H	1.259229000	-0.437480000	12.611881000
H	1.562409000	2.516683000	10.289799000
H	1.239786000	0.838660000	9.836117000
H	0.421017000	1.539695000	11.239147000
H	5.363974000	0.943494000	18.094567000
H	7.315560000	-1.041453000	16.864207000
H	5.624238000	-1.360631000	17.254262000
H	6.053000000	-0.925487000	19.665790000
H	7.158559000	-2.165400000	19.076453000
H	8.990089000	-0.520557000	18.881400000
H	8.329620000	-0.454700000	20.510796000
H	8.689720000	1.849798000	19.551311000
H	7.004508000	1.552446000	19.969604000
H	8.208823000	1.421548000	17.137221000

H	7.107714000	2.652207000	17.760562000
C	10.406464000	-1.353171000	12.785164000
C	11.129071000	-2.532974000	13.461019000
O	9.371547000	-0.723738000	13.529735000
H	9.831936000	-1.826486000	11.979208000
H	11.378215000	-3.277946000	12.705181000
C	11.317486000	-0.316950000	12.116750000
H	10.706770000	0.485578000	11.705105000
H	12.071069000	0.086487000	12.789679000
Cl	12.221077000	-1.054675000	10.710870000
H	10.483328000	-2.962065000	14.224719000
Cl	12.716647000	-2.157224000	14.272050000
C	12.553579000	2.627515000	15.902254000
C	11.726627000	3.009205000	14.834399000
C	10.693708000	2.180094000	14.385906000
C	10.524909000	0.947787000	15.013878000
C	11.333865000	0.582656000	16.080993000
C	12.355313000	1.405761000	16.547264000
C	9.421475000	-0.090146000	14.805709000
O	9.898534000	-1.198770000	15.814543000
C	10.891983000	-0.743466000	16.597579000
O	11.322221000	-1.328654000	17.573205000
O	8.244394000	0.327558000	15.130933000
H	13.345801000	3.294999000	16.232719000
H	11.885384000	3.972668000	14.355332000
H	10.028940000	2.490555000	13.584946000
H	12.969061000	1.092262000	17.386949000
C	1.245159000	5.106904000	14.327542000
C	1.530518000	5.885673000	15.625677000
H	1.350539000	5.270546000	16.514963000
H	2.566088000	6.242431000	15.663677000
H	0.873124000	6.761644000	15.688846000
C	-0.241524000	4.677091000	14.348617000
H	-0.899233000	5.552267000	14.439620000
H	-0.522396000	4.143069000	13.434634000

H	-0.440273000	4.010620000	15.195985000
C	1.476952000	6.067646000	13.136470000
H	1.262085000	5.582910000	12.178145000
H	0.830308000	6.952134000	13.216893000
H	2.518915000	6.406554000	13.109479000

64

26

**7<sup>PA</sup> E = -1645.9411708**

C	15.212859000	-0.553075000	15.553341000
C	14.152023000	-1.354280000	14.770232000
O	14.760617000	0.048172000	16.777736000
H	15.411670000	0.336965000	14.946617000
H	14.149557000	-1.030789000	13.729281000
C	16.567990000	-1.224733000	15.796976000
H	17.148855000	-0.611113000	16.485578000
H	16.472152000	-2.240517000	16.174830000
Cl	17.544318000	-1.324025000	14.257224000
H	13.171419000	-1.199497000	15.240132000
Cl	14.406395000	-3.160071000	14.680656000
C	14.034071000	-4.721950000	18.768775000
C	15.199483000	-3.976425000	18.966756000
C	15.220284000	-2.623433000	18.625131000
C	14.090185000	-2.017673000	18.056650000
C	12.916744000	-2.761113000	17.864033000
C	12.902947000	-4.108996000	18.232233000
C	14.113898000	-0.523287000	17.860569000
O	11.908667000	-0.974855000	16.705500000
C	11.675435000	-2.110073000	17.227942000
O	10.612754000	-2.756366000	17.274766000
O	13.810360000	0.236880000	18.749118000
H	14.010952000	-5.776519000	19.038268000
H	16.084378000	-4.440155000	19.398030000
H	16.112710000	-2.030846000	18.818890000
H	11.972239000	-4.647113000	18.077869000

100

**8TS<sup>ECH</sup>** E=-3570.534643, Imaginary frequency =123.84i

Al	5.438394000	0.996553000	14.593596000
O	4.248195000	1.979201000	13.591336000
N	4.256324000	1.998163000	16.448603000
C	7.090574000	1.964271000	15.174677000
C	4.700571000	-0.803812000	15.054057000
C	3.136427000	2.664443000	13.690468000
C	2.566893000	3.002982000	14.952401000
C	3.167886000	2.647200000	16.225072000
C	2.452520000	3.104046000	12.503936000
C	1.281343000	3.839786000	12.654048000
C	0.702665000	4.187165000	13.894532000
C	1.371218000	3.748518000	15.024305000
C	2.986551000	2.739336000	11.102204000
C	4.429216000	3.267975000	10.910609000
C	2.960468000	1.201028000	10.932471000
C	2.126775000	3.340100000	9.970581000
C	4.637370000	1.899935000	17.871091000
C	5.242773000	0.532517000	18.224985000
C	5.657255000	0.469569000	19.704267000
C	6.619399000	1.606256000	20.078202000
C	6.013641000	2.973399000	19.728890000
C	5.602867000	3.044052000	18.249755000
H	7.558350000	1.541276000	16.076037000
H	7.854915000	1.940084000	14.388093000
H	6.887357000	3.021903000	15.392187000
H	4.071722000	-1.156944000	14.220951000
H	5.457947000	-1.584706000	15.211913000
H	4.049605000	-0.803579000	15.935947000
H	2.592631000	3.014868000	17.091104000
H	0.770729000	4.169677000	11.756684000
H	0.988651000	3.976128000	16.015604000
H	4.783700000	3.028204000	9.898922000
H	4.458100000	4.359065000	11.024381000
H	5.113983000	2.824904000	11.633809000

H	3.335714000	0.921017000	9.938754000
H	3.575830000	0.714716000	11.690458000
H	1.936116000	0.818548000	11.021380000
H	2.102708000	4.436169000	10.007129000
H	2.555623000	3.052460000	9.003415000
H	1.093758000	2.972377000	9.991960000
H	3.728239000	2.029927000	18.487454000
H	6.114665000	0.346966000	17.587294000
H	4.520987000	-0.259748000	18.002696000
H	4.759919000	0.535531000	20.339453000
H	6.115824000	-0.504600000	19.915769000
H	7.562232000	1.477532000	19.527347000
H	6.869852000	1.560658000	21.146793000
H	6.725815000	3.778216000	19.954915000
H	5.132002000	3.149799000	20.364639000
H	6.491535000	2.984321000	17.613035000
H	5.120477000	4.006036000	18.031748000
C	10.691996000	-4.031936000	9.866393000
C	9.215699000	-4.425990000	10.058984000
O	11.294831000	-3.234186000	10.907864000
H	10.688982000	-3.318202000	9.035844000
H	8.684690000	-4.274839000	9.120110000
C	11.670321000	-5.148090000	9.492874000
H	12.686342000	-4.753070000	9.513358000
H	11.580616000	-6.011986000	10.149561000
Cl	11.377057000	-5.739622000	7.797471000
H	8.767981000	-3.808208000	10.841790000
Cl	8.888707000	-6.165915000	10.492206000
C	10.084982000	-6.919056000	14.380124000
C	11.288627000	-6.866146000	13.674428000
C	11.619744000	-5.716299000	12.957774000
C	10.742431000	-4.624034000	12.919872000
C	9.536501000	-4.669670000	13.639368000
C	9.227299000	-5.820970000	14.369565000
C	11.230114000	-3.355179000	12.274190000

O	8.657377000	-2.714081000	12.635767000
C	8.549552000	-3.506789000	13.643287000
O	7.747673000	-3.425521000	14.586056000
O	11.733307000	-2.467769000	12.918944000
H	9.821207000	-7.811606000	14.943187000
H	11.973844000	-7.710413000	13.689822000
H	12.576291000	-5.657636000	12.442869000
H	8.296943000	-5.820744000	14.928623000
C	6.340968000	-0.827679000	12.192660000
C	7.558915000	-0.899063000	12.991108000
O	6.366966000	0.407129000	12.894018000
H	5.533815000	-1.508064000	12.471946000
H	8.456016000	-0.416260000	12.637307000
H	7.491054000	-1.261260000	14.004657000
C	6.415941000	-0.571370000	10.698643000
H	5.582147000	0.062503000	10.396778000
H	7.357178000	-0.092867000	10.424420000
Cl	6.280672000	-2.096879000	9.712872000
C	-0.599547000	5.005252000	13.935816000
C	-1.061708000	5.289929000	15.377610000
H	-1.261614000	4.364400000	15.929758000
H	-0.314462000	5.864985000	15.936694000
H	-1.989242000	5.875097000	15.363593000
C	-0.388235000	6.364257000	13.226499000
H	-0.089835000	6.233906000	12.180777000
H	-1.313038000	6.956531000	13.238702000
H	0.396225000	6.945327000	13.725268000
C	-1.729120000	4.228767000	13.217495000
H	-2.664029000	4.804924000	13.227471000
H	-1.476551000	4.020933000	12.172246000
H	-1.914649000	3.267782000	13.711036000
100			
<b>9ECH</b>	E = - 3570.5991469		
Al	5.325196000	0.385216000	15.062810000
O	4.631025000	1.823455000	14.169020000

N	3.883704000	2.235520000	16.966641000
C	6.864981000	0.833016000	16.260446000
C	3.916599000	-0.923018000	15.627623000
C	3.577231000	2.553816000	13.911215000
C	2.703931000	3.025300000	14.941468000
C	2.928823000	2.848591000	16.375334000
C	3.289244000	2.954255000	12.556360000
C	2.140702000	3.703828000	12.316272000
C	1.237329000	4.127848000	13.311930000
C	1.560037000	3.781712000	14.613565000
C	4.219526000	2.557231000	11.386266000
C	5.666402000	3.036762000	11.657911000
C	4.205916000	1.022412000	11.186556000
C	3.779838000	3.194939000	10.050059000
C	3.900634000	2.305915000	18.421675000
C	3.893739000	0.895066000	19.039028000
C	4.001477000	0.941981000	20.571263000
C	5.239326000	1.728958000	21.027612000
C	5.249284000	3.140066000	20.420547000
C	5.140981000	3.095082000	18.888497000
H	6.677463000	0.612927000	17.320575000
H	7.783652000	0.293266000	15.985421000
H	7.098181000	1.905808000	16.198975000
H	3.233178000	-1.151258000	14.794929000
H	4.353433000	-1.885616000	15.940591000
H	3.293866000	-0.575781000	16.460969000
H	2.159938000	3.357877000	16.988644000
H	1.921130000	3.985359000	11.292953000
H	0.928903000	4.100797000	15.438842000
H	6.315698000	2.761646000	10.815713000
H	5.698426000	4.129012000	11.763899000
H	6.064957000	2.584858000	12.565501000
H	4.796244000	0.758757000	10.297045000
H	4.636250000	0.498209000	12.040479000
H	3.180700000	0.665932000	11.022805000

H	3.756276000	4.290670000	10.100217000
H	4.497021000	2.915490000	9.269113000
H	2.792667000	2.844518000	9.724528000
H	3.002681000	2.842578000	18.794701000
H	4.732444000	0.326986000	18.619446000
H	2.979446000	0.370896000	18.735095000
H	3.100288000	1.417627000	20.989014000
H	4.028430000	-0.078854000	20.975422000
H	6.144666000	1.193038000	20.707348000
H	5.276267000	1.783347000	22.124600000
H	6.161411000	3.676076000	20.716037000
H	4.404384000	3.713728000	20.832670000
H	6.032799000	2.621973000	18.460362000
H	5.094830000	4.111277000	18.476175000
C	8.733856000	-4.172557000	9.745144000
C	8.950861000	-5.603312000	9.269020000
O	9.877018000	-3.335268000	9.481590000
H	8.529284000	-4.215825000	10.820465000
H	8.036005000	-6.179918000	9.408188000
C	7.599661000	-3.422656000	9.040621000
H	7.494348000	-2.430828000	9.479143000
H	7.804467000	-3.335424000	7.973465000
Cl	6.004805000	-4.261574000	9.217920000
H	9.764366000	-6.069687000	9.822872000
Cl	9.388817000	-5.722711000	7.508988000
C	11.961740000	-5.742750000	13.556769000
C	12.268998000	-6.004008000	12.220642000
C	11.827686000	-5.135007000	11.222600000
C	11.064371000	-4.004530000	11.545778000
C	10.751769000	-3.745864000	12.891544000
C	11.212713000	-4.615963000	13.885922000
C	10.797378000	-3.016291000	10.436497000
O	9.062293000	-2.188165000	12.386811000
C	9.919784000	-2.582070000	13.341664000
O	10.003825000	-2.097298000	14.450654000

O	11.472881000	-2.029394000	10.290850000
H	12.304772000	-6.413837000	14.339329000
H	12.860521000	-6.875576000	11.953130000
H	12.099288000	-5.316567000	10.185782000
H	10.963610000	-4.386871000	14.916656000
C	6.933257000	-1.486596000	13.592444000
C	8.140850000	-1.103414000	12.717861000
O	6.116214000	-0.369941000	13.576900000
H	7.296901000	-1.757749000	14.596944000
H	7.781011000	-0.751118000	11.749266000
H	8.696963000	-0.307620000	13.215589000
C	6.086975000	-2.651463000	13.052797000
H	5.153197000	-2.687241000	13.611122000
H	5.873721000	-2.548556000	11.986836000
Cl	6.837510000	-4.330056000	13.265097000
C	-0.011100000	4.940412000	12.927325000
C	-0.868685000	5.306311000	14.153695000
H	-1.221251000	4.412893000	14.681659000
H	-0.312002000	5.924267000	14.867615000
H	-1.750707000	5.876748000	13.836794000
C	0.409824000	6.257169000	12.231765000
H	0.997630000	6.066874000	11.327567000
H	-0.472082000	6.844193000	11.940623000
H	1.022858000	6.870763000	12.902140000
C	-0.893813000	4.117178000	11.958860000
H	-1.785405000	4.687012000	11.663067000
H	-0.350633000	3.848726000	11.046612000
H	-1.224614000	3.185870000	12.432874000

110

**10TS<sup>ECH</sup>** E = -4223.2122597,Imaginary frequency =439.51i

Al	5.267561000	0.363304000	14.758210000
O	5.036238000	1.994435000	13.725486000
N	3.995391000	2.057448000	16.558153000
C	6.795865000	0.986014000	15.933804000
C	3.371472000	-0.270230000	14.515797000

C	4.127204000	2.914839000	13.545233000
C	3.297498000	3.423351000	14.604915000
C	3.308247000	2.980067000	15.996199000
C	3.924974000	3.503289000	12.234879000
C	2.987823000	4.516517000	12.076118000
C	2.181042000	5.030417000	13.111515000
C	2.364283000	4.454396000	14.355442000
C	4.710050000	2.985022000	11.014783000
C	6.227187000	3.198158000	11.235214000
C	4.364904000	1.490907000	10.794932000
C	4.350892000	3.716368000	9.703473000
C	3.782677000	1.885524000	17.993059000
C	3.652743000	0.393365000	18.345749000
C	3.500640000	0.174702000	19.859187000
C	4.647477000	0.827606000	20.645662000
C	4.765684000	2.321343000	20.307069000
C	4.924947000	2.544963000	18.795132000
H	6.590331000	0.770216000	16.991515000
H	7.770846000	0.513895000	15.728270000
H	6.943863000	2.071643000	15.859514000
H	3.335156000	-1.052853000	13.742211000
H	2.951849000	-0.720263000	15.425448000
H	2.687501000	0.528416000	14.199932000
H	2.594865000	3.552803000	16.619146000
H	2.858255000	4.937723000	11.085299000
H	1.773547000	4.792294000	15.202857000
H	6.804399000	2.730208000	10.427703000
H	6.459711000	4.271416000	11.240487000
H	6.549006000	2.781625000	12.189436000
H	4.969636000	1.068683000	9.984854000
H	4.528512000	0.908998000	11.702011000
H	3.306356000	1.391495000	10.522111000
H	4.573551000	4.789828000	9.750382000
H	4.946311000	3.290949000	8.886531000
H	3.293985000	3.596021000	9.436010000

H	2.842483000	2.388783000	18.299656000
H	4.538441000	-0.135212000	17.972803000
H	2.796791000	-0.029695000	17.807446000
H	2.545294000	0.604690000	20.198996000
H	3.450896000	-0.900235000	20.079657000
H	5.592051000	0.325079000	20.390165000
H	4.499841000	0.690259000	21.726078000
H	5.613017000	2.769289000	20.844179000
H	3.862413000	2.841291000	20.662755000
H	5.880862000	2.132478000	18.452782000
H	4.947246000	3.618455000	18.566025000
C	11.184613000	-2.860150000	10.698419000
C	12.670076000	-2.762370000	10.373049000
O	10.481063000	-3.684817000	9.749950000
H	10.783339000	-1.840511000	10.689887000
H	13.182805000	-2.202123000	11.155667000
C	10.862877000	-3.521922000	12.040510000
H	9.782634000	-3.548918000	12.180141000
H	11.264137000	-4.534765000	12.079420000
Cl	11.565878000	-2.604222000	13.434309000
H	12.816653000	-2.266407000	9.414454000
Cl	13.489999000	-4.378094000	10.253728000
C	10.628380000	0.544364000	6.801157000
C	11.451460000	-0.574688000	6.666409000
C	11.153809000	-1.745728000	7.363980000
C	10.038883000	-1.807356000	8.211036000
C	9.213175000	-0.678302000	8.347828000
C	9.512364000	0.486668000	7.632377000
C	9.675319000	-3.155026000	8.781959000
O	8.168537000	-1.421150000	10.324767000
C	8.014340000	-0.632558000	9.245596000
O	7.048622000	0.065313000	9.023036000
O	8.789441000	-3.829199000	8.322312000
H	10.854388000	1.459197000	6.260484000
H	12.318647000	-0.542889000	6.012301000

