# An experimental and DFT study of the reaction between dichloroethylene carbonate and triethylamine in dimethyl carbonate

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## 1. Detailed analysis conditions for gas chromatography-mass spectrometry and gas chromatography.

Test conditions for Thermo Fisher Trace GC 1300 MS ISQ LT system: Maintain the temperature at 40°C for 4 minutes, then increase to 200°C at 10°C/min. Set the injector temperature to 200°C, with an injection volume of 20uL and a split ratio 20:1. Use He as the carrier gas. Set the EI ionization source voltage to 70eV, operate in full scan mode, and maintain the ion source temperature at 220°C and the transfer line temperature at 280°C. TG-BOND column:30m×0.25mm×2.5μm。

Test conditions for Agilent 7820A GC system: Column oven maintained at 90°C; injector port temperature is set to 150°C, while the detector temperature is set to 250°C; injection volume of 1mL without splitting; the carrier gas is He gas; TCD detector. Initially, the gas passes through a Porapak-QS column. Given that the retention times of air and CO are within 1 minute, at 1 minute, promptly switch the six-way valve to direct air and CO to the MolSieve 5A column for storage. Concurrently, the gas continues to flow through the Porapak-QS column. After a runtime of 60 minutes, $CO_2$, chloromethane, and chloroethane are fully eluted from the column and detected by the detector. Subsequently, the valve is switched to the MolSieve 5A column, the stored air and CO are released, and the detector is channeled through, with an operational time of 10 minutes. This process allows for the detection and analysis of air, CO, $CO_2$, chloromethane, and chloroethane in the gas. An external standard method was adopted for the test. The gas standard samples were $CO_2$, CO, chloromethane, and chloroethane. Therefore, only these four components in the gas were tested. In the standard samples, the concentration of $CO_2$ was 19.90%, the concentration of CO was 3.02%, the concentration of chloromethane was 5.00%, and the concentration of chloroethane was 4.95%. Porapak-QS column: OD 1/8inch, ID 2mm, Length 2m. MolSieve 5A column: OD 1/8inch, ID 2mm, Length 2.44m.

Test conditions for the Shimadzu GC-2014C system: Maintain at 60°C for 5

minutes, then increase to 260°C at a rate of 20°C/min and maintain for 10 minutes; set the injector temperature to 280°C and the detector temperature to 300°C; use an injection volume of 1uL with a split ratio of 30:1; employ high-purity nitrogen gas as the carrier gas. The internal standard method is used for quantitative analysis, with chlorobenzene as the internal standard substance. SH-5 column:30m×0.53mm×1.5μm。

## 2 Tables S1-S8.

**Table S1.** The amount of dichloroethylene carbonate in the chlorinated solution

| cis-DCEC[a]/wt% | trans-DCEC/wt% | EC[b]/wt% | CEC[c]/wt% | Other substance/wt% |
|---|---|---|---|---|
| 1.06 | 7.29 | 4.28 | 83.72 | 3.65 |

[a]DCEC refers to the dichloroethylene carbonate. [b]EC refers to the ethylene carbonate. [c]CEC refers to the chloroethylene cabonate.

**Table S2.** Gibbs free energy barriers for removing the first HCl molecule from DCEC.

| Label | Reactant (kcal/mol) | Transition state (kcal/mol) | Product (kcal/mol) |
|---|---|---|---|
| syn-1 | 0.00 | 30.4 | -4.3 |
| syn-2 | 0.00 | 30.7 | -6.2 |
| anti-1 | 0.00 | 26.1 | −8.5 |
| anti-2 | 0.00 | 25.8 | −8.6 |

"syn" indicates a syn-elimination reaction, while "anti" denotes a trans-elimination; the "1" and "2" labels indicate that TEA is the first and second conformer, respectively.

**Table S3.** The molar gas composition

| Base | solvent | CO/% | $CO_2$/% | chloromethane/% | Chloroethane/% |
|---|---|---|---|---|---|
| TEA | MeCN | 11.50 | 81.76 | --- | 3.49 |
| TPA | DEC | 4.96 | 62.15 | --- | 0.06 |

"---" indicates a compound was not detected in the gas chromatograph.

**Table S4.** DCEC reacts with TEA or TPA in different solvents.

| Base | solvent | temperature<br>℃ | time<br>hr | conv[a] (%) | chloromethane<br>mmol | chloroethane<br>mmol | ethyl chloroacetate<br>mmol | chloropropane<br>mmol | gas<br>L |
|---|---|---|---|---|---|---|---|---|---|
| TEA | MeCN | 75 | 12 | 100.0 | --- | 32.598 | --- | --- | 1.080 |
| TPA | DEC | 90 | 12 | / | --- | 0.973 | 0.241 | 1.138 | 0.208 |

[a]Conv refers to th fact that DCEC and TPA cannot be separated in gas chromatography, making it impossible to calculate the conversion of DCEC.

"---" indicates a compound was not detected in the gas chromatograph.

**Table S5.** Peak positions and possible chemical structural formulas of the mass spectrum of *N,N*-dipropyl chloroacetamide

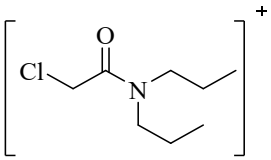
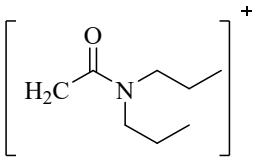
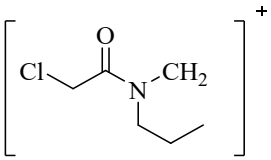
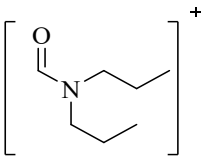
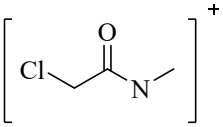
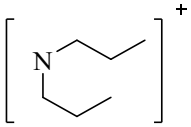
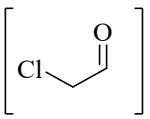
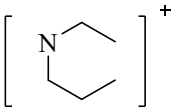
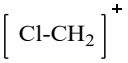
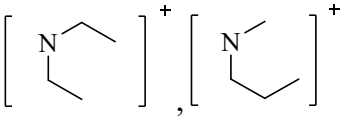
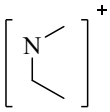
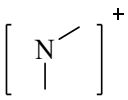
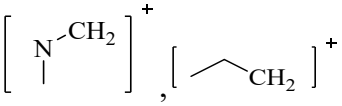
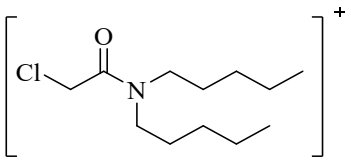
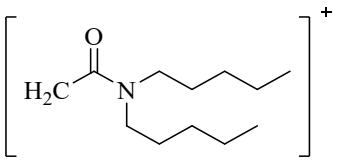
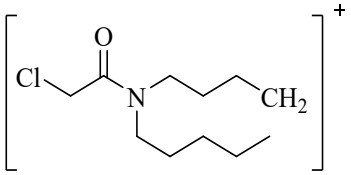
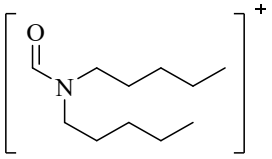
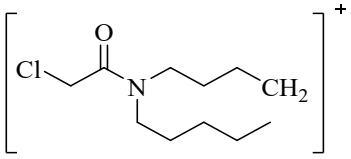
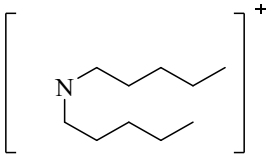
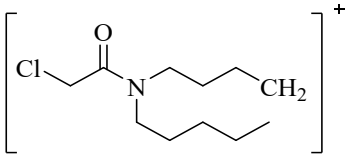
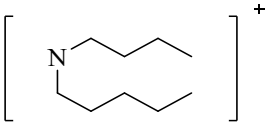
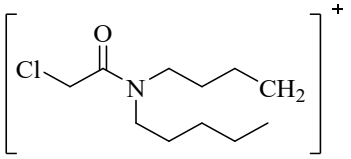
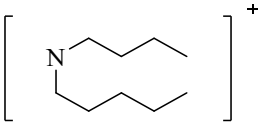
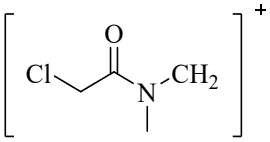
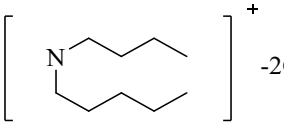
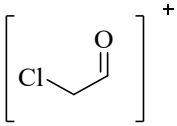
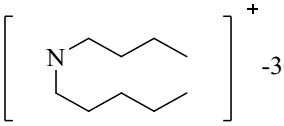
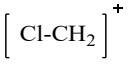
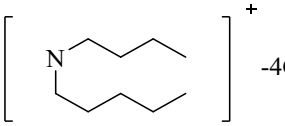
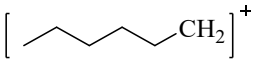
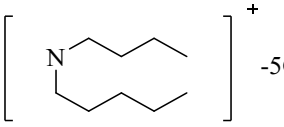
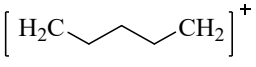
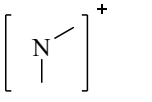
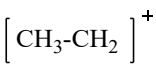
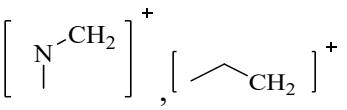
| Peak positions | Possible chemical structural formulas | Peak positions | Possible chemical structural formulas |
|---|---|---|---|
| 177,179 |  | 142 |  |
| 148,150 |  | 128 |  |
| 106,108 |  | 100 |  |
| 77,79 |  | 86 |  |
| 49,51 |  | 72 |  |
| | | 58 |  |
| | | 44 |  |
| | | 43 |  |

**Table S6.** Peak positions and possible chemical structural formulas of the mass spectrum of *N,N*-diamyl chloroacetamide

| Peak positions | Possible chemical structural formulas | Peak positions | Possible chemical structural formulas |
|---|---|---|---|

| | | | |
|---|---|---|---|
| 233 |  | 198,199 |  |
| 218 |  | 184,185 |  |
| 204,206 |  -$CH_2$ | 156,158 |  |
| 190,192 |  -$2CH_2$ | 142 |  |
| 176,178 |  -$3CH_2$ | 128 |  -$CH_2$ |
| 120,122 |  | 114 |  -$2CH_2$ |
| 77,79 |  | 100 |  -$3CH_2$ |
| 49,51 |  | 86 |  -$4CH_2$ |
| 71 |  | 72 |  -$5CH_2$ |
| 56 |  | 44 |  |
| 29 |  | 43 |  |

The chemical structural formulas on the left mainly comprise fragment ions that include the chloro element, as indicated in Table S4 to S6. These fragment ions adhere

to the [M+2] rule. Conversely, the formulas on the right mainly consist of fragment ions lacking the chloro element, as detailed in Table S4 to S6. When the fragment ion has more carbons, the [M+1] rule becomes relevant.

**Table S7.** The molar gas composition and the molar ratio between the collected $CO_2$ and the consumed DCEC in different conditions.

| Base | CO/% | $CO_2$/% | chloromethane/% | $CO_2$: DCEC[a] |
|---|---|---|---|---|
| TPA | 4.47 | 82.25 | 2.73 | 1.132:1 |
| TAA | 8.64 | 64.32 | 1.25 | 0.162:1 |

[a]$CO_2$: DCEC denotes the molar ratio between the collected $CO_2$ and the fed DCEC, with TPA as the base.

**Table S8.** DCEC reacts with TPA and TAA in different reaction conditions.

| Base | temperature | time | conv[a] (%) | chloromethane[b] | methyl chloroacetate | chloroalkane[c] | gas |
|---|---|---|---|---|---|---|---|
| | ℃ | hr | | mmol | mmol | mmol | L |
| TPA | 90 | 12 | / | 15.8 | 3.0 | 11.7 | 2.888 |
| TAA | 80 | 24 | 67% | 4.1 | 1.3 | 4.8 | 0.352 |

Reaction conditions: TPA 209 mmol, DCEC 95.6 mmol, DMC 140.5 mL; TAA 145.3 mmol, DCEC 62.4 mol, DMC 140.5 mL. [a]Conv refers to the fact that DCEC and TPA cannot be separated in gas chromatography, making it impossible to calculate the conversion of DCEC. [b]Chloromethane refers to the chloromethane in the liquid phase. [c]Chloroalkane refers to 1-chloropropane for TPA and 1-chloropentane for TAA.

