Electronic Supplementary information

Bifunctional Picolinate Ionic Liquid as Metal-/Halide-Free Sustainable Catalyst for CO_2 Cycloaddition to Epoxides

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Page: 113

Figure: 66 (S1 – S66)

Table: 3 (S1 – S3)

Index Page no.

Abbreviation:

Entry	Reagents (Abbreviation)	CAS no.	Producer	Purity
1.	Picolinic acid [PA]	98-98-6	SRL	99.9%
2.	Tetra methyl ammonium hydroxide [TMA][OH]	75-59-2	Sigma-Aldrich	25% H_2O
3.	Tetra ethyl ammonium hydroxide [TEA][OH]	77-98-5	Sigma-Aldrich	20% H_2O
4.	Tetra propyl ammonium hydroxide [TPA][OH]	4499-86-9	Sigma-Aldrich	25% H_2O
5.	Tetra butyl ammonium hydroxide [TMA][OH]	2052-49-5	Sigma-Aldrich	20% H_2O
6.	Benzoic acid [BA]	65-85-0	Sigma-Aldrich	99 %
7.	Propylene oxide [PO]	115-07-1	Spectrochem	99%
8.	Carbon dioxide [CO_2]	124-38-9	-	99.9 %

Experiment details:

Materials & Methods

Picolinic acid (>99 %), Tetramethyl ammonium hydroxide (25% in H_2O), Tetraethyl ammonium hydroxide (20% in H_2O), Tetrapropyl ammonium hydroxide (25% in H_2O), Tetrabutyl ammonium hydroxide (25% in H_2O). Benzaldehyde and other substituted benzaldehyde brought from Sigma Aldrich with purity ≥ 99 %. Propylene oxide and epoxides derivatives are purchased from TCI with purity ≥ 99 % and Carbon dioxide with 99.99 % purity was provided by local Vendors. Methanol with purity ≥ 99 %, Ethyl acetate with purity ≥ 99 %, Acetonitrile with purity ≥ 99 % and Deionized water used for experiments. All chemicals were used without further purification.

^{1}H and ^{13}C NMR data obtained from (Bruker AV-600 and 500) MHz spectrometer. Positive (+) Electrospray Ionization Process mass spectrometry was conducted in (Agilent AdvanceBio 6545XT-LC/Q-TOF and a Brucker Micro-TOF QII spectrometer). The characteristic band was analysed by Fourier transform infrared spectroscopy using KBr pellets as internal standard (FTIR; Perkin–Elmer GX FTIR spectrometer). The decomposition temperature of the catalyst was studied by thermal gravimetric analysis (TGA; NETZ5CH; DMA 242 E Artemis). Gas Chromatography was performed for analysis of conversion and selectivity for targeted product. (Shimadzu 2014). Viscosity was measured in (Anton Paar, AMVn). CO_2 cycloaddition reactions were conducted in a 50 mL stainless steel high pressure stirred reactor (KLB Instruments Co. Pvt Ltd.).

Preparation of Picolinate RTILs

Tetramethyl picolinate, [TMA][P]

The Picolinate RTIL **[TMA][P]** was prepared by environmentally free procedure, by neutralization of picolinic acid [PA] (0.123 gm, 1 mmol) in methanol by treating with 25% aqueous tetra methyl ammonium hydroxide solution [TMA][OH] (0.364 ml, 1 mmol) in 1:1

molar ratio at room temperature and reaction mixture was stirred for 2 hr. Upon completion of the reaction, the reaction mixture was passed through anhydrous sodium sulphate to remove the byproduct water. Subsequently, methanol was removed by rotary evaporation, resulting in a pale-yellow coloured viscous room temperature ionic liquid.

Tetraethyl picolinate, [TEA][P]

[TEA][P] was prepared by neutralization of a solution of picolinic acid [PA] (0.123 gm, 1.0 mmol) in methanol by treating it with 20% aqueous tetraethylammonium hydroxide solution [TEA][OH] (0.651 ml, 1 mmol) i.e. 1:1 molar ratio at room temperature. The reaction mixture was stirred for 2 hr. **[TEA][P]** was obtained as a viscous pale orange coloured liquid at room temperature.

Tetrapropyl picolinate, [TPA][P]

[TPA][P] was prepared by the same procedure as discussed above, with the use of 25% aqueous solution of tetrapropylammonium hydroxide solution [TPA][OH] (1.036 ml, 1.0 mmol) in place of tetraethylammonium hydroxide solution. **[TPA][P]** was obtained as a viscous light orange coloured liquid at room temperature.

Tetrabutyl picolinate, [TBA][P]

[TBA][P] was prepared by the same procedure discussed above, with the use of 20% aqueous tetrabutylammonium hydroxide solution [TBA][OH] (1.015 ml, 1.0 mmol) instead of tetrapropylammonium hydroxide solution at room temperature. **[TBA][P]** was obtained as a light red viscous liquid at room temperature.

Preparation of Benzoate RTIL

The synthesis of tetramethylammonium benzoate [**TMA**][**Bz**] was achieved in the same procedure mentioned above, by the neutralization of benzoic acid (BA, 1 mmol) in methanol,

by treating with 25% aqueous tetra methyl ammonium hydroxide solution [TMA][OH] (0.364 ml, 1 mmol) in 1:1 molar ratio at room temperature and reaction mixture was stirred for 2 hr.

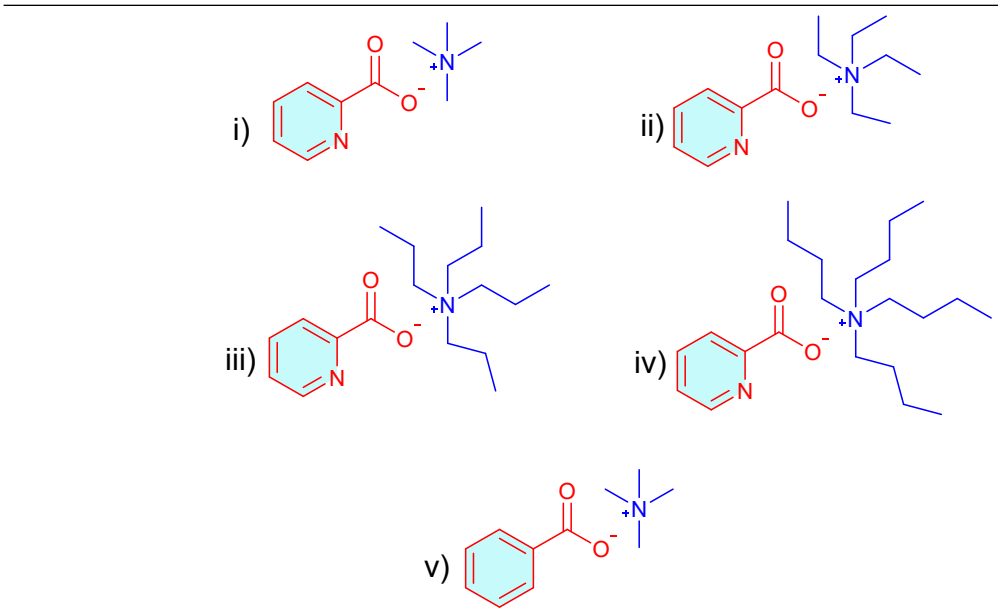


Figure S1: Picolinate and benzoate-based room temperature ionic liquids (RTILs).

Potentiometric titration:

The basic sites in **[TMA][P]** were quantified using potentiometric titration in Compact Titrator G10s from Mettler Toledo with different standard of acid as titrant. The electrode (DGi115-SC) was first calibrated using three buffer solutions of pH 4.02, 7.00 and 10.02 at 25 ± 0.5 °C and the slope was found in the standard range, i.e., -55 mV/pH to -65 mV/ pH. A calibration curve was prepared using different known standard of inorganic acids, **[TMA][P]** and melamine, **Figure 2c**. 50 mg of each acid and base were dispersed in a 50 mL DI water and the potential were recorded with respect to time. **[TMA][P]** potential was recorded at -26.65 mV. The positive potential value validates the acidic nature of acids, whereas negative potential value in melamine and **[TMA][P]** corroborate their basic nature. Unfortunately, we are unable to quantify the total basic sites in it, using standard protocol with KHP buffer and titrating it with different standard of organic and inorganic acid. This may be attributed to the adsorption of the CO_2 and moisture on the surface of the basic N- sites. However, the value of the potential

as depicted from the potential curve of **[TMA][P]** give the clear implication that it may be use as a basic catalyst for CO_2 cycloaddition reaction.

General Procedure for the cycloaddition of CO_2 into epoxide to cyclic carbonate.

The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TMA][P]** (0.6 mol%, 141.30 mg) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. Then mixture was work-up using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC)/^{1}H NMR.

Recyclability Experiment: Chemical fixation of CO_2

Considering the paucity of recyclable homogeneous catalytic systems, we wanted to explore the recyclability of our picolinate-based IL catalyst, despite the low catalyst loading of 0.6%. During the cycloaddition experiments, the ionic liquid (IL) catalyst and the cyclic carbonate product were separated by the classical solvent phase separation technique, using water and ethyl acetate. The ILs are soluble in water, while the product cyclic carbonates are soluble in ethyl acetate. The organic layer was collected and dried over Na_2SO_4. The solvents were removed under reduced pressure to recover the cyclic carbonate (from ethyl acetate layer) and IL from the water layer. The recovered IL was re-used for subsequent catalytic cycles, with comparable yield and selectivity of the desired cyclic carbonate product.

Recycling organocatalysts through phase separation is challenging due to potential catalyst loss; therefore, we also employed the direct reuse method to assess the efficiency of the catalyst

across multiple cycles.[1] To further improve upon the green aspects of the process by directly re-using the homogeneous catalyst under solvent-free conditions, we have precluded the cyclic carbonate separation step and added fresh stocks of the epoxide starting material in the same reaction vessel periodically, after the completion of the previous cycle to ascertain the recyclability of the IL catalyst. Aliquots were removed after each catalytic cycle to ascertain the conversion and purity of the product through GC analysis.

This approach eliminates the need for solvents for extraction/ purification steps, minimizes catalyst loss, and ensures the catalyst remains active in the reaction medium. This approach eliminates the need for solvents for extraction/ purification steps, minimizes catalyst loss, and ensures the catalyst remains active in the reaction medium.

However, this process showed a decrease in the yield of cyclic carbonate over successive catalytic cycles. This decrease in the yield could be ascribed to several factors:

(i) Increase in the volume of the reaction mixture in the batch process: We have conducted the catalytic transformations in a 50 mL high pressure reactor with 8.37 mL (120 mmol) propylene oxide and 146.30 mg of the IL (i.e. 0.6 mol%) in the first cycle, under solvent-free protocol, and to ensure proper overhead stirring and mixing of the reactants and the catalyst. With each subsequent step, further 8.37 mL of the propylene oxide was further added to the reaction vessel. Thus, there is a substantial increase of the volume of the reaction mixture (i.e. product+ added reactant) in each step. This reduces the effective volume of CO_2 gas (initial pressure constant at 10 bar) available for the reaction (Table S1), which is expected to reduce the product yield in subsequent catalytic cycles.

(ii) Reduced CO_2 utilization in each subsequent cycle: Each catalytic cycle revealed less CO_2 consumption compared to the previous catalytic cycle (Table S1), which could be a reason for the reduced product yield. The solubility of CO_2 in propylene carbonate (PC) is less compared

to propylene oxide (PO), and the overall solubility of CO_2 in the PO-PC binary mixture was reduced.[2] This is expected to reduce the conversion of propylene oxide to the propylene carbonate product, and thus the consumption of CO_2 was less in each subsequent catalytic cycle.

(iii) Increase in the viscosity of the reaction medium: The higher viscosity of PC (viscosity ~ 2.5 centipoise at 25°C) compared to PO (viscosity ~ 0.28 centipoise at 25°C) enhances the overall viscosity of the reaction mixture, and thus the interaction of PO and CO_2 becomes sluggish, which affects the reaction rate and overall yield of the propylene carbonate from the cycloaddition of CO_2 to propylene oxide.

We surmise that the above factors contribute towards a decrease in the observed yield of the propylene carbonate product, though the IL-based catalytic system remains active.

Table S1: Recyclability study of [TMA][P]**.**

Reaction cycles	**Propylene oxide**	**[TMA][P] loading**	**Time**	**Temp**	**Initial CO_2 pressure**	**Final CO_2 pressure**	**Conv. / Sel.**
Cycle-1	120 mmol (8.37 ml)	0.6 mol % (141.30 mg)	9 h	120 ºC	10 Bar	0.2 Bar	99 % / 99 %
Cycle-2	120 mmol (8.37 ml)	-	9 h	120 ºC	10 Bar	2.2 Bar	89 % / 99 %
Cycle-3	120 mmol (8.37 ml)	-	9 h	120 ºC	10 Bar	3.4 Bar	76 % / 99 %

Characterisation:

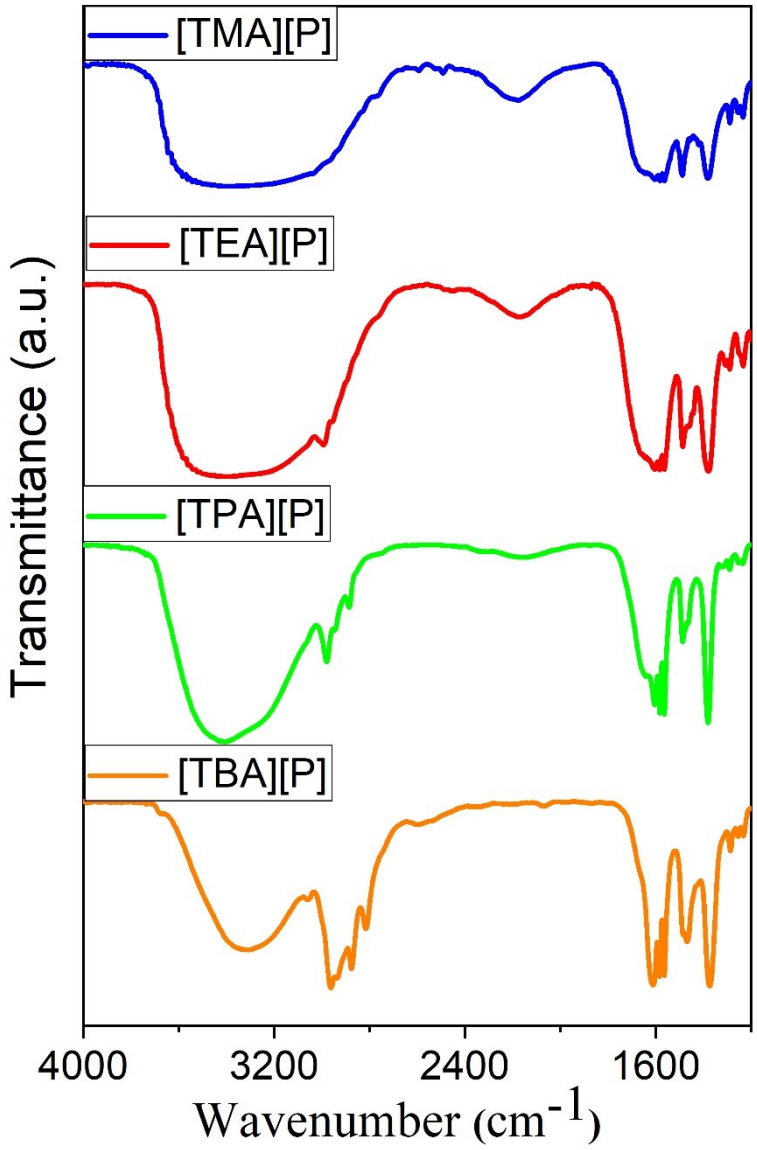


Figure S2: FTIR spectra of Picolinate RTILs.

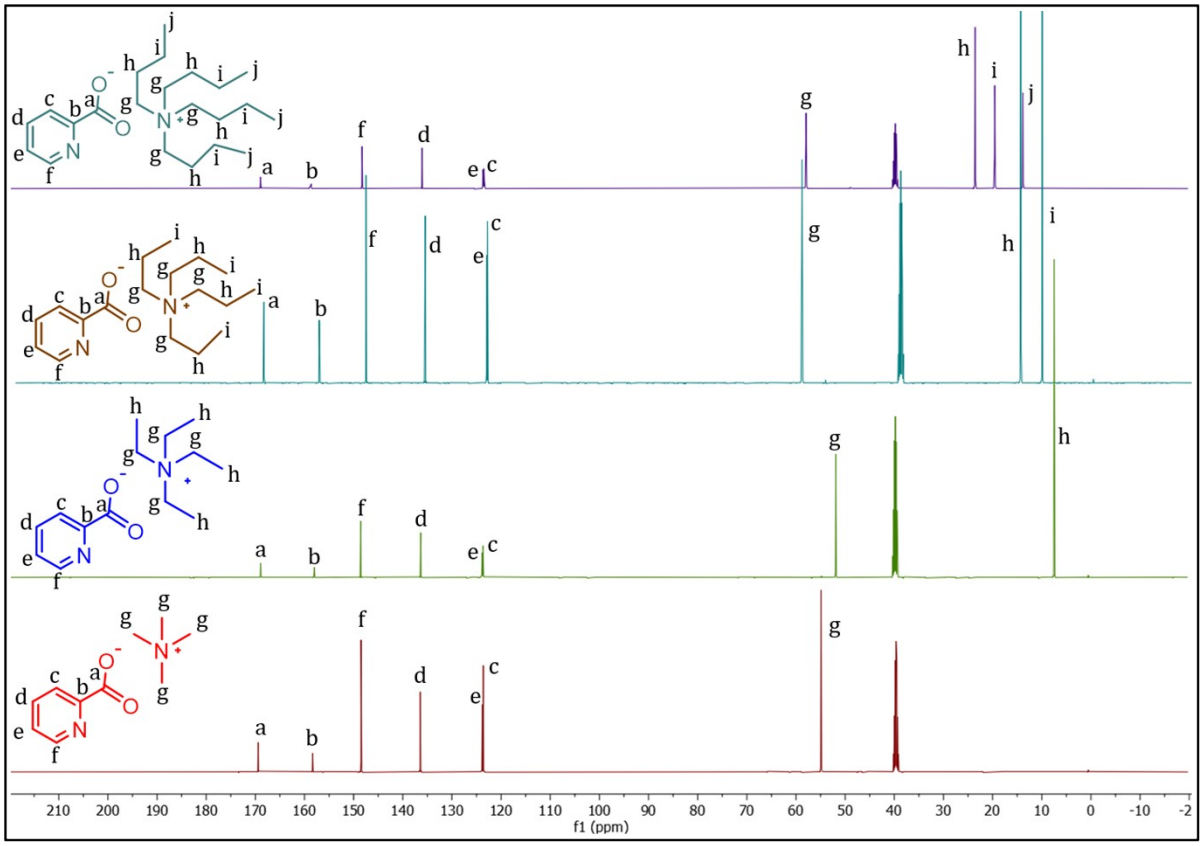


Figure S3. ^{13}C NMR spectra of RTILs.

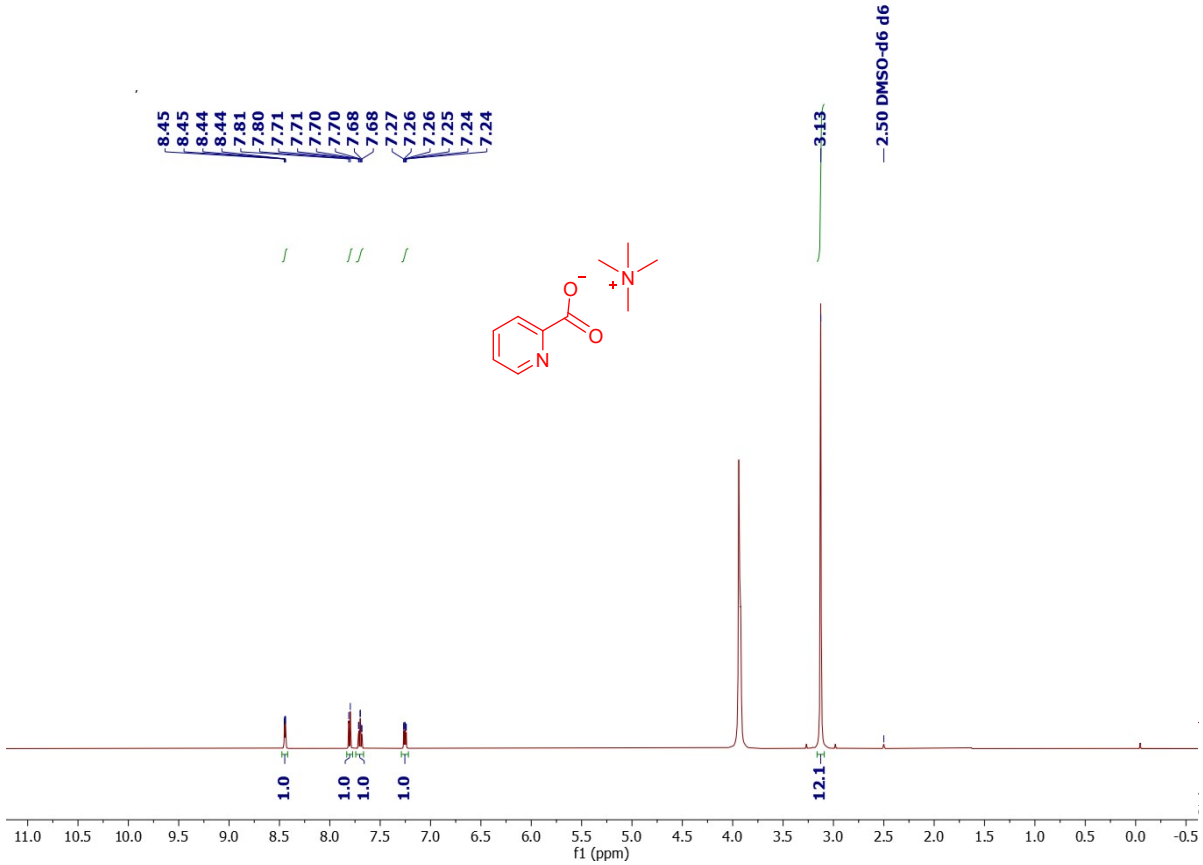


Figure S4: ^{1}H-NMR of [TMA][P].