H	11.771159000	-2.630254000	7.229292000
H	8.856107000	1.342316000	7.751138000
C	7.148991000	-0.277243000	12.354500000
C	7.106962000	-1.429257000	11.323835000
O	6.298115000	-0.672005000	13.396899000
H	6.762784000	0.628970000	11.879688000
H	7.244334000	-2.386885000	11.827482000
H	6.138993000	-1.422402000	10.820345000
C	8.545092000	0.065174000	12.915740000
H	8.416897000	0.728148000	13.767884000
H	9.128667000	-0.806518000	13.217998000
Cl	9.634318000	0.979173000	11.749615000
C	6.614058000	-2.293370000	15.981620000
C	6.883556000	-2.432231000	14.552930000
O	5.460269000	-1.588377000	15.650096000
H	7.376610000	-1.716559000	16.525167000
H	6.263620000	-3.123770000	13.998082000
H	7.822071000	-2.137131000	14.111476000
C	6.232117000	-3.548699000	16.754621000
H	5.784387000	-3.264941000	17.709328000
H	5.524569000	-4.154262000	16.186440000
Cl	7.671258000	-4.619162000	17.132846000
C	1.164214000	6.147176000	12.822428000
C	0.387991000	6.569993000	14.084085000
H	-0.182665000	5.734910000	14.506318000
H	1.058972000	6.949756000	14.863273000
H	-0.322977000	7.368563000	13.836935000
C	0.135702000	5.661145000	11.772711000
H	-0.593696000	6.450642000	11.543718000
H	0.622275000	5.372814000	10.834925000
H	-0.411226000	4.786617000	12.143479000
C	1.894345000	7.395849000	12.272489000
H	2.448406000	7.167842000	11.355735000
H	1.179366000	8.197788000	12.041590000
H	2.612808000	7.778884000	13.006496000

110

**11<sup>ECH</sup>** E= -4223.3160468

Al	4.494935000	0.880363000	14.276336000
O	3.247878000	2.134752000	13.194591000
N	3.408116000	1.704728000	15.914932000
C	5.996317000	2.116887000	13.703407000
C	3.493204000	-0.614471000	13.377901000
C	2.902408000	3.345795000	13.431309000
C	2.823392000	3.830355000	14.781009000
C	2.964212000	2.930345000	15.887589000
C	2.526270000	4.267993000	12.373320000
C	2.188696000	5.563101000	12.724621000
C	2.141215000	6.062315000	14.056687000
C	2.440268000	5.163581000	15.060758000
C	2.516149000	3.792120000	10.907856000
C	3.934280000	3.337477000	10.486269000
C	1.528546000	2.608908000	10.754056000
C	2.071627000	4.899857000	9.931973000
C	3.212148000	1.028582000	17.221714000
C	2.834036000	-0.449891000	17.041853000
C	2.607045000	-1.125929000	18.403497000
C	3.835118000	-0.982617000	19.315631000
C	4.224636000	0.493458000	19.490774000
C	4.437962000	1.191906000	18.138103000
H	6.949366000	1.969218000	14.233541000
H	6.210300000	2.016572000	12.627500000
H	5.724118000	3.172483000	13.849975000
H	3.575327000	-0.535606000	12.283732000
H	3.827822000	-1.623287000	13.654101000
H	2.416680000	-0.553548000	13.601450000
H	2.589700000	3.341034000	16.835971000
H	1.931826000	6.255131000	11.929151000
H	2.390943000	5.460262000	16.105835000
H	3.924419000	2.983611000	9.446135000
H	4.644014000	4.171486000	10.553353000

H	4.289058000	2.531393000	11.128815000
H	1.525853000	2.251070000	9.715352000
H	1.810757000	1.782948000	11.408718000
H	0.507112000	2.923177000	11.005106000
H	2.749742000	5.762103000	9.948386000
H	2.071238000	4.502123000	8.909790000
H	1.057113000	5.258123000	10.147049000
H	2.360860000	1.520960000	17.722897000
H	3.643513000	-0.948827000	16.501086000
H	1.931701000	-0.521254000	16.422335000
H	1.734387000	-0.675980000	18.903808000
H	2.365259000	-2.186960000	18.255845000
H	4.678730000	-1.527699000	18.869288000
H	3.642830000	-1.443946000	20.294470000
H	5.132452000	0.578684000	20.103577000
H	3.426024000	1.008444000	20.048366000
H	5.297589000	0.773846000	17.608227000
H	4.633958000	2.262038000	18.291778000
C	12.553714000	-2.798970000	11.573817000
C	13.961492000	-2.452461000	11.102854000
O	12.158580000	-4.125012000	11.168839000
H	11.875072000	-2.051350000	11.148464000
H	14.256712000	-1.485395000	11.510975000
C	12.379218000	-2.834934000	13.094742000
H	11.343364000	-3.068383000	13.339079000
H	13.038080000	-3.581165000	13.539218000
Cl	12.766805000	-1.241576000	13.858269000
H	14.002925000	-2.416642000	10.015282000
Cl	15.214936000	-3.655672000	11.629983000
C	11.428370000	-1.909313000	6.553354000
C	12.527882000	-2.691196000	6.910254000
C	12.502263000	-3.431616000	8.092391000
C	11.384889000	-3.391161000	8.937464000
C	10.278244000	-2.602408000	8.575410000
C	10.309230000	-1.873391000	7.380828000

C	11.358564000	-4.364477000	10.091720000
O	9.288990000	-2.704500000	10.713123000
C	9.040373000	-2.479495000	9.406775000
O	7.955480000	-2.182046000	8.954906000
O	10.758376000	-5.407129000	10.026968000
H	11.441419000	-1.331942000	5.633353000
H	13.402001000	-2.735703000	6.266272000
H	13.342977000	-4.070347000	8.350508000
H	9.438763000	-1.279314000	7.123434000
C	7.755911000	-1.170593000	11.997559000
C	8.162927000	-2.610485000	11.621416000
O	6.668968000	-1.245036000	12.903775000
H	7.337553000	-0.691247000	11.109141000
H	8.489578000	-3.172309000	12.497534000
H	7.297654000	-3.102564000	11.173503000
C	8.866415000	-0.256999000	12.541860000
H	8.402318000	0.638462000	12.953578000
H	9.497496000	-0.727995000	13.297645000
Cl	10.000330000	0.341233000	11.233079000
C	6.796401000	-0.677365000	15.310789000
C	6.886403000	-1.768668000	14.224811000
O	5.529447000	-0.183715000	15.501650000
H	7.532327000	0.107869000	15.054040000
H	6.086717000	-2.496958000	14.403157000
H	7.851289000	-2.285247000	14.289913000
C	7.220696000	-1.273401000	16.668722000
H	7.129624000	-0.516765000	17.445821000
H	6.613662000	-2.143422000	16.928643000
Cl	8.979607000	-1.839459000	16.745494000
C	1.751582000	7.528516000	14.307947000
C	1.749973000	7.880680000	15.807585000
H	1.027719000	7.273240000	16.365292000
H	2.737849000	7.732063000	16.258364000
H	1.475120000	8.933920000	15.944973000
C	0.332167000	7.802041000	13.754673000

H	0.045539000	8.850445000	13.915255000
H	0.270460000	7.600659000	12.679943000
H	-0.407347000	7.165053000	14.253805000
C	2.758762000	8.467387000	13.601028000
H	2.789137000	8.288017000	12.521037000
H	2.488085000	9.520578000	13.758255000
H	3.771463000	8.312170000	13.990460000

85

**5TS<sup>ECH</sup>** E = -3037.5286467,Imaginary frequency =405.43i

Al	7.256641000	0.808665000	15.168298000
O	5.796991000	1.142818000	13.905798000
N	5.721346000	1.695469000	16.803733000
C	7.865900000	2.766883000	15.006379000
C	6.464301000	-1.020619000	15.622483000
C	4.713092000	1.846287000	13.872685000
C	4.104806000	2.395642000	15.053787000
C	4.626299000	2.238045000	16.402400000
C	4.040057000	2.090697000	12.611717000
C	2.868409000	2.833431000	12.608583000
C	2.259115000	3.377792000	13.763345000
C	2.903747000	3.133355000	14.963132000
C	4.628078000	1.525951000	11.301769000
C	6.054843000	2.084883000	11.077731000
C	4.667823000	-0.020352000	11.370043000
C	3.791774000	1.905445000	10.062275000
C	5.965444000	1.719883000	18.246587000
C	6.204934000	0.302782000	18.799697000
C	6.479990000	0.332415000	20.311442000
C	7.662791000	1.250938000	20.653458000
C	7.446985000	2.663132000	20.088687000
C	7.163111000	2.631369000	18.578935000
H	8.389728000	2.947153000	14.053087000
H	6.976725000	3.412351000	14.978414000
H	8.508526000	3.186565000	15.797347000
H	6.281678000	-1.613446000	14.710294000

H	7.077558000	-1.649272000	16.286402000
H	5.478398000	-0.925043000	16.098184000
H	3.956302000	2.667443000	17.167594000
H	2.380085000	3.011647000	11.656308000
H	2.491315000	3.516291000	15.893387000
H	6.485974000	1.662815000	10.159042000
H	6.025783000	3.176179000	10.964943000
H	6.704172000	1.845295000	11.920484000
H	5.136471000	-0.432811000	10.466422000
H	5.230744000	-0.354343000	12.242213000
H	3.650654000	-0.426992000	11.439924000
H	3.735870000	2.991427000	9.917339000
H	4.259987000	1.477180000	9.167560000
H	2.768453000	1.514005000	10.116640000
H	5.077004000	2.137550000	18.760745000
H	7.055805000	-0.137613000	18.268583000
H	5.334888000	-0.326863000	18.579665000
H	5.584056000	0.689214000	20.843937000
H	6.671566000	-0.685725000	20.676115000
H	8.581462000	0.827376000	20.221206000
H	7.816985000	1.292161000	21.740820000
H	8.323130000	3.293560000	20.292293000
H	6.598937000	3.132333000	20.611806000
H	8.036644000	2.254583000	18.036862000
H	6.967295000	3.642076000	18.200808000
C	8.449807000	-0.904365000	12.973816000
C	8.936664000	-2.240020000	13.554525000
O	8.575090000	0.200502000	13.806373000
H	7.378659000	-1.098313000	12.789844000
H	8.591909000	-3.077412000	12.947526000
C	9.087820000	-0.528083000	11.630772000
H	8.631958000	0.389782000	11.264073000
H	10.167619000	-0.405431000	11.721747000
Cl	8.829104000	-1.788269000	10.318933000
H	8.589343000	-2.336363000	14.580734000

Cl	10.769318000	-2.452368000	13.620629000
C	10.092134000	0.955343000	16.490863000
C	10.305365000	0.727674000	15.059692000
O	8.853560000	0.307200000	16.425124000
H	10.046442000	2.015290000	16.778537000
H	10.780018000	-0.186754000	14.732221000
H	10.217703000	1.538505000	14.353510000
C	10.993235000	0.182965000	17.444361000
H	10.572523000	0.205810000	18.451353000
H	11.113950000	-0.850952000	17.118621000
Cl	12.675336000	0.906456000	17.556813000
C	0.957344000	4.186969000	13.638815000
C	0.447286000	4.684859000	15.004608000
H	0.232981000	3.851930000	15.684163000
H	1.175518000	5.342235000	15.493618000
H	-0.481022000	5.254980000	14.872682000
C	-0.152057000	3.309726000	13.010063000
H	-1.086781000	3.877675000	12.902702000
H	0.133220000	2.947846000	12.016995000
H	-0.354049000	2.433166000	13.636374000
C	1.191494000	5.424666000	12.739370000
H	1.526884000	5.136879000	11.737387000
H	0.267449000	6.009415000	12.628217000
H	1.959816000	6.076740000	13.170705000

85

**6<sup>EC</sup>H** E = -3037.6243483

Al	6.952443000	0.994313000	15.070379000
O	5.206924000	1.007182000	13.921144000
N	5.586284000	1.568168000	16.601603000
C	7.519385000	2.579588000	13.953159000
C	6.903979000	-1.000311000	14.756150000
C	4.251967000	1.860176000	13.904176000
C	3.920463000	2.607170000	15.085905000
C	4.538138000	2.298890000	16.342103000
C	3.427147000	2.082872000	12.728001000

C	2.429642000	3.039030000	12.799271000
C	2.115156000	3.806531000	13.955941000
C	2.863819000	3.548276000	15.086616000
C	3.681334000	1.265041000	11.447109000
C	5.114674000	1.527180000	10.925298000
C	3.512174000	-0.243756000	11.753457000
C	2.699179000	1.623186000	10.313946000
C	5.799763000	1.324682000	18.050309000
C	6.291786000	-0.106637000	18.315865000
C	6.479112000	-0.350089000	19.821922000
C	7.433799000	0.680469000	20.444164000
C	6.953120000	2.114474000	20.172602000
C	6.742453000	2.370647000	18.671583000
H	7.708941000	2.291603000	12.907884000
H	6.723624000	3.338673000	13.912811000
H	8.426736000	3.091517000	14.302817000
H	7.047400000	-1.226242000	13.687435000
H	7.666302000	-1.554350000	15.321844000
H	5.925524000	-1.428008000	15.020224000
H	4.000595000	2.714066000	17.206413000
H	1.832066000	3.217707000	11.911138000
H	2.660297000	4.069423000	16.019174000
H	5.304279000	0.929039000	10.023079000
H	5.243502000	2.584730000	10.663221000
H	5.855060000	1.269036000	11.682794000
H	3.709031000	-0.837966000	10.850419000
H	4.202557000	-0.557087000	12.538093000
H	2.486888000	-0.458800000	12.081445000
H	2.787210000	2.672755000	10.007108000
H	2.919747000	1.004749000	9.435243000
H	1.655604000	1.435532000	10.596003000
H	4.820674000	1.428036000	18.549449000
H	7.240209000	-0.246102000	17.788866000
H	5.572682000	-0.821705000	17.897460000
H	5.505275000	-0.292511000	20.334548000

H	6.856979000	-1.367493000	19.989555000
H	8.435236000	0.548147000	20.011273000
H	7.531201000	0.510163000	21.525605000
H	7.670135000	2.840725000	20.579209000
H	6.006022000	2.280490000	20.710698000
H	7.687972000	2.320444000	18.125737000
H	6.322708000	3.373769000	18.514019000
C	10.424384000	-0.961166000	13.085489000
C	10.152168000	-2.420859000	13.471867000
O	9.945362000	0.010830000	13.986217000
H	9.810260000	-0.806585000	12.188273000
H	10.190087000	-3.050769000	12.582945000
C	11.878203000	-0.646330000	12.705961000
H	11.960752000	0.412477000	12.461562000
H	12.581634000	-0.905855000	13.496402000
Cl	12.409685000	-1.571482000	11.225507000
H	9.170764000	-2.490516000	13.941666000
Cl	11.349751000	-3.173543000	14.632699000
C	9.735341000	1.207215000	16.044141000
C	10.380916000	-0.005056000	15.351168000
O	8.396370000	1.035569000	16.325127000
H	9.933960000	2.081856000	15.398757000
H	10.046258000	-0.919192000	15.855662000
H	11.476130000	0.052228000	15.404338000
C	10.412091000	1.461395000	17.405029000
H	9.921457000	2.295444000	17.903615000
H	10.370729000	0.575683000	18.042833000
Cl	12.194635000	1.934413000	17.309502000
C	0.978662000	4.840798000	13.899370000
C	0.784090000	5.564715000	15.245114000
H	0.520571000	4.864955000	16.046698000
H	1.689313000	6.102829000	15.548721000
H	-0.028384000	6.297419000	15.162644000
C	-0.355229000	4.143417000	13.538519000
H	-1.174662000	4.873033000	13.480504000

H	-0.296047000	3.631317000	12.572237000
H	-0.617304000	3.394190000	14.294669000
C	1.295299000	5.910603000	12.826542000
H	1.417876000	5.463871000	11.834112000
H	0.486692000	6.651791000	12.762770000
H	2.225100000	6.437975000	13.068725000

93

**5TS<sup>LA</sup>** E = -2919.2219632, Imaginary frequency =172.69i

Al	7.088520000	0.862278000	15.042885000
O	5.565347000	0.935868000	13.806044000
N	5.858348000	1.879823000	16.589932000
C	7.706600000	2.686326000	14.403860000
C	6.475093000	-0.944958000	15.726381000
C	4.437795000	1.571465000	13.836612000
C	3.976168000	2.266995000	15.007368000
C	4.697247000	2.338575000	16.265044000
C	3.574000000	1.598476000	12.672716000
C	2.365546000	2.274317000	12.751231000
C	1.897099000	2.958419000	13.897591000
C	2.728623000	2.931949000	15.001931000
C	4.019200000	0.921266000	11.360263000
C	5.286934000	1.635881000	10.831908000
C	4.300295000	-0.583504000	11.593502000
C	2.951988000	1.010312000	10.249708000
C	6.265624000	2.085771000	17.987975000
C	6.152910000	0.772919000	18.789672000
C	6.559330000	0.980432000	20.256694000
C	7.975001000	1.566641000	20.367197000
C	8.097333000	2.868251000	19.558950000
C	7.686043000	2.670215000	18.090100000
H	8.138315000	2.662609000	13.390158000
H	6.864013000	3.393465000	14.354493000
H	8.474910000	3.137063000	15.046686000
H	6.520430000	-1.685345000	14.910965000
H	7.070872000	-1.363638000	16.549727000