## 3. Figures S1-S21.

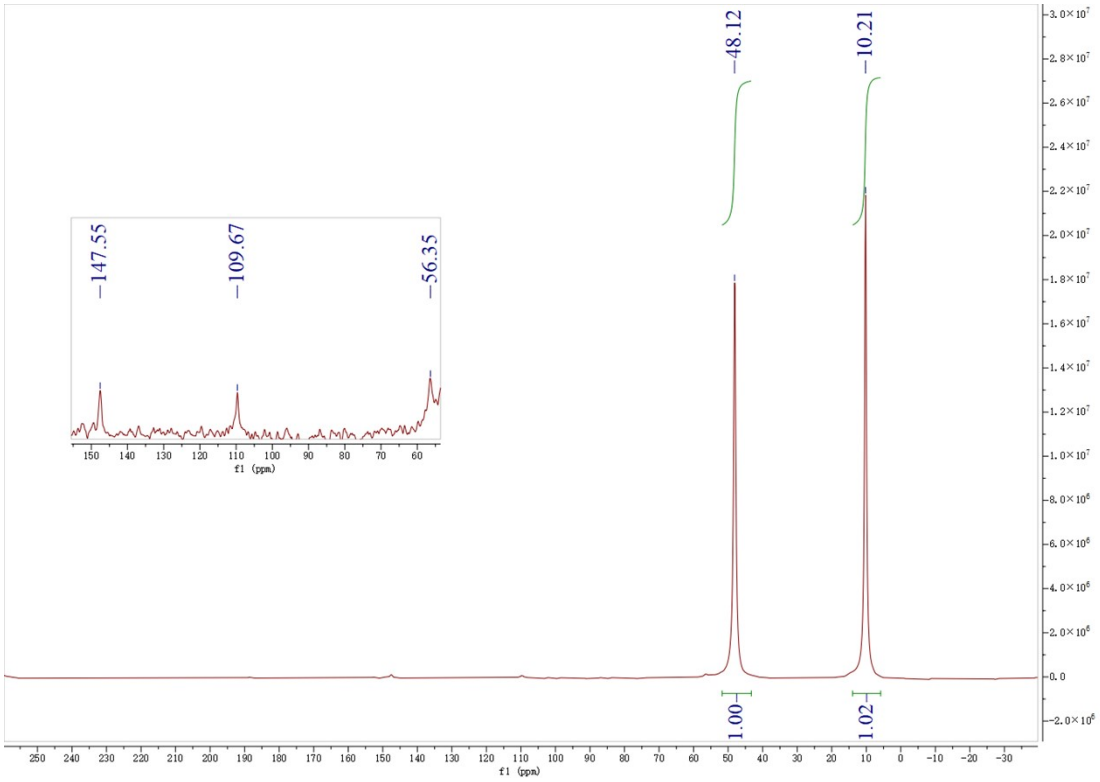



**Fig. S1.** $^{13}$C-ssNMR of the precipitate.

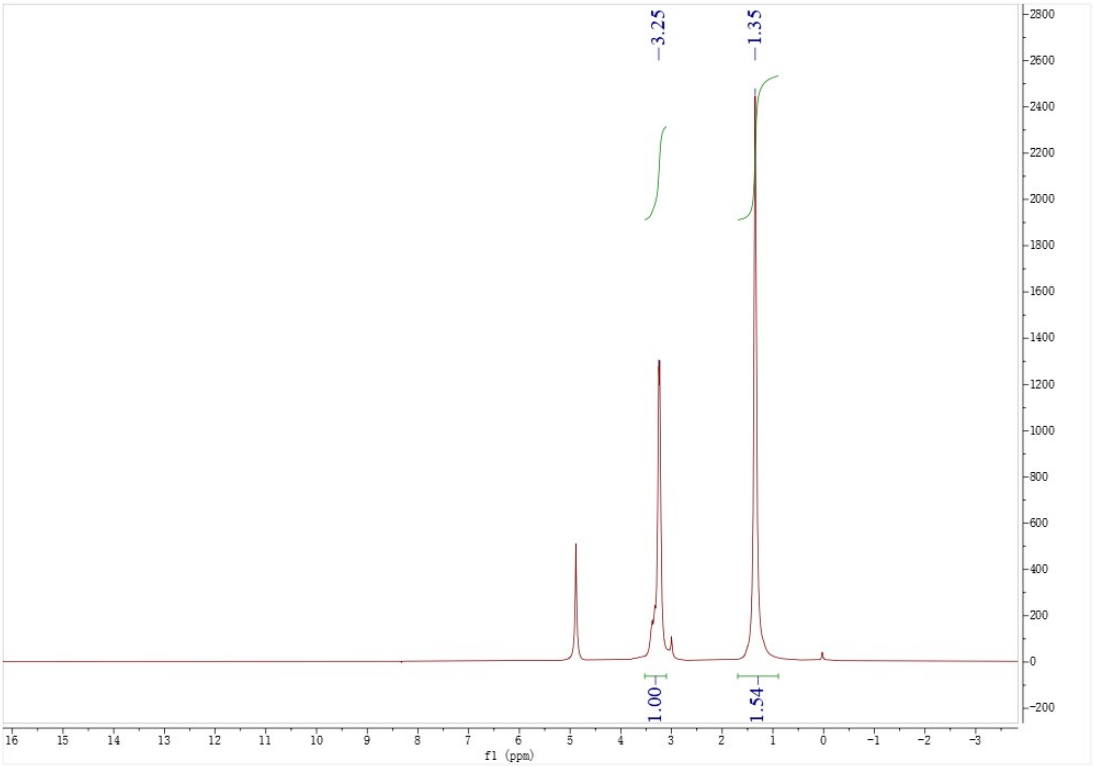


**Fig. S2.** $^{1}$H-NMR of the precipitate.

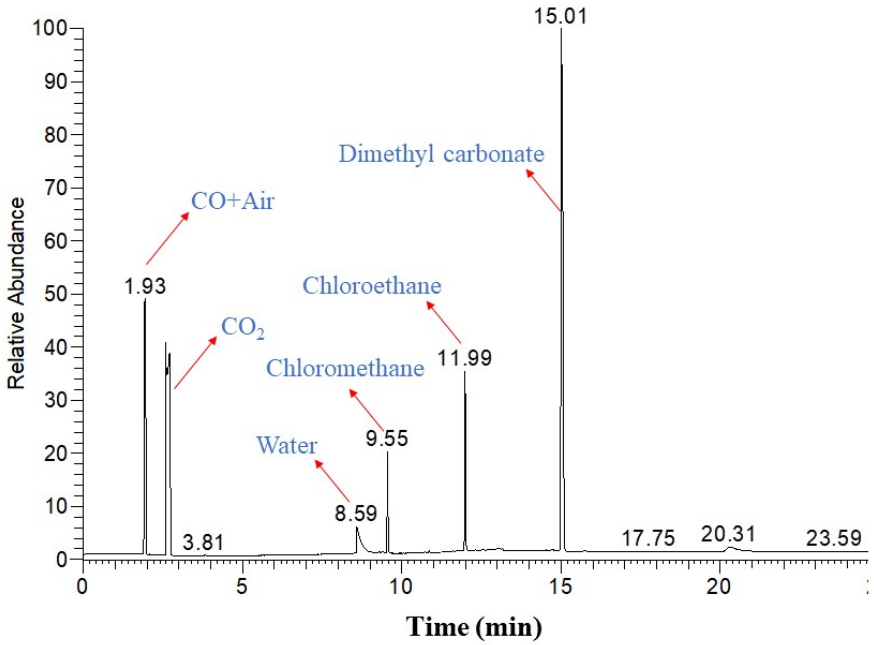



**Fig. S3.** Products of the gas phase collected at the temperature of 75℃

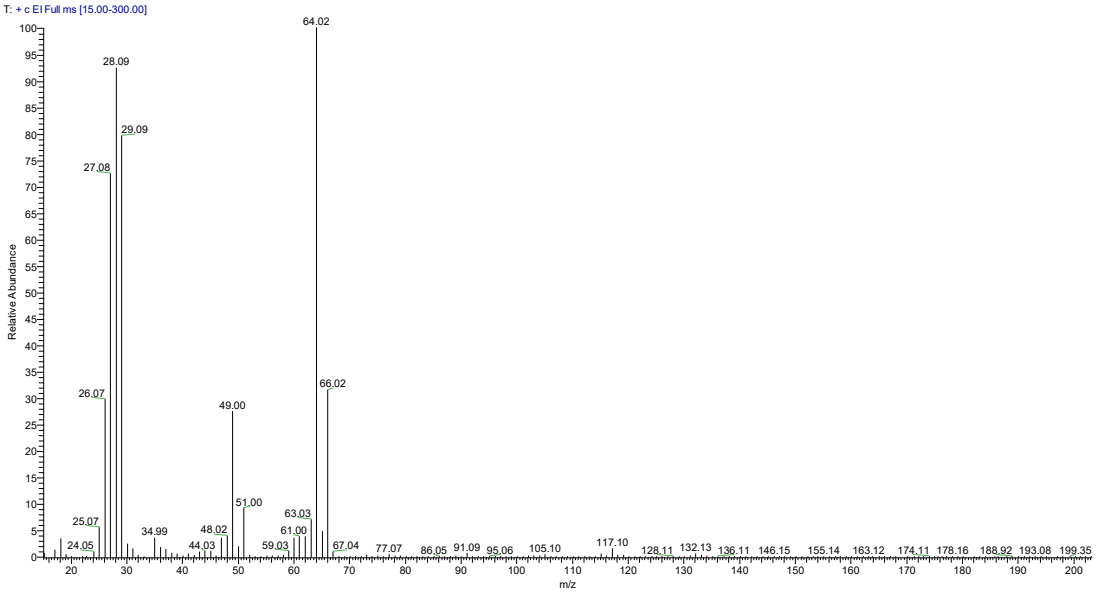



**Fig. S4.** Mass spectrum of chloroethane

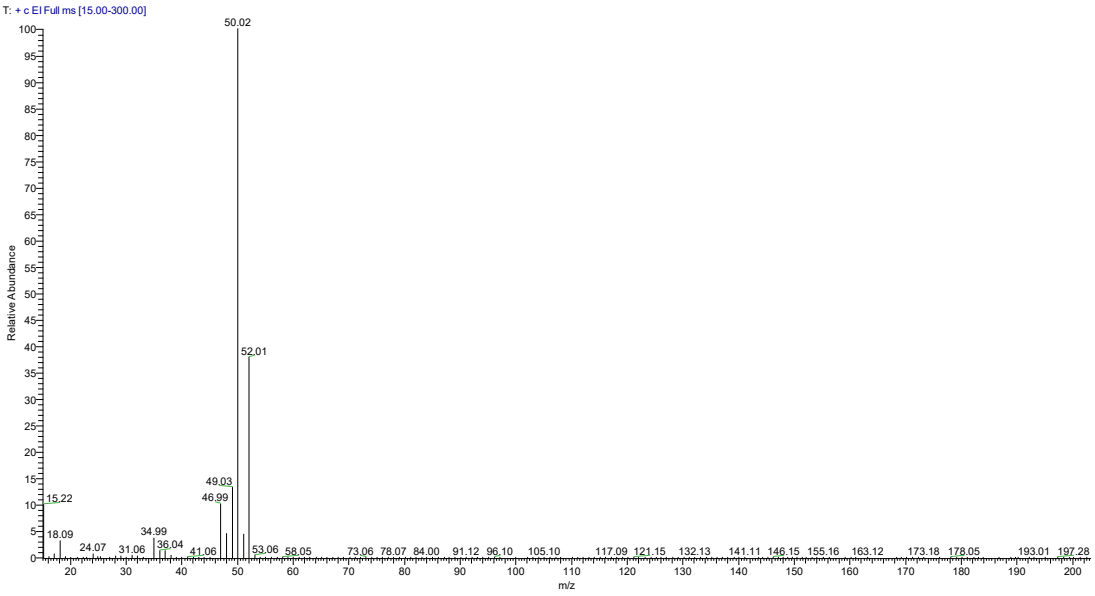



**Fig. S5.** Mass spectrum of chloromethane

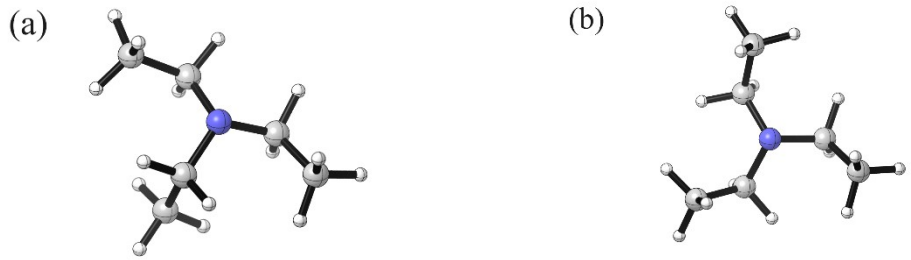



**Fig. S6.** Two stable conformers of TEA: Blue ball, N atom; Grey ball, C atom; White ball, H atom

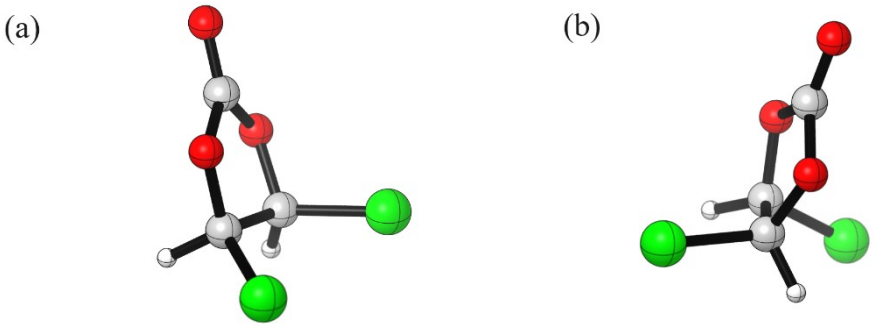



**Fig. S7.** Cis and Trans DCEC (S7a is cis DCEC and S7b is trans DCEC); Green ball, Cl atom; Grey ball, C atom; Red ball, O atom; White ball, H atom