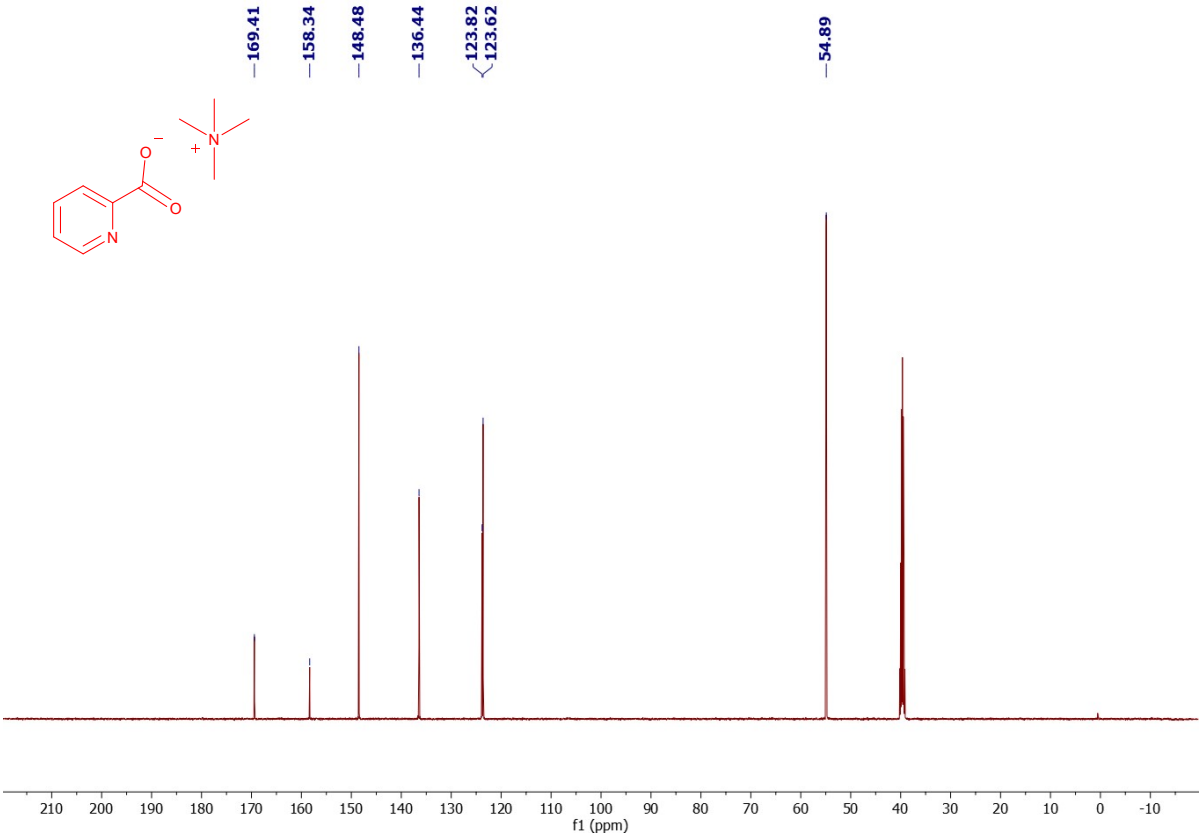


Figure S5: ^{13}C-NMR of [TMA][P].

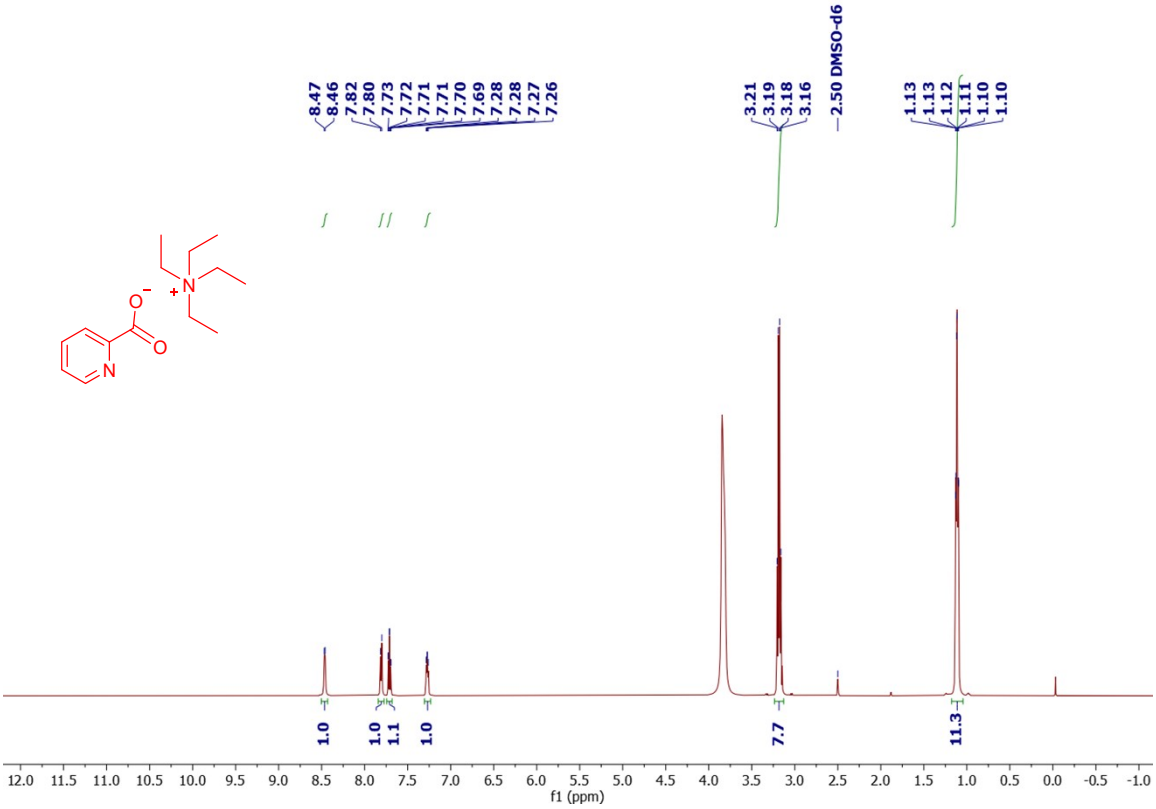


Figure S6: ^{1}H-NMR of [TEA][P]

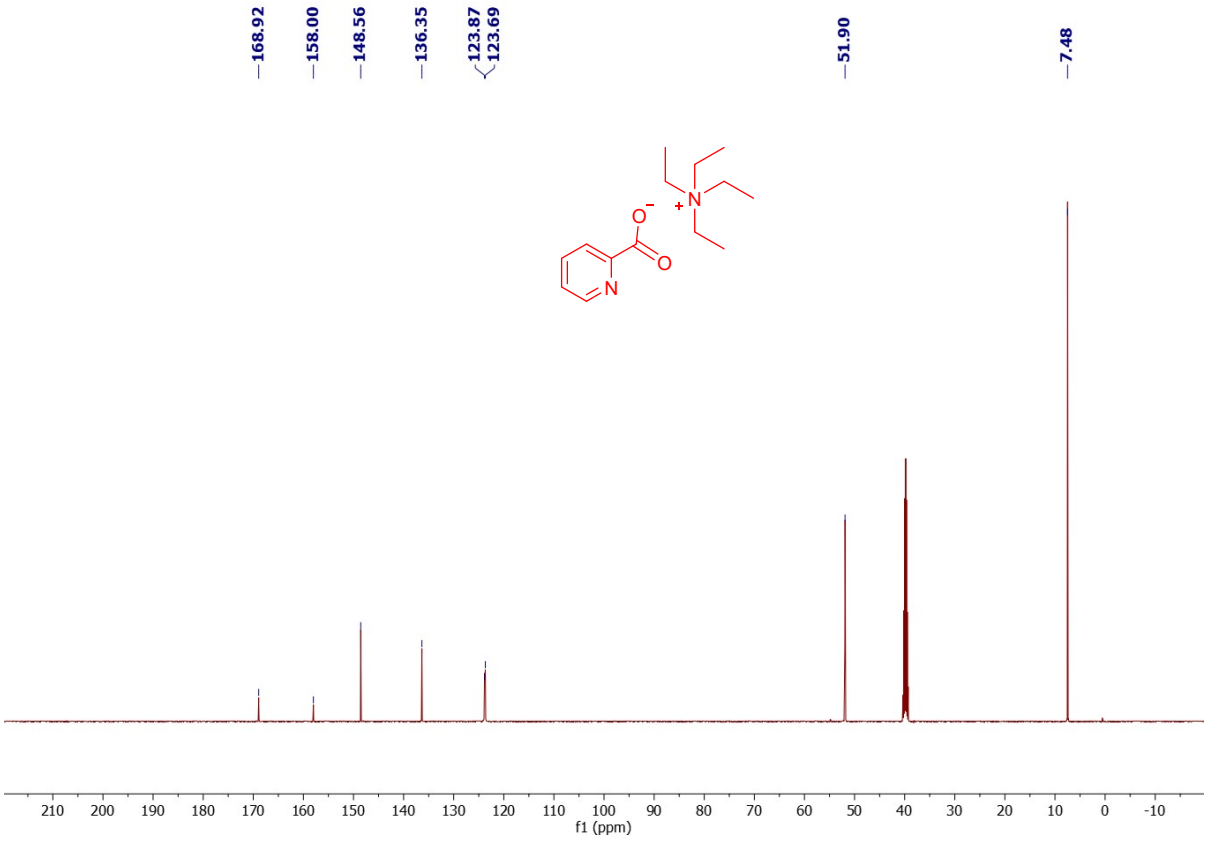


Figure S7: ^{13}C-NMR of [TEA][P].

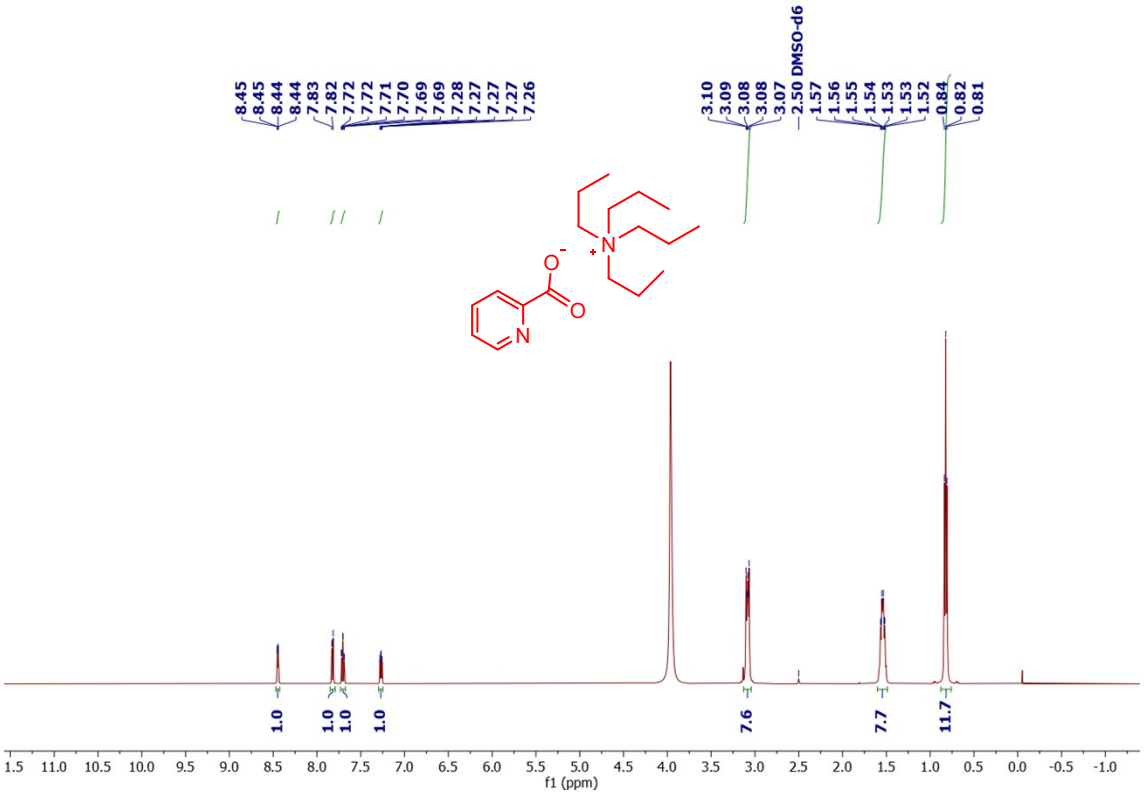


Figure S8: ^{1}H-NMR of [TPA][P].

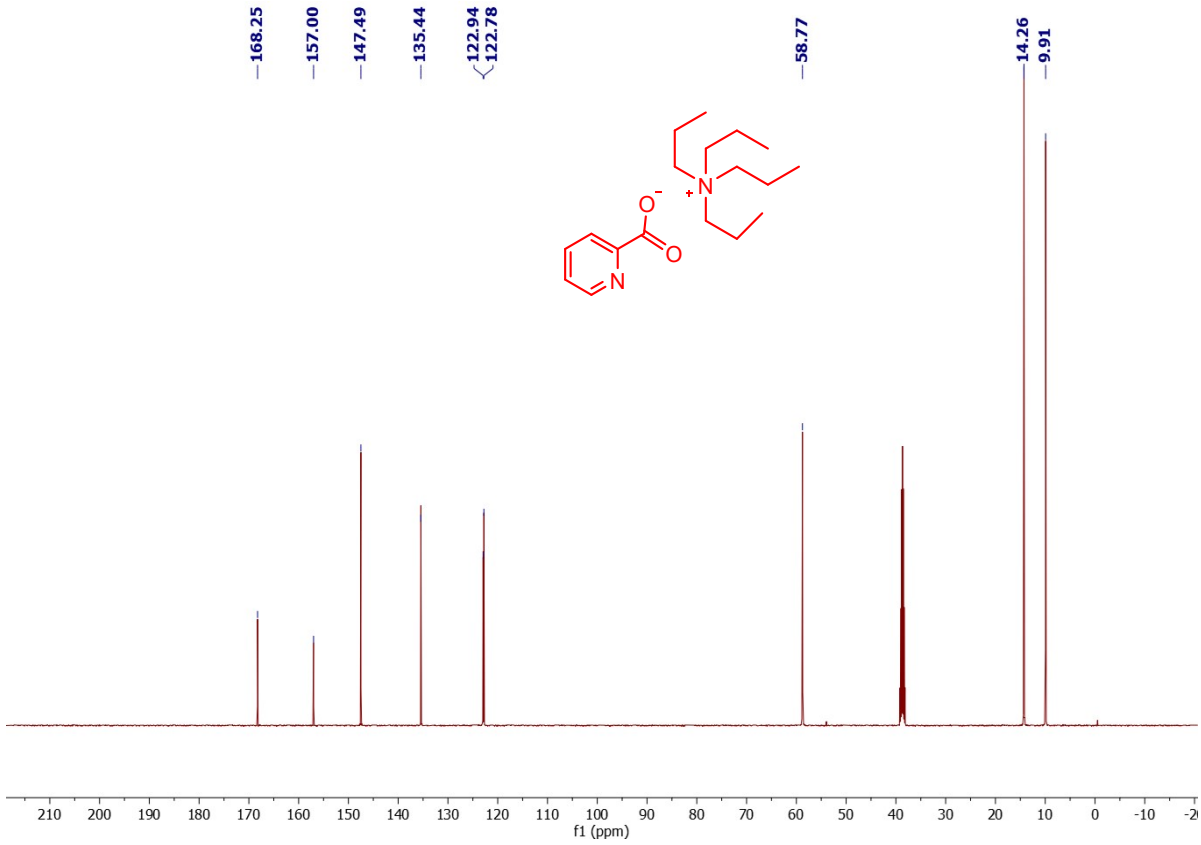


Figure S9: ^{13}C-NMR of [TPA][P].

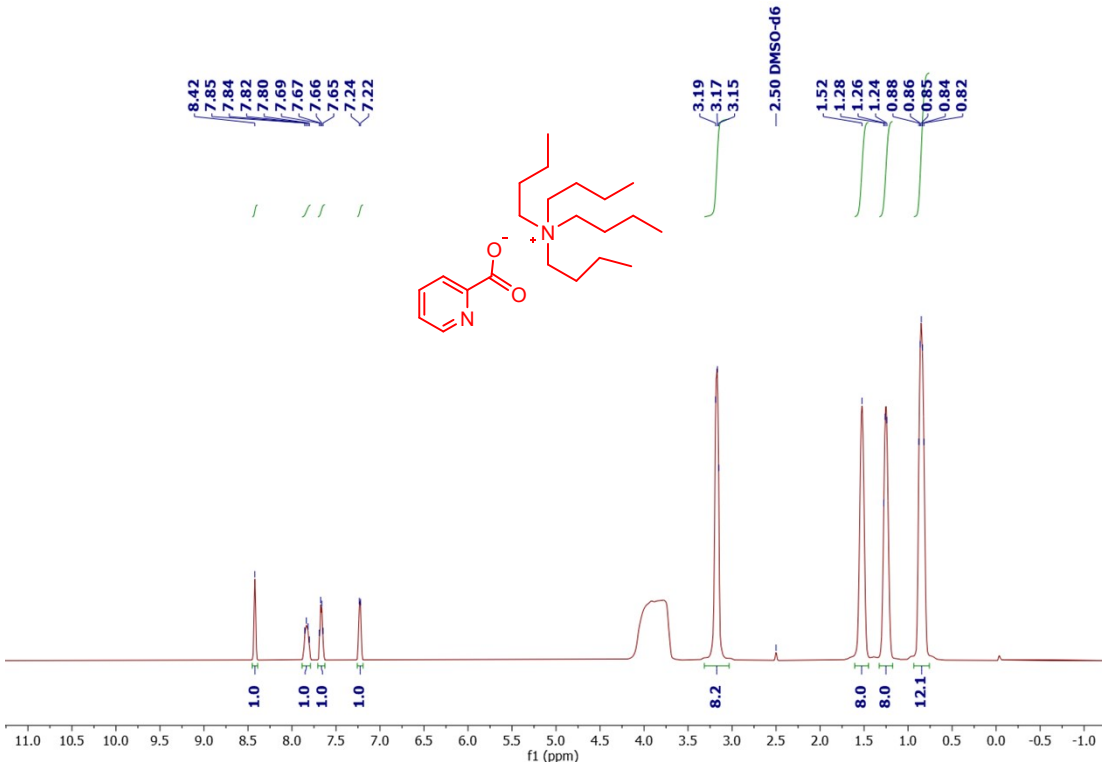


Figure S10: ^{1}H-NMR of [TBA][P].

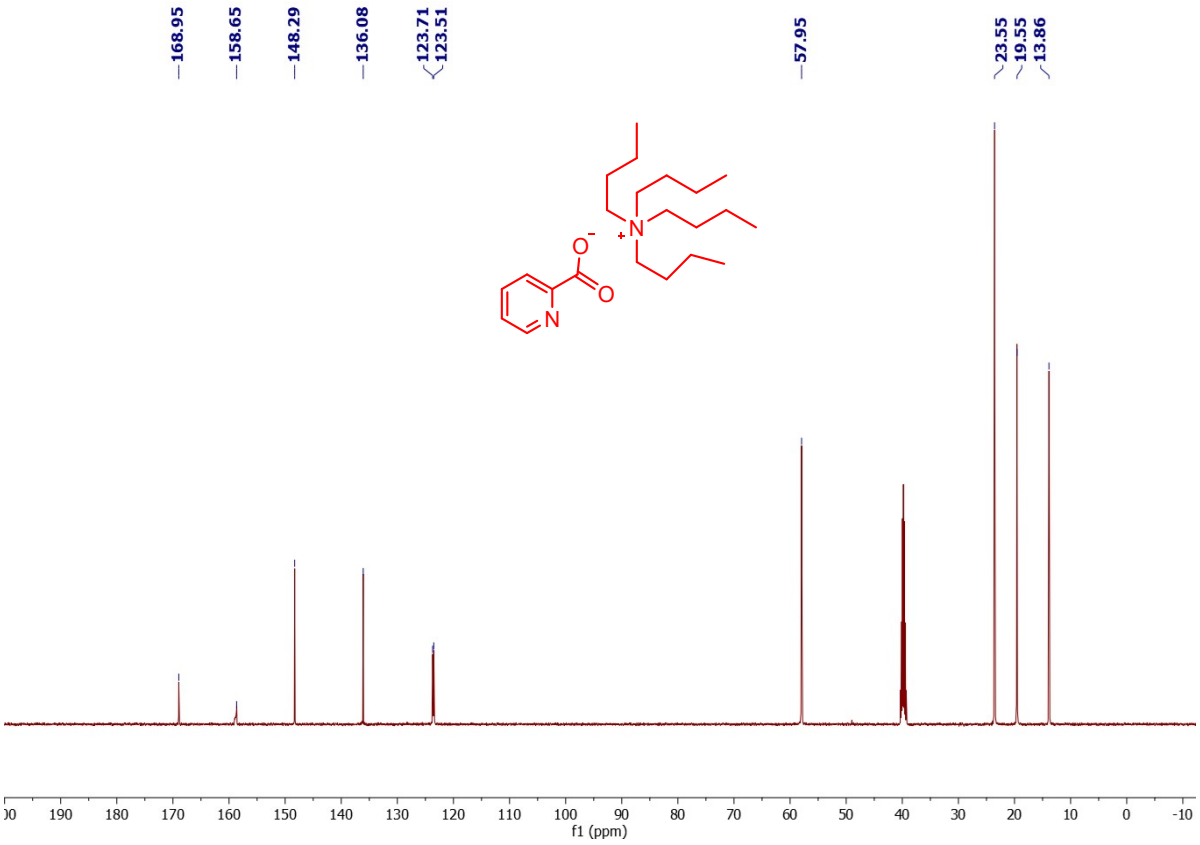


Figure S11: ^{13}C-NMR of [TBA][P]

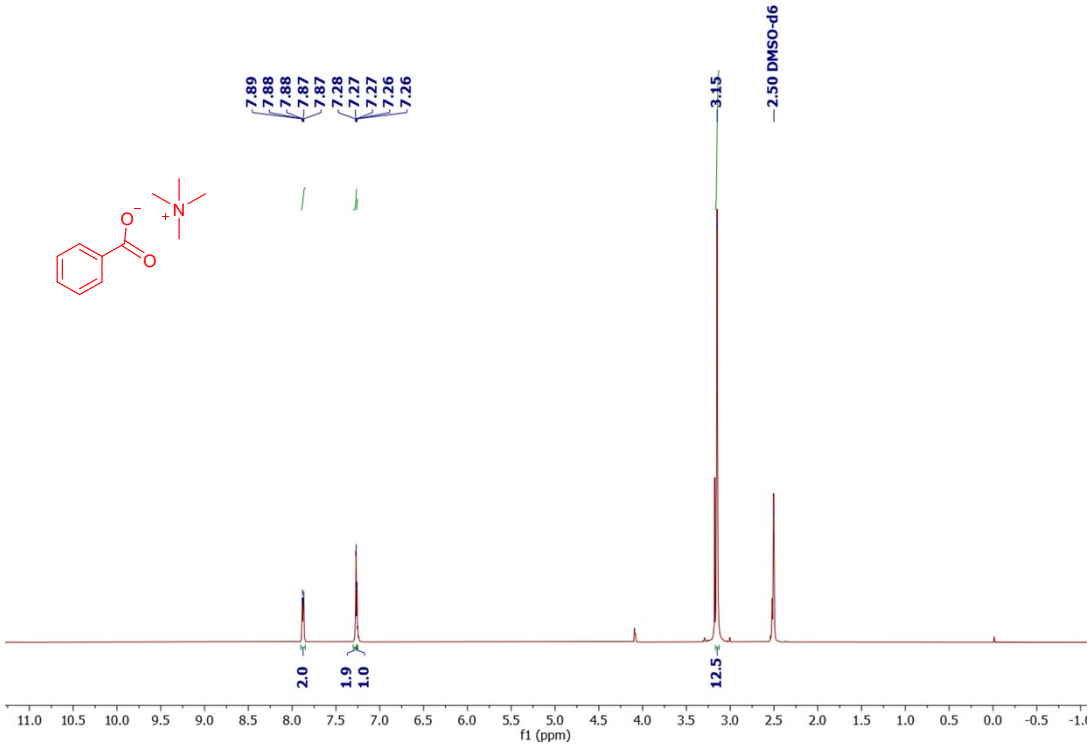


Figure S12: ^{1}H-NMR of [TMA][Bz].