H	5.427340000	-0.925493000	16.062185000
H	4.134044000	2.874244000	17.045172000
H	1.731724000	2.286265000	11.871045000
H	2.435792000	3.436205000	15.919307000
H	5.688976000	1.117381000	9.951361000
H	5.048915000	2.665691000	10.537464000
H	6.062049000	1.678003000	11.597611000
H	4.654890000	-1.050472000	10.664239000
H	5.047016000	-0.727463000	12.374363000
H	3.381978000	-1.100860000	11.899532000
H	2.724975000	2.046978000	9.973275000
H	3.327479000	0.507591000	9.350013000
H	2.014555000	0.517972000	10.536716000
H	5.569466000	2.810754000	18.450352000
H	6.793889000	0.016516000	18.323994000
H	5.123191000	0.397841000	18.723761000
H	5.845885000	1.665557000	20.742266000
H	6.493723000	0.028097000	20.800661000
H	8.698136000	0.833841000	19.981280000
H	8.234403000	1.743494000	21.420377000
H	9.126641000	3.247714000	19.606085000
H	7.459639000	3.638420000	20.022154000
H	8.392573000	1.998633000	17.590125000
H	7.725035000	3.623771000	17.549595000
C	8.529670000	-0.223197000	12.355793000
C	8.267398000	-1.643952000	11.844384000
O	8.594970000	-0.180659000	13.761864000
H	7.619070000	0.323341000	12.067922000
H	7.960274000	-1.636843000	10.798083000
C	9.698854000	0.485207000	11.666525000
H	9.812831000	1.489059000	12.067028000
H	10.629852000	-0.073121000	11.756578000
Cl	9.413288000	0.664897000	9.866851000
H	7.499393000	-2.107193000	12.462987000
Cl	9.712687000	-2.771090000	11.915597000

O	10.581618000	1.239928000	14.396494000
C	11.958566000	0.981705000	14.112043000
C	12.630474000	2.320219000	13.850449000
C	12.612696000	0.215356000	15.263263000
O	13.710880000	0.461144000	15.712056000
O	11.869025000	-0.791663000	15.754410000
C	10.617067000	-1.101522000	15.054422000
C	9.937764000	-2.188335000	15.855090000
C	9.795439000	0.199331000	14.949665000
O	9.041344000	0.534045000	15.903701000
H	12.145461000	2.819108000	13.006156000
H	13.690093000	2.172715000	13.626212000
H	12.545722000	2.960653000	14.732367000
H	10.877355000	-1.463883000	14.056616000
H	9.696195000	-1.816128000	16.852921000
H	10.596899000	-3.059065000	15.934560000
H	9.009001000	-2.477635000	15.360719000
H	12.055219000	0.347737000	13.213448000
C	0.541201000	3.682782000	13.860847000
C	0.203179000	4.354247000	15.205381000
H	0.145628000	3.622645000	16.019639000
H	0.948985000	5.109187000	15.479613000
H	-0.769940000	4.856524000	15.138881000
C	-0.587431000	2.674962000	13.536027000
H	-1.561763000	3.180632000	13.491298000
H	-0.423833000	2.181125000	12.572250000
H	-0.642220000	1.893770000	14.303085000
C	0.564451000	4.783062000	12.772393000
H	0.771754000	4.366098000	11.781040000
H	-0.401619000	5.303882000	12.721508000
H	1.342291000	5.524575000	12.988328000

93

**6<sup>LA</sup>** E = -2919.2581412

AI	6.803917000	0.484717000	14.443666000
O	4.906845000	0.723801000	13.747117000

N	6.083645000	1.547226000	16.116196000
C	7.394011000	1.876003000	13.109331000
C	6.395077000	-1.485577000	14.391561000
C	4.153155000	1.763595000	13.786278000
C	4.293729000	2.717253000	14.847440000
C	5.158891000	2.455476000	15.959350000
C	3.106788000	2.000712000	12.810695000
C	2.356576000	3.158072000	12.929358000
C	2.506036000	4.126532000	13.960815000
C	3.467844000	3.864831000	14.915388000
C	2.864259000	0.984806000	11.677766000
C	4.132756000	0.858629000	10.799861000
C	2.513676000	-0.396863000	12.283359000
C	1.699019000	1.397896000	10.756473000
C	6.621982000	1.482386000	17.497694000
C	6.743262000	0.031896000	17.983517000
C	7.233478000	-0.008142000	19.440994000
C	8.551785000	0.760079000	19.626556000
C	8.452842000	2.199685000	19.097232000
C	7.947843000	2.244759000	17.645026000
H	7.258170000	1.563612000	12.062482000
H	6.763151000	2.770380000	13.225256000
H	8.432644000	2.204617000	13.225107000
H	6.174023000	-1.810435000	13.362049000
H	7.196104000	-2.128488000	14.778012000
H	5.483212000	-1.712401000	14.963933000
H	4.963826000	3.105716000	16.822185000
H	1.589678000	3.344791000	12.184924000
H	3.619978000	4.541723000	15.752437000
H	3.969516000	0.120590000	10.002657000
H	4.373743000	1.818872000	10.327439000
H	4.989520000	0.546046000	11.397307000
H	2.353686000	-1.130894000	11.481873000
H	3.318093000	-0.752440000	12.928923000
H	1.590524000	-0.336621000	12.874205000

H	1.890112000	2.352151000	10.250329000
H	1.565485000	0.635647000	9.979318000
H	0.750691000	1.482971000	11.301619000
H	5.888304000	1.976285000	18.156924000
H	7.438134000	-0.499196000	17.326601000
H	5.769188000	-0.465463000	17.892670000
H	6.462205000	0.431645000	20.093469000
H	7.351672000	-1.051134000	19.764739000
H	9.357223000	0.246646000	19.089238000
H	8.835894000	0.768462000	20.688194000
H	9.433711000	2.686102000	19.158169000
H	7.767538000	2.776391000	19.739484000
H	8.679628000	1.804338000	16.965584000
H	7.799313000	3.286036000	17.328308000
C	9.741847000	-0.587932000	12.633109000
C	9.425092000	-2.005181000	12.174576000
O	10.418456000	-0.626393000	13.872463000
H	8.774822000	-0.084221000	12.729259000
H	8.909206000	-2.003616000	11.214296000
C	10.637818000	0.220397000	11.690581000
H	10.739688000	1.231813000	12.080306000
H	11.615348000	-0.251255000	11.586726000
Cl	9.956083000	0.376922000	10.002053000
H	8.817555000	-2.503518000	12.928636000
Cl	10.913837000	-3.047059000	11.944261000
O	10.300214000	1.553417000	14.777501000
C	11.580985000	1.934659000	15.259771000
C	11.820066000	3.389602000	14.888029000
C	11.593682000	1.724486000	16.778371000
O	11.982443000	2.531291000	17.594643000
O	11.066232000	0.544314000	17.174358000
C	10.817457000	-0.432169000	16.125681000
C	10.258952000	-1.681753000	16.771052000
C	9.901334000	0.164991000	15.004396000
O	8.616432000	0.093416000	15.214584000

H	11.805627000	3.499468000	13.799490000
H	12.784865000	3.729512000	15.274880000
H	11.034436000	4.018839000	15.314869000
H	11.782581000	-0.667291000	15.666596000
H	9.289602000	-1.485304000	17.230464000
H	10.952278000	-2.057436000	17.531529000
H	10.125988000	-2.446408000	16.001064000
H	12.370688000	1.306735000	14.810386000
C	1.605299000	5.372958000	13.972931000
C	0.119117000	4.950847000	14.065337000
H	-0.537193000	5.831741000	14.062076000
H	-0.174738000	4.313673000	13.224416000
H	-0.067634000	4.388914000	14.987892000
C	1.820068000	6.187137000	12.674333000
H	1.591122000	5.594306000	11.782344000
H	1.174733000	7.076057000	12.660150000
H	2.861503000	6.518723000	12.592816000
C	1.909410000	6.297676000	15.166747000
H	1.742952000	5.790914000	16.124424000
H	2.945146000	6.655433000	15.147411000
H	1.252596000	7.175821000	15.136857000

93

**7<sup>LA</sup>** E = -2919.2585473

Al	6.684619000	1.304332000	14.526504000
O	5.160160000	2.296504000	13.594197000
N	5.690715000	2.003279000	16.280645000
C	7.900942000	2.613888000	13.618654000
C	5.822270000	-0.421477000	13.953702000
C	3.904829000	2.228484000	13.856213000
C	3.456352000	2.011699000	15.201781000
C	4.385763000	2.058857000	16.290639000
C	2.888370000	2.413406000	12.837819000
C	1.561147000	2.301603000	13.214075000
C	1.105525000	2.056533000	14.539978000
C	2.077187000	1.941040000	15.512911000

C	3.301934000	2.708738000	11.383201000
C	4.130138000	4.016469000	11.333395000
C	4.148759000	1.539211000	10.825207000
C	2.086795000	2.891073000	10.452029000
C	6.310291000	2.377188000	17.574778000
C	6.779857000	1.168438000	18.400733000
C	7.345558000	1.625627000	19.755749000
C	8.479897000	2.647237000	19.580069000
C	8.034381000	3.837276000	18.715484000
C	7.451830000	3.383202000	17.366471000
H	7.673523000	2.658904000	12.543439000
H	7.725659000	3.633718000	13.996241000
H	8.973295000	2.410401000	13.717071000
H	6.052904000	-0.600558000	12.891773000
H	6.162017000	-1.315311000	14.489563000
H	4.725827000	-0.402081000	14.025274000
H	3.908064000	2.228401000	17.265271000
H	0.803802000	2.414084000	12.445218000
H	1.806466000	1.788181000	16.554771000
H	4.442165000	4.226868000	10.301382000
H	3.531276000	4.866886000	11.684454000
H	5.020475000	3.934408000	11.958600000
H	4.458904000	1.756128000	9.793830000
H	5.039338000	1.379402000	11.433498000
H	3.565889000	0.609884000	10.815317000
H	1.446230000	3.724633000	10.766165000
H	2.439246000	3.110323000	9.436864000
H	1.468969000	1.986309000	10.396478000
H	5.538028000	2.892468000	18.170920000
H	7.537948000	0.636699000	17.819678000
H	5.934621000	0.483254000	18.552481000
H	6.541474000	2.080130000	20.355940000
H	7.702632000	0.757589000	20.326525000
H	9.335486000	2.153976000	19.099438000
H	8.830292000	2.999561000	20.560059000

H	8.877345000	4.520150000	18.546473000
H	7.273546000	4.414153000	19.264506000
H	8.225304000	2.910840000	16.754737000
H	7.078273000	4.245923000	16.801644000
C	8.089017000	-2.132488000	16.613472000
C	8.169421000	-2.431254000	18.105064000
O	9.269267000	-1.472359000	16.208243000
H	7.227357000	-1.465238000	16.482109000
H	7.265084000	-2.926552000	18.458808000
C	7.920672000	-3.365842000	15.721155000
H	7.801568000	-3.045509000	14.688174000
H	8.771916000	-4.039417000	15.823261000
Cl	6.432011000	-4.344254000	16.137328000
H	8.334665000	-1.505709000	18.655623000
Cl	9.556485000	-3.534164000	18.561309000
O	8.885111000	-0.804926000	13.977708000
C	10.037164000	-1.267249000	13.283018000
C	9.590662000	-1.898505000	11.973749000
C	10.968369000	-0.075682000	13.053796000
O	11.569829000	0.151195000	12.027901000
O	11.053601000	0.764099000	14.107513000
C	10.578076000	0.265915000	15.387417000
C	10.753373000	1.394586000	16.378831000
C	9.110823000	-0.298579000	15.307786000
O	8.127242000	0.491780000	15.668103000
H	8.946058000	-2.759385000	12.175111000
H	10.459931000	-2.222051000	11.394969000
H	9.029502000	-1.171843000	11.379943000
H	11.226073000	-0.571377000	15.666051000
H	10.146975000	2.253517000	16.086164000
H	11.805337000	1.696462000	16.422549000
H	10.438395000	1.059440000	17.370744000
H	10.570775000	-2.015402000	13.894412000
C	-0.402876000	1.952712000	14.820623000
C	-0.700242000	1.694538000	16.309871000

H	-0.247957000	0.758149000	16.655834000
H	-0.326866000	2.506893000	16.944247000
H	-1.783285000	1.620405000	16.467975000
C	-1.007743000	0.784104000	14.005813000
H	-2.088591000	0.702310000	14.184605000
H	-0.856840000	0.920502000	12.929661000
H	-0.541007000	-0.166681000	14.287365000
C	-1.108525000	3.269638000	14.416582000
H	-0.963400000	3.498624000	13.355475000
H	-2.189786000	3.204466000	14.599353000
H	-0.714494000	4.113755000	14.994538000

93

**8TS<sup>LA</sup>** E = -2919.2330777, Imaginary frequency =202.19i

Al	6.642559000	1.110119000	14.974894000
O	5.242770000	1.556997000	13.780263000
N	5.396892000	2.039977000	16.676920000
C	7.681047000	2.811450000	14.830138000
C	5.897011000	-0.650671000	15.592099000
C	3.979128000	1.854933000	13.927711000
C	3.417960000	2.224790000	15.193991000
C	4.166294000	2.325735000	16.438259000
C	3.090453000	1.850668000	12.789059000
C	1.754551000	2.180779000	12.982247000
C	1.184941000	2.536911000	14.224080000
C	2.048974000	2.553605000	15.304135000
C	3.614309000	1.485521000	11.384776000
C	4.713231000	2.490323000	10.961319000
C	4.165555000	0.039342000	11.392636000
C	2.513768000	1.541303000	10.304426000
C	5.864069000	2.253898000	18.053734000
C	6.364687000	0.940636000	18.685800000
C	6.839870000	1.167189000	20.130187000
C	7.926204000	2.250353000	20.202161000
C	7.439695000	3.557596000	19.559253000
C	6.964555000	3.330348000	18.115366000

H	7.925233000	2.999580000	13.774653000
H	7.085537000	3.672390000	15.162212000
H	8.634480000	2.831805000	15.369843000
H	6.130548000	-1.450394000	14.875648000
H	6.237195000	-0.986282000	16.578929000
H	4.800219000	-0.587293000	15.650028000
H	3.555512000	2.702759000	17.274514000
H	1.098499000	2.166229000	12.119191000
H	1.686760000	2.827179000	16.291498000
H	5.137084000	2.206383000	9.988971000
H	4.289455000	3.497876000	10.862581000
H	5.518026000	2.530367000	11.695093000
H	4.583332000	-0.214491000	10.409127000
H	4.944518000	-0.083006000	12.144195000
H	3.360212000	-0.673263000	11.611435000
H	2.079469000	2.543577000	10.204692000
H	2.951744000	1.275736000	9.334680000
H	1.700674000	0.832160000	10.502326000
H	5.012244000	2.614462000	18.661556000
H	7.188421000	0.543545000	18.082268000
H	5.559662000	0.196422000	18.659951000
H	5.986721000	1.469141000	20.758331000
H	7.214329000	0.223529000	20.548452000
H	8.818821000	1.897612000	19.666636000
H	8.227033000	2.424200000	21.244687000
H	8.239268000	4.310133000	19.571333000
H	6.614125000	3.970585000	20.160403000
H	7.806400000	3.011573000	17.493148000
H	6.586466000	4.264821000	17.682676000
C	8.891996000	-2.569653000	15.998553000
C	9.578509000	-2.818054000	17.337392000
O	9.665755000	-1.717671000	15.168404000
H	7.936236000	-2.095478000	16.236952000
H	8.978674000	-3.471296000	17.972039000
C	8.648904000	-3.805460000	15.136960000

H	8.116732000	-3.512757000	14.232680000
H	9.585139000	-4.302159000	14.881299000
Cl	7.613517000	-5.048249000	15.980273000
H	9.748923000	-1.860080000	17.825342000
Cl	11.214470000	-3.621863000	17.183452000
O	8.236171000	0.018452000	13.996350000
C	8.880749000	0.172883000	12.758043000
C	7.911779000	0.263226000	11.585424000
C	9.813389000	1.389351000	12.807798000
O	9.900921000	2.247615000	11.958056000
O	10.567903000	1.483997000	13.934446000
C	10.762960000	0.299676000	14.728481000
C	11.721998000	0.687111000	15.844508000
C	9.473624000	-0.317010000	15.344581000
O	8.955518000	0.112035000	16.382975000
H	7.282134000	-0.631044000	11.564627000
H	8.459103000	0.340938000	10.640149000
H	7.270431000	1.141298000	11.679960000
H	11.223876000	-0.463163000	14.092707000
H	11.239277000	1.407479000	16.509938000
H	12.629573000	1.130226000	15.422248000
H	11.994782000	-0.199623000	16.425556000
H	9.526925000	-0.710975000	12.589287000
C	-0.311039000	2.881438000	14.317835000
C	-0.735610000	3.244244000	15.753518000
H	-0.562130000	2.414899000	16.448795000
H	-0.192777000	4.120039000	16.127410000
H	-1.806459000	3.481082000	15.778289000
C	-1.157992000	1.668611000	13.863308000
H	-2.230414000	1.901471000	13.912709000
H	-0.926807000	1.377243000	12.833215000
H	-0.966619000	0.800033000	14.503886000
C	-0.630399000	4.091100000	13.407027000
H	-0.380186000	3.886910000	12.360543000
H	-1.698854000	4.342195000	13.452687000

H	-0.058328000	4.972801000	13.718287000
93			
<b>9<sup>LA</sup></b>	<b>E = -2919.2675495</b>		
Al	7.101605000	1.677213000	14.905699000
O	5.546647000	2.280679000	14.114370000
N	5.215399000	2.892744000	16.973230000
C	8.260038000	3.158004000	15.583221000
C	6.732437000	0.029000000	15.990600000
C	4.242251000	2.140749000	14.131397000
C	3.475795000	2.249560000	15.335218000
C	4.007011000	2.637207000	16.642803000
C	3.518473000	1.923581000	12.902831000
C	2.140786000	1.730322000	12.964786000
C	1.380743000	1.763331000	14.150473000
C	2.080894000	2.044698000	15.311961000
C	4.242414000	1.910820000	11.537165000
C	4.991692000	3.249660000	11.331125000
C	5.232498000	0.724545000	11.456384000
C	3.262801000	1.762453000	10.352456000
C	5.440451000	3.321508000	18.346516000
C	6.376295000	2.337477000	19.074575000
C	6.703323000	2.810309000	20.499621000
C	7.293361000	4.228748000	20.502961000
C	6.360762000	5.215785000	19.784492000
C	6.032619000	4.744958000	18.359117000
H	7.866660000	4.143878000	15.295550000
H	8.327459000	3.158860000	16.679260000
H	9.291007000	3.098928000	15.207322000
H	6.503643000	-0.809223000	15.314822000
H	7.615431000	-0.261684000	16.581947000
H	5.894827000	0.130914000	16.690455000
H	3.211734000	2.732695000	17.407794000
H	1.610574000	1.543540000	12.038104000
H	1.557392000	2.125715000	16.260849000
H	5.533228000	3.237412000	10.375354000