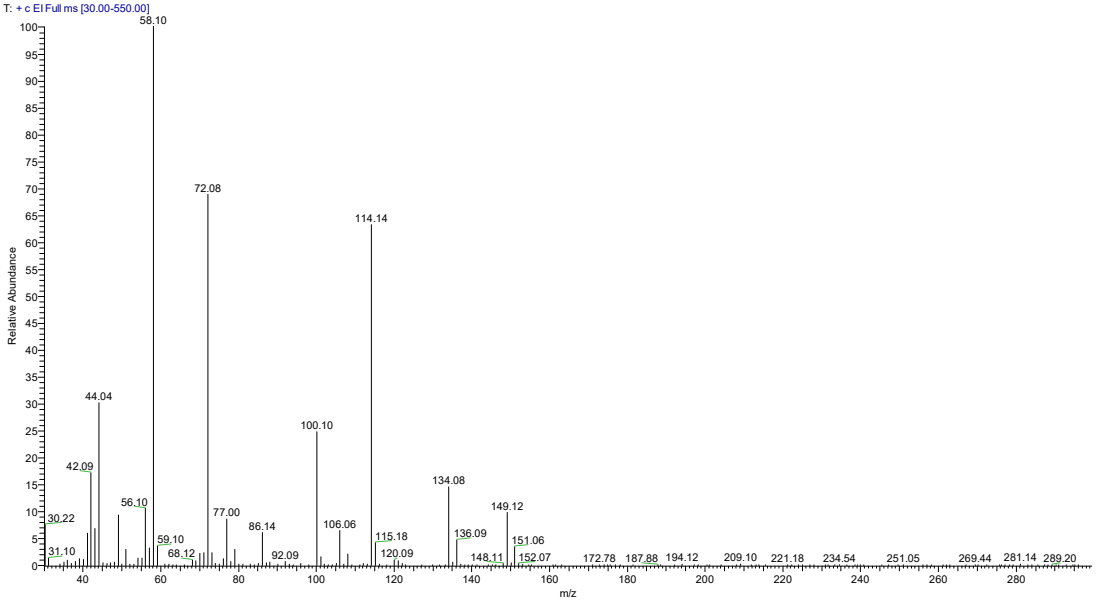



**Fig. S8.** Mass spectrum of *N,N*-diethylchloroacetamide

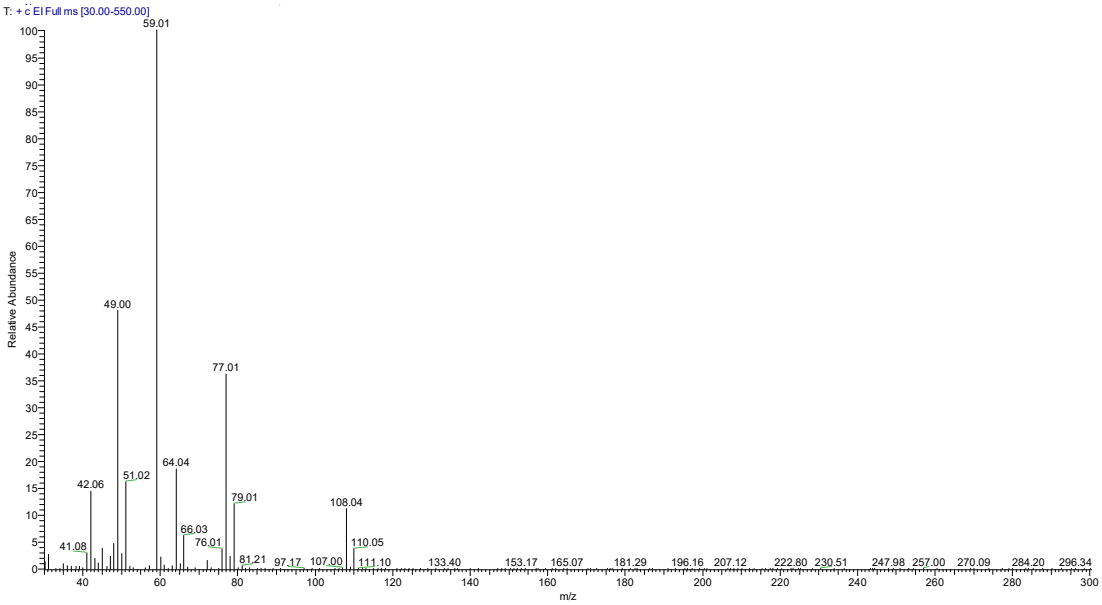



**Fig. S9.** Mass spectrum of methyl chloroacetate

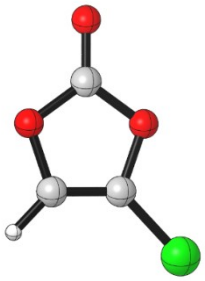


**Fig. S10.** Chlorovinyl carbonate: Green ball, Cl atom; Grey ball, C atom; Red ball, O

atom; White ball, H atom

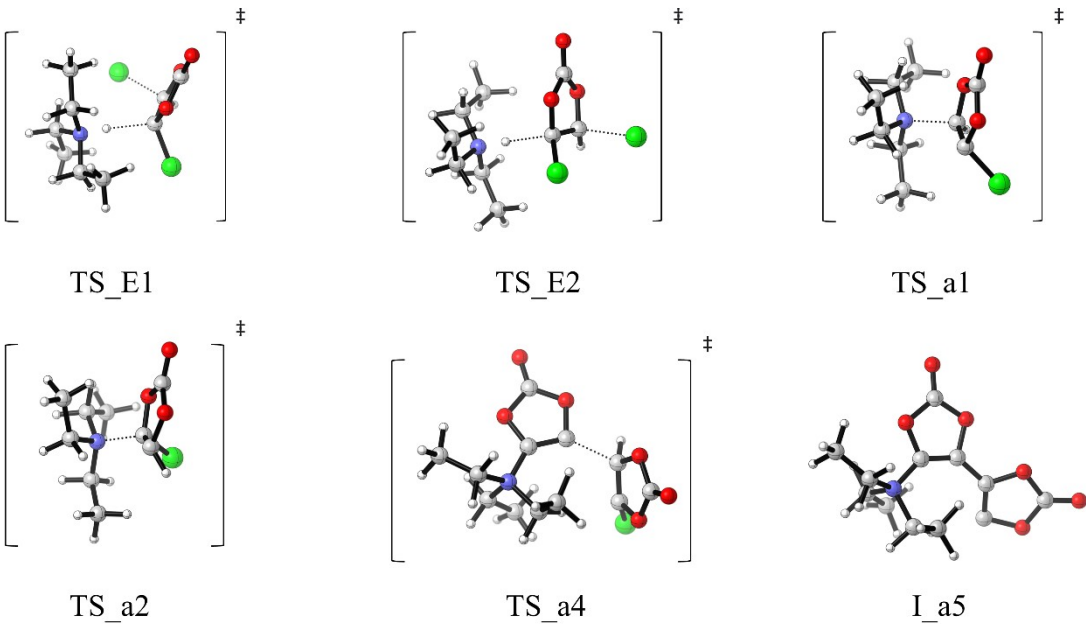



**Fig. S11.** Transition states and intermediates involved in HCl elimination from DCEC and CLVC.

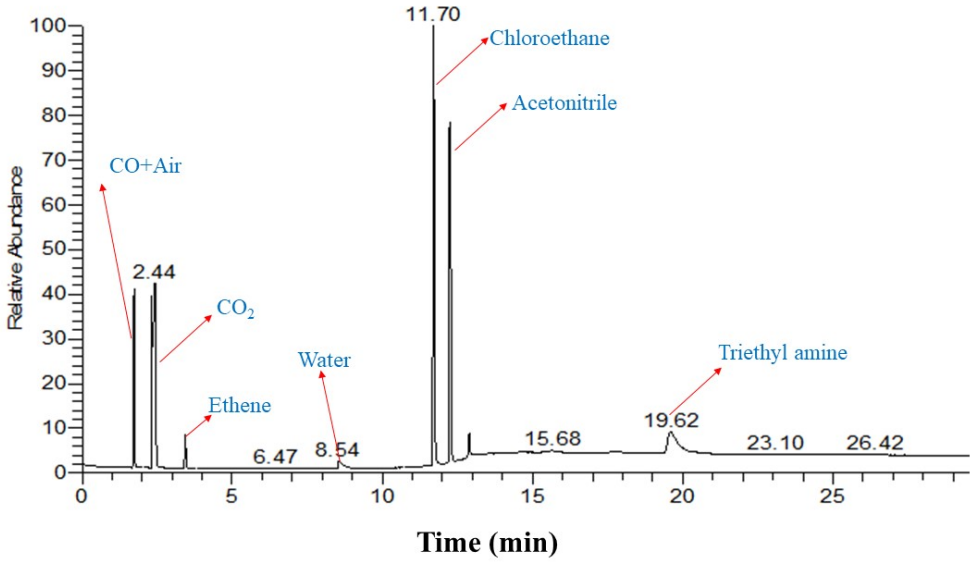



**Fig. S12.** Gas phase collected when DCEC reacts with TEA in the solvent MeCN.

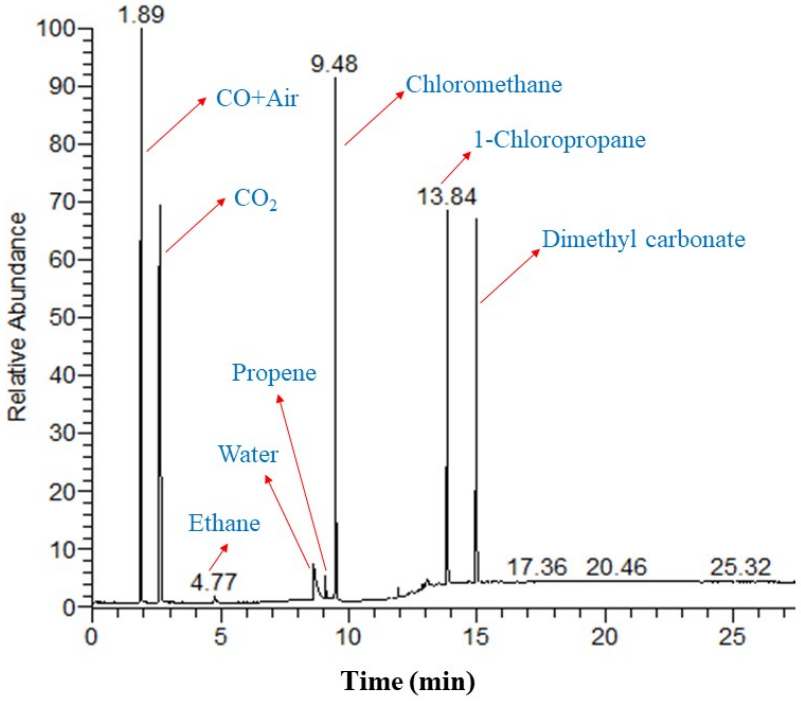