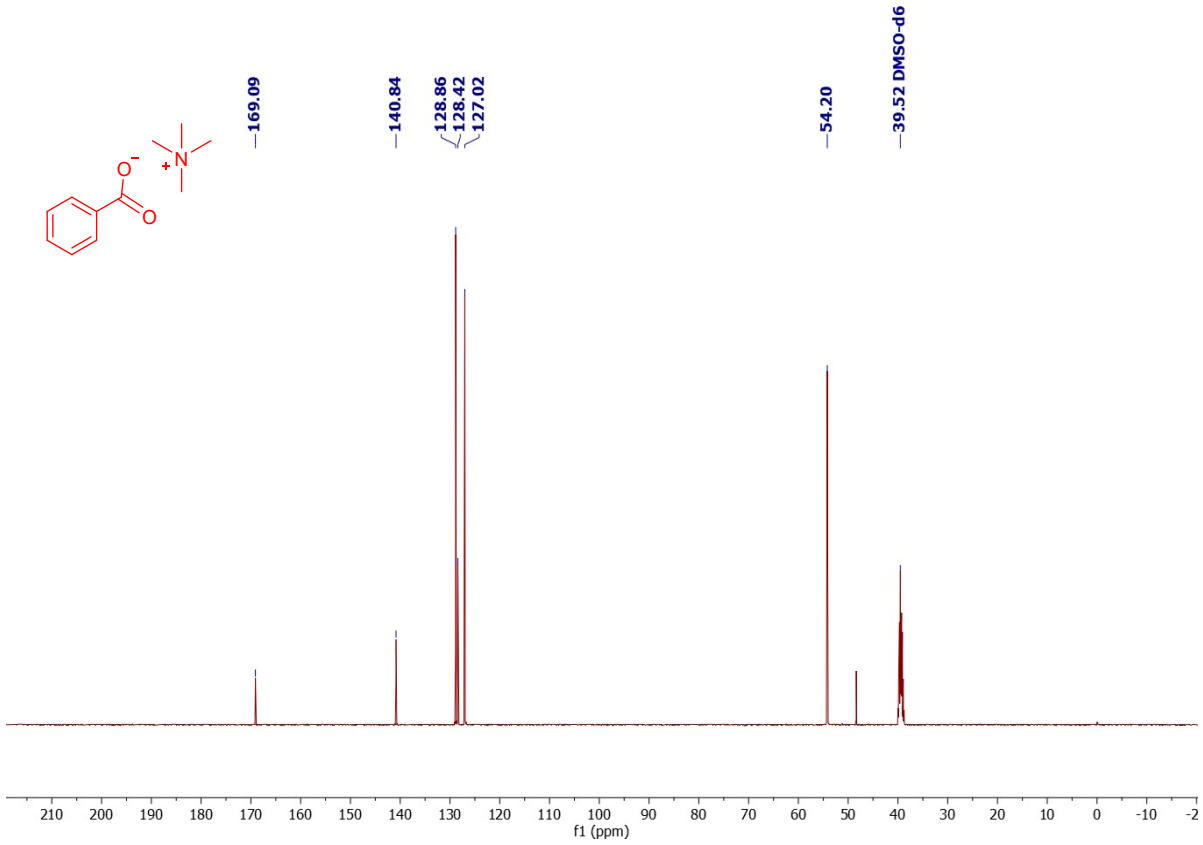


Figure S13: ^{13}C-NMR of [TMA][Bz].

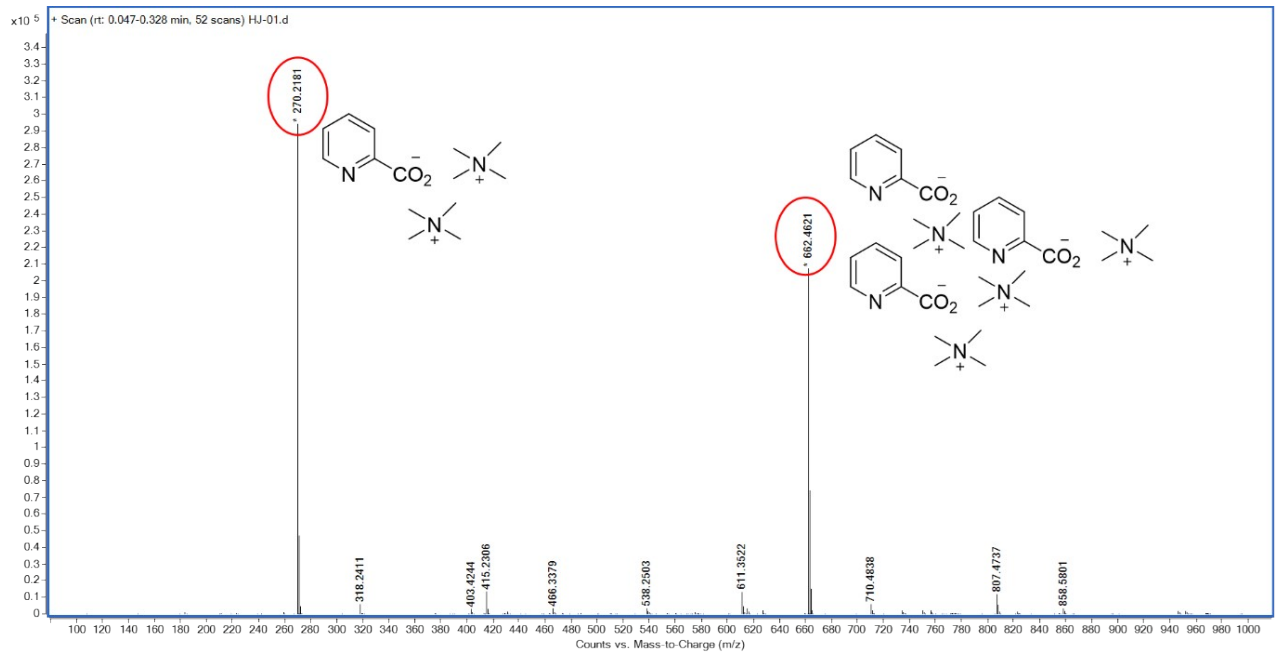


Figure S14: Positive mode ESI mass spectrometry of **[TMA][P]**.

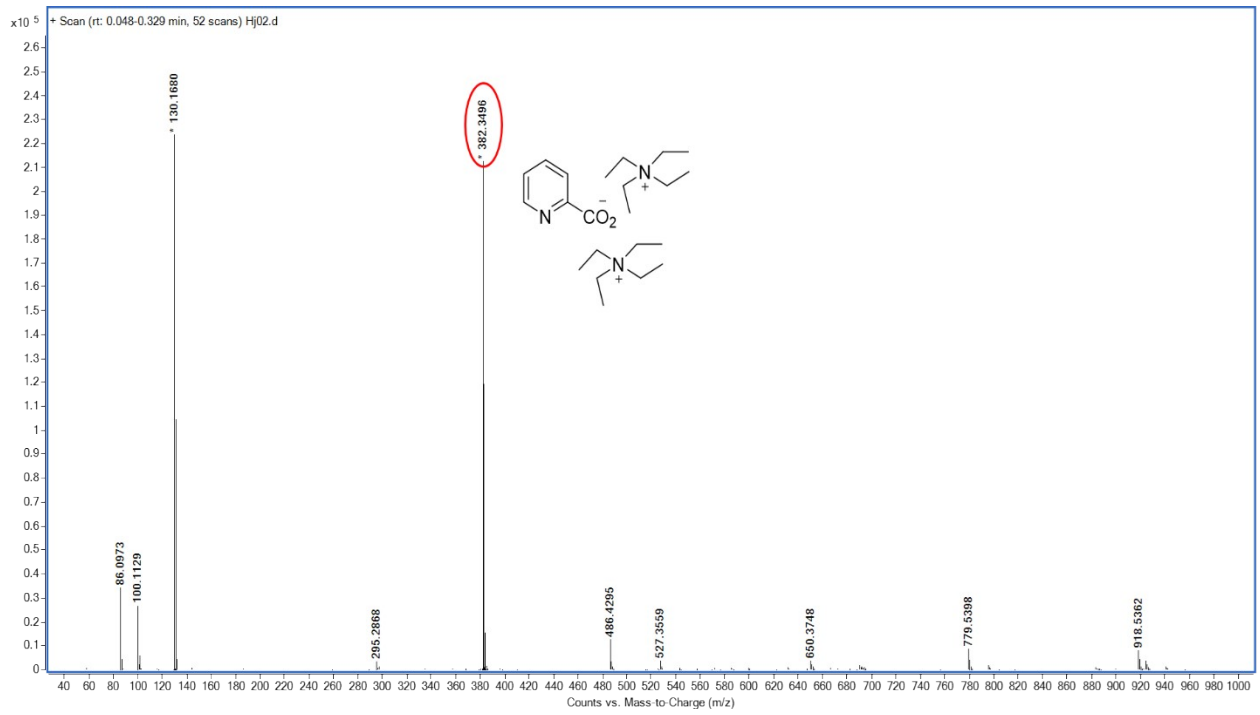


Figure S15: Positive mode ESI mass spectrometry of **[TEA][P]**.

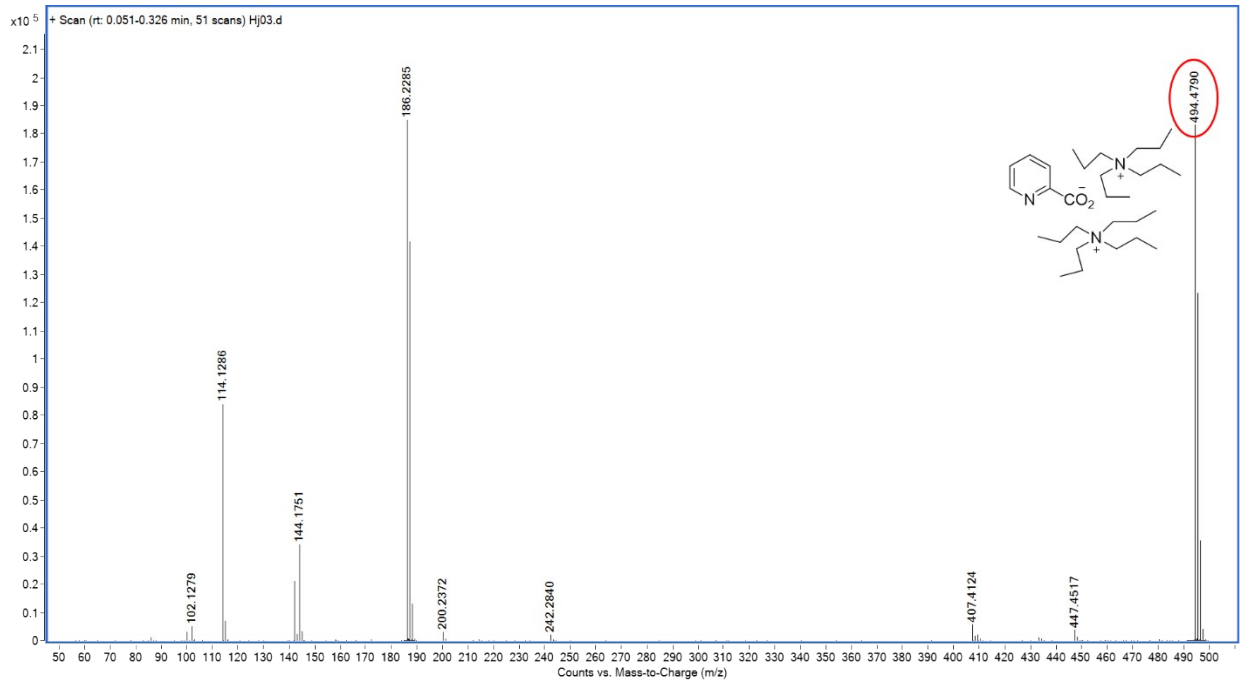


Figure S16: Positive mode ESI mass spectrometry of **[TPA][P]**.

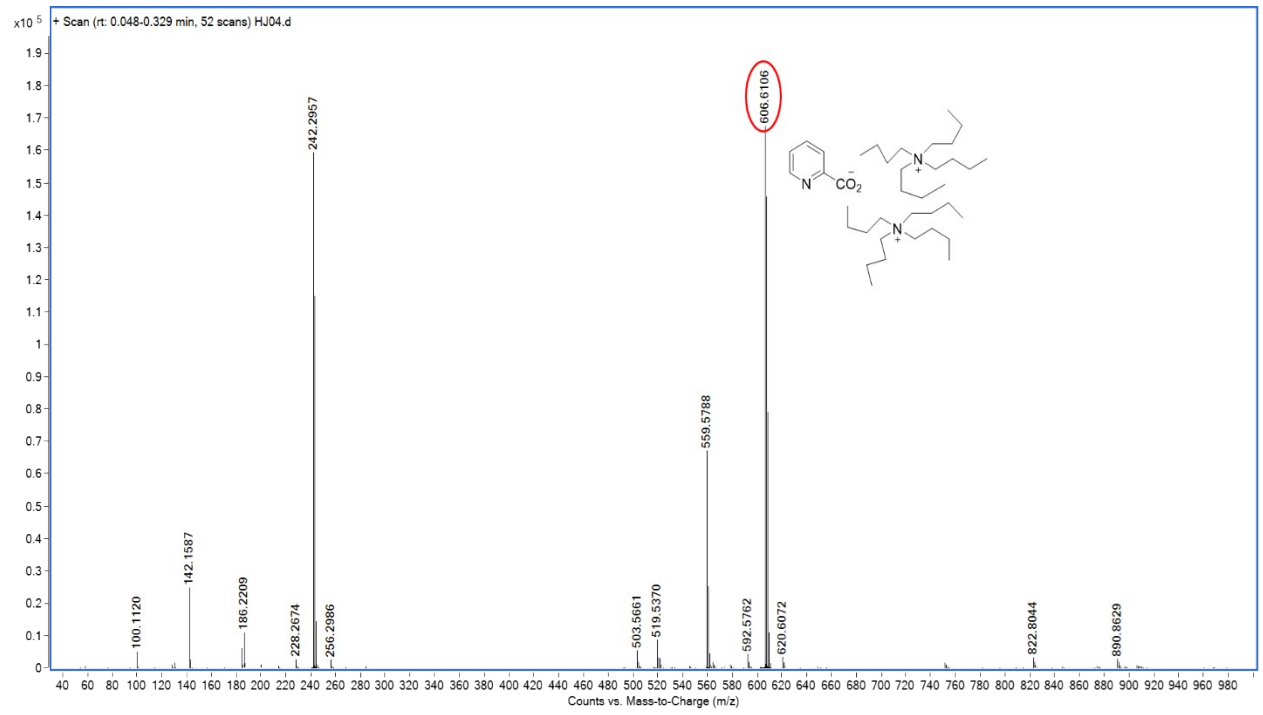


Figure S17: Positive mode ESI mass spectrometry of **[TBA][P]**.

The results of NMR and ESI-MS characterizations for the prepared Picolinate RTILs are as follows:

[TMA][P]: Pale-yellow liquid, ^{1}H NMR (500 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 8.45 (d, 1H), 7.81 (d, 1H), 7.68 (t,1H), 7.27 (t, 1H), 3.13 (s, 12H). ^{13}C NMR (125 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 169.41, 158.34, 148.48, 136.44, 123.82, 123.62, 54.89. +ESI: $\{[TMA]_2[P]\}^+$, 270.21 m/z $\{[TMA_4][P]_3\}^+$, 662.46 m/z.

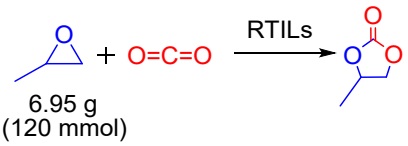
[TEA][P]: Pale-orange liquid, ^{1}H NMR (500 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 8.47 (d, 1H), 7.82 (d, 1H), 7.73 (t,1H), 7.28 (t, 1H), 3.21 (q, 8H), 1.13 (t, 12H). ^{13}C NMR (125 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 168.92, 158, 148.56, 136.35, 123.87, 123.69, 51.90, 7.48. +ESI: $\{[TEA]_2[P]\}^+$, 382.34 m/z.

[TPA][P]: Light orange liquid, ^{1}H NMR (500 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 8.45 (d, 1H), 7.83 (d, 1H), 7.72 (t, 1H), 7.28 (t, 1H), 3.10 (t, 8H) 1.57 (m, 8H), 0.84 (t, 12H).^{13}C NMR (125 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 168.25, 157, 147.49, 135.44, 122.94, 122.78, 58.71, 14.26, 9.91. +ESI: $\{[TPA]_2[P]\}^+$, 494.47 m/z.

[TBA][P]: Light red, ^{1}H NMR (500 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 8.42 (d, 1H), 7.85 (d, 1H), 7.69 (t,1H), 7.24 (t, 1H), 3.19 (t, 8H) 1.52 (m, 8H), 1.26 (m, 8H) 0.86 (t, 12H). ^{13}C NMR (125 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 168.98, 158.65, 148.29, 136.80, 123.71, 123.51, 57.95, 23.55, 19.55, 13.86. +ESI: $\{[TBA]_2[P]\}^+$, 606.61 m/z.

[TMA][Bz]: Light yellow liquid, ^{1}H NMR (500 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 7.89 (d, 2H), 7.27 (t, 2H), 7.26 (t,1H). ^{13}C NMR (125 MHz, DMSO-d6, Me_4Si) $\boldsymbol{\delta}_{ppm}$: 169.09, 140.84, 128.86, 128.82, 127.02, 54.20.

Table S2: Optimization of reaction conditions for picolinate-based RTIL-catalysed for cycloaddition of CO_2 with epoxides.[a]



Entry	Catalyst	Catalyst (mol%)	P_{CO2} (bar)	Time (h)	Temperature (ºC)	PO Conversion (%)	PC Yield (%)	PC Selectivity (%)
1	[TMA][P]	0.6	10	9	120	99	99	99
2	[TEA][P]	0.6	10	9	120	98	93	95
3	[TPA][P]	0.6	10	9	120	98	94	96
4	[TBA][P]	0.6	10	9	120	98	88	90
5	[TMA][Bz]	0.6	10	9	120	83	63	76
6	[TMA][P]	0.6	1	9	120	95	48	49
7	[TMA][P]	0.6	5	9	120	98	79	80
8	[TMA][P]	0.6	15	9	120	99	99	99
9	[TMA][P]	0.6	20	9	120	99	99	99
10	[TMA][P]	0.05	10	9	120	5	5	99
11	[TMA][P]	0.1	10	9	120	35	35	99
12	[TMA][P]	0.2	10	9	120	90	90	99
13	[TMA][P]	0.4	10	9	120	91	91	99
14	[TMA][P]	0.8	10	9	120	99	99	99
15	[TMA][P]	0.6	10	9	80	4	4	99
16	[TMA][P]	0.6	10	9	90	41	41	99
17	[TMA][P]	0.6	10	9	110	84	84	99
18	[TMA][P]	0.6	10	1	120	20	20	99
19	[TMA][P]	0.6	10	3	120	73	73	99
20	[TMA][P]	0.6	10	5	120	80	80	99
21	[TMA][P]	0.6	10	7	120	87	87	99
22	[TMA][P]	0.6	10	15	120	97	97	99
23	none	-	10	9	120	0	0	0
24[b]	Picolinic acid	1	10	9	120	7	4.5	75
25[c]	[TMA][OH]	1	10	9	120	68	68	99
26[d]	Pyridine	1	10	9	120	57	31	54
27	[Bmim][Br]	0.6	10	9	120	62	62	99

[a] Reaction condition: Propylene Oxide (120 mmol, 8.38 ml), 500 rpm, Reaction temperature (120 ºC), Reaction time (9 h), CO_2 pressure (10 bar) and **[TMA][P]** (0.6 mol%, 141.30 mg). [b]Picolinic acid (1 mol%, 147.7 mg),

[c][TMA] [OH] (1 mol%, 107.7 µl), [d]Pyridine (1 mol%, 67.11 µl). All reactions are performed in a high-pressure reactor. Conversion and Selectivity analysis by GC.

Table S3: Comparative study of Ionic liquids under halide free and metal free condition for CO_2 Utilization.

Sr.no	Ionic liquid	Ionic liquid (mol% /mmol)	Epoxide (mmol)	P_{CO2} (bar)	Time	Temperature	Yield/ conversion	Ref
1.	[bmim][MET]	0.5 mol%	430	20	24 h	120 °C	89 %	[3]
2.	$[P_{4444}]$[bzim]	0.25 mmol	5.0	10	2-3 h	100 °C	90 %	[4]
3.	[MOBMIM][Gly]	0.4 mmol	34.5	20	12	110 °C	99 %	[5]
4.	$[P_{66614}]$[2-CNPyr]	1 mol%	1-decanol: propylene oxide 1:1 molar proportions	20	22	120 °C	68-86 %	[6]
5.	[HEBim][Asp]	0.8 mol%	63.83	2.5-20	9-14	90 °C-140°C	90-98 %	[7]
6.	[TMA] [P]	0.6 mol%	120	10	9	120 °C	99 %	**This work**

Computational Studies

All calculations were performed using the density functional theory (DFT) method[8] in the Gaussian 16 suite[9] of quantum chemical program. Using the B3LYP functional,[10] 6-31g(d) basis set,[11] Grimme's D3 dispersion correction,[12] and the Becke Johnson damping method [11] in the gas phase, all the structures were optimized. The single point energy calculation was performed using B3LYP functional and the 6-31++G(d,p) basis set[13] along with Grimme's D3 dispersion correction and Becke Johnson damping scheme. Transition states were characterized by a single imaginary frequency, while all the intermediates were characterized by no imaginary frequency. CYLView software was used to generate 3D images of the transition state structures.[14] All the reported energies are in Gibbs free energies (kcal/mol).