H	4.282385000	4.087127000	11.303978000
H	5.704480000	3.427280000	12.136251000
H	5.700616000	0.697006000	10.461781000
H	6.024207000	0.794545000	12.203666000
H	4.699729000	-0.224931000	11.598038000
H	2.519981000	2.569129000	10.322479000
H	3.830085000	1.801441000	9.414670000
H	2.729236000	0.804252000	10.370098000
H	4.481848000	3.351146000	18.906777000
H	7.298843000	2.235883000	18.490878000
H	5.910882000	1.344490000	19.095916000
H	5.786384000	2.801775000	21.109549000
H	7.399136000	2.106976000	20.976140000
H	8.266216000	4.214799000	19.990490000
H	7.483914000	4.562156000	21.532610000
H	6.814420000	6.215703000	19.753684000
H	5.428941000	5.314884000	20.363060000
H	6.939373000	4.747697000	17.742403000
H	5.323822000	5.432697000	17.880030000
C	8.585714000	-3.525140000	16.430763000
C	9.504316000	-4.730935000	16.584020000
O	8.792292000	-2.875535000	15.166946000
H	8.857005000	-2.829748000	17.232457000
H	9.337983000	-5.213208000	17.547724000
C	7.086415000	-3.804718000	16.474890000
H	6.543302000	-2.864634000	16.374556000
H	6.786668000	-4.505706000	15.695817000
Cl	6.606358000	-4.539364000	18.067080000
H	10.542764000	-4.410953000	16.502503000
Cl	9.246013000	-6.005611000	15.311874000
O	7.958474000	0.938852000	13.462797000
C	9.008430000	1.287416000	12.624156000
C	8.924956000	2.707898000	12.056314000
C	10.388508000	1.069912000	13.292791000
O	11.254314000	1.912046000	13.356412000

O	10.681324000	-0.163386000	13.816961000
C	9.772978000	-1.265497000	13.749799000
C	10.233155000	-2.250756000	12.668855000
C	9.775114000	-1.923525000	15.124592000
O	10.510202000	-1.687439000	16.051378000
H	7.966502000	2.825279000	11.543096000
H	9.737471000	2.899102000	11.346750000
H	8.989578000	3.448400000	12.856974000
H	8.755896000	-0.907711000	13.564799000
H	11.266800000	-2.564379000	12.851583000
H	10.187706000	-1.766482000	11.688344000
H	9.588945000	-3.134625000	12.653460000
H	9.006467000	0.595059000	11.754802000
C	-0.136968000	1.516269000	14.104437000
C	-0.783116000	1.598308000	15.500552000
H	-0.360280000	0.855094000	16.186095000
H	-0.650642000	2.588828000	15.950868000
H	-1.861108000	1.408383000	15.425674000
C	-0.419990000	0.106901000	13.531560000
H	-1.500757000	-0.083614000	13.479218000
H	-0.010649000	-0.008142000	12.522312000
H	0.033528000	-0.666105000	14.162549000
C	-0.817207000	2.574249000	13.202906000
H	-0.425796000	2.546362000	12.180468000
H	-1.901365000	2.404031000	13.151120000
H	-0.648085000	3.583938000	13.594894000

93

**10<sup>LA</sup>, E= -2919.2734472**

Al	7.085524000	2.990168000	15.032488000
O	5.601660000	2.289654000	14.216786000
N	4.799576000	2.285769000	17.045425000
C	6.743273000	4.787278000	15.865667000
C	8.082608000	1.591877000	16.057584000
C	4.745561000	1.310372000	14.105680000
C	4.047696000	0.773323000	15.235260000

C	4.121674000	1.296975000	16.598677000
C	4.434195000	0.761819000	12.807368000
C	3.541294000	-0.303800000	12.734751000
C	2.889794000	-0.883185000	13.842791000
C	3.157981000	-0.309091000	15.073853000
C	5.076512000	1.326393000	11.518011000
C	4.809594000	2.846430000	11.394801000
C	6.602299000	1.066274000	11.516242000
C	4.499689000	0.664945000	10.246398000
C	4.609111000	2.626155000	18.447447000
C	5.946531000	2.560570000	19.209084000
C	5.795387000	3.007647000	20.671516000
C	5.179774000	4.411582000	20.772751000
C	3.840867000	4.481420000	20.022849000
C	3.990589000	4.034567000	18.560392000
H	7.459685000	5.565704000	15.559504000
H	5.741952000	5.152489000	15.596160000
H	6.778795000	4.752252000	16.963130000
H	8.332209000	0.735654000	15.412971000
H	9.042167000	1.978924000	16.437016000
H	7.532840000	1.196243000	16.920897000
H	3.459662000	0.745748000	17.295860000
H	3.326302000	-0.721895000	11.758259000
H	2.669567000	-0.681151000	15.970795000
H	5.218601000	3.219849000	10.446540000
H	3.730492000	3.050698000	11.400707000
H	5.281295000	3.401338000	12.203905000
H	7.028944000	1.372005000	10.550230000
H	7.111465000	1.635367000	12.294441000
H	6.811439000	-0.003216000	11.650486000
H	3.413794000	0.799363000	10.163002000
H	4.958300000	1.129931000	9.365732000
H	4.717623000	-0.409275000	10.196754000
H	3.908989000	1.912553000	18.932488000
H	6.672598000	3.199389000	18.692236000

H	6.341546000	1.538584000	19.158503000
H	5.151024000	2.294777000	21.209597000
H	6.771856000	2.982551000	21.173907000
H	5.875787000	5.141868000	20.334603000
H	5.044996000	4.696575000	21.825665000
H	3.433173000	5.500737000	20.064412000
H	3.110532000	3.833850000	20.532799000
H	4.631769000	4.737081000	18.014123000
H	3.016443000	4.039562000	18.054688000
C	6.225242000	8.659454000	9.666646000
C	6.747010000	9.949879000	9.046086000
O	6.560459000	8.573854000	11.060638000
H	6.720781000	7.839725000	9.134930000
H	6.470731000	10.000418000	7.992342000
C	4.712317000	8.462527000	9.634860000
H	4.458004000	7.518208000	10.115847000
H	4.192874000	9.285328000	10.126299000
Cl	4.098550000	8.383225000	7.928402000
H	7.830694000	9.991237000	9.148924000
Cl	6.084305000	11.448345000	9.834293000
O	8.080664000	3.306846000	13.534315000
C	8.885812000	4.386113000	13.282356000
C	9.891797000	4.063726000	12.156293000
C	8.078586000	5.615255000	12.832367000
O	7.043809000	5.629863000	12.203155000
O	8.700099000	6.786047000	13.201679000
C	7.973476000	7.970336000	12.871714000
C	8.782484000	9.153081000	13.396274000
C	7.792146000	8.076090000	11.358494000
O	8.639404000	7.836976000	10.529674000
H	10.508308000	3.217421000	12.475537000
H	10.540350000	4.917465000	11.923802000
H	9.345491000	3.770888000	11.253679000
H	6.982886000	7.928941000	13.332051000
H	9.763554000	9.181396000	12.912555000

H	8.923519000	9.049392000	14.475910000
H	8.257914000	10.093640000	13.196362000
H	9.465305000	4.720623000	14.162736000
C	1.933329000	-2.071304000	13.642476000
C	1.323977000	-2.559446000	14.970506000
H	2.097851000	-2.889307000	15.673055000
H	0.735910000	-1.773945000	15.458984000
H	0.655610000	-3.409906000	14.785871000
C	0.769735000	-1.660835000	12.708359000
H	1.134455000	-1.331626000	11.729674000
H	0.083582000	-2.503375000	12.544565000
H	0.197414000	-0.833290000	13.143526000
C	2.697109000	-3.257330000	13.006126000
H	3.132483000	-2.984291000	12.039100000
H	3.516423000	-3.583929000	13.656958000
H	2.026454000	-4.112436000	12.843178000

118

**10TS<sup>LA</sup>** E = -4104.9155957 Imaginary frequency =170.96i

Al	4.915807000	1.241896000	15.024618000
O	4.503185000	2.562989000	13.662667000
N	3.695387000	2.364413000	16.438628000
C	6.629871000	2.215149000	15.460959000
C	3.329047000	0.120440000	14.473658000
C	3.483388000	3.346910000	13.518548000
C	2.657004000	3.719387000	14.631366000
C	2.876032000	3.257501000	15.985710000
C	3.152756000	3.905559000	12.225736000
C	2.069404000	4.766283000	12.136343000
C	1.248778000	5.150959000	13.225823000
C	1.575191000	4.613477000	14.456752000
C	3.973316000	3.511835000	10.981100000
C	5.459390000	3.905167000	11.168359000
C	3.851240000	1.985783000	10.746367000
C	3.475376000	4.212032000	9.700033000
C	3.684144000	2.153058000	17.895081000

C	3.286355000	0.708997000	18.258338000
C	3.271029000	0.509500000	19.783688000
C	4.616220000	0.892707000	20.421740000
C	5.017011000	2.327186000	20.045074000
C	5.043733000	2.518806000	18.520782000
H	7.296718000	1.708114000	16.169669000
H	7.208407000	2.387445000	14.540088000
H	6.420390000	3.217550000	15.862464000
H	2.457873000	0.755379000	14.253720000
H	3.529423000	-0.449606000	13.554112000
H	3.013044000	-0.605482000	15.234570000
H	2.228419000	3.759119000	16.720459000
H	1.824825000	5.174639000	11.161605000
H	0.992084000	4.864140000	15.339377000
H	6.047974000	3.572576000	10.304165000
H	5.559585000	4.995336000	11.254512000
H	5.875185000	3.448579000	12.066647000
H	4.462953000	1.681626000	9.889456000
H	4.185476000	1.427297000	11.621213000
H	2.807283000	1.714568000	10.542899000
H	3.544442000	5.304935000	9.771025000
H	4.098287000	3.895986000	8.854770000
H	2.437983000	3.948691000	9.459187000
H	2.926050000	2.827439000	18.335243000
H	3.996142000	0.014032000	17.797920000
H	2.298648000	0.488091000	17.833383000
H	2.473470000	1.125521000	20.229671000
H	3.024467000	-0.534910000	20.017597000
H	5.392692000	0.199180000	20.068538000
H	4.565990000	0.783651000	21.514078000
H	5.999797000	2.574765000	20.469083000
H	4.298488000	3.033016000	20.492478000
H	5.820991000	1.887859000	18.076222000
H	5.292687000	3.556960000	18.266542000
C	10.687849000	-3.010560000	10.466376000

C	12.138523000	-3.095689000	10.008867000
O	9.784609000	-3.513405000	9.464697000
H	10.475688000	-1.957056000	10.679009000
H	12.800384000	-2.777884000	10.815234000
C	10.346613000	-3.853631000	11.696854000
H	9.293350000	-3.722429000	11.942278000
H	10.556021000	-4.907835000	11.515310000
Cl	11.306603000	-3.352726000	13.150029000
H	12.296816000	-2.462688000	9.136468000
Cl	12.648640000	-4.772558000	9.534842000
C	10.385620000	1.175605000	7.401980000
C	10.995863000	0.004733000	6.949881000
C	10.568612000	-1.233245000	7.430789000
C	9.537088000	-1.312998000	8.376263000
C	8.927369000	-0.132798000	8.833898000
C	9.352537000	1.102924000	8.333290000
C	9.003841000	-2.683309000	8.710144000
O	7.975651000	-1.107931000	10.759432000
C	7.843350000	-0.106375000	9.868339000
O	6.986474000	0.749156000	9.907889000
O	7.987196000	-3.112397000	8.228337000
H	10.713125000	2.142683000	7.030874000
H	11.796269000	0.050785000	6.216286000
H	11.015403000	-2.147811000	7.049312000
H	8.861765000	1.998709000	8.698742000
C	7.299665000	-0.102032000	12.997795000
C	7.036726000	-1.131661000	11.878421000
O	6.366792000	-0.388250000	14.012967000
H	7.075356000	0.898651000	12.607414000
H	7.132969000	-2.146176000	12.272205000
H	6.025814000	-0.983943000	11.495512000
C	8.745274000	-0.068551000	13.517905000
H	8.775394000	0.487593000	14.450069000
H	9.177387000	-1.060728000	13.657345000
Cl	9.911620000	0.801589000	12.392179000

O	7.782673000	-0.941584000	16.125698000
C	8.650148000	-2.073496000	16.259346000
C	9.851599000	-1.637263000	17.081173000
C	7.903759000	-3.244537000	16.903023000
O	8.360622000	-3.954478000	17.770460000
O	6.663829000	-3.448264000	16.418933000
C	6.256075000	-2.626916000	15.276009000
C	4.822978000	-2.998271000	14.975505000
C	6.470830000	-1.145212000	15.651395000
O	5.578767000	-0.494478000	16.239111000
H	10.367588000	-0.815559000	16.576526000
H	10.540917000	-2.475469000	17.210090000
H	9.526820000	-1.298233000	18.068597000
H	6.910756000	-2.890385000	14.438504000
H	4.185630000	-2.729455000	15.820116000
H	4.750270000	-4.075164000	14.790122000
H	4.476677000	-2.447638000	14.100509000
H	8.994959000	-2.414694000	15.268134000
C	0.065994000	6.106059000	12.993771000
C	0.576243000	7.449821000	12.420345000
H	1.118330000	7.308452000	11.479332000
H	-0.261106000	8.133517000	12.224629000
H	1.258955000	7.938231000	13.125569000
C	-0.702802000	6.407667000	14.294034000
H	-1.122948000	5.496905000	14.736022000
H	-0.059507000	6.883230000	15.043441000
H	-1.535070000	7.091804000	14.086859000
C	-0.928181000	5.473506000	11.989930000
H	-1.776008000	6.146669000	11.802805000
H	-0.451078000	5.261915000	11.027248000
H	-1.321620000	4.527283000	12.378767000
118			
<b>11<sup>LA</sup></b>	<b>E = -4104.9415676</b>		
Al	4.893663000	2.039135000	13.998315000
O	4.249829000	3.916494000	13.542397000

N	3.987012000	2.461772000	15.843608000
C	6.761718000	2.755412000	13.821409000
C	3.546974000	1.263705000	12.716875000
C	3.057033000	4.365630000	13.711847000
C	2.265106000	3.915789000	14.820842000
C	2.865975000	3.127958000	15.858110000
C	2.476273000	5.373061000	12.845977000
C	1.173143000	5.771479000	13.092104000
C	0.365189000	5.302841000	14.164983000
C	0.951325000	4.397422000	15.027042000
C	3.303501000	5.961543000	11.686387000
C	4.581402000	6.630324000	12.250821000
C	3.703224000	4.843260000	10.693839000
C	2.527783000	7.033176000	10.894747000
C	4.430668000	2.008539000	17.186937000
C	3.930309000	0.601823000	17.554660000
C	4.324920000	0.256246000	19.001515000
C	5.835822000	0.408663000	19.243073000
C	6.350913000	1.787145000	18.799430000
C	5.953988000	2.109365000	17.348771000
H	7.533043000	2.113174000	14.264768000
H	7.029174000	2.919660000	12.764810000
H	6.843355000	3.742714000	14.297752000
H	3.083070000	1.993689000	12.041386000
H	4.004570000	0.483722000	12.096224000
H	2.722884000	0.775302000	13.261258000
H	2.319962000	3.157361000	16.810894000
H	0.730595000	6.503197000	12.424201000
H	0.412067000	4.024827000	15.894501000
H	5.187413000	7.040200000	11.431333000
H	4.320134000	7.457452000	12.923501000
H	5.182866000	5.907151000	12.803719000
H	4.309830000	5.260722000	9.878393000
H	4.278052000	4.065346000	11.197017000
H	2.811790000	4.382570000	10.250268000

H	2.231502000	7.880226000	11.525958000
H	3.167645000	7.425615000	10.095016000
H	1.625282000	6.625858000	10.422541000
H	3.989567000	2.706987000	17.917957000
H	4.352394000	-0.119366000	16.850333000
H	2.837518000	0.563622000	17.444306000
H	3.779062000	0.918507000	19.692851000
H	4.013216000	-0.769305000	19.235869000
H	6.363396000	-0.377715000	18.691397000
H	6.062783000	0.245233000	20.305967000
H	7.442968000	1.835461000	18.906954000
H	5.940849000	2.561664000	19.467215000
H	6.431755000	1.412241000	16.652710000
H	6.286839000	3.117887000	17.075065000
C	12.025837000	-2.817003000	11.798146000
C	13.391713000	-2.559272000	11.173876000
O	11.630786000	-4.200423000	11.692192000
H	11.306097000	-2.172668000	11.280705000
H	13.691865000	-1.527964000	11.362128000
C	11.951137000	-2.559061000	13.305694000
H	10.938836000	-2.755936000	13.657467000
H	12.655864000	-3.197545000	13.838847000
Cl	12.343872000	-0.843919000	13.726348000
H	13.361173000	-2.739088000	10.100305000
Cl	14.702137000	-3.624502000	11.841364000
C	10.613350000	-3.077271000	6.755770000
C	11.738528000	-3.751960000	7.231206000
C	11.778489000	-4.194305000	8.553847000
C	10.700740000	-3.959407000	9.418194000
C	9.569661000	-3.276261000	8.937785000
C	9.534623000	-2.847695000	7.606026000
C	10.733339000	-4.640311000	10.763868000
O	8.705500000	-2.814285000	11.083394000
C	8.378010000	-2.949829000	9.781823000
O	7.262858000	-2.790590000	9.332803000