**Fig. S13.** The gas product collected after DCEC reacts with tripropyl amine in DMC.

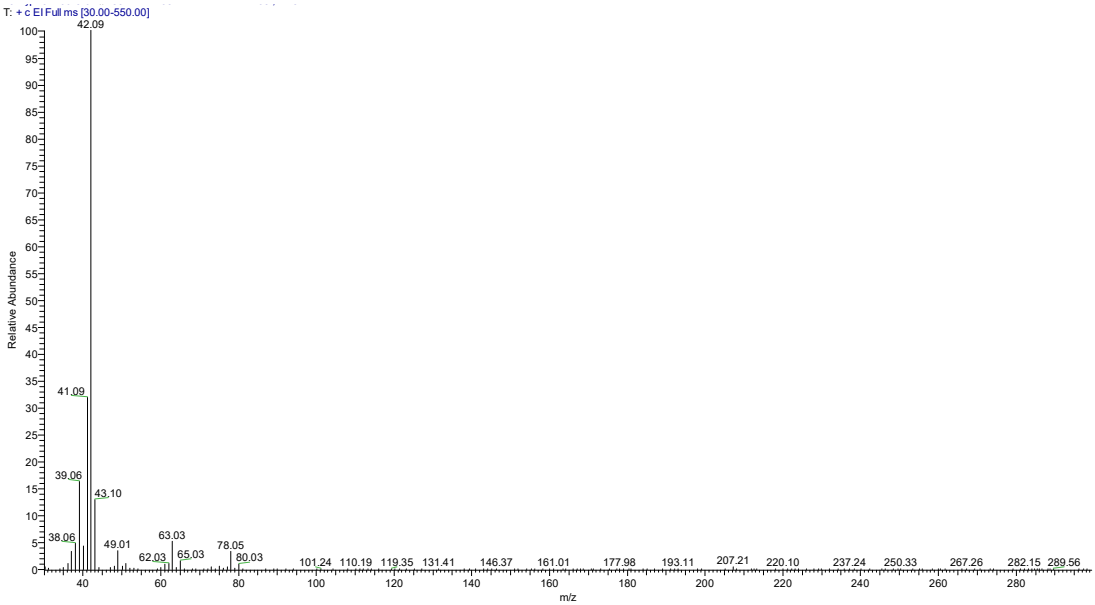



**Fig. S14.** Mass spectrum of 1-chloropropane

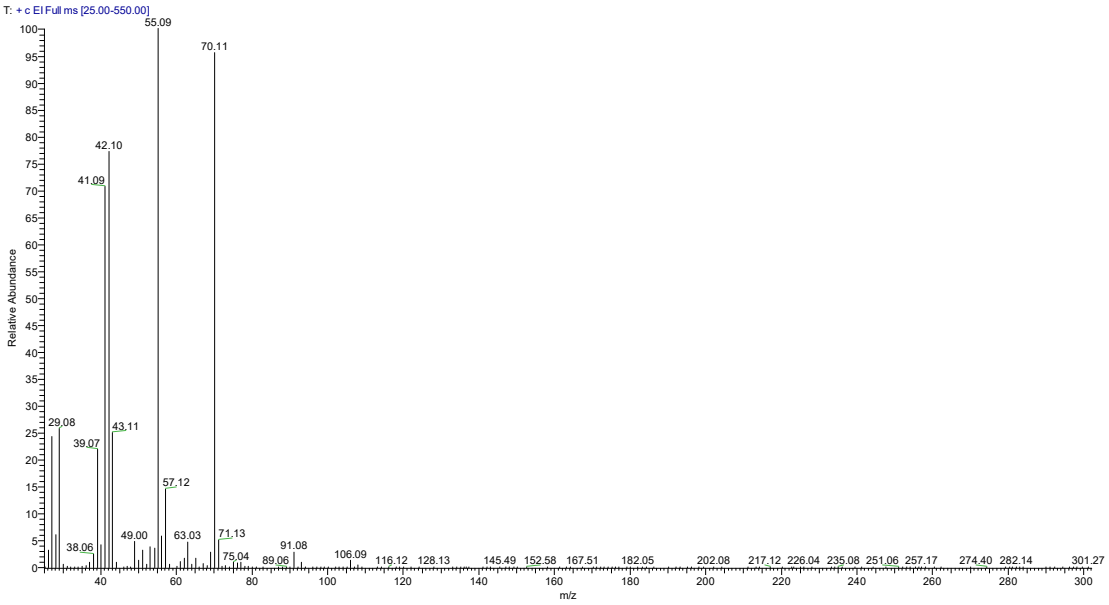



**Fig. S15.** Mass spectrum of 1-chloropentane

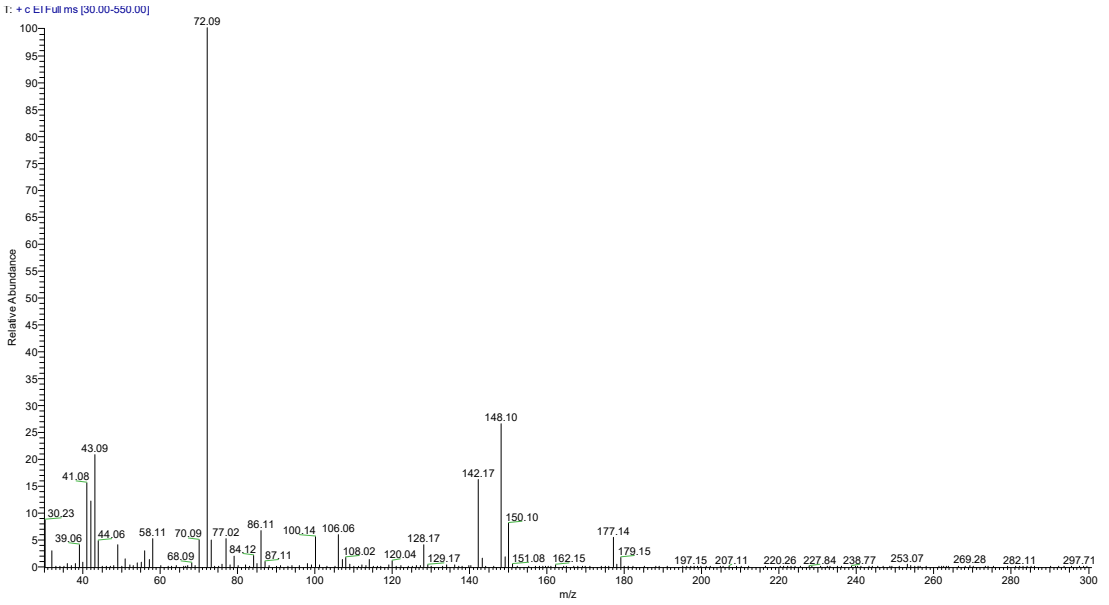



**Fig. S16.** Mass spectrum of *N,N*-dipropyl chloroacetamide

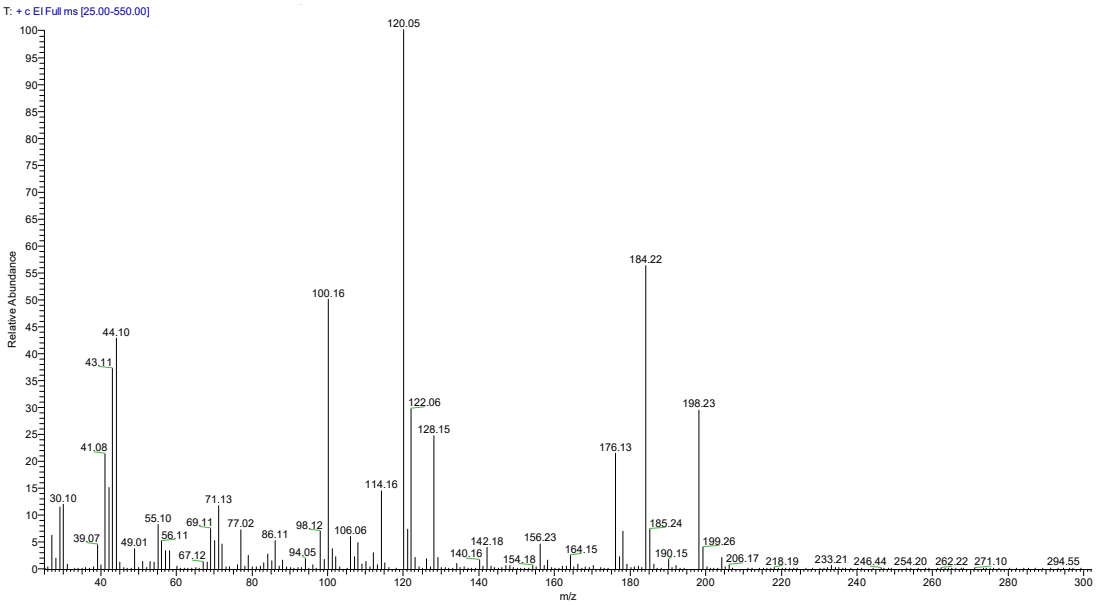



**Fig. S17.** Mass spectrum of *N,N*-diamyl chloroacetamide

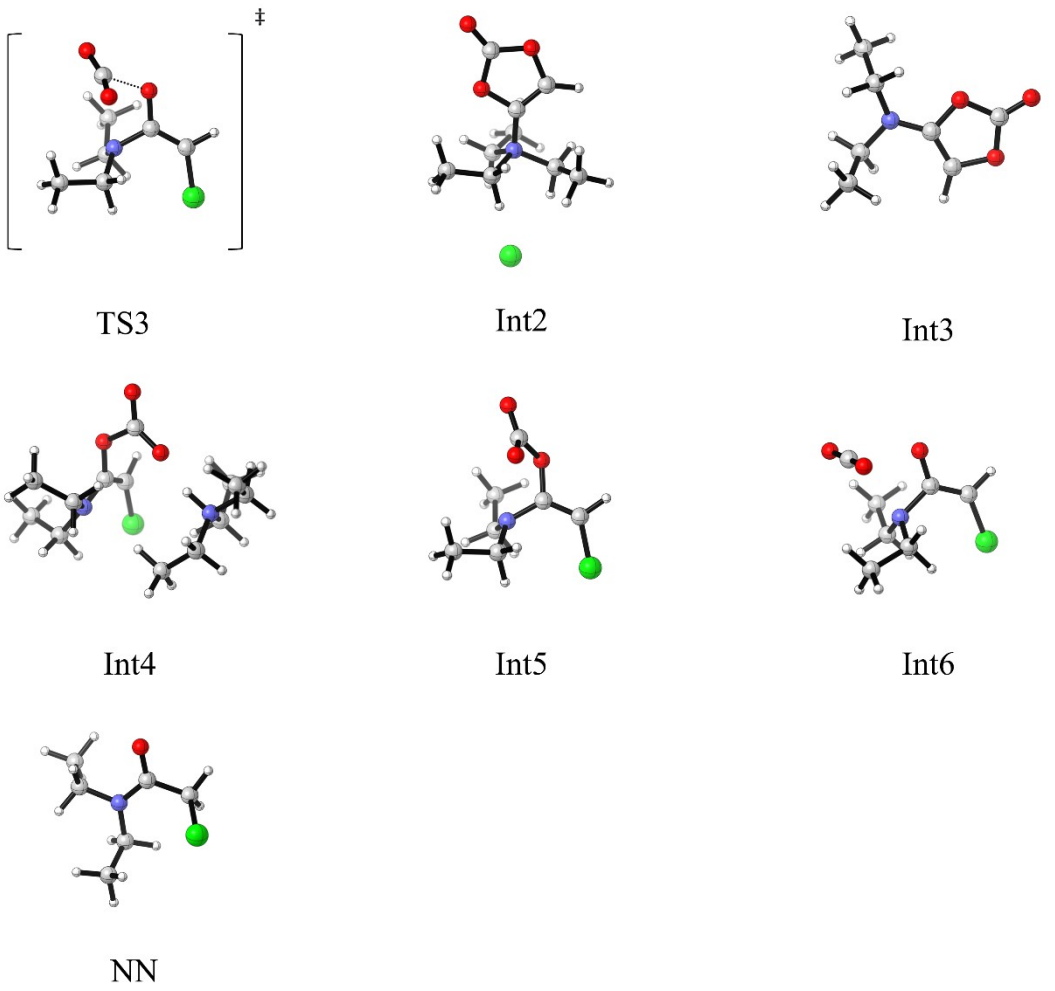



**Fig. S18.** Transition states, intermediates, and minima involved in chloroethane and

*N*,*N*-diethylchloroacetamide formation via I_a2.