The calculated interaction energy of **[TMA][P]** was found to be -25.5 kcal/mol and for **[TEA][P]** it was -14.5 kcal/mol.

Other possible mechanistic pathways considered for the formation of propylene carbonate:

1. Epoxide ring opening mediated by the carboxylate group:

This possible pathway proceeds with a barrier of 33.9 kcal/mol (**TSa2)** for the step-wise mechanism (**Figure S18**) and 33.8 kcal/mol (**TSa3)** for the concerted mechanism (**Figure S19**), which is much higher than the corresponding transition states provided in **Figure 4**.

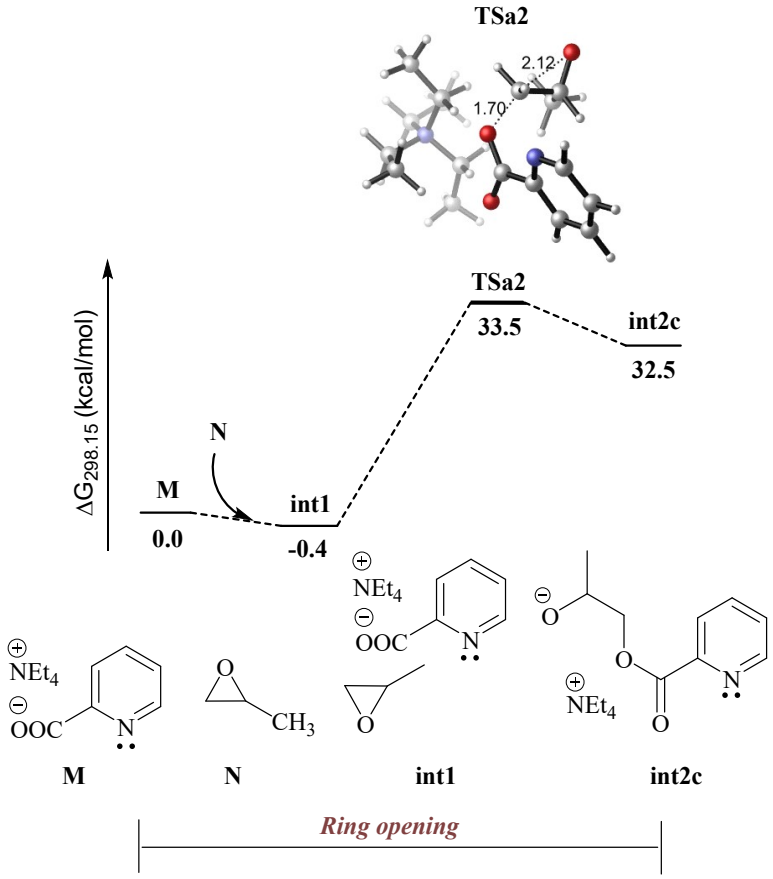


Figure S18. Computed Gibbs free energy profile diagram for the carboxylate group initiated ring opening of epoxide in kcal/mol at the B3LYP-D3(BJ)/6-311++G(d,p)//B3LYP-D3(BJ)/6-31G(d) level of theory. The bond lengths in the transition states are given in Å.

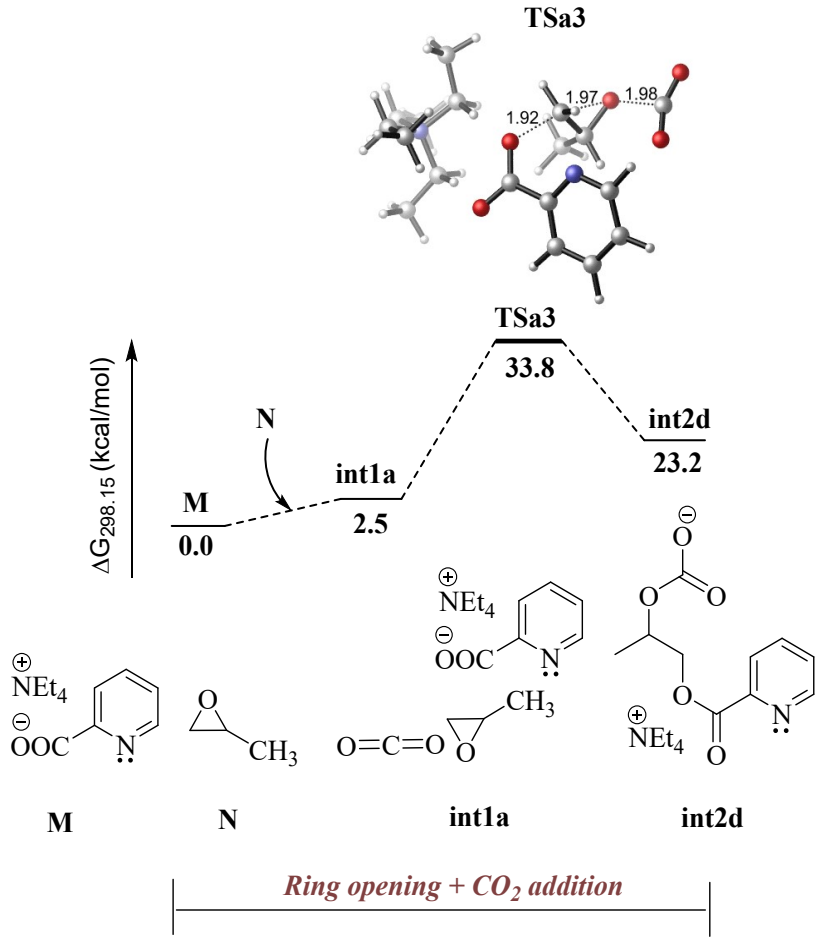


Figure S19. Computed Gibbs free energy profile diagram for the concerted ring opening of epoxide and CO_2 addition in kcal/mol at the B3LYP-D3(BJ)/6-311++G(d,p)//B3LYP-D3(BJ)/6-31G(d) level of theory. The bond lengths in transition states are given in Å.

2. Nucleophilic attack on the methylated carbon:

The mechanism involving nucleophilic attack on the methylated carbon of the epoxide ring was explored in detail **(Figure S20)**. We found that the ring-opening and CO_2 insertion elementary steps were having a barrier close to that of the corresponding steps in **Figure 4**. However, the final ring closing step is found to possess a high energy barrier (**TSc1**)

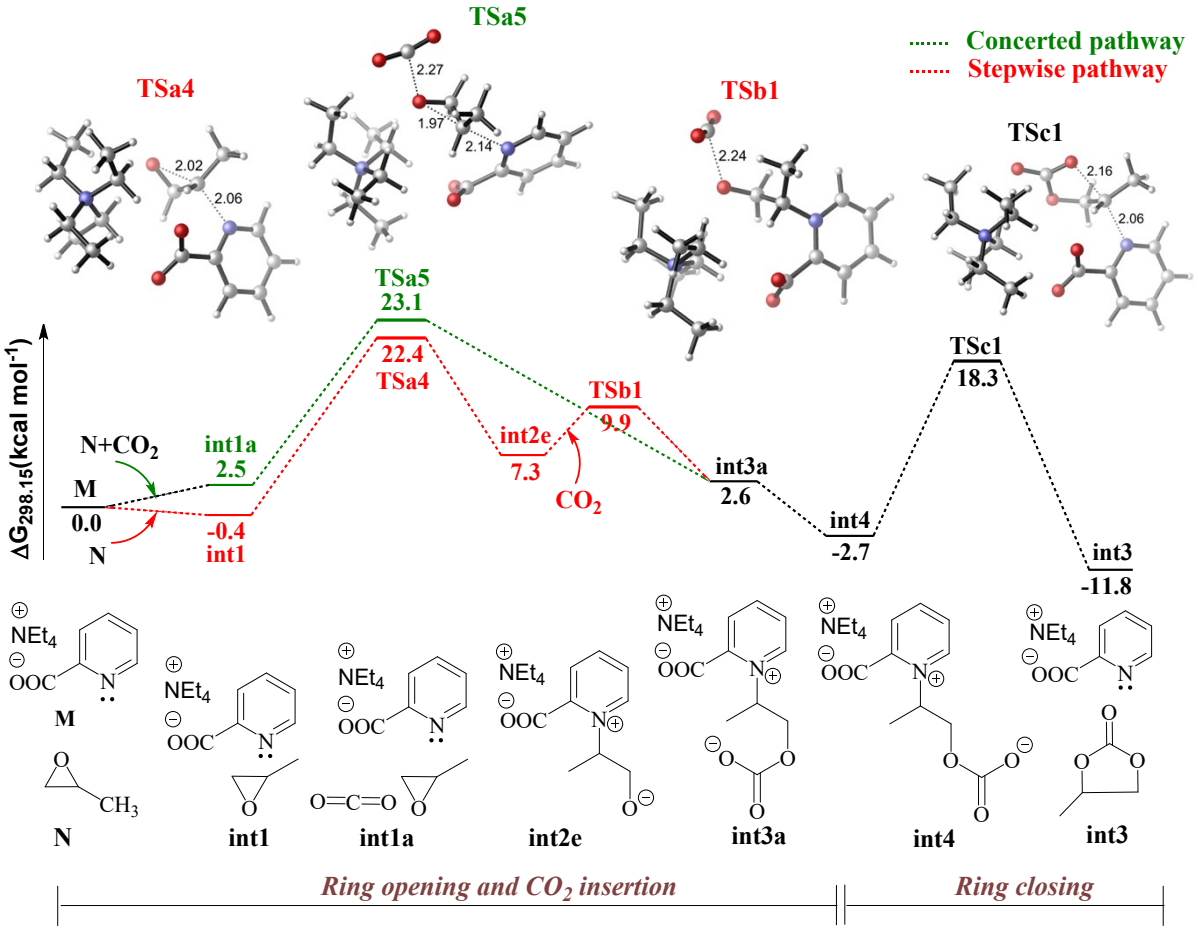


Figure S20. Computed Gibbs free energy profile diagram for the epoxide ring opening by nucleophilic attack on methylated carbon through N-lone pair of **M** in kcal/mol at the B3LYP-D3(BJ)/6-311++G(d,p)//B3LYP-D3(BJ)/6-31G(d) level of theory. The bond lengths in transition states are given in Å.

3. Role of tetraalkylammonium cation in epoxide activation

To investigate the role of the [R_4N] cation in the cycloaddition reaction, a modified system **M_0** was generated by removing the [R_4N] cation from the ionic liquid **M**. From the computed Gibbs free energy profile diagram provided in **Figure S21**, it is evident that the relative free energy of **M_0** is quite high (78.8 kcal/mol with respect to **M**). This reflects in the subsequent ring opening transition state **TSa_0** as well.

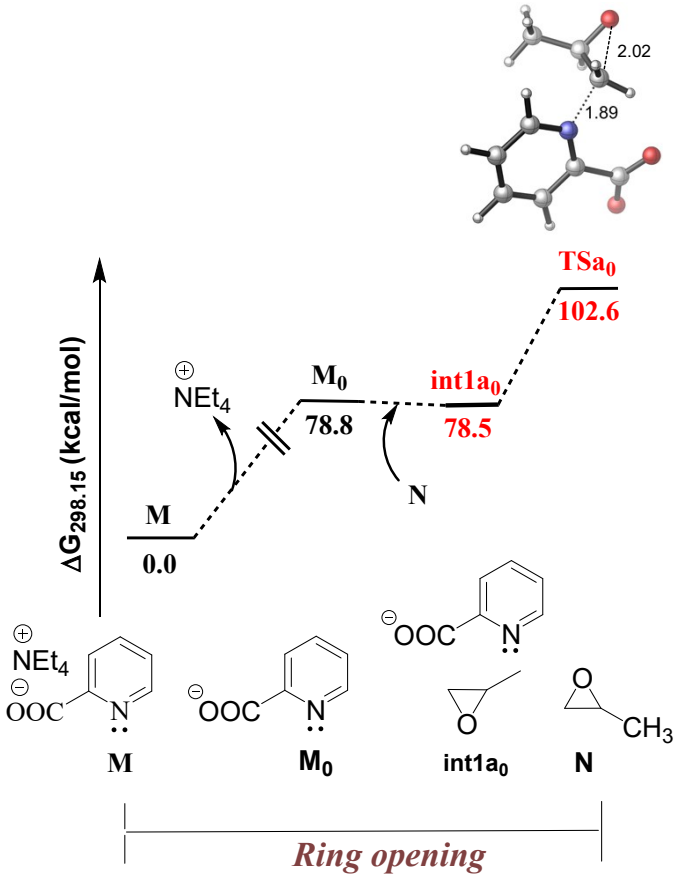


Figure S21. Computed Gibbs free energy profile diagram for the epoxide ring opening elementary step, in the absence of [R_4N] cation, in kcal/mol at the B3LYP-D3(BJ)/6-311++G(d,p)//B3LYP-D3(BJ)/6-31G(d) level of theory. The bond length in the transition state is given in Å.

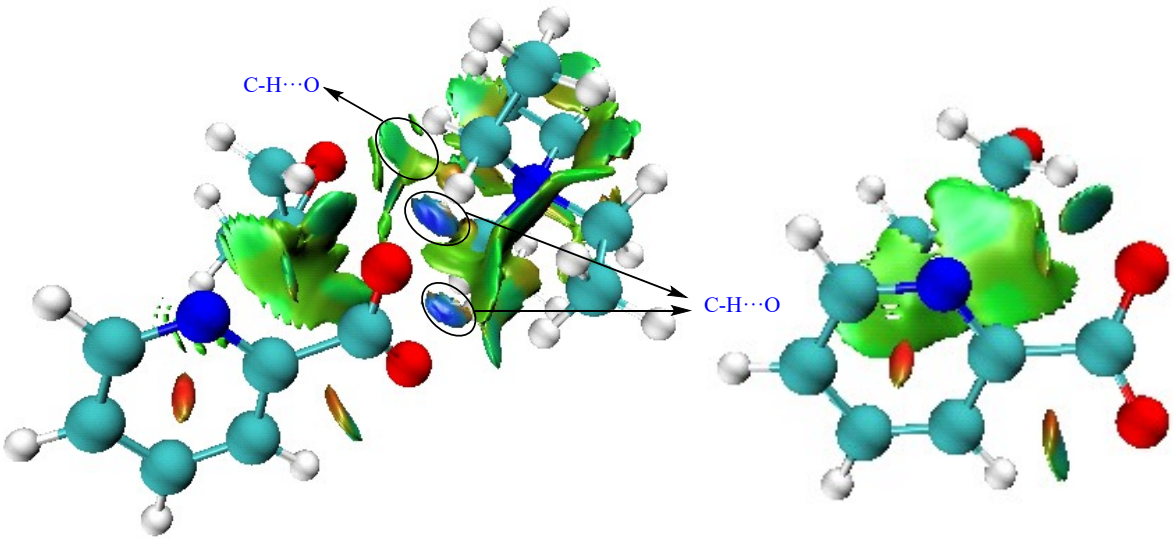


Figure S22. Noncovalent interaction (NCI) plots for **int1a** and **int1a$_0$**. The blue and green regions represent strong and weak interactions, respectively, while the red region denotes repulsive interaction.

4. Effect of alkyl chain of the tetraalkylammonium cation

We have performed additional calculations by substituting the alkyl chain of the cation with a methyl group **(Figure S23).** The corresponding transition state **TSb** exhibited an energy barrier of 24.9 kcal/mol, which was 4 kcal/mol higher than the corresponding transition state **TSa** with ethyl substituent presented in **Figure 4**. Upon substituting the alkyl chain of the cation with a propyl group, we did not obtain a transition state as the cation site was hindered by the bulky propyl group.

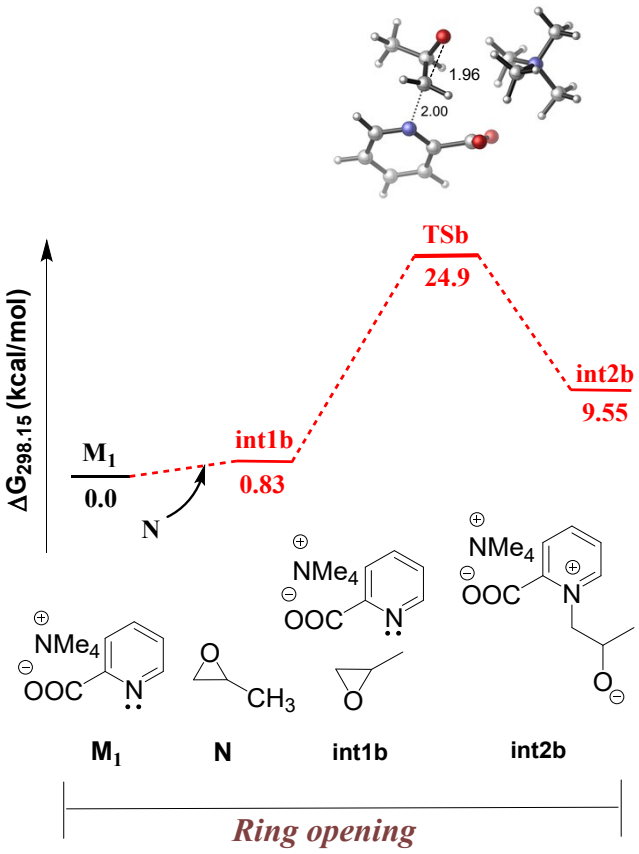


Figure S23. Computed Gibbs free energy profile diagram for the epoxide ring opening elementary step using [TMA][P] as the catalyst in kcal/mol at the B3LYP-D3(BJ)/6-311++G(d,p)//B3LYP-D3(BJ)/6-31G(d) level of theory. The bond length in transition state is given in Å.

5. Carboxylate-Assisted Epoxide Ring-Opening Pathway in [TMA][Bz]

In the case of [TMA][Bz], the ring opening is assisted by the carboxylate group, which occurs via the transition state **TSa5** with an energy barrier of 39.0 kcal/mol (with respect to the separated reactants) (**Figure S24**). The relatively high activation barrier is reflected in the moderate yield product when [TMA][Bz] is employed in the reaction

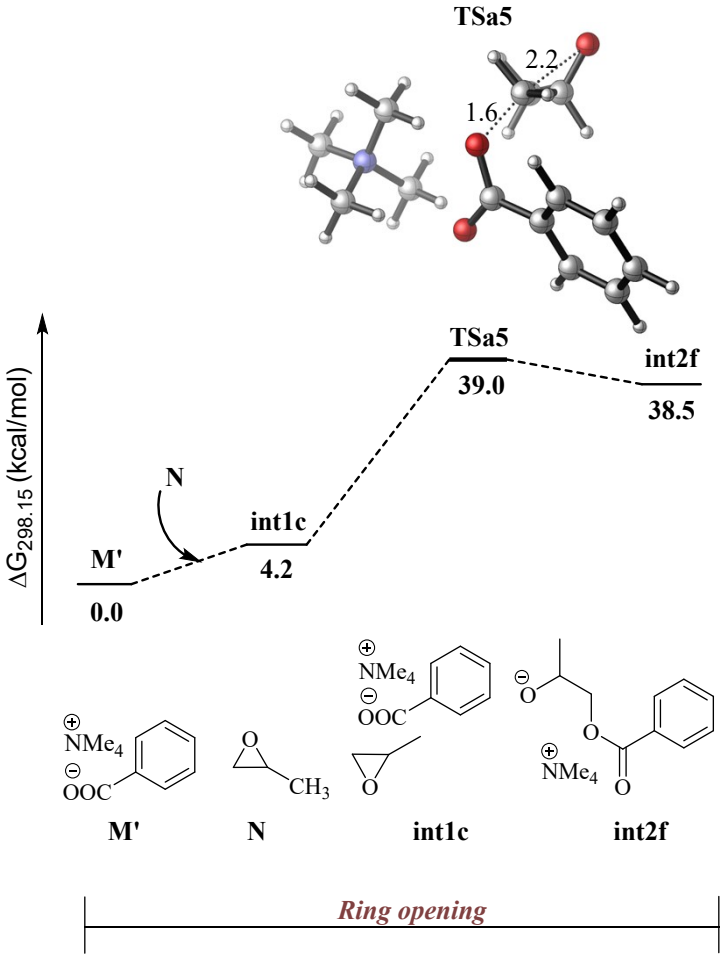
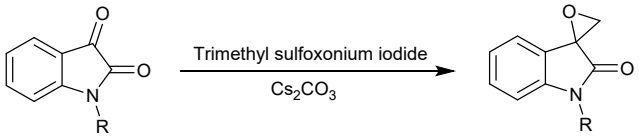


Figure S24. Computed Gibbs free energy profile diagram for the carboxylate group-initiated ring opening of epoxide using [TMA][Bz] in kcal/mol at the B3LYP-D3(BJ)/6-311++G(d,p)//B3LYP-D3(BJ)/ 6-31G(d) level of theory. The bond lengths in the transition states are given in Å.

Typical procedure for synthesis of spiro-epoxyoxindole:



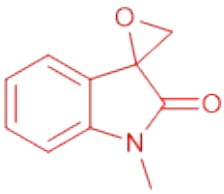
Trimethylsulfoxonium iodide (4.0 mmol) and cesium carbonate (8.0 mmol) were placed in a round-bottom flask containing dry acetonitrile (CH_3CN) and stirred at 50 °C under an inert atmosphere for 1 h to generate the sulfur ylide. Subsequently, a solution of isatin (4.0 mmol) in 20 mL of dry CH_3CN was added dropwise over 10 minutes. The reaction progress was monitored using thin-layer chromatography (TLC). Upon completion, the reaction mixture was filtered through a Celite bed, and the filtrate was evaporated to obtain a concentrated product. The final product was purified using column chromatography with silica gel as the stationary phase and a mobile phase of n-hexane and ethyl acetate in a 90:10 ratio.[15]

^{1}H & ^{13}C NMR spectra of Spirocyclic epoxide derivatives.

1-benzylspiro[indoline-3,2'-oxiran]-2-one

^{1}H NMR (500 MHz, $CDCl_3$) **δ** = 7.34 (d, 4H), 7.29 (m, 2H), 7.13 (d, 1H), 7.06 (t, 1H), 6.83 (d, 1H), 5.02 (q, 2H), 3.67 (d, 1H), 3.49 (d, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) **δ** = 171.9, 144.29, 135.33, 130.35, 128.89, 127.86, 127.45, 122.95, 122.73, 122.21, 109.92, 56.41, 54.34, 44.35.