O	10.096846000	-5.638429000	10.987506000
H	10.575557000	-2.731449000	5.726731000
H	12.581734000	-3.944625000	6.573475000
H	12.638441000	-4.753073000	8.913764000
H	8.647613000	-2.327915000	7.259796000
C	7.323780000	-0.935266000	11.959541000
C	7.636322000	-2.442368000	11.993654000
O	6.180195000	-0.623125000	12.741560000
H	6.994981000	-0.697496000	10.943794000
H	8.004799000	-2.753821000	12.970232000
H	6.738471000	-3.003814000	11.728821000
C	8.522922000	-0.025106000	12.278983000
H	8.163533000	0.955364000	12.580628000
H	9.189382000	-0.421008000	13.041244000
Cl	9.570343000	0.269109000	10.791673000
O	7.429972000	-0.902564000	14.709146000
C	7.721293000	-1.927530000	15.649868000
C	8.894916000	-1.468779000	16.506141000
C	6.521397000	-2.344365000	16.508225000
O	6.608776000	-2.642004000	17.680785000
O	5.343414000	-2.423486000	15.868626000
C	5.338166000	-2.133976000	14.439824000
C	3.889266000	-2.153921000	14.000666000
C	6.051597000	-0.772866000	14.194467000
O	5.414322000	0.236996000	14.712935000
H	9.747970000	-1.224608000	15.865149000
H	9.181767000	-2.251524000	17.212885000
H	8.619343000	-0.572576000	17.068656000
H	5.893955000	-2.941775000	13.948060000
H	3.341144000	-1.352706000	14.499349000
H	3.434304000	-3.119507000	14.246617000
H	3.829093000	-1.988759000	12.922409000
H	8.016959000	-2.854293000	15.115117000
C	-1.072018000	5.826964000	14.322492000
C	-1.058756000	7.364030000	14.503538000

H	-0.592446000	7.868942000	13.650846000
H	-2.080906000	7.753756000	14.604299000
H	-0.496326000	7.643549000	15.402047000
C	-1.783632000	5.213262000	15.543109000
H	-1.848946000	4.121977000	15.466243000
H	-1.266680000	5.457350000	16.478443000
H	-2.805877000	5.604614000	15.616494000
C	-1.898902000	5.473205000	13.062919000
H	-2.926772000	5.850673000	13.152100000
H	-1.461471000	5.906428000	12.157108000
H	-1.943819000	4.387280000	12.921692000

118

**12<sup>LA</sup>** E = -4104.9618338

Al	6.649086000	1.391170000	14.273933000
O	4.990898000	2.407936000	13.652922000
N	5.918883000	1.844688000	16.212203000
C	7.672654000	2.831693000	13.319779000
C	5.756215000	-0.336136000	13.760470000
C	3.791230000	2.363108000	14.105562000
C	3.549618000	2.069846000	15.488148000
C	4.634009000	1.947337000	16.417431000
C	2.637497000	2.645843000	13.272436000
C	1.381808000	2.570793000	13.849818000
C	1.128694000	2.263236000	15.215802000
C	2.234502000	2.036417000	16.010277000
C	2.833021000	3.003969000	11.786777000
C	3.702964000	4.279681000	11.667163000
C	3.527658000	1.832936000	11.049918000
C	1.497874000	3.281502000	11.067617000
C	6.721805000	1.902237000	17.457640000
C	7.114267000	0.506603000	17.974342000
C	7.857402000	0.624172000	19.315991000
C	9.077925000	1.552984000	19.216022000
C	8.698511000	2.928594000	18.643021000
C	7.949044000	2.811802000	17.304229000

H	7.440103000	2.824486000	12.242867000
H	7.360832000	3.826325000	13.673273000
H	8.762573000	2.776597000	13.420731000
H	5.954442000	-0.592682000	12.708520000
H	6.130037000	-1.171968000	14.365098000
H	4.663550000	-0.314619000	13.874085000
H	4.309079000	1.986643000	17.465915000
H	0.519985000	2.764305000	13.219460000
H	2.122844000	1.820446000	17.070061000
H	3.858315000	4.533408000	10.609619000
H	3.206338000	5.132052000	12.148659000
H	4.675514000	4.130747000	12.138465000
H	3.690889000	2.093619000	9.995123000
H	4.489896000	1.602258000	11.508126000
H	2.903692000	0.931087000	11.083119000
H	0.954519000	4.123347000	11.514699000
H	1.697972000	3.537470000	10.020027000
H	0.836379000	2.406352000	11.071337000
H	6.084824000	2.361722000	18.233091000
H	7.732098000	0.010426000	17.220558000
H	6.205256000	-0.097268000	18.099891000
H	7.169559000	1.017531000	20.081744000
H	8.167400000	-0.371284000	19.660983000
H	9.828530000	1.086787000	18.566007000
H	9.546412000	1.671223000	20.203247000
H	9.597473000	3.546106000	18.514783000
H	8.062024000	3.456687000	19.370816000
H	8.598995000	2.396288000	16.529070000
H	7.627438000	3.803367000	16.961598000
O	8.809847000	-0.565147000	13.092370000
C	9.826854000	-0.337294000	12.122266000
C	9.148095000	-0.174583000	10.769336000
C	10.717776000	0.863278000	12.453745000
O	11.167811000	1.621327000	11.624481000
O	11.027211000	1.003915000	13.757064000

C	10.610938000	-0.061195000	14.654633000
C	11.029139000	0.365581000	16.044796000
C	9.087678000	-0.331156000	14.503826000
O	8.311697000	0.569767000	15.035182000
H	8.545883000	-1.061885000	10.551841000
H	9.896713000	-0.039165000	9.984477000
H	8.493816000	0.700777000	10.786556000
H	11.164801000	-0.964087000	14.368274000
H	10.537400000	1.303777000	16.306316000
H	12.114465000	0.506727000	16.085066000
H	10.743670000	-0.404894000	16.765004000
H	10.507157000	-1.210788000	12.078127000
C	-0.319609000	2.212189000	15.730300000
C	-0.391569000	1.871289000	17.230839000
H	0.054104000	0.893179000	17.444899000
H	0.125091000	2.620792000	17.841554000
H	-1.438267000	1.839820000	17.557972000
C	-1.112827000	1.129906000	14.958932000
H	-2.154559000	1.088136000	15.305452000
H	-1.127089000	1.329259000	13.882096000
H	-0.662945000	0.141429000	15.106355000
C	-1.003565000	3.584889000	15.521880000
H	-1.014395000	3.876208000	14.466188000
H	-2.044503000	3.559563000	15.872195000
H	-0.475196000	4.369208000	16.076342000
O	8.842069000	-1.628344000	15.195843000
C	9.172058000	-2.840888000	14.558890000
C	9.670671000	-3.825639000	15.615162000
H	9.103689000	-3.693828000	16.537769000
H	9.604687000	-4.857148000	15.271094000
H	9.940465000	-2.712391000	13.787032000
Cl	11.428440000	-3.569563000	16.060207000
C	7.929963000	-3.433809000	13.874411000
H	7.210441000	-3.841236000	14.588958000
H	7.441999000	-2.668219000	13.271846000

C	12.388423000	-6.820861000	13.887896000
C	13.663887000	-6.106568000	13.475961000
O	11.520300000	-6.848991000	12.732751000
H	11.919270000	-6.219422000	14.673324000
H	14.329570000	-6.008502000	14.333225000
C	12.554349000	-8.260120000	14.376739000
H	11.579299000	-8.672571000	14.633601000
H	13.044273000	-8.876167000	13.622345000
Cl	13.567536000	-8.336853000	15.877119000
H	13.423335000	-5.119963000	13.079839000
Cl	14.597015000	-6.977647000	12.181621000
C	7.836788000	-7.415460000	9.424787000
C	9.122821000	-7.948806000	9.508380000
C	9.897321000	-7.714648000	10.643322000
C	9.398413000	-6.941308000	11.699933000
C	8.112944000	-6.371058000	11.600068000
C	7.339086000	-6.632188000	10.465731000
C	10.180383000	-6.855946000	12.967463000
O	8.402595000	-4.497758000	12.997896000
C	7.512851000	-5.419357000	12.602073000
O	6.342003000	-5.445883000	12.916245000
O	9.698519000	-6.850854000	14.081310000
H	7.222861000	-7.600534000	8.547638000
H	9.521203000	-8.552999000	8.698124000
H	10.890384000	-8.142498000	10.726813000
H	6.346121000	-6.198247000	10.409604000

118

**13TS<sup>LA</sup>** E = -4104.931143, Imaginary frequency = 169.94i

Al	6.714786000	1.165514000	14.952011000
O	5.242056000	1.658946000	13.863256000
N	5.575705000	1.801506000	16.746926000
C	7.691981000	2.906516000	14.853784000
C	6.158932000	-0.731237000	15.274003000
C	3.988885000	1.921762000	14.106527000
C	3.501612000	2.148502000	15.434675000

C	4.329134000	2.103054000	16.628137000
C	3.038784000	2.019067000	13.024119000
C	1.715391000	2.313568000	13.327169000
C	1.217527000	2.536736000	14.631009000
C	2.140490000	2.450439000	15.658038000
C	3.491755000	1.807975000	11.564209000
C	4.538608000	2.883426000	11.184775000
C	4.092526000	0.391520000	11.392153000
C	2.327434000	1.931408000	10.559418000
C	6.129792000	1.807071000	18.110601000
C	6.542837000	0.385429000	18.542110000
C	7.111296000	0.385497000	19.970139000
C	8.293998000	1.356831000	20.099797000
C	7.889417000	2.772216000	19.661332000
C	7.321569000	2.774624000	18.232991000
H	7.854134000	3.207644000	13.809672000
H	7.093063000	3.707868000	15.309717000
H	8.675583000	2.910500000	15.334351000
H	6.101085000	-1.240659000	14.300627000
H	6.845581000	-1.306322000	15.902954000
H	5.158407000	-0.791808000	15.725920000
H	3.777544000	2.359063000	17.545893000
H	1.009171000	2.379533000	12.506984000
H	1.833851000	2.614351000	16.687694000
H	4.900918000	2.718674000	10.161224000
H	4.091616000	3.884767000	11.227440000
H	5.390913000	2.859155000	11.863837000
H	4.435047000	0.249515000	10.358222000
H	4.936153000	0.236240000	12.064494000
H	3.335726000	-0.374204000	11.604820000
H	1.863823000	2.925243000	10.580554000
H	2.711235000	1.770630000	9.544760000
H	1.545003000	1.183450000	10.737520000
H	5.340548000	2.154269000	18.803475000
H	7.300427000	0.011332000	17.846086000

H	5.675274000	-0.282301000	18.472193000
H	6.324794000	0.674043000	20.686067000
H	7.421792000	-0.631872000	20.242396000
H	9.114352000	1.005542000	19.459140000
H	8.671169000	1.367806000	21.132111000
H	8.751614000	3.450010000	19.715670000
H	7.137151000	3.167921000	20.362595000
H	8.099780000	2.468255000	17.527931000
H	7.004629000	3.784694000	17.945710000
O	8.426477000	0.172782000	13.789389000
C	9.089371000	0.656341000	12.651342000
C	8.121949000	1.096893000	11.553847000
C	10.081130000	1.773648000	12.998662000
O	10.238197000	2.797174000	12.372834000
O	10.848129000	1.553274000	14.103961000
C	10.898305000	0.232246000	14.667765000
C	11.978023000	0.286955000	15.744024000
C	9.560908000	-0.199460000	15.302694000
O	9.092665000	0.414990000	16.256649000
H	7.468645000	0.258639000	11.292798000
H	8.668878000	1.419876000	10.662152000
H	7.502354000	1.928053000	11.895983000
H	11.191000000	-0.465444000	13.875732000
H	11.676462000	1.004941000	16.510928000
H	12.933132000	0.597869000	15.309155000
H	12.099761000	-0.692612000	16.218331000
H	9.719038000	-0.148889000	12.211724000
C	-0.272042000	2.855839000	14.843321000
C	-0.615603000	3.067076000	16.330082000
H	-0.400673000	2.172881000	16.926362000
H	-0.055076000	3.905047000	16.760291000
H	-1.684014000	3.290809000	16.438762000
C	-1.139540000	1.687772000	14.316030000
H	-2.208166000	1.904720000	14.449151000
H	-0.966535000	1.504440000	13.250220000

H	-0.909235000	0.760483000	14.853157000
C	-0.647008000	4.148913000	14.080183000
H	-0.456524000	4.054541000	13.005799000
H	-1.711894000	4.384388000	14.211712000
H	-0.060888000	4.999513000	14.446884000
O	9.445611000	-1.621500000	15.402203000
C	9.532016000	-2.469289000	14.264837000
C	10.919652000	-3.151224000	14.215898000
H	11.640949000	-2.587014000	14.804470000
H	10.885787000	-4.184531000	14.563486000
H	9.339273000	-1.904041000	13.352932000
Cl	11.620561000	-3.234078000	12.523269000
C	8.418259000	-3.495730000	14.468471000
H	8.549462000	-4.026679000	15.415702000
H	7.444779000	-3.004924000	14.470592000
C	12.672349000	-6.863604000	12.371769000
C	13.644490000	-6.377115000	11.310825000
O	11.381592000	-6.985139000	11.744008000
H	12.616510000	-6.088362000	13.141882000
H	14.628449000	-6.213487000	11.750062000
C	13.008039000	-8.205502000	13.023222000
H	12.238955000	-8.460887000	13.750965000
H	13.106422000	-8.993082000	12.275891000
Cl	14.577988000	-8.121452000	13.928132000
H	13.272841000	-5.451405000	10.872280000
Cl	13.872160000	-7.553638000	9.942666000
C	6.612558000	-7.459989000	10.435221000
C	7.810995000	-7.956665000	9.921866000
C	9.007441000	-7.703457000	10.588506000
C	9.021810000	-6.942401000	11.766492000
C	7.814524000	-6.416015000	12.268270000
C	6.618028000	-6.699046000	11.603468000
C	10.289725000	-6.795932000	12.536046000
O	8.487510000	-4.444922000	13.373652000
C	7.704420000	-5.526361000	13.479444000

O	6.919756000	-5.736999000	14.379468000
O	10.366117000	-6.584456000	13.729064000
H	5.673531000	-7.660573000	9.926605000
H	7.815372000	-8.547751000	9.010349000
H	9.940860000	-8.103154000	10.208979000
H	5.692678000	-6.304197000	12.010500000

118

**14<sup>LA</sup>** E = -4104.9599631

Al	8.010209000	1.170823000	15.532689000
O	6.589101000	1.246517000	14.332035000
N	5.484589000	2.359553000	16.875489000
C	8.601992000	2.991828000	16.103657000
C	7.614577000	-0.277360000	16.851621000
C	5.358886000	0.817073000	14.164614000
C	4.335274000	0.997057000	15.151340000
C	4.463206000	1.761602000	16.394813000
C	4.969701000	0.187809000	12.924191000
C	3.667907000	-0.288169000	12.788449000
C	2.667871000	-0.169541000	13.772305000
C	3.037188000	0.491544000	14.931390000
C	5.950916000	0.088558000	11.734252000
C	6.348991000	1.520168000	11.300039000
C	7.206111000	-0.732807000	12.110223000
C	5.324048000	-0.597102000	10.500747000
C	5.275210000	3.112607000	18.105343000
C	6.139499000	2.547772000	19.248919000
C	5.995370000	3.377856000	20.534261000
C	6.315519000	4.860236000	20.289202000
C	5.452827000	5.430194000	19.152983000
C	5.597040000	4.601392000	17.867219000
H	9.648122000	3.226361000	15.873359000
H	7.981293000	3.772635000	15.642355000
H	8.487602000	3.108279000	17.190104000
H	7.000269000	-1.073330000	16.402010000
H	8.525319000	-0.741449000	17.253479000

H	7.043473000	0.097543000	17.709483000
H	3.502401000	1.825736000	16.942285000
H	3.398458000	-0.775567000	11.858732000
H	2.308987000	0.655966000	15.720821000
H	7.090021000	1.484520000	10.489675000
H	5.470994000	2.063317000	10.927687000
H	6.769750000	2.079557000	12.135912000
H	7.874139000	-0.804760000	11.238178000
H	7.765635000	-0.284265000	12.930582000
H	6.924563000	-1.752605000	12.401161000
H	4.443039000	-0.061269000	10.127344000
H	6.0614444000	-0.617587000	9.689152000
H	5.035825000	-1.635386000	10.705352000
H	4.213351000	3.045202000	18.424668000
H	7.186708000	2.536048000	18.924891000
H	5.857794000	1.503739000	19.433476000
H	4.965198000	3.291482000	20.914036000
H	6.649613000	2.970800000	21.316641000
H	7.376926000	4.959215000	20.019434000
H	6.168558000	5.441169000	21.210405000
H	5.723634000	6.476446000	18.956585000
H	4.398482000	5.436345000	19.471216000
H	6.621135000	4.676282000	17.482827000
H	4.935887000	4.990461000	17.082107000
O	9.382508000	0.448741000	14.509107000
C	10.324340000	1.108643000	13.713851000
C	9.781668000	2.262148000	12.864934000
C	11.512670000	1.613876000	14.562956000
O	11.889088000	2.761905000	14.604948000
O	12.198808000	0.707848000	15.330884000
C	12.064113000	-0.701114000	15.166351000
C	13.488979000	-1.273429000	15.195008000
C	11.291873000	-1.309048000	16.335444000
O	11.337041000	-0.884014000	17.457755000
H	8.992038000	1.885631000	12.211942000

H	10.577555000	2.693419000	12.247428000
H	9.374112000	3.055882000	13.494396000
H	11.588349000	-0.943627000	14.220096000
H	13.979706000	-0.974118000	16.125766000
H	14.058936000	-0.876415000	14.349704000
H	13.477245000	-2.365170000	15.128057000
H	10.753136000	0.378988000	12.996831000
C	1.254417000	-0.719905000	13.515871000
C	0.307739000	-0.475453000	14.706427000
H	0.674836000	-0.955611000	15.620701000
H	0.183447000	0.593827000	14.912107000
H	-0.684338000	-0.889440000	14.486776000
C	1.322635000	-2.245166000	13.268883000
H	0.323003000	-2.653264000	13.064060000
H	1.966834000	-2.487285000	12.417236000
H	1.730327000	-2.759364000	14.146953000
C	0.640054000	-0.034500000	12.271713000
H	1.248513000	-0.200813000	11.376466000
H	-0.367545000	-0.422987000	12.069283000
H	0.564634000	1.048324000	12.424137000
O	10.720479000	-2.544492000	16.113743000
C	9.954015000	-2.893367000	14.943461000
C	10.689915000	-3.931810000	14.096091000
H	11.364277000	-4.511635000	14.728684000
H	9.984907000	-4.594886000	13.598427000
H	9.672076000	-1.995479000	14.384728000
Cl	11.713691000	-3.247514000	12.744348000
C	8.701529000	-3.547453000	15.544787000
H	8.959776000	-4.454390000	16.096406000
H	8.211609000	-2.842058000	16.217376000
C	9.092920000	-4.503719000	9.944957000
C	9.173603000	-3.276274000	9.053148000
O	7.770763000	-4.514126000	10.528127000
H	9.832395000	-4.378644000	10.742993000
H	10.181863000	-3.170474000	8.653142000