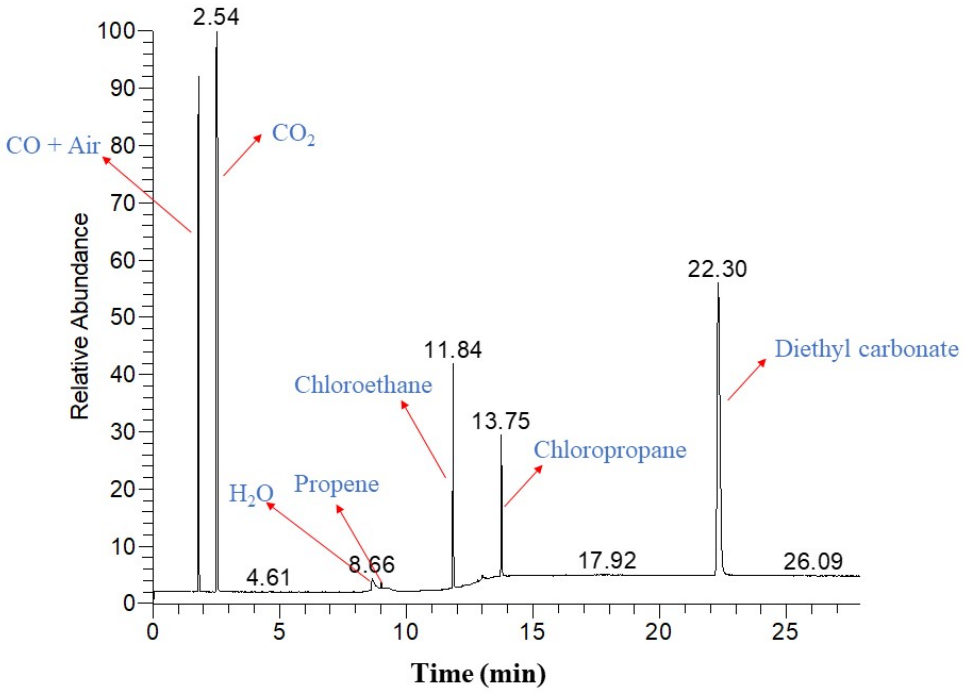



**Fig. S19.** Gas phase collected when DCEC reacts with TPA in the solvent DEC.

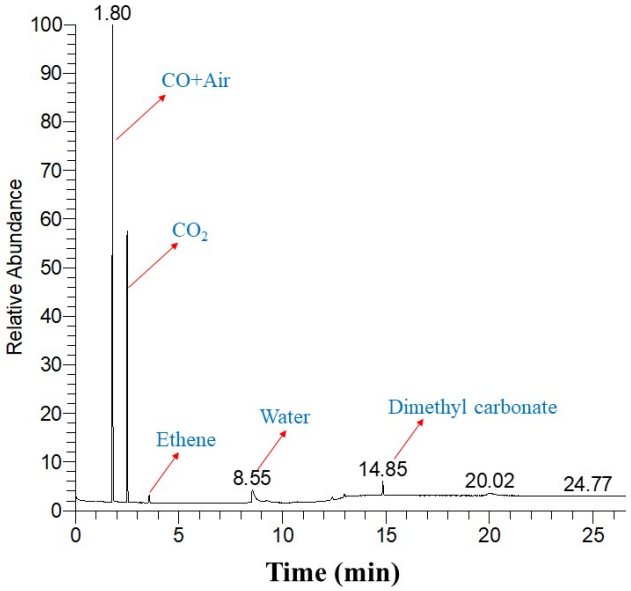



**Fig. S20.** Gas phase collected when TEA, TEA·HCl and DMC are mixed in one pot.

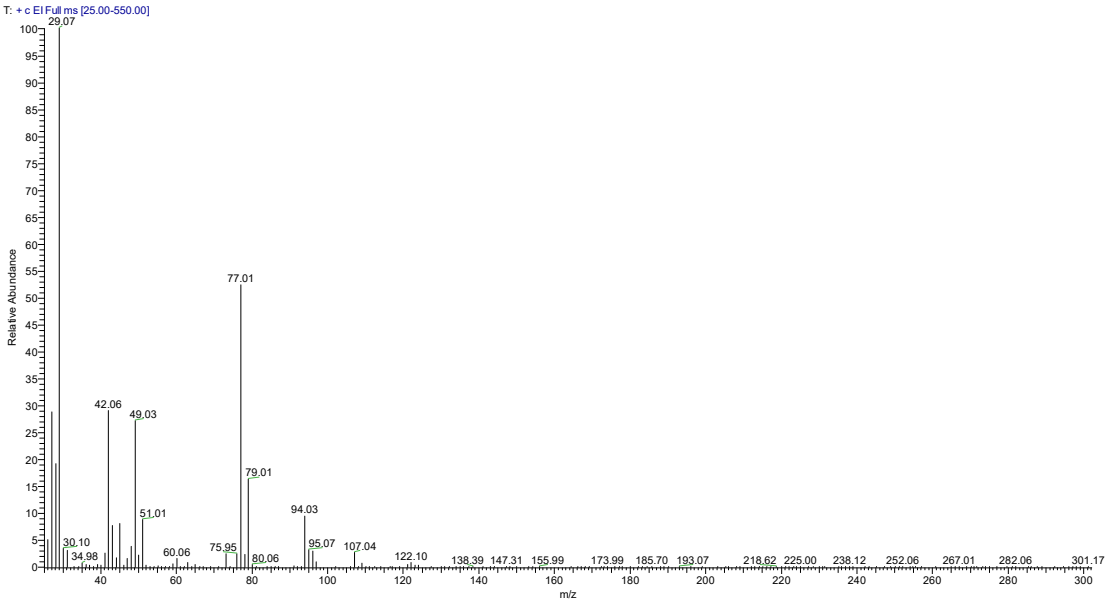



**Fig. S21.** Mass spectrum of ethyl chloroacetate

# 4. Cartesian coordinates

## 4.1 Cartesian coordinates of the structures depicted in Fig. 7

***R_cis***

| | | | |
|---|---|---|---|
| C | -0.36270500 | 0.78097200 | 0.59182300 |
| C | -0.04267200 | -0.71515300 | 0.78472600 |
| C | 1.73302300 | 0.35432700 | -0.11215200 |
| O | 2.81545500 | 0.51251400 | -0.56179600 |
| O | 1.34642500 | -0.73455700 | 0.59909300 |
| O | 0.71604600 | 1.23186200 | -0.20518200 |
| Cl | -0.82590100 | -1.82041200 | -0.39007500 |
| H | -0.33964300 | 1.29141300 | 1.55237600 |
| H | -0.28603900 | -1.07940900 | 1.77518700 |
| Cl | -1.90137000 | 1.18444600 | -0.17291700 |

***R_trans***

| | | | |
|---|---|---|---|
| C | 0.23802900 | -0.21097900 | 1.40908700 |
| C | -0.46244100 | -0.04663400 | 0.05308900 |
| C | 1.77384200 | -0.12584200 | -0.24611800 |
| O | 2.80494200 | -0.12937100 | -0.82569400 |
| O | 0.55793400 | -0.23808200 | -0.86845700 |
| O | 1.60907100 | -0.01134800 | 1.07199500 |
| Cl | -1.14613300 | 1.60570300 | -0.15578300 |
| H | -0.06800100 | 0.52910900 | 2.14032400 |
| H | 0.10563400 | -1.22082000 | 1.79275300 |
| Cl | -1.74267800 | -1.25141800 | -0.21199200 |

***TS_E1***

| | | | |
|---|---|---|---|
| C | 1.78011100 | 0.35500800 | -0.98117800 |
| C | 0.85653500 | -0.62941800 | -0.57705300 |
| H | -0.82624100 | -0.05911800 | 0.00926000 |
| H | 2.07678200 | 0.53246200 | -2.00007900 |

| | | | |
|---|---|---|---|
| C | 2.49734100 | -0.45811000 | 0.95415000 |
| O | 3.15237000 | -0.56796800 | 1.94034800 |
| O | 1.37893600 | -1.11947200 | 0.66222300 |
| O | 2.78173900 | 0.41806700 | -0.05867100 |
| Cl | 0.93144900 | 2.40554700 | -0.86239400 |
| Cl | 0.55114200 | -1.94366100 | -1.73782100 |
| N | -1.79854500 | 0.08209600 | 0.41881800 |
| C | -2.57649100 | -1.16125500 | 0.10626200 |
| H | -2.48665800 | -1.31320200 | -0.96619900 |
| H | -3.62115800 | -0.94650300 | 0.33691500 |
| C | -2.38813700 | 1.28120900 | -0.25395300 |
| H | -1.71998400 | 2.10961900 | -0.03725300 |
| H | -3.35546700 | 1.46961500 | 0.21516400 |
| C | -1.63815800 | 0.27656400 | 1.89527000 |
| H | -1.08713500 | -0.58869100 | 2.25460400 |
| H | -2.63867400 | 0.25028400 | 2.33035600 |
| C | -2.09593100 | -2.40001500 | 0.83778100 |
| H | -2.34259300 | -2.38284600 | 1.89812400 |
| H | -2.59206800 | -3.26390600 | 0.39589800 |
| H | -1.02088800 | -2.54226400 | 0.72481300 |
| C | -2.50600100 | 1.12274100 | -1.75711400 |
| H | -3.28822600 | 0.42475200 | -2.05200000 |
| H | -2.74875300 | 2.09577000 | -2.18337500 |
| H | -1.55528100 | 0.80294100 | -2.18734100 |
| C | -0.89628700 | 1.54186700 | 2.27713300 |
| H | -1.49356800 | 2.43982000 | 2.12600300 |
| H | -0.64700800 | 1.48094000 | 3.33618600 |
| H | 0.03044100 | 1.64703600 | 1.71186900 |

***TS_E2***

| | | | |
|---|---|---|---|
| H | -1.07169900 | -0.05669000 | -0.08274500 |
| N | -2.12405900 | 0.05981900 | -0.22997700 |
| C | -2.44246900 | -0.58316400 | -1.54294500 |
| H | -1.82160100 | -0.08536100 | -2.28408400 |

| | | | |
|---|---|---|---|
| H | -3.48661300 | -0.35883000 | -1.76669100 |
| C | -2.40917700 | 1.52934500 | -0.24298200 |
| H | -2.05302900 | 1.91858700 | 0.70739100 |
| H | -3.49350800 | 1.64672900 | -0.27511300 |
| C | -2.79434800 | -0.63119600 | 0.91682200 |
| H | -2.44831100 | -1.66105500 | 0.89487800 |
| H | -3.86693100 | -0.62443000 | 0.71645600 |
| C | -2.16986200 | -2.07503000 | -1.57763800 |
| H | -2.89511900 | -2.64883300 | -1.00318900 |
| H | -2.23132900 | -2.40716400 | -2.61354300 |
| H | -1.16816800 | -2.30573400 | -1.21128300 |
| C | -1.73464800 | 2.27553000 | -1.37854200 |
| H | -2.18644200 | 2.06757600 | -2.34689200 |
| H | -1.83533100 | 3.34365400 | -1.18893800 |
| H | -0.66831000 | 2.04979400 | -1.43031100 |
| C | -2.47024400 | -0.02080900 | 2.26712200 |
| H | -2.95852600 | 0.93952300 | 2.42426300 |
| H | -2.82430600 | -0.70204900 | 3.04023200 |
| H | -1.39398400 | 0.10104100 | 2.39973100 |
| C | 1.51292500 | -0.10302900 | -0.82730800 |
| C | 0.72581700 | -0.35717600 | 0.32209200 |
| H | 1.30101200 | -0.50865600 | -1.80205500 |
| C | 1.64801900 | 1.66437900 | 0.50373900 |
| O | 1.93836300 | 2.75899400 | 0.87200300 |
| O | 1.11899000 | 0.69001300 | 1.23244100 |
| O | 1.76981000 | 1.24450000 | -0.79610100 |
| Cl | 3.50975700 | -0.94916700 | -0.72471800 |
| Cl | 0.73478500 | -1.92542000 | 1.09664900 |

***CLVC***

| | | | |
|---|---|---|---|
| C | -0.01829900 | 1.32253900 | -0.00018000 |
| C | -0.63185600 | 0.15144900 | -0.00009800 |
| H | -0.35752900 | 2.34095600 | -0.00017100 |
| C | 1.52453700 | -0.25482300 | 0.00000200 |

| | | | |
|---|---|---|---|
| O | 2.56853600 | -0.81936000 | -0.00009400 |
| O | 0.30357700 | -0.85493100 | 0.00005900 |
| O | 1.34184900 | 1.08265600 | 0.00021100 |
| Cl | -2.27061500 | -0.28958000 | 0.00002500 |

***TS_a2***

| | | | |
|---|---|---|---|
| N | 0.96710800 | 0.60432700 | 0.04926300 |
| C | 1.06796000 | 0.96959200 | 1.50532800 |
| H | 0.07796000 | 1.28543000 | 1.81575900 |
| H | 1.72168300 | 1.84401000 | 1.53893700 |
| C | 2.30565200 | 0.14451500 | -0.44871400 |
| H | 2.57804200 | -0.73609800 | 0.11977700 |
| H | 3.01073400 | 0.93693000 | -0.18957300 |
| C | 0.59326500 | 1.83440800 | -0.73073200 |
| H | 0.31313700 | 1.47617900 | -1.71813400 |
| H | 1.50336800 | 2.43036000 | -0.80709400 |
| C | 2.38416600 | -0.16423400 | -1.93261300 |
| H | 2.21432100 | 0.71063300 | -2.55756800 |
| H | 3.39152000 | -0.52776700 | -2.13763300 |
| H | 1.68581500 | -0.94650900 | -2.22516600 |
| C | -0.53170200 | 2.69388100 | -0.18391900 |
| H | -0.28215800 | 3.17574200 | 0.75995100 |
| H | -0.71223200 | 3.48154600 | -0.91617100 |
| H | -1.46623100 | 2.15114100 | -0.06137400 |
| C | 1.57732900 | -0.08417000 | 2.47004500 |
| H | 2.57616500 | -0.44302700 | 2.22618800 |
| H | 1.63051400 | 0.38949600 | 3.45134000 |
| H | 0.90473700 | -0.93464700 | 2.54281400 |
| C | -0.95736500 | -0.51399600 | -1.48037300 |
| C | -0.30868000 | -0.58113500 | -0.25316100 |
| O | -1.24134000 | -0.29838500 | 0.72380900 |
| C | -2.47770900 | -0.18140400 | 0.13247900 |
| O | -3.47045400 | 0.05724900 | 0.75736300 |
| O | -2.35347800 | -0.32712100 | -1.16141700 |

| | | | |
|---|---|---|---|
| Cl | 0.55778600 | -2.20564800 | 0.18164000 |
| H | -0.79481200 | -1.18637600 | -2.30285400 |

***TS_a1***

| | | | |
|---|---|---|---|
| N | 1.38165200 | 0.11236800 | 0.14394800 |
| C | 2.16957800 | -1.02514600 | -0.40085600 |
| H | 1.61558900 | -1.93290000 | -0.18081500 |
| H | 3.11154100 | -1.06694800 | 0.15485000 |
| C | 2.02030500 | 1.40313200 | -0.23355100 |
| H | 1.96193000 | 1.48603600 | -1.31817600 |
| H | 3.08075300 | 1.32993900 | 0.02477800 |
| C | 1.23274000 | 0.02646100 | 1.61398200 |
| H | 0.40504000 | 0.69635100 | 1.85875100 |
| H | 2.14666900 | 0.41863800 | 2.06703000 |
| C | 1.41827300 | 2.64928000 | 0.39370400 |
| H | 1.54874300 | 2.67632800 | 1.47425600 |
| H | 1.93531100 | 3.51351900 | -0.02432700 |
| H | 0.35734700 | 2.75331800 | 0.17289100 |
| C | 0.93308100 | -1.35283300 | 2.17486700 |
| H | 1.76924300 | -2.04315600 | 2.07022000 |
| H | 0.72863400 | -1.23941500 | 3.23966600 |
| H | 0.05119000 | -1.80975200 | 1.72723400 |
| C | 2.45118400 | -0.96560000 | -1.89300500 |
| H | 3.13256900 | -0.15982700 | -2.16248700 |
| H | 2.92447200 | -1.90446700 | -2.18102900 |
| H | 1.53814400 | -0.86887900 | -2.48025200 |
| C | -1.33084400 | 0.59757800 | 0.22168500 |
| C | -0.32432200 | 0.13994400 | -0.64796900 |
| O | -0.55745700 | -1.20176000 | -0.90484000 |
| H | -0.01706300 | 0.70388200 | -1.51891500 |
| C | -1.64893100 | -1.59376600 | -0.18150100 |
| O | -2.04385000 | -2.72006700 | -0.15029300 |
| O | -2.13201500 | -0.56111600 | 0.49141000 |
| Cl | -2.33067600 | 1.95588200 | -0.33562700 |