1-methylspiro[indoline-3,2'-oxiran]-2-one



^{1}H NMR (600 MHz, $CDCl_3$) **δ** = 7.4 (t, 1H), 7.12 (m, 2H), 6.93 (d, 1H), 3.59 (d, 1H), 3.58 (d, 1H), 3.28 (s, 1H). ^{13}C NMR (151 MHz, CDCl3) **δ** = 171.85, 145.21, 130.51, 122.97, 122.81, 122.19, 108.92, 56.47, 54.16, 26.73.

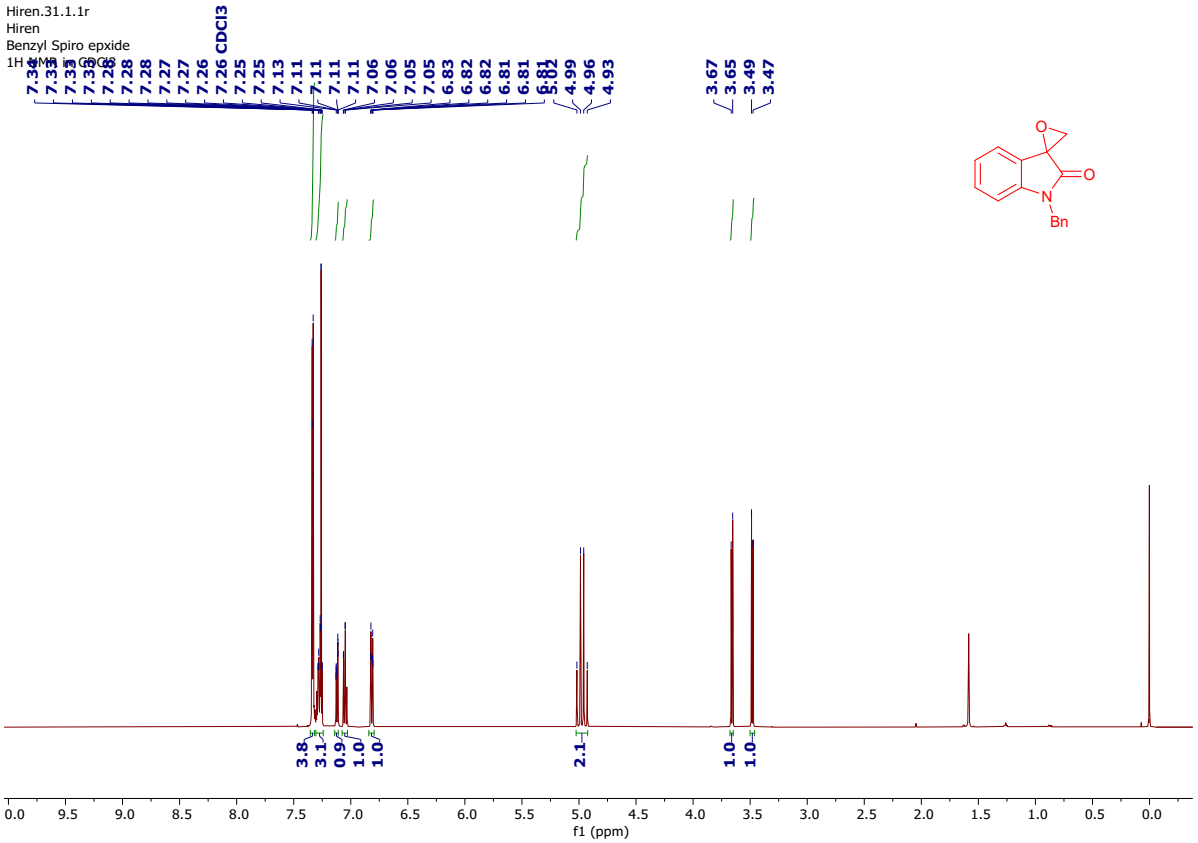


Figure S25: ^{1}H-NMR of 1-benzylspiro[indoline-3,2'-oxiran]-2-one.

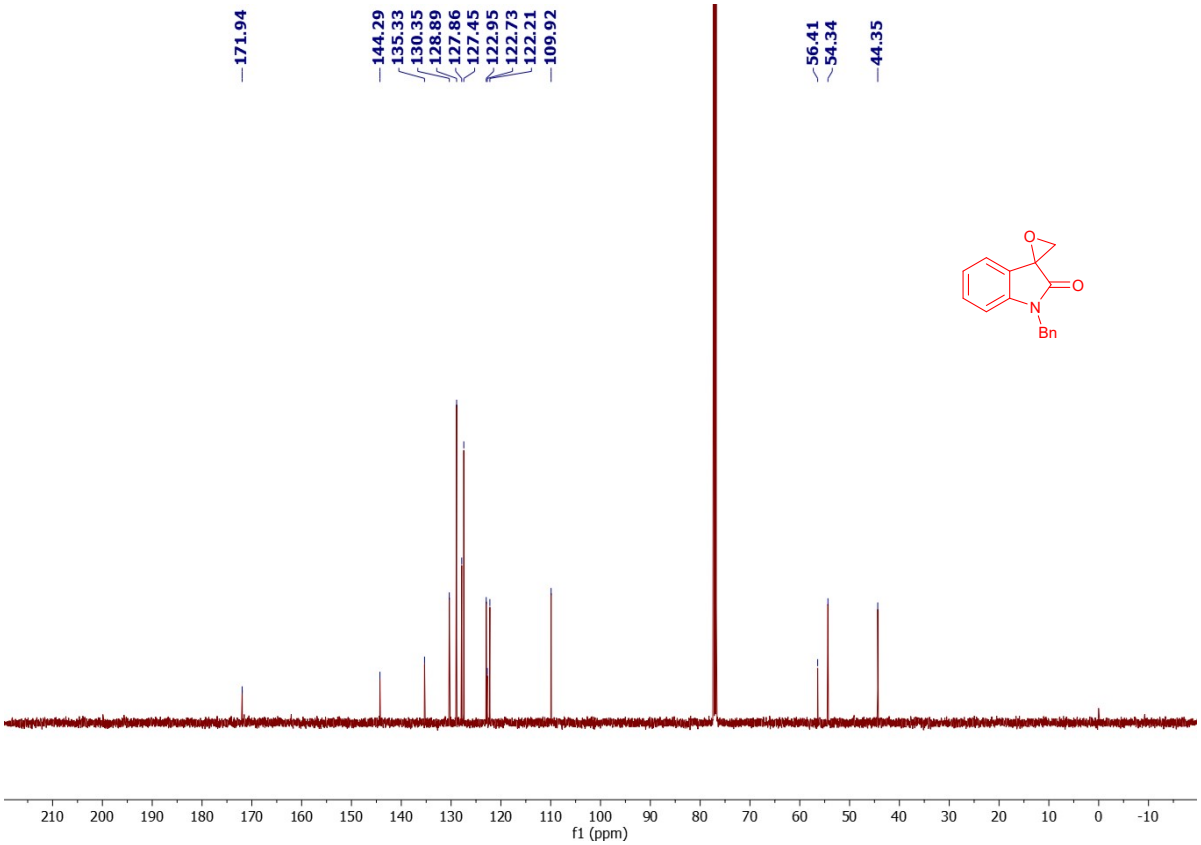


Figure S26: ^{13}C-NMR of 1-benzylspiro[indoline-3,2'-oxiran]-2-one.

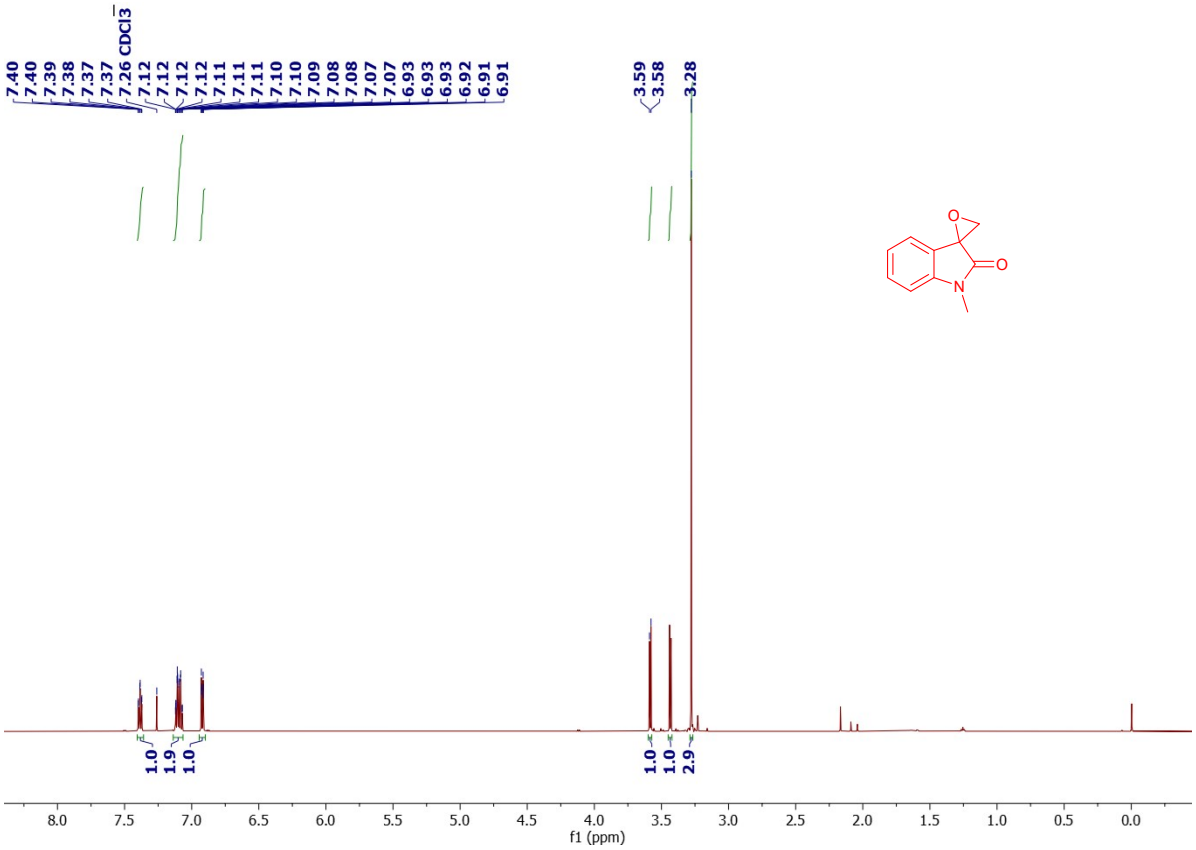


Figure S27: ^{1}H-NMR of 1-methylspiro[indoline-3,2'-oxiran]-2-one.

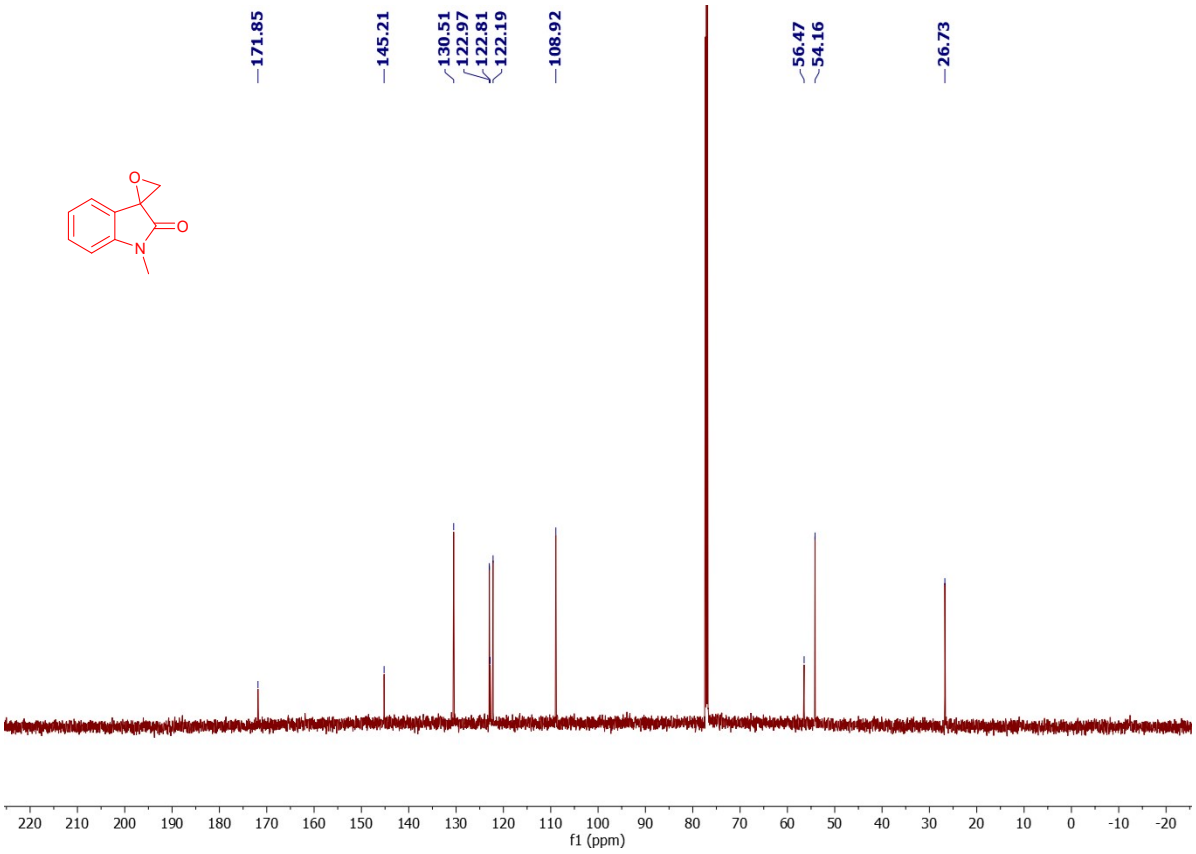
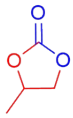


Figure S28: ^{13}C-NMR of 1-methylspiro[indoline-3,2'-oxiran]-2-one

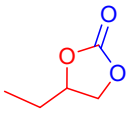
^{1}H & ^{13}C NMR spectra of Cyclic Carbonate derivatives.

Propylene Carbonate:



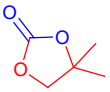
^{1}H NMR (500 MHz, $CDCl_3$, Me_4Si) **δ** ppm:4.8 (m-1H), 4.48 (t-1H), 3.94 (t-1H), 1.37 (d-3H),^{13}C NMR (125 MHz, $CDCl_3$, Me_4Si) **δ** ppm:155.05, 73.6, 70.5, 19.07.

4-ethyl-1,3-dioxolan-2-one



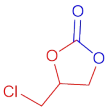
^{1}H NMR (500 MHz, $CDCl_3$, Me_4Si) **δ** ppm:4.67 (m-1H), 4.52 (t-1H), 4.07 (t-1H), 1.80 (m-2H), 1.01 (t-3H),^{13}C NMR (125 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 155.25, 78.13, 69.11, 26.96, 8.52.

4,4-dimethyl-1,3-dioxolan-2-one



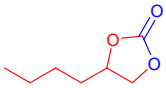
^{1}H NMR (500 MHz, $CDCl_3$, Me_4Si) **δ** ppm:4.1 (s-2H), 1.45 (s-6H), ^{13}C NMR (125 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 154.71, 81.87, 75.4, 25.97.

4-(chloromethyl)-1,3-dioxolan-2-one:



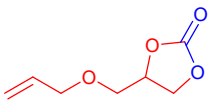
^{1}H NMR (600 MHz, $CDCl_3$, Me_4Si) **δ** ppm:4.94 (m-1H), 4.48 (d-1H), 4.29 (d-1H), 3.74 (d-1H), 3.63 (d-1H),^{13}C NMR (151 MHz, $CDCl_3$, Me4Si) **δ** ppm: 154.8, 74.8, 67, 44.67.

4-butyl-1,3-dioxolan-2-one:



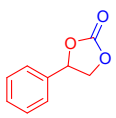
^{1}H NMR (600 MHz, $CDCl_3$, Me_4Si) **δ** ppm:4.63 (m-1H), 4.45 (t-1H), 3.98 (t-1H), 1.69-1.59 (m-2H), 1.36 (m-2H), 1.28 (m-2H), 0.82 (m-3H),^{13}C NMR (151 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 155.2, 77.2, 69.5, 33.4, 26.4, 22.2, 13.7.

4-((allyloxy)methyl)-1,3-dioxolan-2-one:



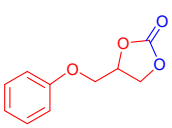
^{1}H NMR (500 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 5.85 (m-1H), 5.26 (d-1H), 5.22 (d-1H), 4.81 (m-1H), 4.48 (t-1H), 4.36 (t-1H), 4.0 (m-2H), 3.67 (d-1H), 3.58 (t-1H) ^{13}C NMR (125 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 155.09, 133.72, 117.75, 75.19, 72.19, 68.85, 66.26.

Styrene Carbonate:



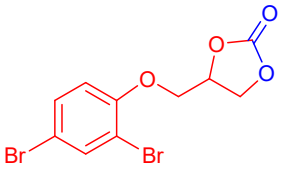
^{1}H NMR (600 MHz, $CDCl_3$, Me_4Si) **δ** ppm:7.4 (d-1H), 7.39 (t-2H), 7.33 (t-2H), 5.65 (t-1H), 4.76 (t-1H), 4.29 (t-1H),^{13}C NMR (151 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 155.1, 136, 129.7, 129.3, 126.1, 76.1, 71.3.

4-(phenoxymethyl)-1,3-dioxolan-2-one:



^{1}H NMR (600 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 7.32 (t-2H), 7.03 (d-1H), 6.92 (d-2H),5.04 (m-1H), 4.62 (t-1H), 4.45 (t-1H), 4.25 (dd-1H), 4.15 (dd-1H), ^{13}C NMR (151 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 157.8, 154.7, 129.8, 122.1, 114.7, 74.2, 66.9, 66.3.

4-((2,4-dibromophenoxy)methyl)-1,3-dioxolan-2-one

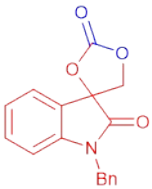


^{1}H NMR (500 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 7.64 (s-1H), 7.36 (d-1H), 6.76 (d-1H), 5.07 (m-2H), 4.63 (d,-1H), 4.27 (dd-1H), 4.15 (dd-1H), ^{13}C NMR (125 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 154.73, 153.52, 135.74, 131.46, 114.95, 114.60, 113.45, 73.99, 68.30, 66.10.

Cyclohexane Carbonate:

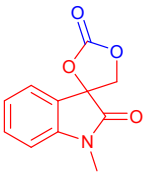
^{1}H NMR (600 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 4.55 (t-2H), 1.75 (m-2H), 1.67 (m-2H), 1.43 (m-2H), 1.28 (m-2H), ^{13}C NMR (151 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 155.4, 75.8, 26.5, 18.9.

1-benzylspiro[indoline-3,4'-[1,3]dioxolane]-2,2'-dione:



^{1}H NMR (500 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 7.47 (d-1H), 7.36 (t-3H), 7.31 (t-3H), 7.17 (t-1H), 4.97 (d-1H), 4.86 (d-1H), 4.79 (d-1H), 4.59 (d-1H), ^{13}C NMR (125 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 171.52, 153.64, 143.56, 134.41, 132.40, 129.08, 128.21, 127.37, 124.98, 124.16, 123.42, 110.43, 70.81, 44.33.

1-methylspiro[indoline-3,4'-[1,3]dioxolane]-2,2'-dione:



^{1}H NMR (600 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 7.48 (dd-2H), 7.2 (t-1H), 6.91 (d-1H), 4.73 (d-1H), 4.54 (d-1H), 3.23 (s-3H), ^{13}C NMR (151 MHz, $CDCl_3$, Me_4Si) **δ** ppm: 171.36, 153.73, 144.45, 132.55, 124.93, 124.24, 123.6, 109.46, 70.85, 26.75.

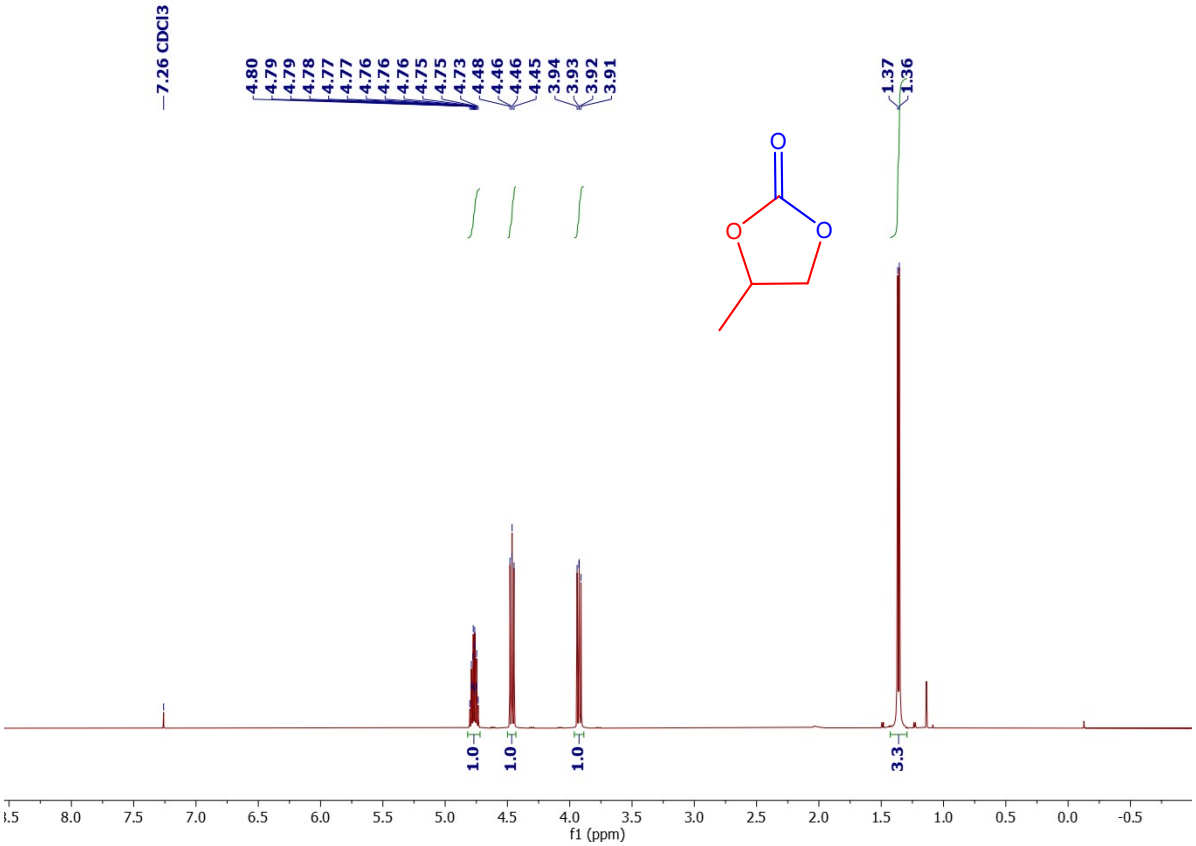


Figure S29: ^{1}H-NMR of Propylene carbonate.