C	9.311587000	-5.850699000	9.255197000
H	9.217790000	-6.654214000	9.984459000
H	8.606063000	-5.990491000	8.436007000
Cl	10.979791000	-5.969783000	8.555771000
H	8.901856000	-2.388947000	9.625532000
Cl	8.047689000	-3.342126000	7.627932000
C	3.559666000	-5.287718000	13.060334000
C	3.858218000	-5.249651000	11.698693000
C	5.183275000	-5.133089000	11.283955000
C	6.221045000	-5.049008000	12.222408000
C	5.916846000	-5.049420000	13.599355000
C	4.584199000	-5.186070000	14.000080000
C	7.630377000	-5.104939000	11.741526000
O	7.791186000	-3.877714000	14.467948000
C	6.908276000	-4.863398000	14.715246000
O	6.840387000	-5.481095000	15.757413000
O	8.541836000	-5.658392000	12.324456000
H	2.530310000	-5.382767000	13.392924000
H	3.064881000	-5.317390000	10.959818000
H	5.427956000	-5.123109000	10.227727000
H	4.364470000	-5.196056000	15.062247000

118

**15<sup>LA</sup>** E = -4104.9743403

Al	7.826076000	1.782459000	13.612088000
O	6.045869000	2.210941000	13.301961000
N	6.671218000	4.071779000	15.513459000
C	8.983178000	3.336470000	13.101911000
C	8.016098000	0.857211000	15.369648000
C	4.839907000	2.242455000	13.803722000
C	4.535382000	2.916671000	15.031952000
C	5.461813000	3.761535000	15.787558000
C	3.737566000	1.633117000	13.095722000
C	2.480239000	1.628155000	13.693282000
C	2.184691000	2.210013000	14.942189000
C	3.233427000	2.861020000	15.570602000

C	3.934392000	0.990034000	11.703196000
C	4.560451000	2.015306000	10.726598000
C	4.838659000	-0.260681000	11.808376000
C	2.599432000	0.535303000	11.072819000
C	7.326322000	5.010829000	16.409982000
C	8.558848000	4.362118000	17.069324000
C	9.331312000	5.360743000	17.945364000
C	9.735031000	6.613893000	17.153677000
C	8.509785000	7.271050000	16.500251000
C	7.735791000	6.273407000	15.624842000
H	9.920301000	3.022911000	12.619887000
H	8.466886000	4.015858000	12.406990000
H	9.265476000	3.942054000	13.972706000
H	7.410467000	-0.061386000	15.393968000
H	9.058469000	0.543188000	15.530184000
H	7.718715000	1.463490000	16.234231000
H	4.988663000	4.198647000	16.689761000
H	1.666812000	1.144536000	13.164495000
H	3.072196000	3.371886000	16.516380000
H	4.714062000	1.551781000	9.742262000
H	3.893800000	2.877220000	10.591215000
H	5.519136000	2.374291000	11.100031000
H	4.914340000	-0.749604000	10.825957000
H	5.847709000	-0.010569000	12.140162000
H	4.404520000	-0.986827000	12.508046000
H	1.885215000	1.361686000	10.968505000
H	2.796592000	0.139313000	10.069177000
H	2.117237000	-0.264871000	11.647656000
H	6.636572000	5.327257000	17.222039000
H	9.210410000	3.969519000	16.279526000
H	8.237861000	3.497768000	17.663037000
H	8.704499000	5.663392000	18.798928000
H	10.220510000	4.876003000	18.370510000
H	10.451042000	6.328260000	16.369212000
H	10.252018000	7.330917000	17.806896000

H	8.816732000	8.138603000	15.900063000
H	7.847226000	7.658634000	17.289971000
H	8.351700000	5.962111000	14.771862000
H	6.836356000	6.744019000	15.207259000
O	8.030521000	0.460941000	12.379384000
C	8.780368000	0.221028000	11.267572000
C	8.654188000	1.295493000	10.158025000
C	10.270325000	0.023196000	11.596224000
O	10.847361000	0.284904000	12.624361000
O	10.930502000	-0.536483000	10.512963000
C	12.326172000	-0.743652000	10.676759000
C	12.605010000	-2.178352000	11.141009000
C	12.991384000	-0.427822000	9.344360000
O	12.455252000	-0.147631000	8.302346000
H	7.597879000	1.383806000	9.886890000
H	9.232860000	1.026455000	9.267138000
H	8.991071000	2.268033000	10.528436000
H	12.709442000	-0.044677000	11.428768000
H	12.187142000	-2.898407000	10.429714000
H	12.127360000	-2.326618000	12.113031000
H	13.679456000	-2.355621000	11.244058000
H	8.480551000	-0.740315000	10.805163000
C	0.762004000	2.120900000	15.520400000
C	0.644685000	2.817062000	16.889669000
H	1.319682000	2.370650000	17.628753000
H	0.876704000	3.886180000	16.821713000
H	-0.379602000	2.722222000	17.271765000
C	0.365093000	0.636791000	15.706913000
H	-0.654474000	0.551542000	16.107994000
H	0.399291000	0.088260000	14.759659000
H	1.049638000	0.137704000	16.402418000
C	-0.244126000	2.795125000	14.556990000
H	-0.234651000	2.323819000	13.568483000
H	-1.267960000	2.728154000	14.950497000
H	0.001170000	3.854865000	14.420683000

O	14.355173000	-0.503716000	9.490381000
C	15.146917000	-0.269413000	8.306311000
C	15.369462000	1.244886000	8.213956000
H	14.418014000	1.755898000	8.355872000
H	16.093576000	1.588658000	8.954858000
H	14.596834000	-0.611887000	7.426392000
Cl	15.972743000	1.776684000	6.584859000
C	16.391473000	-1.120087000	8.544532000
H	16.963531000	-0.752100000	9.402768000
H	16.096338000	-2.152902000	8.746608000
C	19.601966000	3.129980000	6.784143000
C	19.080848000	4.216317000	5.858332000
O	19.693055000	1.916404000	6.009601000
H	18.859121000	2.983998000	7.574545000
H	18.950582000	5.147136000	6.410355000
C	20.969100000	3.391717000	7.417363000
H	21.254075000	2.542641000	8.037340000
H	21.726031000	3.581256000	6.655974000
Cl	20.916877000	4.840934000	8.503382000
H	18.130608000	3.905663000	5.424136000
Cl	20.198338000	4.579480000	4.472671000
C	20.135191000	-2.694155000	4.189807000
C	20.619498000	-1.448860000	3.789095000
C	20.386068000	-0.324811000	4.579498000
C	19.655811000	-0.431030000	5.770546000
C	19.139619000	-1.684265000	6.156907000
C	19.402383000	-2.808676000	5.371022000
C	19.535077000	0.745255000	6.680828000
O	17.217500000	-1.067751000	7.371336000
C	18.283845000	-1.892000000	7.373285000
O	18.483115000	-2.754005000	8.200805000
O	19.363947000	0.682398000	7.880873000
H	20.323943000	-3.576037000	3.584050000
H	21.188127000	-1.352013000	2.868670000
H	20.779360000	0.642195000	4.287279000

H	19.016445000	-3.771190000	5.691591000
111			
<b>15TS<sup>LA</sup></b> E = -3453.5935799, Imaginary frequency =216.80i			
Al	7.473937000	2.070251000	15.133183000
O	6.070988000	1.896166000	13.876314000
N	4.899894000	2.584258000	16.602070000
C	7.633514000	3.922693000	15.844776000
C	7.273504000	0.312448000	16.064082000
C	4.979063000	1.166244000	13.783055000
C	3.986981000	1.107082000	14.820795000
C	3.995337000	1.843159000	16.086996000
C	4.693747000	0.413088000	12.580172000
C	3.545994000	-0.372989000	12.524782000
C	2.593214000	-0.475617000	13.554097000
C	2.840917000	0.295309000	14.674923000
C	5.605550000	0.490650000	11.336324000
C	5.592047000	1.943038000	10.805464000
C	7.042763000	0.035368000	11.676459000
C	5.123337000	-0.413056000	10.179321000
C	4.590426000	3.155008000	17.907556000
C	5.586146000	2.641752000	18.966184000
C	5.320726000	3.264931000	20.345636000
C	5.326923000	4.800098000	20.283095000
C	4.332383000	5.314693000	19.230913000
C	4.601697000	4.694851000	17.850492000
H	8.580741000	4.396953000	15.566777000
H	6.799952000	4.561332000	15.524753000
H	7.608773000	3.891432000	16.941604000
H	7.802112000	-0.491138000	15.532224000
H	7.729424000	0.364757000	17.062378000
H	6.232441000	-0.009732000	16.183293000
H	3.055152000	1.693974000	16.652409000
H	3.365406000	-0.946151000	11.623491000
H	2.136846000	0.291850000	15.502366000
H	6.220605000	2.030046000	9.907902000

H	4.571196000	2.228577000	10.519760000
H	5.949167000	2.650928000	11.553690000
H	7.6655583000	0.037793000	10.771119000
H	7.505069000	0.689989000	12.412601000
H	7.032562000	-0.988415000	12.072104000
H	4.124004000	-0.138250000	9.821136000
H	5.813586000	-0.302832000	9.334105000
H	5.110578000	-1.474533000	10.456132000
H	3.574245000	2.844276000	18.231016000
H	6.604293000	2.879612000	18.636187000
H	5.524151000	1.547927000	19.017550000
H	4.342169000	2.925666000	20.719936000
H	6.068648000	2.909936000	21.067256000
H	6.337956000	5.145176000	20.021493000
H	5.094441000	5.224809000	21.269692000
H	4.378785000	6.410407000	19.166437000
H	3.309125000	5.065694000	19.552877000
H	5.577085000	5.024292000	17.474687000
H	3.851599000	5.033195000	17.123823000
C	5.673425000	8.510030000	11.148226000
C	6.204487000	9.914866000	10.885009000
O	6.247210000	7.939036000	12.336287000
H	5.971161000	7.901379000	10.287064000
H	5.742318000	10.328160000	9.987583000
C	4.167856000	8.398303000	11.371903000
H	3.903430000	7.361534000	11.579778000
H	3.838307000	9.038738000	12.190392000
Cl	3.249592000	8.902738000	9.890174000
H	7.286049000	9.879575000	10.763030000
Cl	5.861071000	11.079008000	12.237414000
O	8.960966000	2.400723000	13.508781000
C	9.201897000	3.439093000	12.578727000
C	9.197534000	2.951681000	11.125389000
C	8.213901000	4.605579000	12.713286000
O	7.072577000	4.644657000	12.309014000

O	8.805108000	5.681410000	13.304428000
C	7.932637000	6.789193000	13.540141000
C	8.716743000	7.810108000	14.359962000
C	7.485172000	7.387491000	12.208911000
O	8.143392000	7.439908000	11.196280000
H	9.911412000	2.129745000	11.006951000
H	9.488188000	3.763529000	10.445792000
H	8.207887000	2.598186000	10.838430000
H	7.050185000	6.443542000	14.082516000
H	9.607629000	8.134918000	13.813317000
H	9.025123000	7.349969000	15.302594000
H	8.091945000	8.682767000	14.576152000
H	10.177412000	3.877390000	12.809625000
O	11.065674000	3.171906000	14.724449000
C	12.357336000	3.208510000	14.107559000
C	13.067139000	4.452844000	14.614354000
C	13.134703000	1.925784000	14.414745000
O	14.306915000	1.893743000	14.716932000
O	12.411747000	0.795261000	14.312288000
C	11.046780000	0.922740000	13.792654000
C	10.421863000	-0.451046000	13.882925000
C	10.304687000	1.988045000	14.631281000
O	9.654579000	1.666690000	15.643361000
H	12.476814000	5.338172000	14.360659000
H	14.059946000	4.531994000	14.163991000
H	13.180480000	4.402351000	15.700641000
H	11.127440000	1.248093000	12.750439000
H	10.321408000	-0.742166000	14.930524000
H	11.042542000	-1.180727000	13.352568000
H	9.426703000	-0.431402000	13.433719000
H	12.256361000	3.268027000	13.009858000
C	1.364921000	-1.386198000	13.390090000
C	0.450372000	-1.359337000	14.629514000
H	0.978387000	-1.696694000	15.528723000
H	0.059862000	-0.353587000	14.823196000

H	-0.407692000	-2.025718000	14.476093000
C	0.528415000	-0.928872000	12.171032000
H	1.114238000	-0.955723000	11.246005000
H	-0.347115000	-1.577993000	12.032091000
H	0.173425000	0.099203000	12.308302000
C	1.823326000	-2.847557000	13.168633000
H	2.456371000	-2.941601000	12.279865000
H	2.403098000	-3.206011000	14.026969000
H	0.958637000	-3.512466000	13.036575000

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**16<sup>LA</sup>** E = -3453.6390667

Al	7.486377000	1.886500000	15.514564000
O	6.063784000	1.542421000	14.405537000
N	4.963027000	2.109304000	17.091208000
C	7.531561000	3.839417000	15.938233000
C	7.806548000	0.423698000	16.833975000
C	4.927747000	0.913694000	14.236685000
C	3.986893000	0.715398000	15.297224000
C	4.078507000	1.307933000	16.631746000
C	4.565984000	0.426242000	12.928647000
C	3.388245000	-0.302479000	12.790669000
C	2.491702000	-0.580457000	13.842133000
C	2.816292000	-0.039827000	15.075147000
C	5.460785000	0.705044000	11.700374000
C	5.656498000	2.230449000	11.522567000
C	6.831366000	0.010112000	11.869613000
C	4.840326000	0.176280000	10.389180000
C	4.744997000	2.627171000	18.434702000
C	5.949585000	2.319536000	19.343405000
C	5.776877000	2.928870000	20.743505000
C	5.522554000	4.442313000	20.675221000
C	4.322246000	4.759409000	19.770441000
C	4.494869000	4.148077000	18.371329000
H	8.239915000	4.366807000	15.289856000
H	6.533607000	4.276375000	15.800658000

H	7.832086000	4.042893000	16.977486000
H	8.302233000	-0.425599000	16.342304000
H	8.483221000	0.746496000	17.640580000
H	6.898026000	0.041560000	17.314646000
H	3.223594000	1.027439000	17.277503000
H	3.138346000	-0.684001000	11.807316000
H	2.151884000	-0.175150000	15.924489000
H	6.299016000	2.436583000	10.657789000
H	4.689995000	2.722607000	11.351157000
H	6.123484000	2.670012000	12.402984000
H	7.448547000	0.180099000	10.976839000
H	7.371786000	0.396294000	12.732694000
H	6.699184000	-1.073557000	11.987015000
H	3.859581000	0.622890000	10.183490000
H	5.501681000	0.434689000	9.553578000
H	4.727380000	-0.915027000	10.390523000
H	3.846735000	2.158998000	18.890166000
H	6.853755000	2.718038000	18.867718000
H	6.088295000	1.234367000	19.409683000
H	4.928518000	2.445620000	21.253058000
H	6.665057000	2.719148000	21.354365000
H	6.417367000	4.939421000	20.272855000
H	5.361274000	4.850724000	21.682649000
H	4.180820000	5.845884000	19.690437000
H	3.407148000	4.360508000	20.235223000
H	5.344210000	4.615740000	17.858260000
H	3.607582000	4.341486000	17.754647000
C	6.372708000	8.912397000	10.125693000
C	6.577039000	10.345116000	10.605239000
O	6.429507000	7.976492000	11.215059000
H	7.195838000	8.697512000	9.435338000
H	6.524850000	11.033619000	9.760909000
C	5.034849000	8.620546000	9.451937000
H	4.979568000	7.564514000	9.188545000
H	4.196925000	8.888438000	10.095610000

Cl	4.858218000	9.569293000	7.914941000
H	7.546605000	10.431540000	11.094150000
Cl	5.326951000	10.887280000	11.805393000
O	9.172145000	2.729178000	12.472459000
C	9.778114000	3.783821000	11.730803000
C	10.212541000	3.311485000	10.345863000
C	8.699649000	4.864732000	11.609394000
O	7.938442000	4.996957000	10.672570000
O	8.662444000	5.659227000	12.702586000
C	7.559927000	6.573573000	12.753369000
C	7.619744000	7.278056000	14.105934000
C	7.670711000	7.582030000	11.612831000
O	8.696517000	8.035907000	11.162412000
H	10.973207000	2.529638000	10.432559000
H	10.630891000	4.141633000	9.764349000
H	9.353159000	2.911133000	9.802212000
H	6.626419000	6.017722000	12.637396000
H	8.562301000	7.825557000	14.204743000
H	7.552264000	6.531594000	14.901917000
H	6.785923000	7.981730000	14.198278000
H	10.613356000	4.210362000	12.293803000
O	10.373889000	3.333259000	14.373534000
C	11.720119000	3.278631000	14.830999000
C	11.856943000	4.253704000	15.991302000
C	12.175378000	1.867391000	15.213069000
O	12.891749000	1.620161000	16.157306000
O	11.775498000	0.890433000	14.377970000
C	10.987754000	1.279470000	13.220343000
C	10.534758000	-0.007622000	12.562088000
C	9.817809000	2.196936000	13.670284000
O	8.923559000	1.538812000	14.369672000
H	11.544544000	5.250688000	15.666919000
H	12.892655000	4.288162000	16.339193000
H	11.217702000	3.938649000	16.820178000
H	11.649468000	1.843214000	12.547672000