***I_a2***

| | | | |
|---|---|---|---|
| N | -1.29500600 | 0.13488200 | 0.11368200 |
| C | -1.50211700 | 0.05413600 | 1.63062600 |
| H | -1.31439600 | -0.97849300 | 1.90750700 |
| H | -2.56213900 | 0.26061400 | 1.76868300 |
| C | -1.25036500 | 1.61943200 | -0.27939000 |
| H | -0.30876900 | 1.99168400 | 0.12368600 |
| H | -2.09594500 | 2.06494300 | 0.24241700 |
| C | -2.46845900 | -0.55155200 | -0.57425900 |
| H | -2.25534100 | -0.52837500 | -1.63913300 |
| H | -3.32878000 | 0.08930600 | -0.38643000 |
| C | -1.31108200 | 1.90966300 | -1.75917700 |
| H | -2.23651400 | 1.58598900 | -2.23273300 |
| H | -1.25178800 | 2.99369500 | -1.85881100 |
| H | -0.45330600 | 1.50145200 | -2.29066900 |
| C | -2.71133600 | -1.97246700 | -0.11471000 |
| H | -3.08795200 | -2.02550200 | 0.90471200 |
| H | -3.46649000 | -2.40395300 | -0.77105400 |
| H | -1.81293800 | -2.58525100 | -0.19789400 |
| C | -0.65300400 | 1.00334100 | 2.45329700 |
| H | -1.00695600 | 2.03017500 | 2.38903100 |
| H | -0.73898100 | 0.68485900 | 3.49231700 |
| H | 0.39773600 | 0.97512600 | 2.17098700 |
| C | 0.43435800 | -0.84476800 | -1.45535800 |
| C | -0.07064200 | -0.53009600 | -0.27512800 |
| O | 0.78697600 | -0.92172700 | 0.70838900 |
| C | 1.88701800 | -1.43256100 | 0.09028900 |
| O | 2.84307400 | -1.86745200 | 0.63637700 |
| O | 1.65928600 | -1.42014400 | -1.24327600 |
| Cl | 2.23800700 | 1.89898900 | -0.06220800 |
| H | 0.10056400 | -0.73943800 | -2.46992600 |

***I_a1***

| | | | |
|---|---|---|---|
| N | -1.26565300 | 0.04592500 | -0.07582200 |
| C | -2.04508000 | -0.89912500 | 0.81422600 |
| H | -1.52880300 | -1.85187500 | 0.78164200 |
| H | -3.01448200 | -1.01802600 | 0.33050800 |
| C | -1.95796700 | 1.39983100 | -0.03898900 |
| H | -1.79731500 | 1.79645400 | 0.96051900 |
| H | -3.01997000 | 1.17819700 | -0.14179000 |
| C | -1.29325100 | -0.46581500 | -1.50196100 |
| H | -0.54488000 | 0.12710800 | -2.02426000 |
| H | -2.27949700 | -0.20441200 | -1.88333900 |
| C | -1.52997400 | 2.42228300 | -1.07325000 |
| H | -1.78435300 | 2.11871500 | -2.08729500 |
| H | -2.07897100 | 3.33880000 | -0.85321100 |
| H | -0.46292700 | 2.62373200 | -1.02924400 |
| C | -1.05210500 | -1.94976000 | -1.70447200 |
| H | -1.85342200 | -2.56611200 | -1.30071500 |
| H | -1.02155000 | -2.11564200 | -2.78154400 |
| H | -0.10526400 | -2.30123200 | -1.30107100 |
| C | -2.21185000 | -0.45882800 | 2.25563000 |
| H | -2.80641400 | 0.44689700 | 2.36010900 |
| H | -2.73973700 | -1.25892900 | 2.77449100 |
| H | -1.25608800 | -0.32239000 | 2.76035600 |
| C | 1.14835700 | 0.75890000 | -0.55954200 |
| C | 0.16827600 | 0.23375200 | 0.47461600 |
| O | 0.65126800 | -1.01811500 | 0.90642100 |
| H | 0.04784000 | 0.88278200 | 1.33468900 |
| C | 1.69374300 | -1.38056500 | 0.11026000 |
| O | 2.25118900 | -2.43117200 | 0.20876200 |
| O | 1.93244600 | -0.43809600 | -0.79214300 |
| Cl | 2.28854600 | 1.87879300 | 0.43455700 |

***TS_a3***

| | | | |
|---|---|---|---|
| N | 1.67350600 | 1.08670000 | 0.32097600 |
| C | 2.31654600 | 1.54833800 | -0.96600500 |

| | | | |
|---|---|---|---|
| H | 2.82950200 | 0.69051200 | -1.38574400 |
| H | 3.07173600 | 2.27541300 | -0.66470700 |
| C | 0.84595700 | 2.21731700 | 0.86997100 |
| H | 0.03345600 | 2.35486300 | 0.16656400 |
| H | 1.46744000 | 3.11548700 | 0.85611800 |
| C | 2.80700000 | 0.85669800 | 1.30920200 |
| H | 2.35622700 | 0.38445900 | 2.17350600 |
| H | 3.16935300 | 1.85117300 | 1.57734500 |
| C | 0.29160900 | 1.96403600 | 2.25707800 |
| H | 1.05406400 | 2.03701800 | 3.03069700 |
| H | -0.46901100 | 2.71665800 | 2.46956300 |
| H | -0.16669100 | 0.97701700 | 2.31149100 |
| C | 3.95592600 | 0.00114500 | 0.81542000 |
| H | 4.55552600 | 0.49186000 | 0.05001100 |
| H | 4.60584500 | -0.18990700 | 1.67042200 |
| H | 3.61818000 | -0.96470900 | 0.44581300 |
| C | 1.41607900 | 2.16549400 | -2.01487900 |
| H | 0.99775200 | 3.12044300 | -1.69916100 |
| H | 2.03160600 | 2.35884700 | -2.89432300 |
| H | 0.62017000 | 1.48801300 | -2.31329200 |
| C | 1.12088500 | -1.26461500 | 0.99026500 |
| C | 0.67863200 | -0.14813600 | 0.12710500 |
| O | 0.88267300 | -0.62539300 | -1.23910700 |
| H | -1.26653500 | 0.17200800 | 0.03022000 |
| C | 1.39842600 | -1.85131800 | -1.20595500 |
| O | 1.66492200 | -2.50938900 | -2.17740400 |
| O | 1.59060900 | -2.24125100 | 0.05891800 |
| Cl | -0.64388400 | -2.29351400 | 1.62758400 |
| N | -2.29768500 | 0.29207400 | -0.27795600 |
| C | -2.64590800 | 1.75258500 | -0.24474600 |
| H | -2.23220300 | 2.14261600 | 0.68331700 |
| H | -3.73239400 | 1.80912300 | -0.17067100 |
| C | -2.37654200 | -0.26908000 | -1.66581400 |
| H | -1.57455300 | 0.20479500 | -2.22705000 |

| | | | |
|---|---|---|---|
| H | -3.33075600 | 0.04774700 | -2.08980800 |
| C | -3.20208000 | -0.44904200 | 0.65963000 |
| H | -2.85343900 | -1.47548300 | 0.67949900 |
| H | -4.20042900 | -0.41269100 | 0.21835400 |
| C | -2.22631800 | -1.77654700 | -1.73227600 |
| H | -3.12817300 | -2.29540600 | -1.41010600 |
| H | -2.02981900 | -2.05407700 | -2.76752500 |
| H | -1.39473800 | -2.12268900 | -1.11989900 |
| C | -3.20029400 | 0.09634200 | 2.07282800 |
| H | -3.64502000 | 1.08767100 | 2.15310400 |
| H | -3.78486800 | -0.58231800 | 2.69401400 |
| H | -2.18835900 | 0.11427900 | 2.47567700 |
| C | -2.17915700 | 2.58258300 | -1.42342600 |
| H | -2.70177400 | 2.32594600 | -2.34323300 |
| H | -2.39563000 | 3.62729200 | -1.19924500 |
| H | -1.11139000 | 2.49580900 | -1.60066100 |

***I_a3***

| | | | |
|---|---|---|---|
| N | -0.99623700 | 0.10855800 | -0.05360500 |
| C | -1.15602400 | 0.79434900 | -1.40340000 |
| H | -0.42167500 | 1.59427500 | -1.41993400 |
| H | -2.15173300 | 1.23748400 | -1.39671400 |
| C | -1.94779100 | -1.08054200 | 0.00327600 |
| H | -1.52219400 | -1.82768800 | -0.65874200 |
| H | -2.88225500 | -0.71311200 | -0.41963400 |
| C | -1.39019100 | 1.08142500 | 1.05504000 |
| H | -1.07804800 | 0.60167500 | 1.97874000 |
| H | -2.47916700 | 1.11646000 | 1.03104600 |
| C | -2.17361400 | -1.67517300 | 1.37848200 |
| H | -2.73821400 | -1.01760500 | 2.03757900 |
| H | -2.76009100 | -2.58386200 | 1.23810900 |
| H | -1.23240900 | -1.95372600 | 1.84751400 |
| C | -0.82818800 | 2.48648300 | 0.96743200 |
| H | -1.21835100 | 3.03974900 | 0.11467600 |

| | | | |
|---|---|---|---|
| H | -1.15175300 | 3.00776500 | 1.86911300 |
| H | 0.25777900 | 2.49910900 | 0.93943400 |
| C | -0.95930800 | -0.12015800 | -2.59240400 |
| H | -1.77047300 | -0.83662200 | -2.70988300 |
| H | -0.93144300 | 0.50239600 | -3.48657500 |
| H | -0.01520700 | -0.66057200 | -2.52495700 |
| C | 0.84841900 | -1.61384000 | 0.20132600 |
| C | 0.36470900 | -0.37218800 | 0.09834700 |
| O | 1.33396400 | 0.63038300 | 0.03095400 |
| C | 2.50963500 | -0.02767700 | 0.12224700 |
| O | 3.58556400 | 0.50322700 | 0.11079100 |
| O | 2.26334800 | -1.33382400 | 0.22742800 |

***TS_a4***

| | | | |
|---|---|---|---|
| N | 1.55323100 | -1.10976000 | 0.09579100 |
| C | 1.92317100 | -1.30983500 | 1.56096700 |
| H | 2.83313500 | -0.73745700 | 1.71906200 |
| H | 2.15654800 | -2.36930200 | 1.66309300 |
| C | 0.23394300 | -1.82535600 | -0.17752600 |
| H | -0.53147700 | -1.25876000 | 0.35418400 |
| H | 0.34195100 | -2.79823300 | 0.30003500 |
| C | 2.62989400 | -1.72768400 | -0.79590900 |
| H | 2.41300400 | -1.36726200 | -1.79830000 |
| H | 2.43676600 | -2.79926000 | -0.76349700 |
| C | -0.13349900 | -1.98114200 | -1.63972700 |
| H | 0.50848000 | -2.68430500 | -2.16755900 |
| H | -1.14776800 | -2.38068200 | -1.66919000 |
| H | -0.13519200 | -1.02769200 | -2.16539100 |
| C | 4.07265400 | -1.45077300 | -0.42385200 |
| H | 4.35573100 | -1.91202300 | 0.52066800 |
| H | 4.68529700 | -1.90407600 | -1.20383300 |
| H | 4.30080800 | -0.38906600 | -0.39120600 |
| C | 0.85031100 | -0.87644100 | 2.53546600 |
| H | -0.02612600 | -1.52104000 | 2.51355800 |

| | | | |
|---|---|---|---|
| H | 1.27834000 | -0.92453800 | 3.53647200 |
| H | 0.53315500 | 0.15031600 | 2.35357500 |
| C | 0.27428600 | 1.00598900 | -0.44487000 |
| C | 1.36615100 | 0.29565700 | -0.17390900 |
| O | 2.50149500 | 1.08502100 | -0.04722400 |
| C | 2.08308900 | 2.35214200 | -0.27240500 |
| O | 2.78405800 | 3.31667000 | -0.26173400 |
| O | 0.76156800 | 2.32473900 | -0.51123800 |
| C | -2.29092700 | 0.11564100 | 0.66906700 |
| C | -1.70889000 | 1.10907500 | -0.07283200 |
| H | -1.56812500 | 2.12232100 | 0.27656500 |
| O | -2.21631400 | 0.98702000 | -1.37228300 |
| O | -3.05137100 | -0.69116400 | -0.21941100 |
| C | -2.98915500 | -0.12069200 | -1.42458700 |
| O | -3.50608000 | -0.53533500 | -2.42043300 |
| Cl | -2.90353900 | 0.24436900 | 2.28650000 |