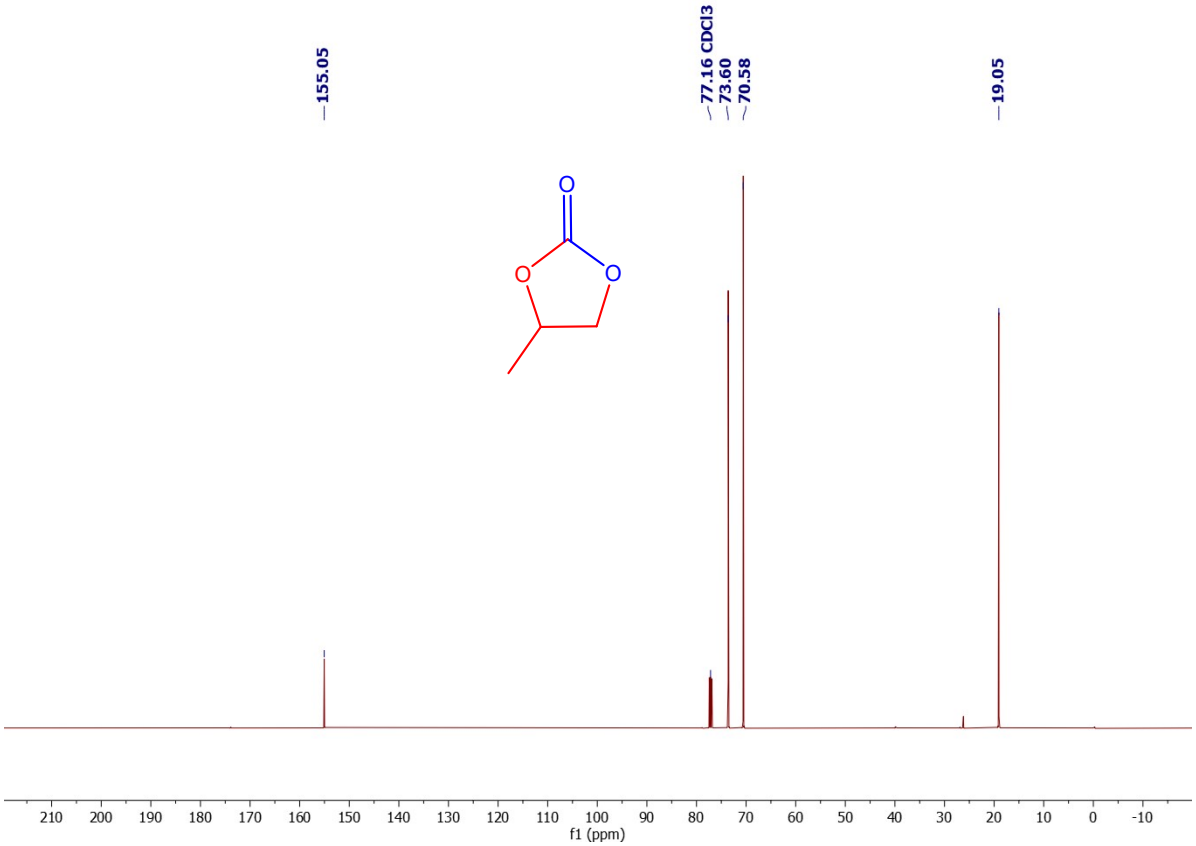


Figure S30: ^{13}C-NMR of Propylene carbonate.

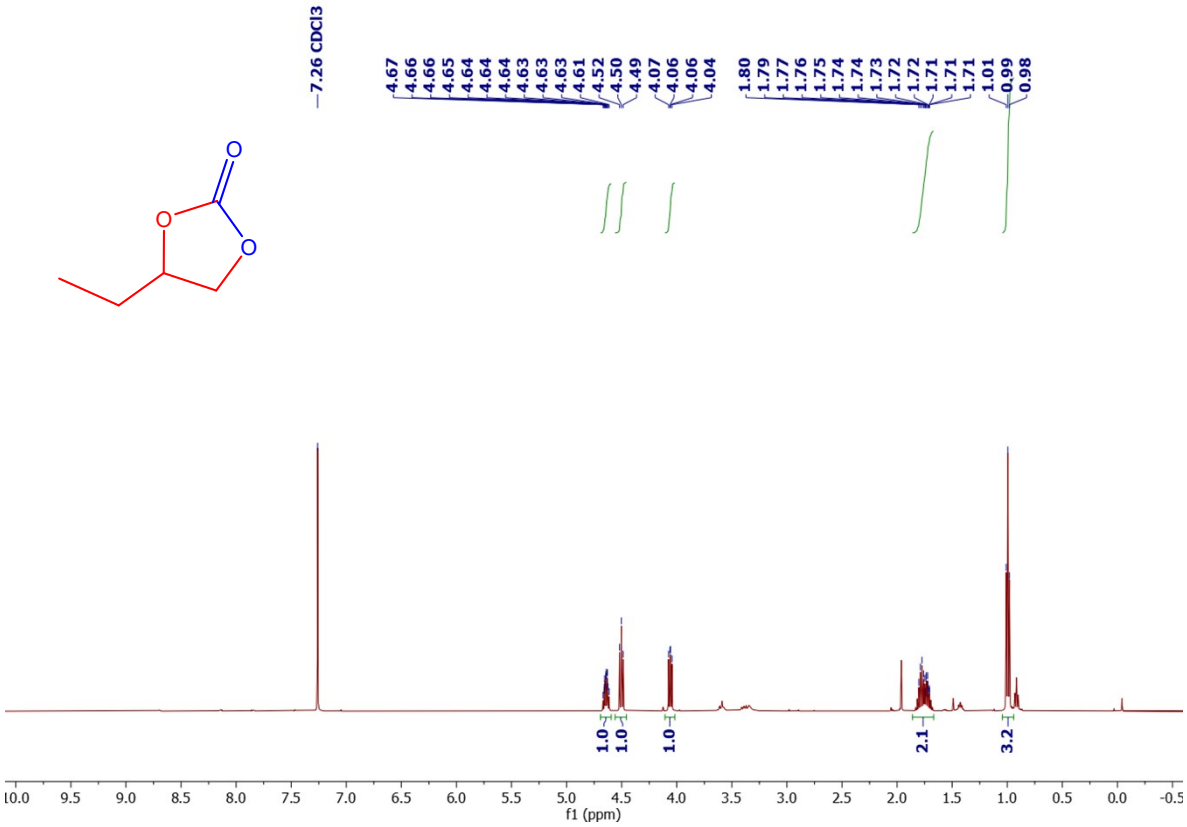


Figure S31: ^{1}H-NMR of 4-ethyl-1,3-dioxolan-2-one

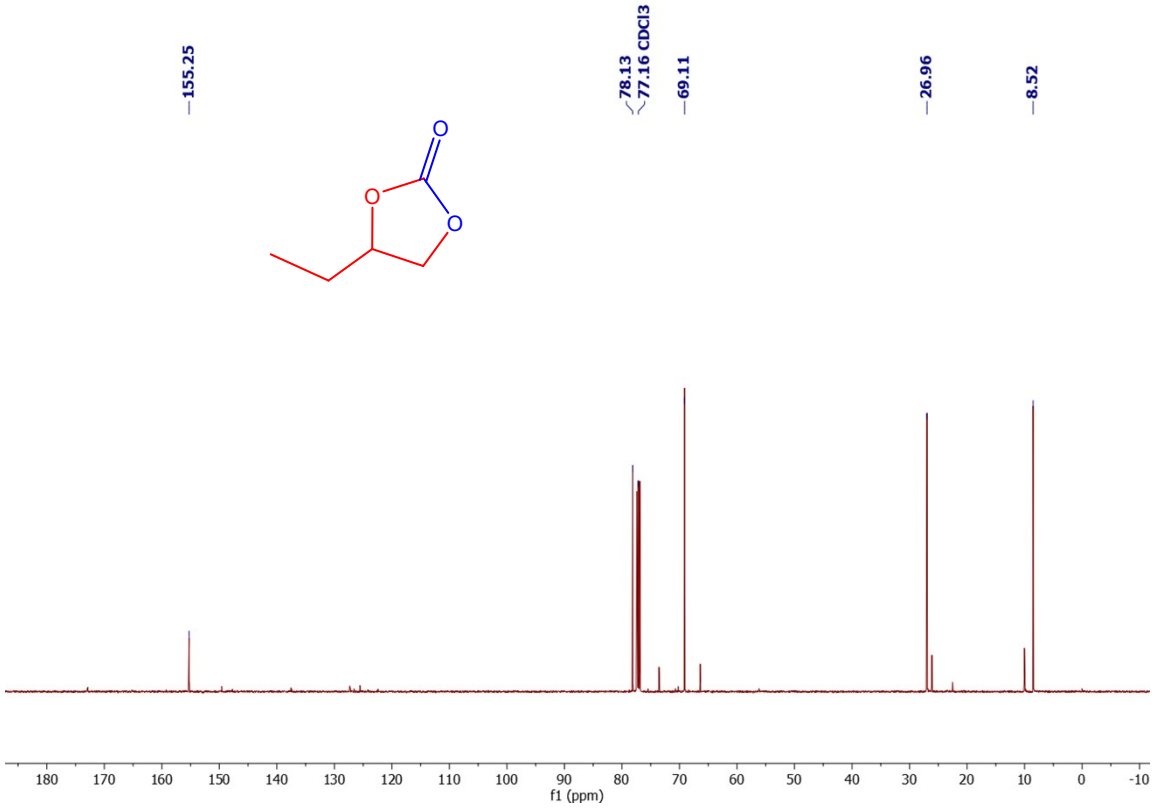


Figure S32: ^{13}C-NMR of 4-ethyl-1,3-dioxolan-2-one

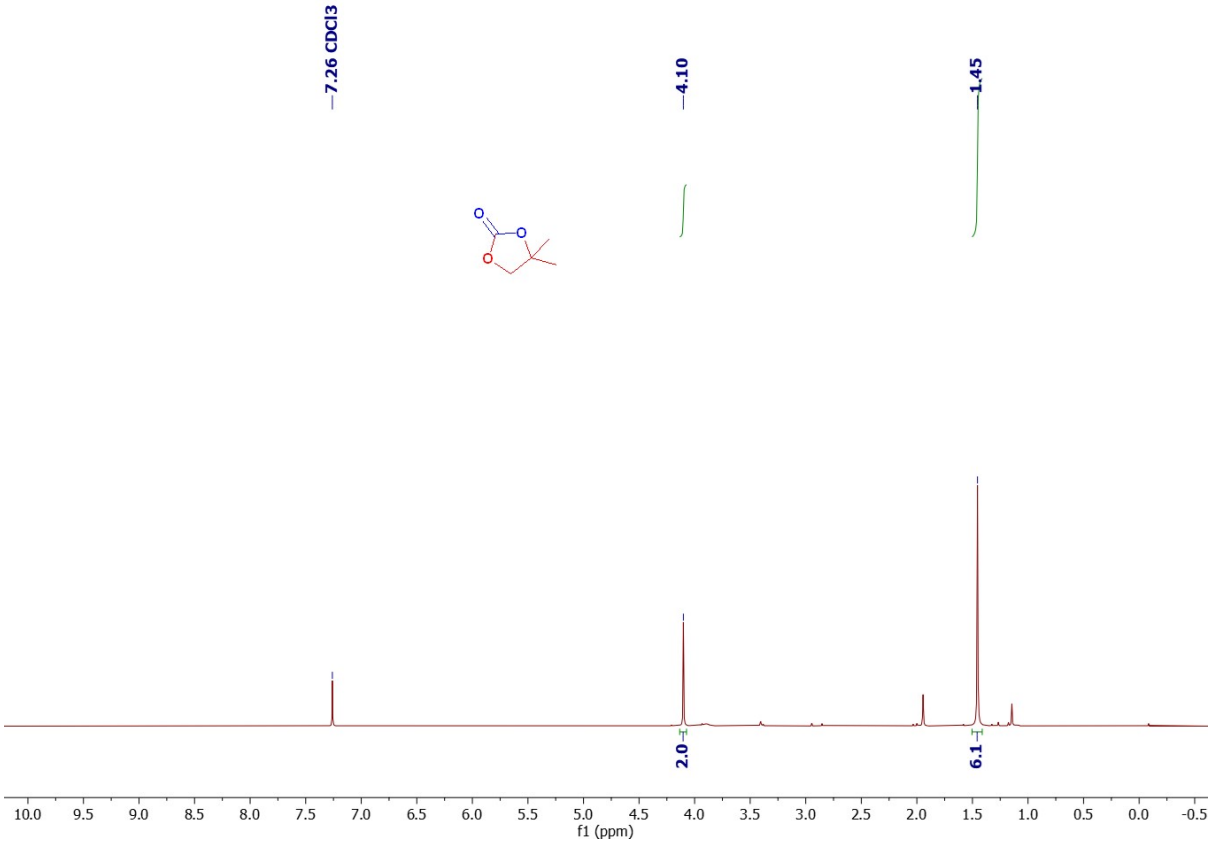


Figure S33: ^{1}H-NMR of 4,4-dimethyl-1,3-dioxolan-2-one

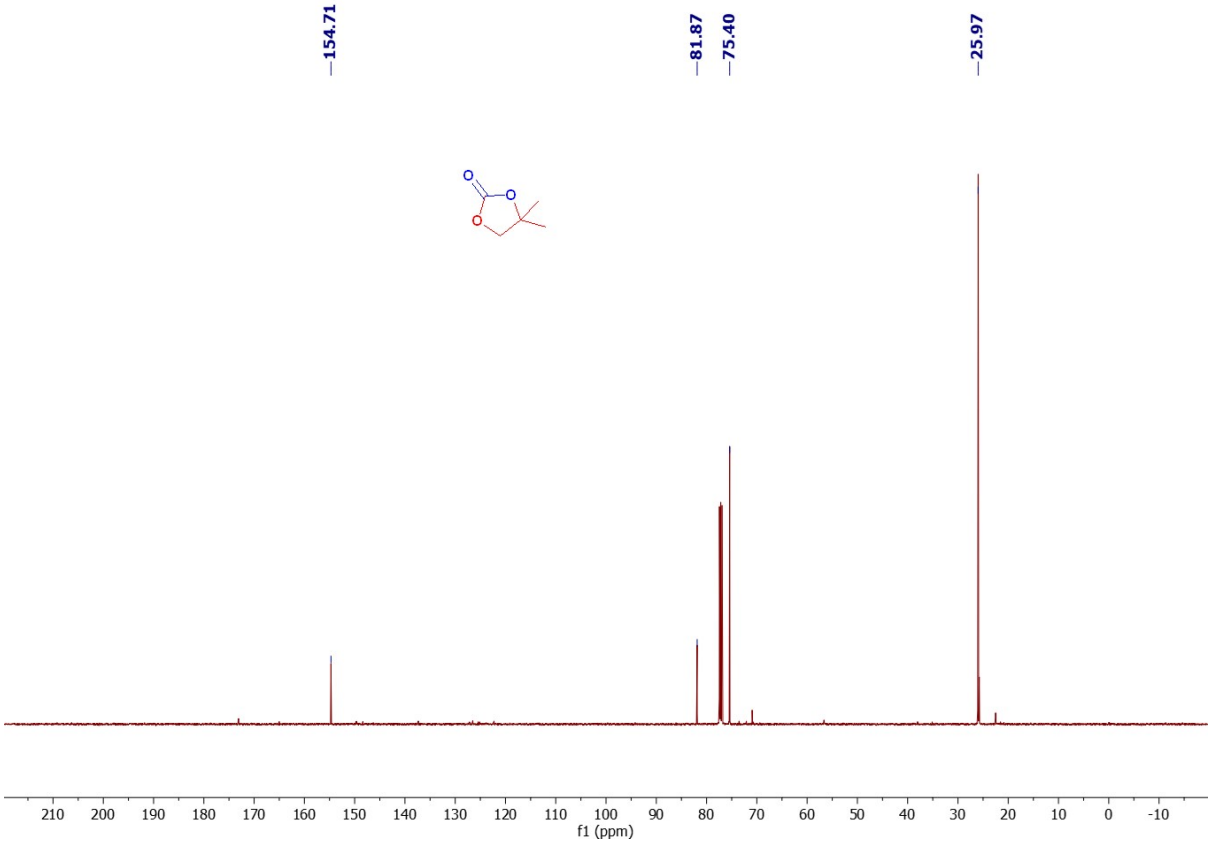


Figure S34: ^{13}C-NMR of 4,4-dimethyl-1,3-dioxolan-2-one

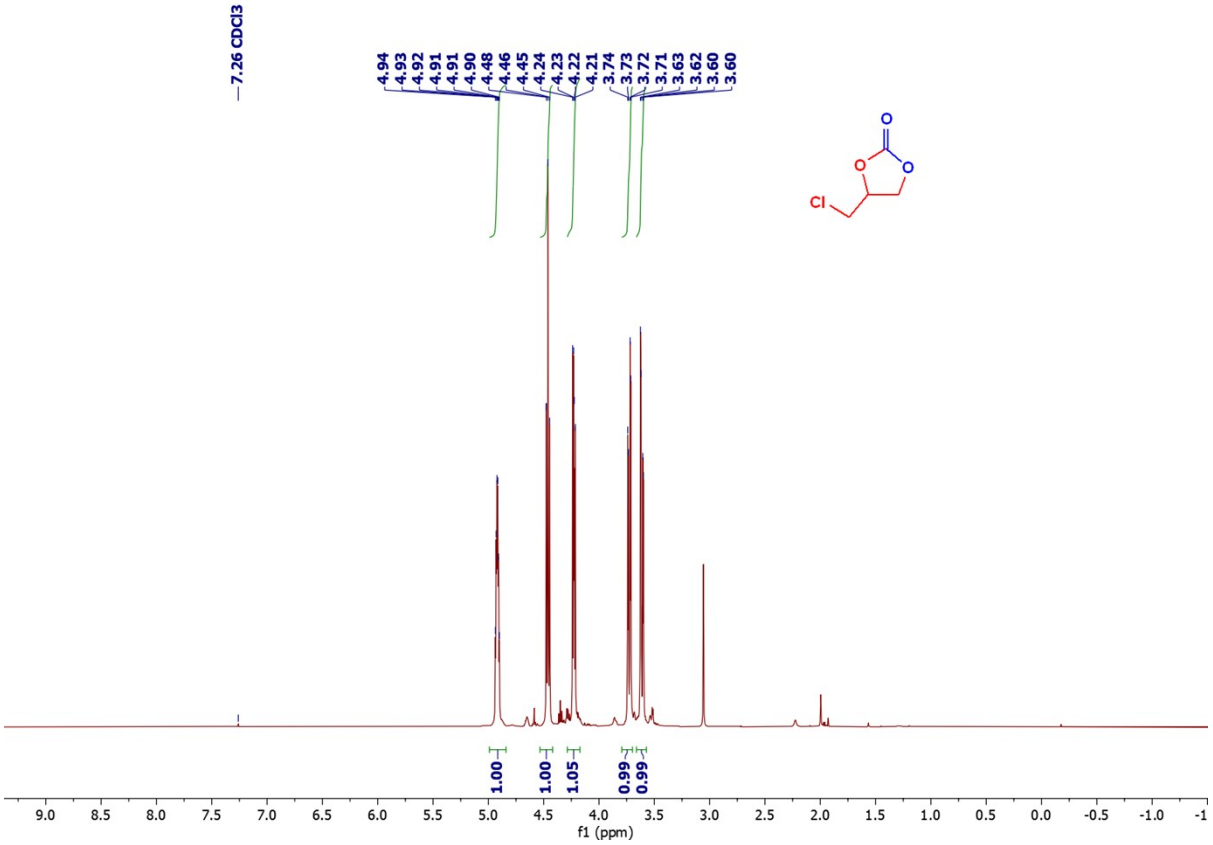


Figure S35: ^{1}H-NMR of 4-(chloromethyl)-1,3-dioxolan-2-one.

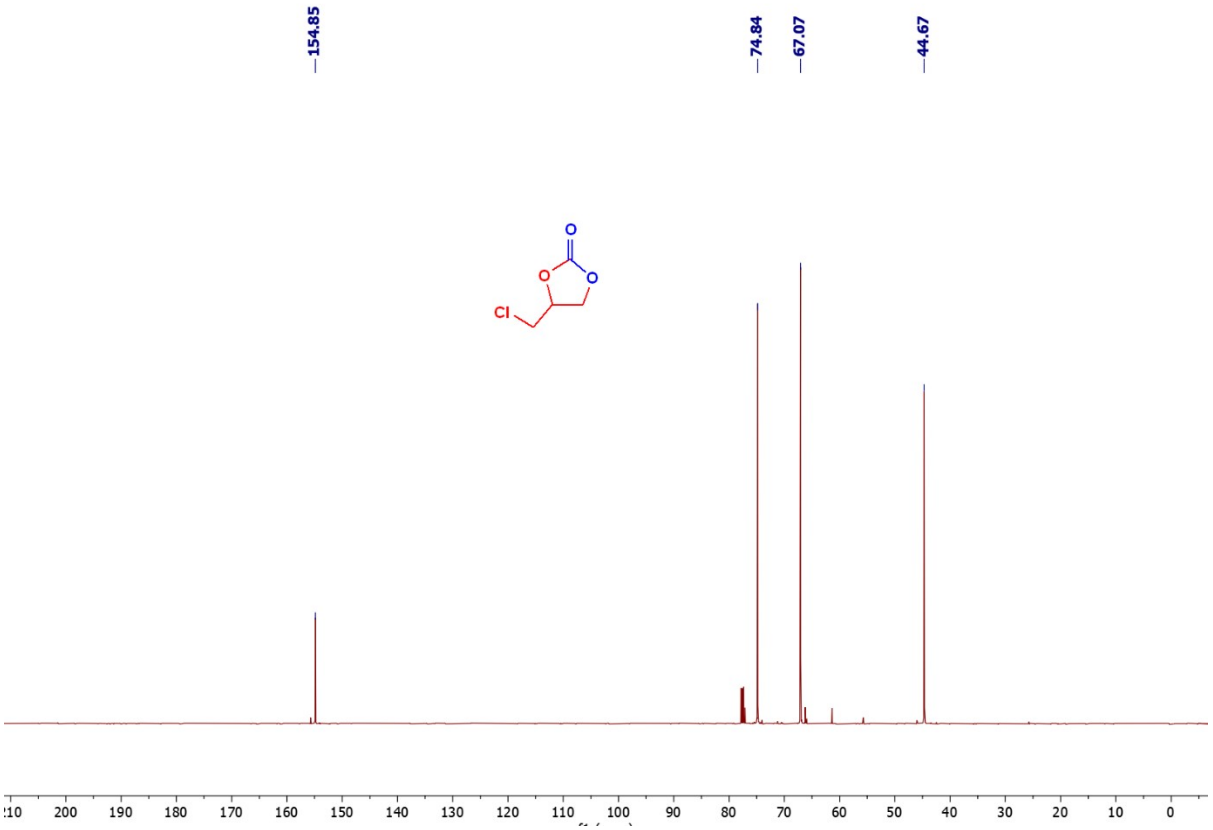


Figure S36: ^{13}C-NMR of 4-(chloromethyl)-1,3-dioxolan-2-one.