H	9.894526000	-0.561024000	13.251845000
H	11.402447000	-0.621093000	12.296594000
H	9.960892000	0.217225000	11.659949000
H	12.400797000	3.595362000	14.015546000
C	1.228998000	-1.419404000	13.580833000
C	0.382939000	-1.611005000	14.853914000
H	0.948670000	-2.120682000	15.642211000
H	0.030947000	-0.653371000	15.254541000
H	-0.500120000	-2.221794000	14.628147000
C	0.342312000	-0.722962000	12.520840000
H	0.876068000	-0.585303000	11.574554000
H	-0.558656000	-1.316780000	12.313991000
H	0.026533000	0.267079000	12.869866000
C	1.630691000	-2.820790000	13.061719000
H	2.213402000	-2.756666000	12.136710000
H	2.243277000	-3.347430000	13.802555000
H	0.740602000	-3.431266000	12.856166000

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**17<sup>LA</sup>** E = -3453.6390792

Al	7.359690000	1.963627000	15.233263000
O	6.053270000	1.187447000	14.202302000
N	4.708901000	2.418886000	16.530858000
C	7.237919000	3.951155000	15.058996000
C	7.674061000	0.984559000	16.943551000
C	4.980591000	0.437248000	14.169088000
C	3.975786000	0.476528000	15.187971000
C	3.921198000	1.441469000	16.286379000
C	4.757357000	-0.4444432000	13.050115000
C	3.647556000	-1.284051000	13.073626000
C	2.692824000	-1.319040000	14.109939000
C	2.881524000	-0.412448000	15.139717000
C	5.724810000	-0.461208000	11.845634000
C	5.830154000	0.955472000	11.230194000
C	7.121857000	-0.951768000	12.290355000
C	5.246548000	-1.404790000	10.721086000

C	4.351201000	3.288463000	17.642791000
C	5.501926000	3.376376000	18.662386000
C	5.179306000	4.354834000	19.802457000
C	4.821657000	5.749800000	19.267591000
C	3.673912000	5.672383000	18.249419000
C	3.996659000	4.692474000	17.110821000
H	7.959059000	4.328130000	14.325379000
H	6.226849000	4.237300000	14.740087000
H	7.436827000	4.475351000	16.006306000
H	8.247976000	0.066438000	16.752449000
H	8.277598000	1.580479000	17.645937000
H	6.759172000	0.696256000	17.474813000
H	3.040270000	1.287757000	16.939788000
H	3.502517000	-1.959177000	12.238051000
H	2.163640000	-0.350682000	15.953325000
H	6.522672000	0.953609000	10.379609000
H	4.848837000	1.288637000	10.867183000
H	6.196349000	1.673541000	11.962911000
H	7.794572000	-0.998208000	11.423103000
H	7.565057000	-0.282319000	13.026223000
H	7.054685000	-1.960066000	12.719783000
H	4.256638000	-1.127072000	10.338211000
H	5.952023000	-1.345948000	9.883686000
H	5.208676000	-2.452993000	11.042887000
H	3.457074000	2.895233000	18.171363000
H	6.408451000	3.697376000	18.135303000
H	5.713420000	2.377256000	19.060213000
H	4.332051000	3.968447000	20.390478000
H	6.031337000	4.418513000	20.492368000
H	5.706055000	6.185391000	18.779946000
H	4.554882000	6.421929000	20.095109000
H	3.460442000	6.668442000	17.838159000
H	2.757439000	5.346622000	18.765674000
H	4.846469000	5.063131000	16.524453000
H	3.147295000	4.611670000	16.420146000

C	6.184878000	6.889339000	7.883842000
C	6.232133000	8.412936000	7.911617000
O	6.216421000	6.334461000	9.209356000
H	7.081209000	6.562396000	7.345309000
H	6.203282000	8.807065000	6.895008000
C	4.940277000	6.273337000	7.251026000
H	4.992373000	5.187102000	7.321804000
H	4.029382000	6.634673000	7.728409000
Cl	4.828240000	6.693892000	5.489107000
H	7.143533000	8.740668000	8.410107000
Cl	4.839610000	9.159895000	8.806096000
O	9.219427000	2.004641000	12.169654000
C	9.808174000	2.837495000	11.175065000
C	10.387800000	2.011638000	10.029736000
C	8.669532000	3.726661000	10.666126000
O	7.987196000	3.504218000	9.686453000
O	8.477482000	4.799665000	11.465369000
C	7.310499000	5.577764000	11.169879000
C	7.203066000	6.655875000	12.244668000
C	7.443730000	6.206048000	9.785009000
O	8.467072000	6.607932000	9.282516000
H	11.193386000	1.367777000	10.395629000
H	10.791208000	2.662556000	9.244997000
H	9.607216000	1.386631000	9.588799000
H	6.433791000	4.925653000	11.173738000
H	8.090326000	7.296455000	12.226157000
H	7.124728000	6.178547000	13.225167000
H	6.314159000	7.270906000	12.069790000
H	10.561798000	3.489574000	11.626179000
O	10.217679000	3.260946000	13.856186000
C	11.518637000	3.468345000	14.394099000
C	11.485556000	4.752398000	15.210215000
C	12.035416000	2.282734000	15.214071000
O	12.683560000	2.395185000	16.230507000
O	11.778402000	1.068809000	14.692493000

C	11.065134000	1.020206000	13.427254000
C	10.758463000	-0.440636000	13.167970000
C	9.801354000	1.919651000	13.507089000
O	8.901872000	1.423755000	14.323783000
H	11.135778000	5.574953000	14.579453000
H	12.481688000	4.983451000	15.596521000
H	10.798379000	4.640657000	16.052962000
H	11.740127000	1.414812000	12.654702000
H	10.101574000	-0.817456000	13.954383000
H	11.685407000	-1.024011000	13.155188000
H	10.248927000	-0.549904000	12.207655000
H	12.245273000	3.589558000	13.565902000
C	1.515692000	-2.307183000	14.044196000
C	0.587080000	-2.189703000	15.267823000
H	1.122634000	-2.391732000	16.202480000
H	0.139439000	-1.191963000	15.342572000
H	-0.231148000	-2.916270000	15.187777000
C	0.669311000	-2.036749000	12.777179000
H	1.265092000	-2.137512000	11.863828000
H	-0.169482000	-2.743160000	12.709639000
H	0.259523000	-1.020146000	12.794676000
C	2.052901000	-3.757539000	13.992831000
H	2.700619000	-3.917415000	13.124373000
H	2.640377000	-3.985077000	14.889801000
H	1.226050000	-4.478539000	13.932251000

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**18TS<sup>LA</sup>** E = -3453.5989106, Imaginary frequency =177.82i

Al	6.723538000	1.227071000	14.987745000
O	5.259661000	1.836500000	13.925894000
N	5.605392000	1.800245000	16.815692000
C	7.728617000	2.959709000	14.966876000
C	6.055670000	-0.657341000	15.172168000
C	4.020592000	2.135324000	14.190375000
C	3.545721000	2.307478000	15.531858000
C	4.372607000	2.159637000	16.717737000

C	3.070324000	2.329494000	13.120108000
C	1.760834000	2.660005000	13.444940000
C	1.276642000	2.831986000	14.761702000
C	2.198742000	2.651812000	15.777569000
C	3.510752000	2.180053000	11.648933000
C	4.597876000	3.232491000	11.322399000
C	4.057199000	0.752658000	11.398473000
C	2.349604000	2.399991000	10.657211000
C	6.158469000	1.700644000	18.175970000
C	6.493759000	0.236009000	18.523304000
C	7.071672000	0.122762000	19.942960000
C	8.305819000	1.020457000	20.116117000
C	7.973846000	2.478987000	19.767234000
C	7.399086000	2.596773000	18.346547000
H	7.893759000	3.309808000	13.938103000
H	7.142781000	3.747550000	15.462251000
H	8.712785000	2.927243000	15.445693000
H	5.972154000	-1.073037000	14.157454000
H	6.698564000	-1.330465000	15.747823000
H	5.050549000	-0.685940000	15.617713000
H	3.832821000	2.384750000	17.650566000
H	1.055164000	2.798520000	12.633201000
H	1.901783000	2.771036000	16.816217000
H	4.951471000	3.108848000	10.289949000
H	4.189978000	4.246504000	11.420250000
H	5.449406000	3.138778000	11.996436000
H	4.393192000	0.654345000	10.357218000
H	4.894753000	0.532568000	12.061122000
H	3.270430000	0.007050000	11.571373000
H	1.925111000	3.408505000	10.732330000
H	2.723693000	2.277552000	9.633557000
H	1.539130000	1.674794000	10.800587000
H	5.388521000	2.049455000	18.889655000
H	7.222616000	-0.139631000	17.798342000
H	5.588600000	-0.376225000	18.425480000

H	6.307438000	0.411061000	20.682897000
H	7.328919000	-0.923867000	20.152484000
H	9.100313000	0.665327000	19.445790000
H	8.691913000	0.949434000	21.142826000
H	8.870851000	3.106405000	19.854486000
H	7.247563000	2.870166000	20.497967000
H	8.156271000	2.293849000	17.617821000
H	7.132226000	3.637152000	18.123458000
O	8.358666000	0.258580000	13.761867000
C	9.058255000	0.768751000	12.660557000
C	8.127548000	1.316399000	11.580164000
C	10.105442000	1.810595000	13.076639000
O	10.324574000	2.854015000	12.504152000
O	10.849157000	1.490247000	14.171992000
C	10.807863000	0.144953000	14.678969000
C	11.858833000	0.080544000	15.781267000
C	9.430053000	-0.236351000	15.257711000
O	8.970207000	0.373278000	16.224720000
H	7.436464000	0.526769000	11.269873000
H	8.700176000	1.658858000	10.712162000
H	7.547059000	2.158049000	11.962484000
H	11.081456000	-0.535594000	13.864334000
H	11.577753000	0.769966000	16.581400000
H	12.841275000	0.361253000	15.387966000
H	11.910119000	-0.931695000	16.194648000
H	9.650539000	-0.044745000	12.183008000
C	-0.197875000	3.199652000	14.999152000
C	-0.527759000	3.343287000	16.497037000
H	-0.347898000	2.409813000	17.042580000
H	0.068324000	4.132753000	16.969136000
H	-1.585706000	3.604357000	16.623611000
C	-1.114681000	2.098823000	14.413786000
H	-2.173082000	2.351982000	14.563804000
H	-0.952380000	1.966689000	13.338741000
H	-0.921500000	1.134978000	14.898698000

C	-0.521854000	4.546799000	14.309700000
H	-0.338800000	4.503526000	13.230747000
H	-1.575729000	4.818242000	14.459625000
H	0.100072000	5.351290000	14.719014000
C	5.321490000	-7.323492000	13.643928000
C	4.867581000	-8.021832000	12.366952000
O	5.253446000	-5.893493000	13.518317000
H	6.366688000	-7.612916000	13.799304000
H	4.922089000	-9.103969000	12.491980000
C	4.502812000	-7.626573000	14.895679000
H	4.888624000	-7.047830000	15.734622000
H	3.446231000	-7.405216000	14.744514000
Cl	4.626343000	-9.379901000	15.347950000
H	5.501318000	-7.712422000	11.536800000
Cl	3.156030000	-7.630719000	11.902571000
O	9.245829000	-1.641926000	15.303100000
C	9.333167000	-2.453508000	14.136450000
C	10.537687000	-3.394262000	14.228044000
C	8.055627000	-3.294077000	14.093847000
O	7.701200000	-4.068315000	14.955783000
O	7.369418000	-3.109307000	12.939590000
C	6.101626000	-3.774511000	12.885337000
C	5.421117000	-3.337975000	11.591308000
C	6.307634000	-5.286267000	12.906871000
O	7.225722000	-5.886051000	12.397945000
H	11.469811000	-2.821188000	14.255674000
H	10.570626000	-4.072927000	13.367021000
H	10.462127000	-3.992002000	15.140996000
H	5.513744000	-3.483054000	13.758744000
H	6.033411000	-3.614558000	10.727359000
H	5.286736000	-2.253027000	11.600969000
H	4.439927000	-3.815341000	11.502183000
H	9.361477000	-1.840264000	13.236865000

111

**19<sup>LA</sup>** E = -3453.6390667

Al	7.486377000	1.886500000	15.514564000
O	6.063784000	1.542421000	14.405537000
N	4.963027000	2.109304000	17.091208000
C	7.531561000	3.839417000	15.938233000
C	7.806548000	0.423698000	16.833975000
C	4.927747000	0.913694000	14.236685000
C	3.986893000	0.715398000	15.297224000
C	4.078507000	1.307933000	16.631746000
C	4.565984000	0.426242000	12.928647000
C	3.388245000	-0.302479000	12.790669000
C	2.491702000	-0.580457000	13.842133000
C	2.816292000	-0.039827000	15.075147000
C	5.460785000	0.705044000	11.700374000
C	5.656498000	2.230449000	11.522567000
C	6.831366000	0.010112000	11.869613000
C	4.840326000	0.176280000	10.389180000
C	4.744997000	2.627171000	18.434702000
C	5.949585000	2.319536000	19.343405000
C	5.776877000	2.928870000	20.743505000
C	5.522554000	4.442313000	20.675221000
C	4.322246000	4.759409000	19.770441000
C	4.494869000	4.148077000	18.371329000
H	8.239915000	4.366807000	15.289856000
H	6.533607000	4.276375000	15.800658000
H	7.832086000	4.042893000	16.977486000
H	8.302233000	-0.425599000	16.342304000
H	8.483221000	0.746496000	17.640580000
H	6.898026000	0.041560000	17.314646000
H	3.223594000	1.027439000	17.277503000
H	3.138346000	-0.684001000	11.807316000
H	2.151884000	-0.175150000	15.924489000
H	6.299016000	2.436583000	10.657789000
H	4.689995000	2.722607000	11.351157000
H	6.123484000	2.670012000	12.402984000
H	7.448547000	0.180099000	10.976839000

H	7.371786000	0.396294000	12.732694000
H	6.699184000	-1.073557000	11.987015000
H	3.859581000	0.622890000	10.183490000
H	5.501681000	0.434689000	9.553578000
H	4.727380000	-0.915027000	10.390523000
H	3.846735000	2.158998000	18.890166000
H	6.853755000	2.718038000	18.867718000
H	6.088295000	1.234367000	19.409683000
H	4.928518000	2.445620000	21.253058000
H	6.665057000	2.719148000	21.354365000
H	6.417367000	4.939421000	20.272855000
H	5.361274000	4.850724000	21.682649000
H	4.180820000	5.845884000	19.690437000
H	3.407148000	4.360508000	20.235223000
H	5.344210000	4.615740000	17.858260000
H	3.607582000	4.341486000	17.754647000
C	6.372708000	8.912397000	10.125693000
C	6.577039000	10.345116000	10.605239000
O	6.429507000	7.976492000	11.215059000
H	7.195838000	8.697512000	9.435338000
H	6.524850000	11.033619000	9.760909000
C	5.034849000	8.620546000	9.451937000
H	4.979568000	7.564514000	9.188545000
H	4.196925000	8.888438000	10.095610000
Cl	4.858218000	9.569293000	7.914941000
H	7.546605000	10.431540000	11.094150000
Cl	5.326951000	10.887280000	11.805393000
O	9.172145000	2.729178000	12.472459000
C	9.778114000	3.783821000	11.730803000
C	10.212541000	3.311485000	10.345863000
C	8.699649000	4.864732000	11.609394000
O	7.938442000	4.996957000	10.672570000
O	8.662440000	5.659227000	12.702586000
C	7.559927000	6.573573000	12.753369000
C	7.619744000	7.278056000	14.105934000

C	7.670711000	7.582030000	11.612831000
O	8.696517000	8.035907000	11.162412000
H	10.973207000	2.529638000	10.432559000
H	10.630891000	4.141633000	9.764349000
H	9.353159000	2.911133000	9.802212000
H	6.626419000	6.017722000	12.637396000
H	8.562301000	7.825557000	14.204743000
H	7.552264000	6.531594000	14.901917000
H	6.785923000	7.981730000	14.198278000
H	10.613356000	4.210362000	12.293803000
O	10.373889000	3.333259000	14.373534000
C	11.720119000	3.278631000	14.830999000
C	11.856943000	4.253704000	15.991302000
C	12.175378000	1.867391000	15.213069000
O	12.891749000	1.620161000	16.157306000
O	11.775498000	0.890433000	14.377970000
C	10.987754000	1.279470000	13.220343000
C	10.534758000	-0.007622000	12.562088000
C	9.817809000	2.196936000	13.670284000
O	8.923559000	1.538812000	14.369672000
H	11.544544000	5.250688000	15.666919000
H	12.892655000	4.288162000	16.339193000
H	11.217702000	3.938649000	16.820178000
H	11.649468000	1.843214000	12.547672000
H	9.894526000	-0.561024000	13.251845000
H	11.402447000	-0.621093000	12.296594000
H	9.960892000	0.217225000	11.659949000
H	12.400797000	3.595362000	14.015546000
C	1.228998000	-1.419404000	13.580833000
C	0.382939000	-1.611005000	14.853914000
H	0.948670000	-2.120682000	15.642211000
H	0.030947000	-0.653371000	15.254541000
H	-0.500120000	-2.221794000	14.628147000
C	0.342312000	-0.722962000	12.520840000
H	0.876068000	-0.585303000	11.574554000

H	-0.558656000	-1.316780000	12.313991000
H	0.026533000	0.267079000	12.869866000
C	1.630691000	-2.820790000	13.061719000
H	2.213402000	-2.756666000	12.136710000
H	2.243277000	-3.347430000	13.802555000
H	0.740602000	-3.431266000	12.856166000