***I_a4***

| | | | |
|---|---|---|---|
| N | -1.64731300 | -1.02031500 | 0.22751500 |
| C | -1.97873600 | -1.78943600 | -1.05252900 |
| H | -2.74643700 | -1.20660800 | -1.55536800 |
| H | -2.42274300 | -2.72226900 | -0.70729000 |
| C | -0.58350500 | -1.78012800 | 1.02128900 |
| H | 0.32435400 | -1.75721500 | 0.40505700 |
| H | -0.96202100 | -2.79962200 | 1.07718800 |
| C | -2.91120600 | -0.95675700 | 1.11071900 |
| H | -2.72936400 | -0.16511800 | 1.83182800 |
| H | -2.90491800 | -1.90720200 | 1.63886800 |
| C | -0.31181700 | -1.20696300 | 2.39516800 |
| H | -1.13030200 | -1.35353800 | 3.09823100 |
| H | 0.56511300 | -1.72231400 | 2.78498100 |
| H | -0.06556200 | -0.14512800 | 2.35522600 |
| C | -4.24528800 | -0.77072400 | 0.41586900 |
| H | -4.52899600 | -1.63713900 | -0.17818200 |

| | | | |
|---|---|---|---|
| H | -4.98595300 | -0.66591200 | 1.20968300 |
| H | -4.28917800 | 0.12363700 | -0.19841900 |
| C | -0.81453800 | -2.04505800 | -1.97955800 |
| H | -0.02158300 | -2.62859300 | -1.51959700 |
| H | -1.20973000 | -2.60110700 | -2.83039000 |
| H | -0.38209900 | -1.12064700 | -2.35843900 |
| C | -0.03285100 | 0.90345300 | -0.41888000 |
| C | -1.18891500 | 0.31380900 | -0.10562400 |
| O | -2.20587300 | 1.23095400 | -0.19588900 |
| C | -1.66000800 | 2.41918200 | -0.55721000 |
| O | -2.25523000 | 3.43045500 | -0.71680400 |
| O | -0.33817700 | 2.22789100 | -0.69624000 |
| C | 1.92525900 | -0.78032300 | -0.36975000 |
| C | 1.43243500 | 0.63167500 | -0.62987600 |
| H | 1.65407600 | 0.96417900 | -1.64271000 |
| O | 2.15380400 | 1.48779600 | 0.28592200 |
| O | 2.50351300 | -0.59219000 | 0.94321900 |
| C | 2.71296300 | 0.69908600 | 1.22242100 |
| O | 3.28528700 | 1.11411300 | 2.18701100 |
| Cl | 3.42101100 | -0.97248500 | -1.51607500 |

***TS_a5***

| | | | |
|---|---|---|---|
| N | -2.62842100 | 0.18349700 | 0.85672400 |
| C | -2.25377500 | -0.74619400 | 2.00366700 |
| H | -2.36979200 | -1.75513800 | 1.61479100 |
| H | -3.01102300 | -0.58157000 | 2.77010200 |
| C | -2.42555500 | 1.63427400 | 1.29767300 |
| H | -1.34043900 | 1.75849900 | 1.42205900 |
| H | -2.93665400 | 1.70935300 | 2.25720100 |
| C | -4.12704300 | 0.00452200 | 0.56714900 |
| H | -4.30516200 | 0.47727600 | -0.39327800 |
| H | -4.61598800 | 0.59858200 | 1.33632900 |
| C | -2.92960700 | 2.65285900 | 0.30095900 |
| H | -4.01524100 | 2.69357900 | 0.22208200 |

| | | | |
|---|---|---|---|
| H | -2.57955500 | 3.62831300 | 0.63896800 |
| H | -2.50229400 | 2.48406500 | -0.68832600 |
| C | -4.67240000 | -1.41045300 | 0.58672300 |
| H | -4.67391900 | -1.84378500 | 1.58517800 |
| H | -5.71069800 | -1.34395500 | 0.25944600 |
| H | -4.15113300 | -2.07439100 | -0.09723800 |
| C | -0.86533200 | -0.55201000 | 2.56554300 |
| H | -0.73378300 | 0.41333400 | 3.04763200 |
| H | -0.70584100 | -1.33469700 | 3.30816400 |
| H | -0.10043500 | -0.64616900 | 1.79852100 |
| C | -0.58156800 | 0.14517300 | -0.75547300 |
| C | -1.83594400 | -0.10431300 | -0.32872700 |
| O | -2.49762400 | -0.88887800 | -1.27039800 |
| C | -1.65351500 | -1.08000400 | -2.29676300 |
| O | -1.89323700 | -1.69250300 | -3.28876700 |
| O | -0.49615500 | -0.46563800 | -2.00701000 |
| C | 0.58029100 | 1.80522000 | 0.66331300 |
| C | 0.69810200 | 0.66420300 | -0.28023500 |
| H | 1.56798000 | -0.59366400 | 0.13105700 |
| O | 1.38669700 | 1.22217800 | -1.46607400 |
| O | 0.72713100 | 2.92523300 | -0.23514900 |
| C | 1.30477500 | 2.54688700 | -1.38593000 |
| O | 1.68397000 | 3.30769500 | -2.23770400 |
| Cl | 2.31375600 | 1.89426800 | 1.63958700 |
| N | 2.27985200 | -1.57293200 | 0.20776100 |
| C | 2.77252700 | -1.75840400 | -1.19135900 |
| H | 1.90402000 | -1.65215000 | -1.83965400 |
| H | 3.13995000 | -2.78446700 | -1.27954600 |
| C | 3.41118100 | -1.33054400 | 1.14847400 |
| H | 3.82023600 | -0.35723200 | 0.89215500 |
| H | 4.17301400 | -2.09126500 | 0.95377600 |
| C | 1.50016300 | -2.76410500 | 0.64156700 |
| H | 1.16723000 | -2.57870800 | 1.65915300 |
| H | 2.19483700 | -3.60855600 | 0.67330100 |

| | | | |
|---|---|---|---|
| C | 3.02693500 | -1.33335700 | 2.61703200 |
| H | 2.82707300 | -2.33367900 | 3.00017800 |
| H | 3.86216900 | -0.92260800 | 3.18475600 |
| H | 2.16632100 | -0.69049400 | 2.79967600 |
| C | 0.29196500 | -3.11208800 | -0.20623800 |
| H | 0.53275100 | -3.28094200 | -1.25433600 |
| H | -0.14206500 | -4.03180600 | 0.18628800 |
| H | -0.47010700 | -2.33816000 | -0.13314900 |
| C | 3.84313100 | -0.77328500 | -1.62473100 |
| H | 4.79864600 | -0.95627800 | -1.13492300 |
| H | 3.99169000 | -0.88859100 | -2.69870800 |
| H | 3.53212200 | 0.25381300 | -1.44107500 |

***I_a5***

| | | | |
|---|---|---|---|
| N | 1.62861300 | -0.88214000 | -0.06097200 |
| C | 2.21609000 | -1.16691000 | 1.31955500 |
| H | 2.84565400 | -0.31245200 | 1.55473700 |
| H | 2.85380900 | -2.04073200 | 1.18633600 |
| C | 0.72899800 | -2.04603700 | -0.46656600 |
| H | -0.11200300 | -2.05308500 | 0.22802900 |
| H | 1.34109200 | -2.93119500 | -0.29994900 |
| C | 2.76483400 | -0.80169700 | -1.09572700 |
| H | 2.32815900 | -0.31743100 | -1.96542700 |
| H | 2.97422400 | -1.83927400 | -1.34828400 |
| C | 0.21612000 | -1.98556300 | -1.88874500 |
| H | 0.99069300 | -2.15087000 | -2.63602000 |
| H | -0.52192300 | -2.78143300 | -1.98963100 |
| H | -0.29428800 | -1.04668700 | -2.09979400 |
| C | 4.04829400 | -0.11387100 | -0.67489800 |
| H | 4.57880600 | -0.66297100 | 0.10087400 |
| H | 4.68933100 | -0.10031100 | -1.55731300 |
| H | 3.89629000 | 0.91287000 | -0.35612000 |
| C | 1.18681500 | -1.38369000 | 2.40500100 |
| H | 0.60085600 | -2.28828400 | 2.26182700 |

| | | | |
|---|---|---|---|
| H | 1.72680700 | -1.47128100 | 3.34811600 |
| H | 0.49879300 | -0.54308400 | 2.48642800 |
| C | -0.40708700 | 0.70444300 | 0.04871900 |
| C | 0.88466100 | 0.35487700 | -0.02790700 |
| O | 1.67270100 | 1.48693900 | 0.03686300 |
| C | 0.83765300 | 2.55422800 | 0.06814700 |
| O | 1.17497900 | 3.68998700 | 0.08482500 |
| O | -0.42758300 | 2.09270100 | 0.07568200 |
| C | -2.01099700 | -1.11929100 | 0.75790100 |
| C | -1.66642500 | 0.04414900 | 0.15570100 |
| O | -2.76618700 | 0.71641700 | -0.40557300 |
| O | -3.40577300 | -1.15498900 | 0.53210500 |
| C | -3.82525600 | -0.06751000 | -0.14758000 |
| O | -4.95298600 | 0.16424900 | -0.47498000 |

**4.2 Cartesian coordinates of the structures depicted in Fig. 10**

***Int2***

| | | | |
|---|---|---|---|
| C | 1.08742200 | 0.31337200 | -0.04215800 |
| C | 1.84836900 | 1.39489600 | -0.01587700 |
| C | 3.17536100 | -0.36641600 | -0.02990700 |
| O | 4.13364500 | -1.05964000 | -0.03234600 |
| O | 3.15884800 | 0.98609600 | -0.01462700 |
| O | 1.88285900 | -0.80056900 | -0.04429700 |
| Cl | -4.09277500 | -0.34259800 | 0.10343900 |
| N | -0.33133900 | 0.10098900 | -0.01452700 |
| C | -0.81723900 | -0.62914200 | -1.27921900 |
| H | -0.36632100 | -0.09272200 | -2.11041800 |
| H | -1.89615600 | -0.46796500 | -1.27054900 |
| C | -1.05181900 | 1.44828900 | 0.05937800 |
| H | -0.58217700 | 1.99708600 | 0.87138900 |
| H | -2.07199200 | 1.18596900 | 0.34401600 |
| C | -0.70455400 | -0.72156300 | 1.22327600 |
| H | -0.14836100 | -1.65066400 | 1.14126000 |

| | | | |
|---|---|---|---|
| H | -1.77107200 | -0.91863600 | 1.10112500 |
| C | -0.51981600 | -2.11092400 | -1.35922300 |
| H | -1.07464600 | -2.68123000 | -0.61672900 |
| H | -0.86825400 | -2.43554600 | -2.34034400 |
| H | 0.53931800 | -2.34549900 | -1.28570900 |
| C | -1.06063800 | 2.25209500 | -1.22616900 |
| H | -1.73116900 | 1.82232400 | -1.96735600 |
| H | -1.44212100 | 3.24192000 | -0.97571500 |
| H | -0.07546200 | 2.37969300 | -1.67323600 |
| C | -0.40286400 | -0.03341200 | 2.53534300 |
| H | -1.05194200 | 0.82068500 | 2.71832900 |
| H | -0.58678500 | -0.76031800 | 3.32617200 |
| H | 0.63910200 | 0.28082300 | 2.61391000 |
| H | 1.65644100 | 2.45105700 | 0.00458400 |

***TS1***

| | | | |
|---|---|---|---|
| C | -1.02974600 | 0.39537700 | -0.06655600 |
| C | -1.80573400 | 0.86200500 | -1.04795500 |
| C | -3.02599000 | -0.53411100 | 0.14716800 |
| O | -3.92118300 | -1.19668400 | 0.56432500 |
| O | -3.05975800 | 0.27397800 | -0.92023600 |
| O | -1.77887200 | -0.48171900 | 0.68899600 |
| Cl | 3.58726000 | -0.56497000 | -0.00352000 |
| N | 0.29790600 | 0.53062500 | 0.24831000 |
| C | 0.96874700 | 1.59112700 | -0.52550300 |
| H | 0.70000100 | 1.45830100 | -1.57488500 |
| H | 2.03461100 | 1.38456000 | -0.44254800 |
| C | 1.12029200 | -1.74049200 | -0.85262800 |
| H | 0.25304500 | -1.85870900 | -0.22017600 |
| H | 2.03155200 | -2.22628200 | -0.53999900 |
| C | 0.65106400 | 0.52723200 | 1.69073500 |
| H | -0.04319200 | 1.17810900 | 2.23035900 |
| H | 1.64000600 | 0.97811300 | 1.74207700 |
| C | 0.64244900 | 3.00857100 | -0.07124900 |

| | | | |
|---|---|---|---|
| H | 0.98541000 | 3.18639800 | 0.94847400 |
| H | 1.15526400 | 3.71723100 | -0.72233200 |
| H | -0.42694900 | 3.21956100 | -0.11627200 |
| C | 0.98157900 | -1.29270100 | -2.21534200 |
| H | 1.91660000 | -0.93534000 | -2.63964100 |
| H | 0.72806100 | -2.23607800 | -2.73941900 |
| H | 0.14405000 | -0.61800100 | -2.38438800 |
| C | 0.71663300 | -0.84407000 | 2.33997000 |
| H | 1.50688200 | -1.43930300 | 1.88353900 |
| H | 0.96706200 | -0.71253200 | 3.39376900 |
| H | -0.22872300 | -1.38033100 | 2.28641600 |
| H | -1.66970500 | 1.57219100 | -1.83983300 |

***Int3***

| | | | |
|---|---|---|---|
| C | 0.23204900 | -0.26793700 | -0.09774100 |
| C | 0.91050000 | -1.40159900 | -0.31324200 |
| C | 2.38979200 | 0.19404400 | 0.07526600 |
| O | 3.40239000 | 0.80049700 | 0.25357700 |
| O | 2.27924400 | -1.09762300 | -0.22816700 |
| O | 1.14511500 | 0.73620900 | 0.15480600 |
| N | -1.06908600 | 0.08413400 | -0.14980500 |
| C | -2.02866500 | -0.93809800 | -0.53764100 |
| H | -1.61294600 | -1.48603200 | -1.38689700 |
| H | -2.91826900 | -0.42260900 | -0.90291900 |
| C | -1.56036200 | 1.26474900 | 0.55873300 |
| H | -0.79688200 | 1.60203600 | 1.25804800 |
| H | -2.42374300 | 0.96468200 | 1.15796300 |
| C | -2.40234200 | -1.89995600 | 0.58623100 |
| H | -2.85381900 | -1.36605800 | 1.42420900 |
| H | -3.12472000 | -2.63330900 | 0.22488000 |
| H | -1.52768100 | -2.43685900 | 0.95591500 |
| C | -1.94068000 | 2.39183900 | -0.38987700 |
| H | -2.69967100 | 2.06352600 | -1.10246700 |
| H | -2.34475100 | 3.23675200 | 0.17067500 |

| | | | |
|---|---|---|---|
| H | -1.06812900 | 2.73215000 | -0.94889100 |
| H | 0.63848100 | -2.41413500 | -0.53398500 |