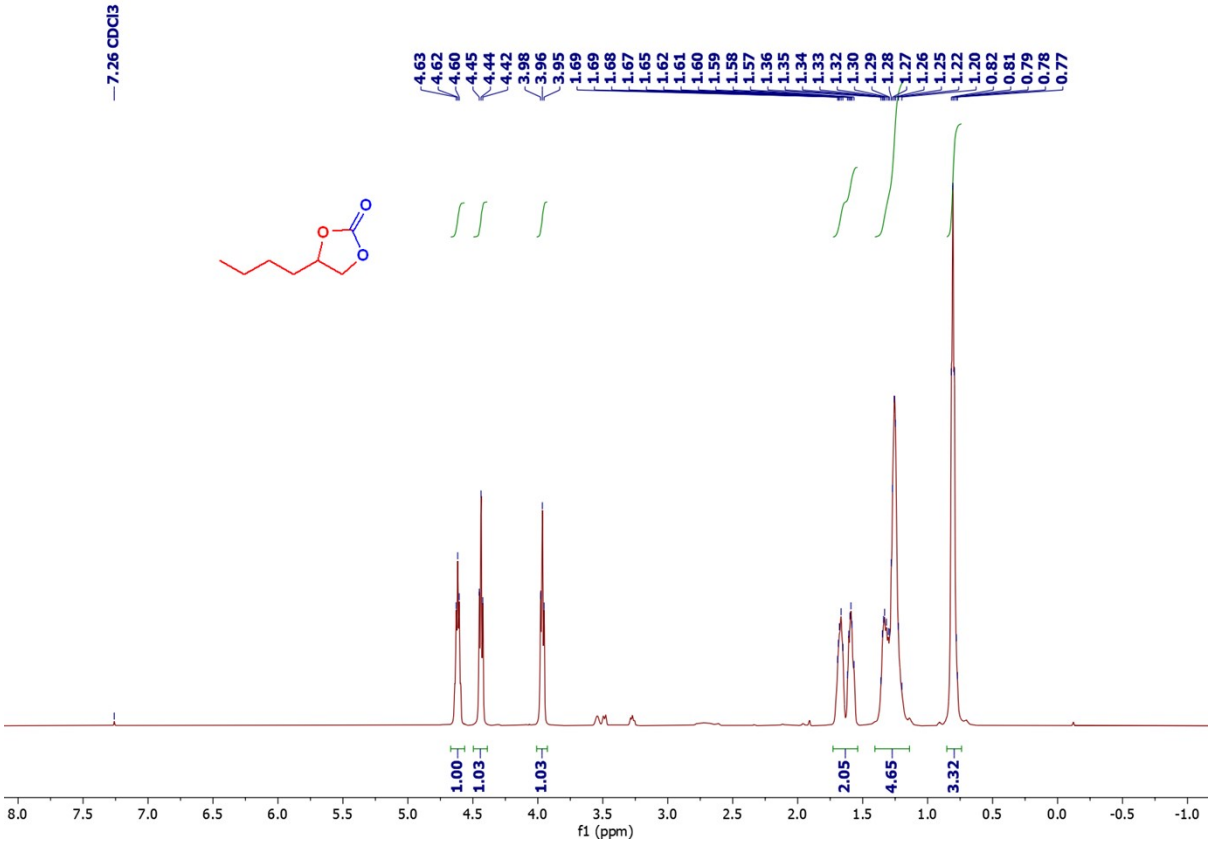


Figure S37: [1]H-NMR of 4-butyl-1,3-dioxolan-2-one.

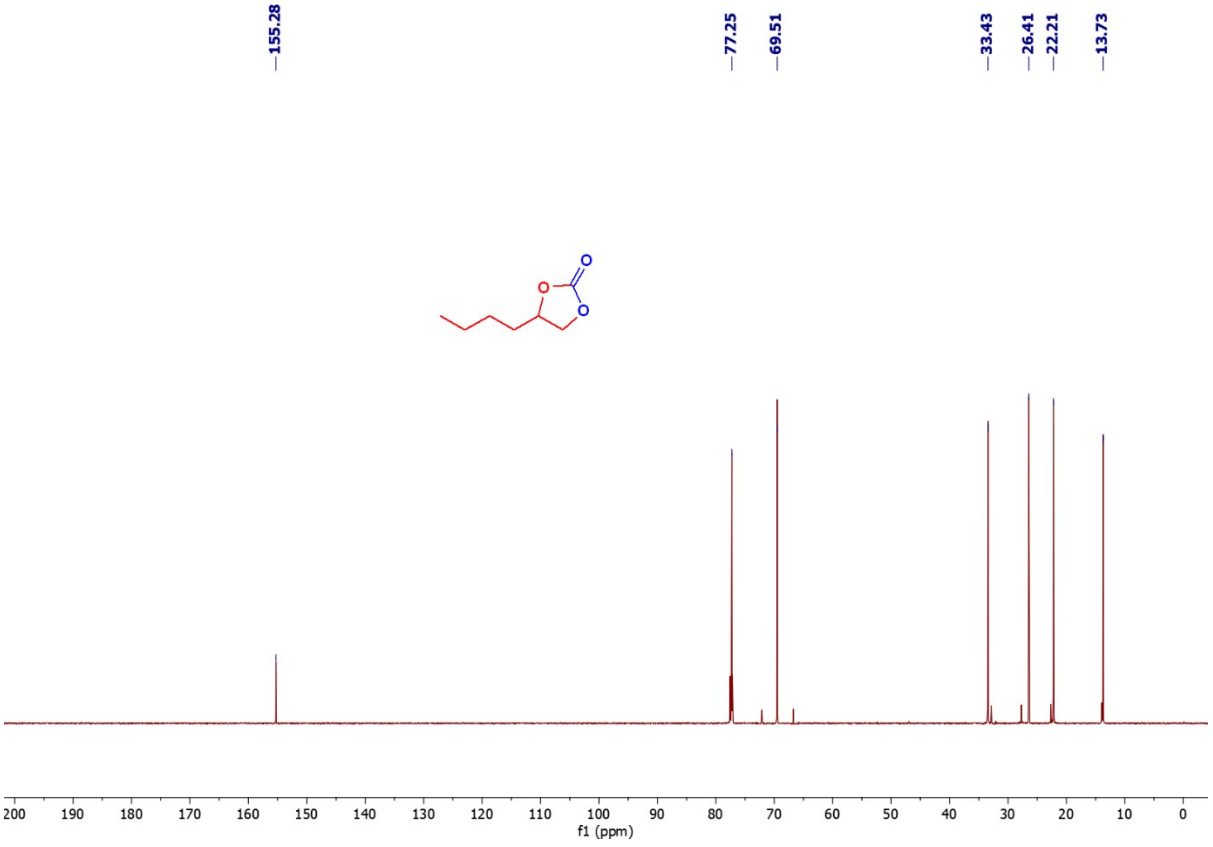


Figure S38: [13]C-NMR 4-butyl-1,3-dioxolan-2-one.

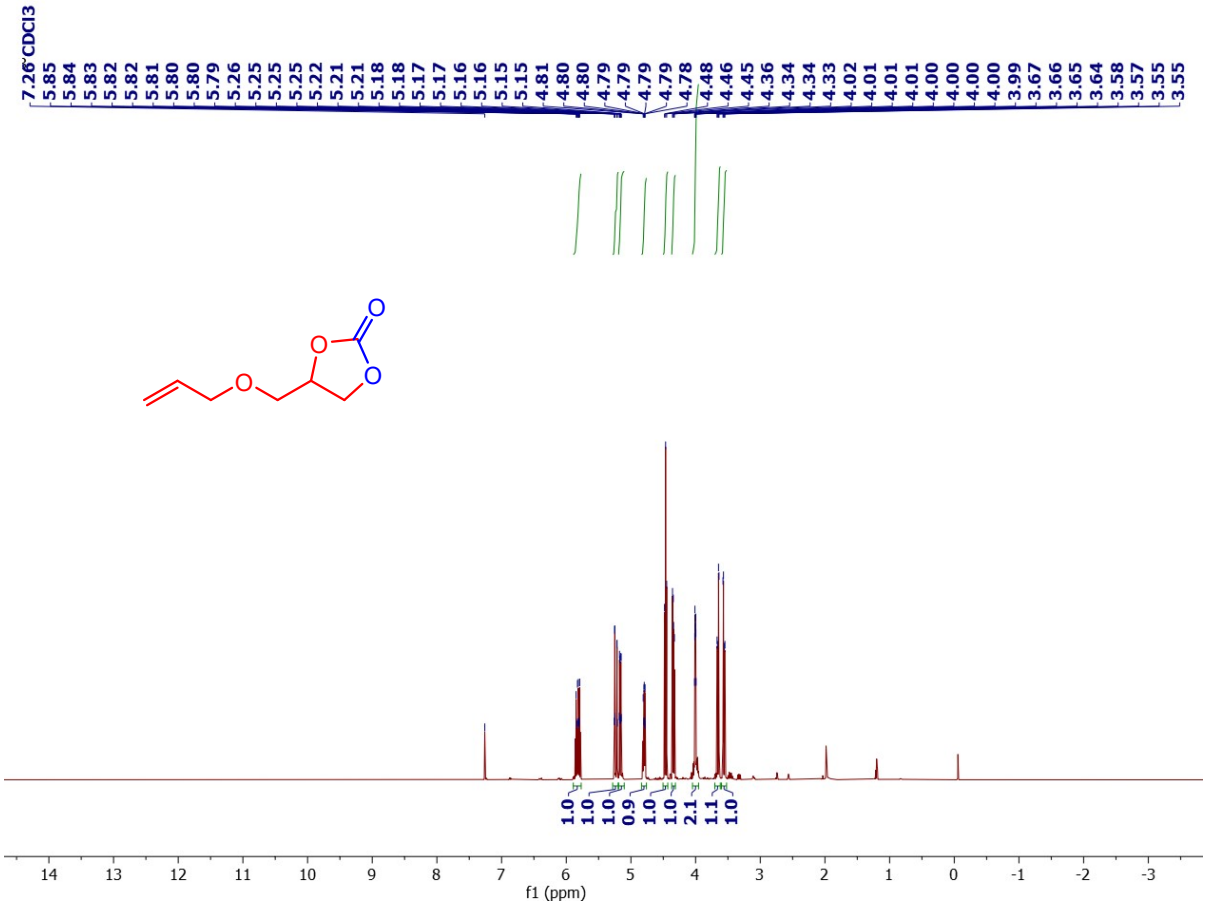


Figure S39: [1]H-NMR of 4-((allyloxy)methyl)-1,3-dioxolan-2-one:

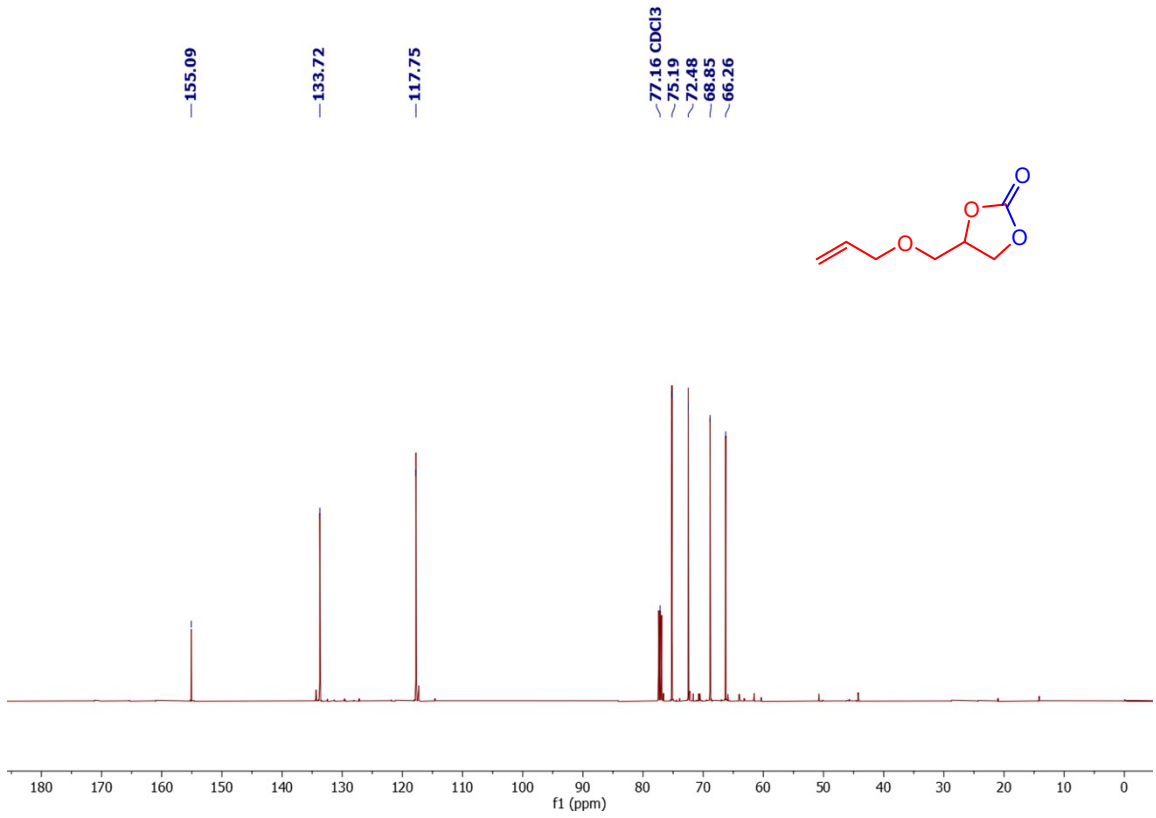


Figure S40: [13]C-NMR of 4-((allyloxy)methyl)-1,3-dioxolan-2-one:

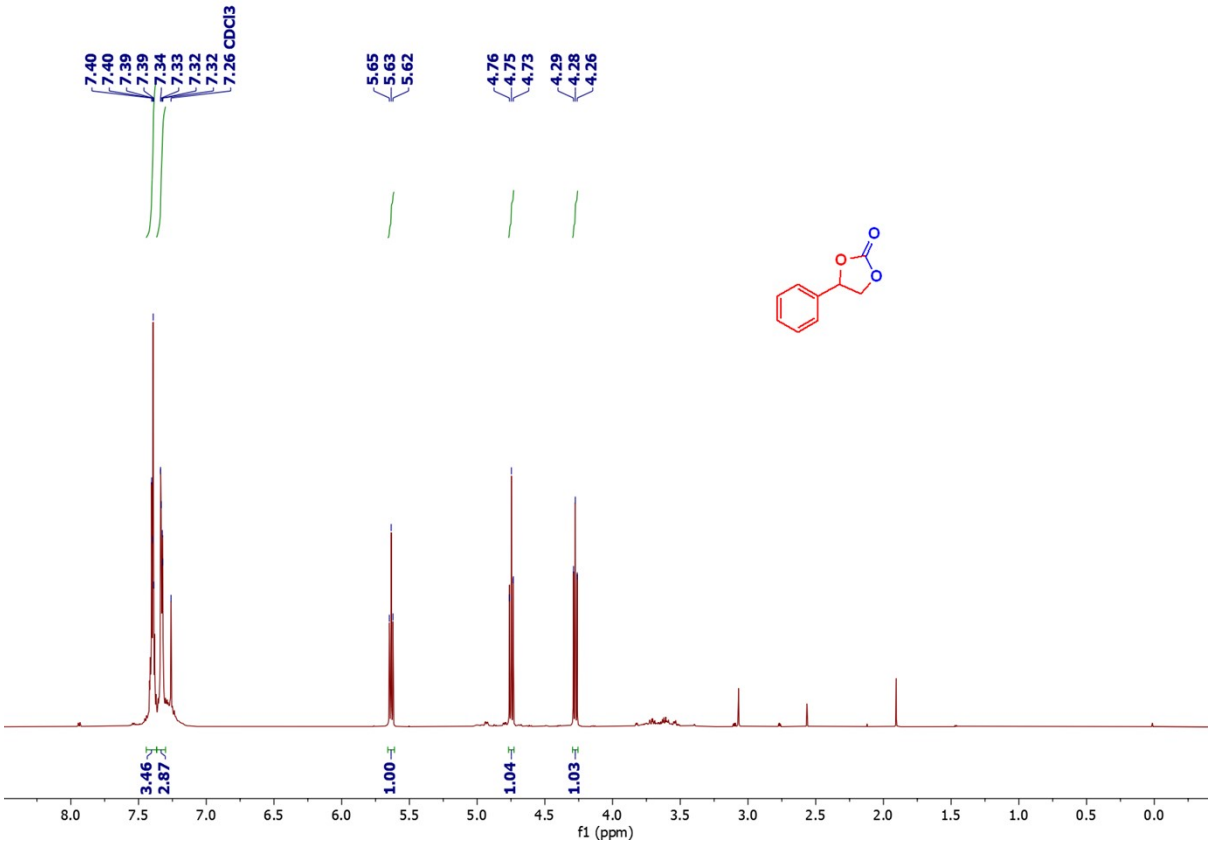


Figure S41: ^{1}H-NMR of Styrene carbonate.

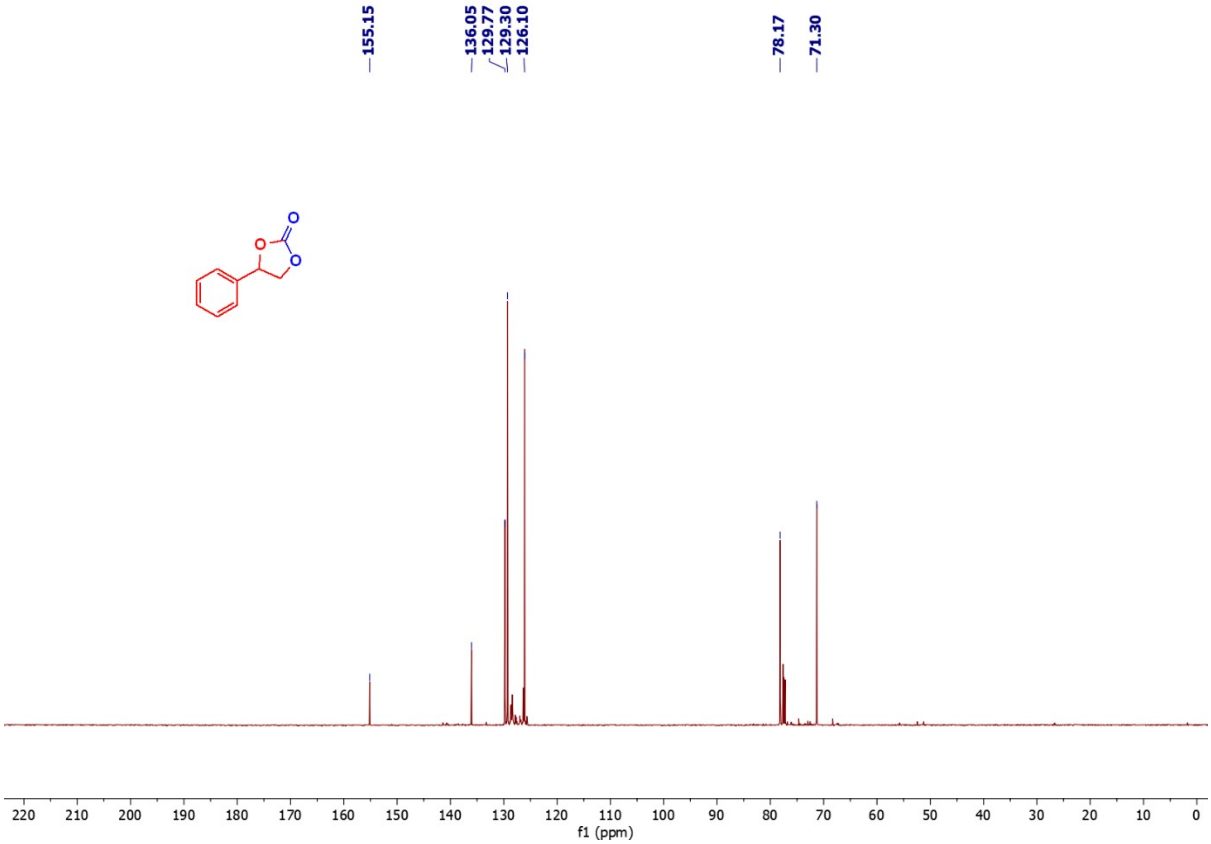


Figure S42: ^{13}C-NMR of Styrene carbonate.