111

**20<sup>LA</sup>** E = -3453.6578929

Al	8.166916000	0.865278000	15.311812000
O	6.687816000	1.741358000	14.632209000
N	6.215128000	1.716962000	17.550144000
C	9.371067000	2.147236000	16.253012000
C	7.626013000	-0.904359000	16.092741000
C	5.922101000	2.801073000	14.657556000
C	5.405507000	3.350800000	15.875261000
C	5.585572000	2.776368000	17.209251000
C	5.527892000	3.437648000	13.423633000
C	4.731403000	4.577690000	13.483112000
C	4.256299000	5.160122000	14.674958000
C	4.605912000	4.512163000	15.848022000
C	5.986085000	2.881627000	12.055955000
C	7.525156000	2.981426000	11.927125000
C	5.534845000	1.409253000	11.896870000
C	5.379801000	3.664351000	10.870665000
C	6.167569000	1.353782000	18.959116000
C	5.429189000	0.010282000	19.127541000
C	5.416625000	-0.457908000	20.590869000
C	6.838367000	-0.540964000	21.167052000
C	7.576881000	0.796649000	21.007535000
C	7.589873000	1.265334000	19.544187000
H	9.791081000	2.877686000	15.545070000
H	8.878781000	2.718223000	17.049636000
H	10.229710000	1.628933000	16.706378000
H	8.037684000	-1.782017000	15.572428000
H	7.958576000	-0.988534000	17.137404000

H	6.533727000	-1.018159000	16.102649000
H	5.065630000	3.363510000	17.991853000
H	4.454852000	5.055787000	12.550506000
H	4.255128000	4.887901000	16.805588000
H	7.836683000	2.673885000	10.918571000
H	7.854124000	4.018063000	12.074935000
H	8.036739000	2.341001000	12.646315000
H	5.873064000	1.013214000	10.929431000
H	5.943529000	0.787433000	12.693011000
H	4.439770000	1.336218000	11.924416000
H	5.707152000	4.711026000	10.851242000
H	5.710352000	3.202738000	9.932383000
H	4.282867000	3.647512000	10.878178000
H	5.609310000	2.118300000	19.540562000
H	5.924654000	-0.737096000	18.496259000
H	4.404369000	0.114121000	18.748020000
H	4.824337000	0.245042000	21.197375000
H	4.915834000	-1.432606000	20.668758000
H	7.396504000	-1.325433000	20.635417000
H	6.806601000	-0.838043000	22.224682000
H	8.605786000	0.710645000	21.381781000
H	7.081427000	1.555988000	21.632727000
H	8.176090000	0.571022000	18.930396000
H	8.078715000	2.243139000	19.457709000
O	9.076399000	0.486158000	13.763964000
C	9.088929000	-0.716119000	13.098734000
C	9.294833000	-0.513489000	11.581499000
C	10.198523000	-1.639449000	13.629479000
O	11.057010000	-1.372297000	14.436279000
O	10.125168000	-2.886169000	13.043150000
C	11.155841000	-3.794154000	13.421844000
C	10.780102000	-5.165160000	12.861076000
C	12.539951000	-3.378510000	12.918456000
O	13.566800000	-3.836492000	13.369627000
H	8.478740000	0.105142000	11.198853000

H	9.313450000	-1.465188000	11.040767000
H	10.237048000	0.014676000	11.397836000
H	11.240209000	-3.829685000	14.511808000
H	10.692425000	-5.122790000	11.770473000
H	9.817075000	-5.479200000	13.273917000
H	11.543047000	-5.901787000	13.130364000
H	8.154145000	-1.293576000	13.226119000
C	3.393280000	6.432556000	14.623900000
C	2.974649000	6.909667000	16.027629000
H	2.375747000	6.154862000	16.550158000
H	3.844943000	7.142974000	16.651597000
H	2.367340000	7.819985000	15.947872000
C	2.105085000	6.163592000	13.809559000
H	1.482688000	7.067269000	13.752642000
H	2.332726000	5.849822000	12.785289000
H	1.511370000	5.368321000	14.275191000
C	4.186954000	7.577481000	13.950066000
H	4.490020000	7.313479000	12.931329000
H	3.581215000	8.492425000	13.893458000
H	5.096992000	7.804007000	14.517422000
C	15.380712000	4.138312000	11.513018000
C	15.834461000	4.824464000	12.796829000
O	14.170993000	3.386333000	11.714102000
H	16.180948000	3.444695000	11.232784000
H	16.764275000	5.366875000	12.619833000
C	15.056733000	5.064618000	10.344262000
H	14.690819000	4.479117000	9.501034000
H	14.319084000	5.816810000	10.623719000
Cl	16.539586000	5.946608000	9.781092000
H	15.986604000	4.077620000	13.575445000
Cl	14.634632000	6.024307000	13.435311000
O	12.474083000	-2.523025000	11.874928000
C	13.722617000	-2.022298000	11.351702000
C	14.036912000	-2.696774000	10.026144000
C	13.579629000	-0.505549000	11.217198000

O	13.872669000	0.122647000	10.220583000
O	13.123021000	0.036638000	12.354497000
C	12.949144000	1.466043000	12.360304000
C	12.270419000	1.843319000	13.674534000
C	14.315195000	2.130837000	12.222566000
O	15.377259000	1.658103000	12.552672000
H	14.170469000	-3.771071000	10.184039000
H	14.955273000	-2.281530000	9.602323000
H	13.226111000	-2.535720000	9.309918000
H	12.337461000	1.754181000	11.501297000
H	12.877888000	1.510416000	14.521025000
H	11.282758000	1.375098000	13.741978000
H	12.152305000	2.930435000	13.723581000
H	14.504667000	-2.227475000	12.090342000

108

<b>15TS<sup>PA</sup></b>	E = -3452.1929369, Imaginary frequency =189.89i		
Al	6.614932000	2.483789000	15.229380000
O	5.151345000	2.776986000	14.093998000
N	5.094341000	2.182436000	16.933325000
C	6.992552000	4.322350000	15.910202000
C	6.850555000	0.497170000	15.209204000
C	3.874933000	2.495071000	14.134807000
C	3.232992000	2.010001000	15.319723000
C	3.8764444000	1.918271000	16.620204000
C	3.045818000	2.699118000	12.971719000
C	1.710139000	2.318024000	13.033454000
C	1.079651000	1.772147000	14.172711000
C	1.868175000	1.652303000	15.303006000
C	3.619192000	3.350406000	11.695114000
C	4.163662000	4.759441000	12.034873000
C	4.746221000	2.471258000	11.107211000
C	2.554553000	3.526866000	10.592142000
C	5.440762000	2.088848000	18.359363000
C	6.763004000	1.331562000	18.572866000
C	7.134761000	1.267315000	20.063154000

C	7.200163000	2.666746000	20.692381000
C	5.879959000	3.423432000	20.483931000
C	5.501788000	3.493645000	18.996086000
H	6.072114000	4.830046000	16.229647000
H	7.696138000	4.339611000	16.752626000
H	7.429553000	4.915550000	15.098538000
H	6.997805000	0.142682000	14.180286000
H	7.738456000	0.188044000	15.771730000
H	5.984321000	-0.046965000	15.612016000
H	3.190985000	1.599954000	17.422607000
H	1.102339000	2.454386000	12.146240000
H	1.445931000	1.277956000	16.231710000
H	4.559221000	5.239458000	11.129480000
H	3.358343000	5.393767000	12.427205000
H	4.966923000	4.710397000	12.769049000
H	5.166253000	2.941552000	10.207222000
H	5.544821000	2.334540000	11.834357000
H	4.359736000	1.484607000	10.821845000
H	1.724310000	4.166147000	10.916306000
H	3.018424000	4.007777000	9.722428000
H	2.139684000	2.569192000	10.254192000
H	4.640548000	1.530030000	18.880792000
H	7.566757000	1.824624000	18.015040000
H	6.675247000	0.321848000	18.157491000
H	6.390458000	0.664158000	20.607391000
H	8.097233000	0.753025000	20.178312000
H	8.018329000	3.232615000	20.224415000
H	7.435363000	2.597106000	21.763598000
H	5.950012000	4.439013000	20.896791000
H	5.080482000	2.914077000	21.044647000
H	6.237128000	4.095806000	18.453534000
H	4.530210000	3.989359000	18.869101000
C	8.218236000	5.041901000	6.091680000
C	9.318215000	6.011491000	5.670577000
O	7.915316000	5.186325000	7.489930000

H	8.609356000	4.033797000	5.915849000
H	9.545719000	5.887294000	4.611049000
C	6.877732000	5.215957000	5.383057000
H	6.153569000	4.503954000	5.779497000
H	6.497454000	6.231885000	5.491859000
Cl	7.032862000	4.886569000	3.605196000
H	10.215069000	5.829252000	6.262696000
Cl	8.871010000	7.755092000	5.911767000
O	8.505128000	2.667259000	14.029094000
C	8.851352000	2.594428000	12.686899000
C	8.466540000	1.260195000	12.013553000
C	8.278845000	3.780958000	11.900767000
O	7.467126000	4.592417000	12.277819000
O	8.829746000	3.830576000	10.638665000
C	8.340327000	4.867357000	9.788797000
C	8.973216000	6.225481000	10.125500000
C	8.699204000	4.474972000	8.362709000
O	9.566600000	3.716274000	8.008400000
H	8.946326000	0.451843000	12.570177000
H	8.801212000	1.232269000	10.970983000
H	7.384437000	1.104347000	12.045360000
H	7.252514000	4.939353000	9.883019000
H	10.064598000	6.151060000	10.079987000
H	8.672989000	6.510641000	11.135254000
H	8.634712000	6.990756000	9.420178000
H	9.942279000	2.700759000	12.568357000
C	-0.403244000	1.369516000	14.117445000
C	-0.905082000	0.815140000	15.464298000
H	-0.345409000	-0.076650000	15.768767000
H	-0.820370000	1.558837000	16.265159000
H	-1.962125000	0.533557000	15.382541000
C	-0.604995000	0.272469000	13.044970000
H	-1.661773000	-0.020115000	12.979337000
H	-0.290323000	0.615031000	12.053410000
H	-0.017144000	-0.620006000	13.288517000

C	-1.271578000	2.598186000	13.755746000
H	-0.989858000	3.022554000	12.786266000
H	-2.333723000	2.323032000	13.704017000
H	-1.159013000	3.387477000	14.508072000
C	12.761665000	5.488858000	14.654787000
C	11.564233000	5.881955000	15.275540000
C	10.524577000	4.974061000	15.492345000
C	10.709270000	3.661475000	15.064317000
C	11.893315000	3.275871000	14.447367000
C	12.938967000	4.171845000	14.230003000
C	9.850718000	2.443134000	15.285650000
O	10.634950000	1.349958000	14.603580000
C	11.824271000	1.816772000	14.156888000
O	12.669018000	1.126183000	13.624424000
O	9.296430000	2.162601000	16.332257000
H	13.556162000	6.218215000	14.512705000
H	11.448242000	6.913166000	15.601968000
H	9.599073000	5.273245000	15.971540000
H	13.858509000	3.839562000	13.756384000

108

**16<sup>PA</sup>** E = -3452.2401667

Al	4.068620000	3.222581000	13.956135000
O	2.313791000	2.793293000	13.614568000
N	4.032321000	2.366452000	15.792593000
C	4.233490000	5.185969000	14.060357000
C	5.236118000	2.179456000	12.750454000
C	1.471300000	1.975517000	14.196526000
C	1.788557000	1.371799000	15.448219000
C	3.019802000	1.638768000	16.153406000
C	0.201846000	1.680326000	13.596829000
C	-0.642978000	0.806465000	14.271583000
C	-0.349140000	0.189341000	15.511409000
C	0.874537000	0.496140000	16.076919000
C	-0.197310000	2.312949000	12.247339000
C	-0.219807000	3.856419000	12.372120000

C	0.805899000	1.888402000	11.146756000
C	-1.600615000	1.868448000	11.786947000
C	5.145537000	2.487490000	16.769324000
C	6.498970000	2.074323000	16.170356000
C	7.600476000	2.140524000	17.243148000
C	7.672451000	3.535587000	17.880488000
C	6.311546000	3.987393000	18.430916000
C	5.214951000	3.909854000	17.354434000
H	3.628080000	5.642657000	14.855161000
H	5.277025000	5.488003000	14.213649000
H	3.908287000	5.642393000	13.113180000
H	4.918432000	2.306507000	11.704368000
H	6.277955000	2.517957000	12.807214000
H	5.225586000	1.099505000	12.954045000
H	3.085364000	1.153522000	17.134422000
H	-1.600536000	0.577362000	13.818314000
H	1.168967000	0.067294000	17.030421000
H	-0.500020000	4.306278000	11.410726000
H	-0.958172000	4.172792000	13.119396000
H	0.755940000	4.245919000	12.665079000
H	0.526950000	2.344618000	10.188007000
H	1.822362000	2.197424000	11.393523000
H	0.798143000	0.799255000	11.016167000
H	-2.382248000	2.161164000	12.498478000
H	-1.832818000	2.347988000	10.828988000
H	-1.662733000	0.784233000	11.634024000
H	4.918987000	1.797565000	17.598785000
H	6.768983000	2.748888000	15.349615000
H	6.422892000	1.061973000	15.753135000
H	7.401164000	1.383116000	18.019660000
H	8.565892000	1.915491000	16.779305000
H	8.011105000	4.243896000	17.115915000
H	8.426703000	3.543704000	18.677371000
H	6.370765000	5.014585000	18.814563000
H	6.024292000	3.351760000	19.284278000

H	5.438103000	4.620728000	16.551124000
H	4.236135000	4.183282000	17.772275000
C	12.853749000	5.605758000	7.259489000
C	14.139042000	5.055333000	6.651967000
O	12.957433000	5.730986000	8.688199000
H	12.066199000	4.880721000	7.026423000
H	14.038922000	4.977661000	5.568740000
C	12.439725000	6.998073000	6.791461000
H	11.533017000	7.305253000	7.312339000
H	13.232386000	7.726931000	6.961258000
Cl	12.069942000	7.008405000	5.015681000
H	14.353145000	4.074686000	7.075177000
Cl	15.589989000	6.100030000	6.973258000
O	8.783640000	3.867052000	12.969087000
C	9.943159000	3.226627000	12.429902000
C	9.450395000	2.031179000	11.615967000
C	10.708841000	4.181257000	11.519346000
O	10.229395000	4.971371000	10.735849000
O	12.049743000	4.003824000	11.660841000
C	12.861558000	4.904259000	10.905030000
C	14.300104000	4.712532000	11.379096000
C	12.727614000	4.601124000	9.415506000
O	12.514439000	3.518356000	8.924645000
H	8.919403000	1.344463000	12.280174000
H	10.297391000	1.507577000	11.159303000
H	8.769101000	2.363814000	10.826823000
H	12.523449000	5.928106000	11.081789000
H	14.621567000	3.679779000	11.213461000
H	14.353010000	4.932387000	12.448764000
H	14.970728000	5.388565000	10.839043000
H	10.571675000	2.893970000	13.257169000
C	-1.371919000	-0.762162000	16.156029000
C	-0.871386000	-1.328761000	17.498179000
H	0.053624000	-1.903993000	17.376755000
H	-0.685769000	-0.534657000	18.230576000

H	-1.626155000	-2.001059000	17.923014000
C	-1.647344000	-1.953177000	15.207348000
H	-2.383757000	-2.636959000	15.649280000
H	-2.040378000	-1.620599000	14.240668000
H	-0.728390000	-2.518799000	15.015567000
C	-2.695801000	-0.006007000	16.420723000
H	-3.126819000	0.395613000	15.497418000
H	-3.439592000	-0.675588000	16.871925000
H	-2.533964000	0.834748000	17.105060000
C	12.516798000	6.965321000	14.691402000
C	11.512572000	7.434399000	13.837185000
C	10.361612000	6.671768000	13.633863000
C	10.217909000	5.426916000	14.265511000
C	11.219462000	4.956466000	15.126862000
C	12.360155000	5.738354000	15.334602000
C	8.912275000	4.690621000	14.057856000
O	10.080087000	2.918523000	15.383314000
C	11.066540000	3.593902000	15.820791000
O	11.900524000	3.300630000	16.695010000
O	7.900714000	5.001187000	14.652268000
H	13.410933000	7.563136000	14.859595000
H	11.617380000	8.397073000	13.341217000
H	9.574736000	7.035826000	12.978468000
H	13.104164000	5.344986000	16.021337000

44

**17<sup>PA</sup>** E = -2180.3368365

C	19.594319000	3.410853000	8.455770000
C	20.889620000	2.907553000	7.828964000
O	19.707136000	3.522174000	9.883723000
H	18.827736000	2.664248000	8.220615000
H	20.780185000	2.835608000	6.746210000
C	19.132136000	4.794851000	8.008946000
H	18.221496000	5.066460000	8.542464000
H	19.902968000	5.546513000	8.179560000
Cl	18.743853000	4.815807000	6.236206000

H	21.139377000	1.930977000	8.241890000
Cl	22.310720000	3.995162000	8.142620000
O	15.524289000	1.695256000	14.099805000
C	16.680413000	1.027392000	13.596101000
C	16.182401000	-0.184429000	12.809461000
C	17.468238000	1.949607000	12.671487000
O	17.009049000	2.726134000	11.861131000
O	18.806656000	1.767886000	12.835179000
C	19.631969000	2.666113000	12.092254000
C	21.064659000	2.456882000	12.576146000
C	19.507452000	2.377718000	10.599333000
O	19.326631000	1.295620000	10.093616000
H	15.638752000	-0.844419000	13.490718000
H	17.025758000	-0.733353000	12.375976000
H	15.512706000	0.133197000	12.003528000
H	19.302166000	3.691479000	12.275792000
H	21.378399000	1.423170000	12.401906000
H	21.108874000	2.665000000	13.648518000
H	21.746088000	3.133226000	12.049755000
H	17.292495000	0.706729000	14.441351000
C	19.285489000	4.764870000	15.823713000
C	18.286526000	5.241205000	14.967207000
C	17.128918000	4.487777000	14.768171000
C	16.970887000	3.244354000	15.401217000
C	17.968333000	2.765821000	16.263898000
C	19.115027000	3.541155000	16.469362000
C	15.650177000	2.534865000	15.184730000
O	16.854674000	0.706804000	16.517017000
C	17.822188000	1.396627000	16.957074000
O	18.666231000	1.119763000	17.832019000
O	14.638317000	2.876013000	15.750752000
H	20.185788000	5.354276000	15.991120000
H	18.400156000	6.201516000	14.467901000
H	16.344219000	4.858796000	14.113446000
H	19.853234000	3.140898000	17.158580000

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