***TS2***

| | | | |
|---|---|---|---|
| C | 0.49792000 | 0.64277600 | -0.57691700 |
| C | 1.48028600 | -0.26482100 | -0.25951600 |
| O | 1.13869300 | -1.58969600 | -0.30320200 |
| O | -0.64783800 | -0.78245300 | -1.29447200 |
| H | 0.16136000 | 1.26130500 | -1.37824400 |
| C | -0.13273100 | -1.83603400 | -0.80029600 |
| O | -0.58097400 | -2.95606200 | -0.69919900 |
| H | -1.98632100 | -0.14128800 | -0.35217100 |
| N | -2.77869000 | 0.17137800 | 0.24280700 |
| C | -4.02938000 | -0.21525000 | -0.48549200 |
| H | -3.99328900 | 0.29487900 | -1.44430800 |
| H | -4.86712300 | 0.18667600 | 0.08606900 |
| C | -2.64475500 | 1.65504600 | 0.40863500 |
| H | -1.65671200 | 1.82675100 | 0.83057300 |
| H | -3.40220000 | 1.96449300 | 1.13001300 |
| C | -2.65472900 | -0.55862500 | 1.54837700 |
| H | -2.58768400 | -1.61443700 | 1.29663400 |
| H | -3.58759700 | -0.39323400 | 2.08903000 |
| C | -4.15531500 | -1.71074400 | -0.70717800 |
| H | -4.40612000 | -2.24942800 | 0.20520700 |
| H | -4.95676100 | -1.88328700 | -1.42500500 |
| H | -3.23414300 | -2.12636900 | -1.12025600 |
| C | -2.76160600 | 2.41961700 | -0.89524400 |
| H | -3.78295400 | 2.47197200 | -1.26974200 |
| H | -2.41405100 | 3.43731300 | -0.72095000 |
| H | -2.12485100 | 1.98334500 | -1.66711700 |
| C | -1.45143100 | -0.14951800 | 2.37584000 |
| H | -1.56999700 | 0.83451300 | 2.82630400 |
| H | -1.33343300 | -0.87536100 | 3.17997700 |
| H | -0.53844100 | -0.14379600 | 1.77930100 |

| | | | |
|---|---|---|---|
| Cl | 1.00956000 | 2.62172000 | 0.51098400 |
| N | 2.71220100 | -0.07597700 | 0.23257000 |
| C | 3.61594200 | 0.98835400 | -0.20976200 |
| H | 4.61884000 | 0.63069100 | 0.02700600 |
| H | 3.43807100 | 1.89587200 | 0.36857200 |
| C | 3.25498600 | -1.02073600 | 1.21270100 |
| H | 2.42562900 | -1.48493500 | 1.74316300 |
| H | 3.80995600 | -0.43026700 | 1.94508200 |
| C | 3.54084300 | 1.28736000 | -1.69565400 |
| H | 4.33928500 | 1.98286200 | -1.95801900 |
| H | 3.66705900 | 0.37718300 | -2.28539500 |
| H | 2.59346000 | 1.75236900 | -1.96557700 |
| C | 4.15210500 | -2.08692200 | 0.59939400 |
| H | 4.98537800 | -1.63808200 | 0.05518800 |
| H | 4.56733000 | -2.72031800 | 1.38529600 |
| H | 3.58636100 | -2.71380200 | -0.08934700 |

***Int4***

| | | | |
|---|---|---|---|
| C | -1.07350000 | -1.01302500 | -1.37507700 |
| C | -1.37626000 | 0.08499100 | -0.66356000 |
| O | -1.25264000 | 1.27376200 | -1.33555400 |
| O | 0.91471000 | 1.48433300 | -0.68696600 |
| H | -0.82601400 | -0.94185600 | -2.42043900 |
| C | 0.00713100 | 1.93393600 | -1.41728500 |
| O | 0.00130100 | 2.88464200 | -2.18022500 |
| H | 1.68975200 | 0.27131600 | 0.05528300 |
| N | 2.43428200 | -0.33431400 | 0.48458700 |
| C | 3.73339200 | 0.36306400 | 0.21598500 |
| H | 3.79149100 | 0.48433300 | -0.86216200 |
| H | 4.52925000 | -0.31392900 | 0.53136700 |
| C | 2.37607500 | -1.66164700 | -0.20069100 |
| H | 1.40251600 | -2.08421500 | 0.02862200 |
| H | 3.14312800 | -2.29355400 | 0.25060900 |
| C | 2.15522200 | -0.44087300 | 1.95020000 |

| | | | |
|---|---|---|---|
| H | 2.11298100 | 0.57874800 | 2.32440200 |
| H | 3.01488100 | -0.93629800 | 2.40516500 |
| C | 3.85298600 | 1.72053300 | 0.88115700 |
| H | 3.98409000 | 1.65142200 | 1.96017700 |
| H | 4.73164300 | 2.22050500 | 0.47376200 |
| H | 2.98064500 | 2.33517100 | 0.65738000 |
| C | 2.52955200 | -1.56467800 | -1.70648000 |
| H | 3.55051900 | -1.34768900 | -2.01706800 |
| H | 2.24577900 | -2.52331600 | -2.14049900 |
| H | 1.86201000 | -0.80219300 | -2.11099400 |
| C | 0.85753200 | -1.15372300 | 2.27787300 |
| H | 0.91663200 | -2.22959800 | 2.11994500 |
| H | 0.63423800 | -0.98597900 | 3.33158600 |
| H | 0.02862200 | -0.75531700 | 1.68934800 |
| Cl | -1.07750400 | -2.66063900 | -0.76939000 |
| N | -1.87597300 | 0.17810300 | 0.60861300 |
| C | -2.88359500 | -0.76219500 | 1.10079300 |
| H | -3.17832000 | -0.40072100 | 2.08627900 |
| H | -2.44272600 | -1.74842200 | 1.25138200 |
| C | -1.75128800 | 1.43711100 | 1.33828500 |
| H | -0.82286000 | 1.91841500 | 1.03735400 |
| H | -1.63263500 | 1.18093100 | 2.39492500 |
| C | -4.11292900 | -0.87785700 | 0.20928700 |
| H | -4.83179400 | -1.56540400 | 0.65871000 |
| H | -4.59348100 | 0.09293400 | 0.07906800 |
| H | -3.84868700 | -1.26332600 | -0.77635100 |
| C | -2.92720100 | 2.39057700 | 1.16624500 |
| H | -3.85685200 | 1.94194300 | 1.52255600 |
| H | -2.75508700 | 3.30263300 | 1.74131700 |
| H | -3.04998400 | 2.65861400 | 0.11705800 |

***Int5***

| | | | |
|---|---|---|---|
| C | 0.96113500 | -1.59084200 | 0.01184800 |
| C | 0.04483700 | -0.63607200 | 0.17201500 |

| | | | |
|---|---|---|---|
| O | -1.20609800 | -1.04467000 | 0.50668800 |
| O | -3.37968000 | -0.74143700 | 0.11795800 |
| H | 0.70494500 | -2.63797400 | -0.01189000 |
| C | -2.28047400 | -0.72929300 | -0.43160900 |
| O | -1.92998000 | -0.54887900 | -1.59728700 |
| Cl | 2.68387300 | -1.28678700 | -0.14192400 |
| N | 0.23466400 | 0.75137200 | 0.10553100 |
| C | 0.55645400 | 1.40943900 | 1.37106200 |
| H | 0.55472300 | 2.48437600 | 1.18190200 |
| H | 1.57788200 | 1.14500900 | 1.68889600 |
| C | 0.94340000 | 1.28755200 | -1.05160900 |
| H | 0.90998300 | 0.53418300 | -1.83761200 |
| H | 2.00242500 | 1.46572300 | -0.82073600 |
| C | -0.41983500 | 1.10719400 | 2.49597200 |
| H | -0.14691300 | 1.69090600 | 3.37744400 |
| H | -1.44039900 | 1.36173600 | 2.20648600 |
| H | -0.40413500 | 0.05201200 | 2.76930400 |
| C | 0.30463000 | 2.57091300 | -1.56633100 |
| H | 0.32028500 | 3.36278800 | -0.81468500 |
| H | 0.84957200 | 2.93486500 | -2.44049400 |
| H | -0.73168100 | 2.38869300 | -1.85159800 |

***TS3***

| | | | |
|---|---|---|---|
| C | 1.35777900 | -1.45282600 | -0.29387800 |
| C | 0.21335800 | -0.83244500 | 0.09195000 |
| O | -0.83846000 | -1.51165200 | 0.38941500 |
| O | -3.24623200 | -0.64515100 | 0.54031200 |
| H | 1.42654100 | -2.52222800 | -0.41242500 |
| C | -2.55257900 | -0.70769300 | -0.40542400 |
| O | -2.28333200 | -0.61539900 | -1.54629000 |
| Cl | 2.91925100 | -0.64311700 | -0.56412100 |
| N | 0.09727700 | 0.60324600 | 0.20082400 |
| C | 0.65806800 | 1.16727700 | 1.42393600 |
| H | 0.42232800 | 2.23460400 | 1.42878000 |

| | | | |
|---|---|---|---|
| H | 1.75713300 | 1.08840800 | 1.42755800 |
| C | 0.40087800 | 1.38188200 | -0.99445600 |
| H | 0.30805000 | 0.71909600 | -1.85523100 |
| H | 1.43733800 | 1.74799200 | -0.98726500 |
| C | 0.10580500 | 0.53892800 | 2.69314900 |
| H | 0.54813600 | 1.02337800 | 3.56656800 |
| H | -0.97825700 | 0.64936900 | 2.74300800 |
| H | 0.33791300 | -0.52589100 | 2.74121500 |
| C | -0.55521300 | 2.55648700 | -1.16525400 |
| H | -0.50031800 | 3.24642800 | -0.32022900 |
| H | -0.30933900 | 3.11960300 | -2.06915600 |
| H | -1.58211300 | 2.19746600 | -1.24617200 |

***Int6***

| | | | |
|---|---|---|---|
| C | 1.72770600 | -0.92750300 | -0.97858900 |
| C | 0.41215100 | -0.78050900 | -0.62511900 |
| O | -0.48840600 | -1.55913100 | -1.05272100 |
| O | -2.99020500 | -1.01856100 | 0.51093300 |
| H | 2.06455100 | -1.71945400 | -1.62810100 |
| C | -2.78521600 | -0.38244600 | -0.43563800 |
| O | -2.74972600 | 0.29125500 | -1.37796300 |
| Cl | 3.09325400 | 0.08396700 | -0.41599500 |
| N | -0.03085400 | 0.29676900 | 0.26309200 |
| C | 0.43073600 | 0.20008500 | 1.64334400 |
| H | -0.13309500 | 0.92876600 | 2.23138300 |
| H | 1.49324500 | 0.47139900 | 1.73864800 |
| C | 0.09921000 | 1.62796600 | -0.31805500 |
| H | -0.17563300 | 1.54082300 | -1.37047900 |
| H | 1.13698100 | 1.99235200 | -0.28684600 |
| C | 0.20821100 | -1.17826600 | 2.24587300 |
| H | 0.53775000 | -1.18484000 | 3.28722600 |
| H | -0.84697100 | -1.45115600 | 2.20884100 |
| H | 0.77526500 | -1.93796100 | 1.70534100 |
| C | -0.80670600 | 2.66406700 | 0.33710400 |

| | | | |
|---|---|---|---|
| H | -0.50558200 | 2.88567800 | 1.36246800 |
| H | -0.76288900 | 3.59980100 | -0.22472100 |
| H | -1.84282700 | 2.32090900 | 0.35099200 |

***NN***

| | | | |
|---|---|---|---|
| C | -1.38395200 | -0.98759700 | -0.70213700 |
| C | -0.02874100 | -0.99938900 | -0.00434900 |
| O | 0.34197600 | -2.04275900 | 0.52210500 |
| H | -1.74358500 | -2.00966600 | -0.71724100 |
| Cl | -2.61829000 | -0.01945300 | 0.19762500 |
| N | 0.72567600 | 0.11809500 | -0.01316700 |
| C | 2.05226300 | 0.04930200 | 0.59856300 |
| H | 1.98886700 | -0.58245000 | 1.48255000 |
| H | 2.31564800 | 1.05422200 | 0.92783500 |
| C | 0.37318300 | 1.38142000 | -0.65562600 |
| H | -0.45602100 | 1.22395600 | -1.34035500 |
| H | 1.22554400 | 1.68739300 | -1.26757400 |
| C | 3.10501300 | -0.48695300 | -0.36227600 |
| H | 4.08486200 | -0.48894500 | 0.11785000 |
| H | 2.86620200 | -1.50825000 | -0.65966800 |
| H | 3.16894100 | 0.13223300 | -1.25934500 |
| C | 0.01732500 | 2.48274200 | 0.33478100 |
| H | 0.84865700 | 2.70476400 | 1.00510800 |
| H | -0.22735800 | 3.39731200 | -0.20762100 |
| H | -0.84514500 | 2.19409500 | 0.93498100 |
| H | -1.34176300 | -0.59571200 | -1.71454500 |