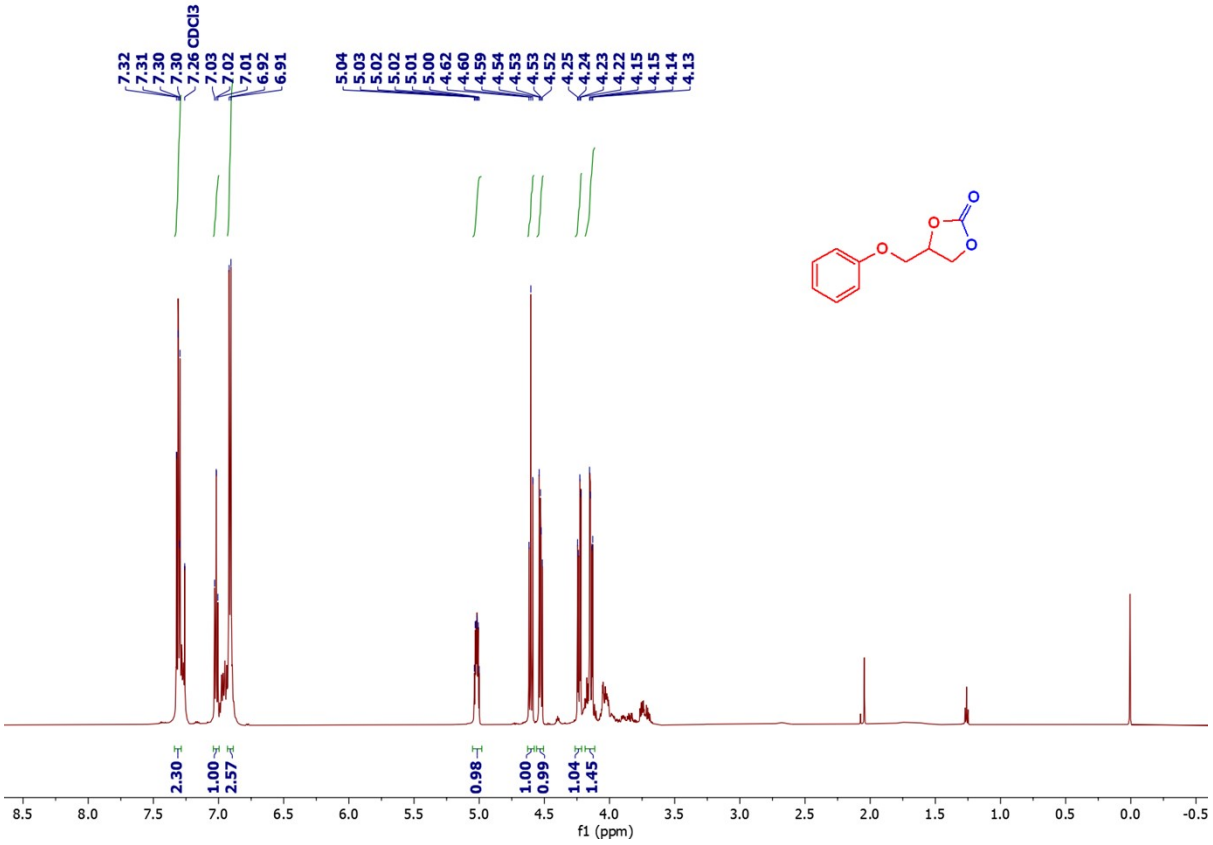


Figure S43: [1]H-NMR of 4-(phenoxymethyl)-1,3-dioxolan-2-one.

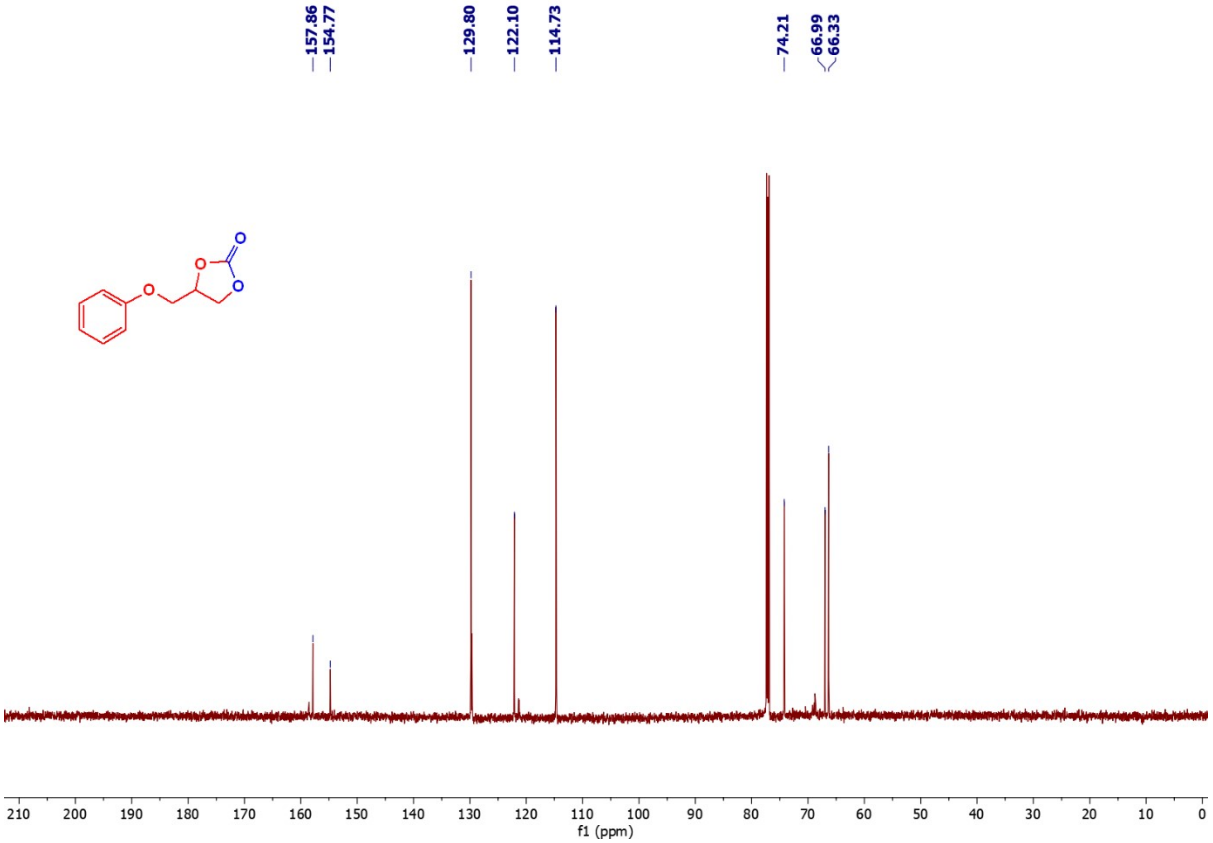


Figure S44: [13]C-NMR of 4-(phenoxymethyl)-1,3-dioxolan-2-one.

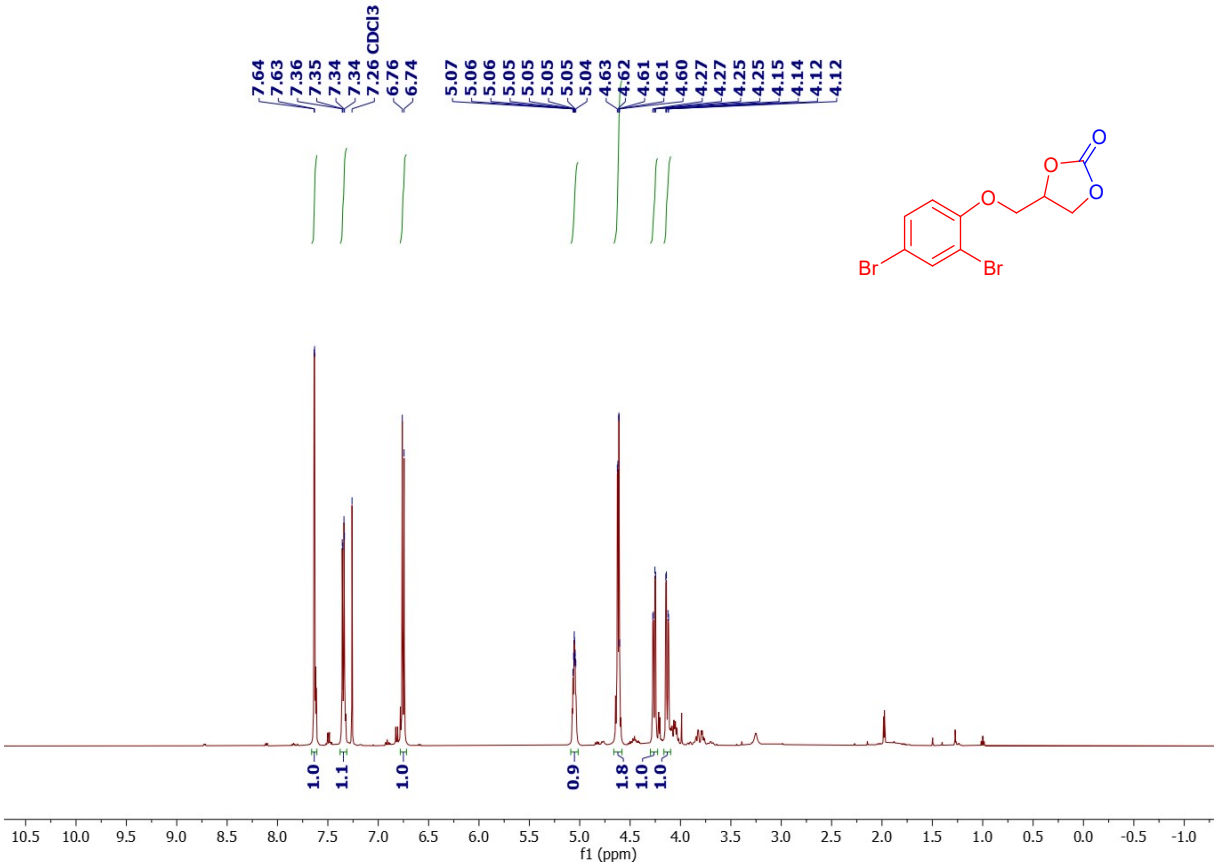


Figure S45: [1]H-NMR of 4-((2,4-dibromophenoxy)methyl)-1,3-dioxolan-2-one

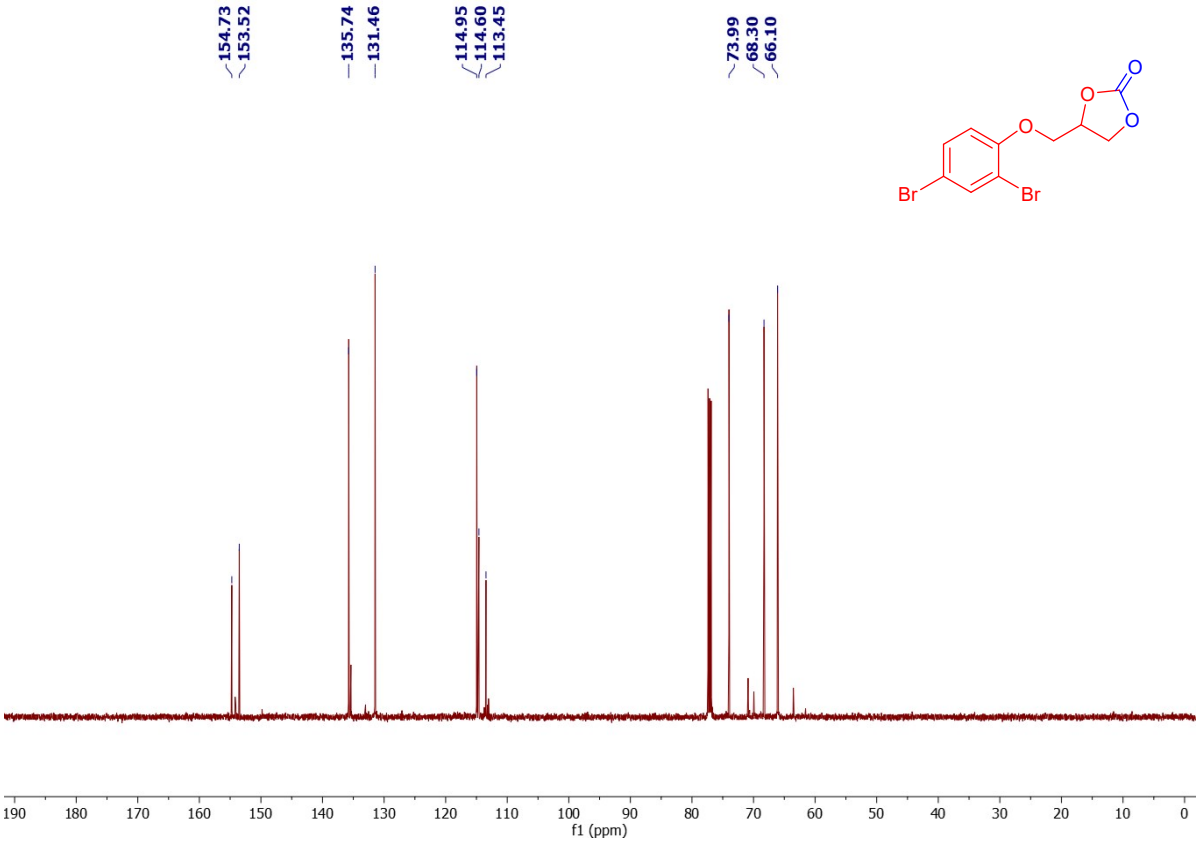


Figure S46: [13]C-NMR of 4-((2,4-dibromophenoxy)methyl)-1,3-dioxolan-2-one

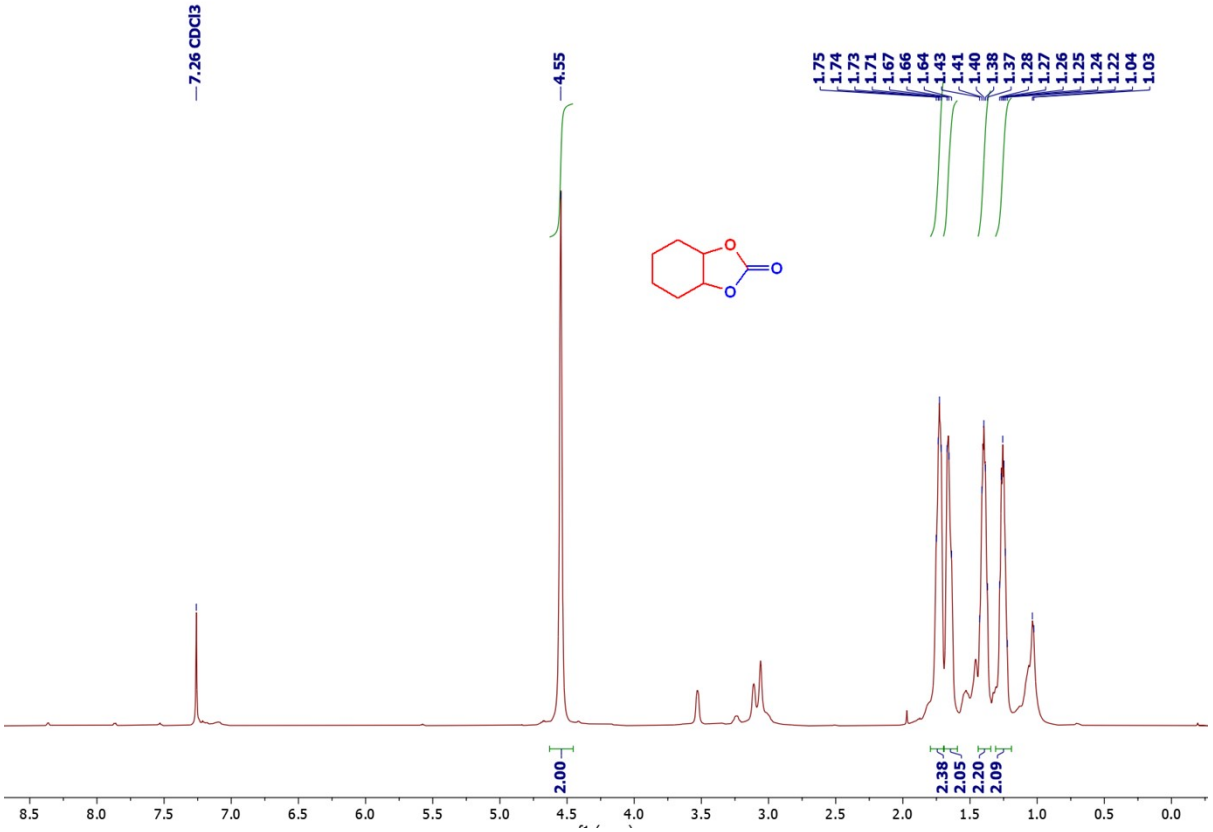


Figure S47: ^{1}H-NMR of Cyclohexane carbonate.

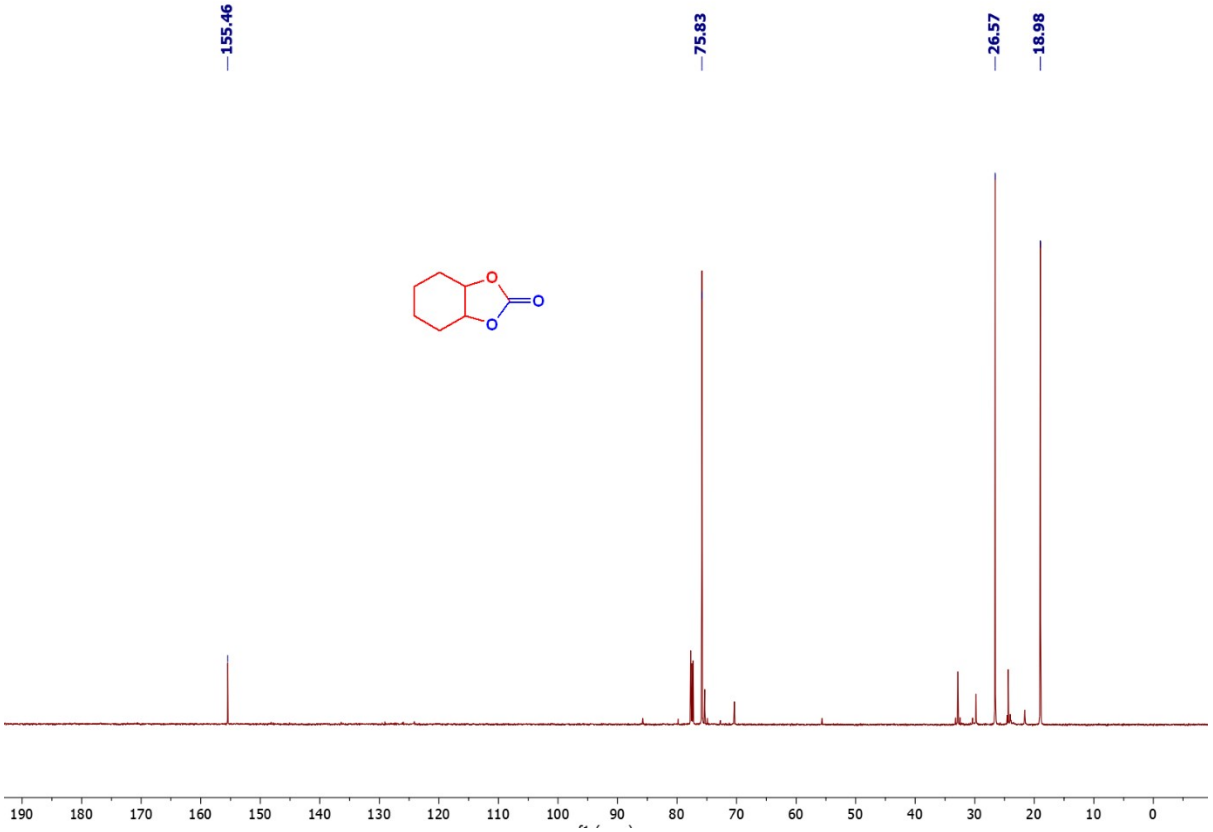


Figure S48: ^{13}C-NMR of Cyclohexane carbonate.

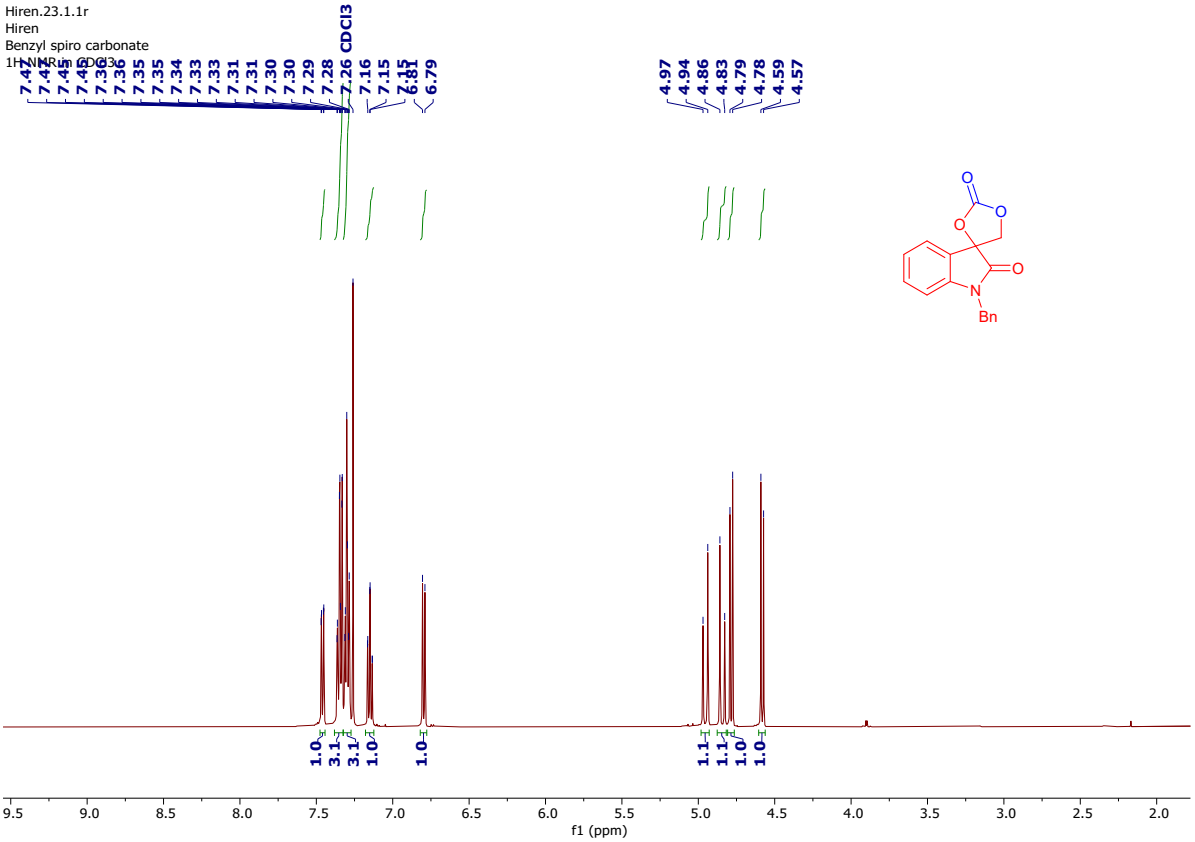


Figure S49: [1]H-NMR of 1-benzylspiro[indoline-3,4'-[1,3]dioxolane]-2,2'-dione:

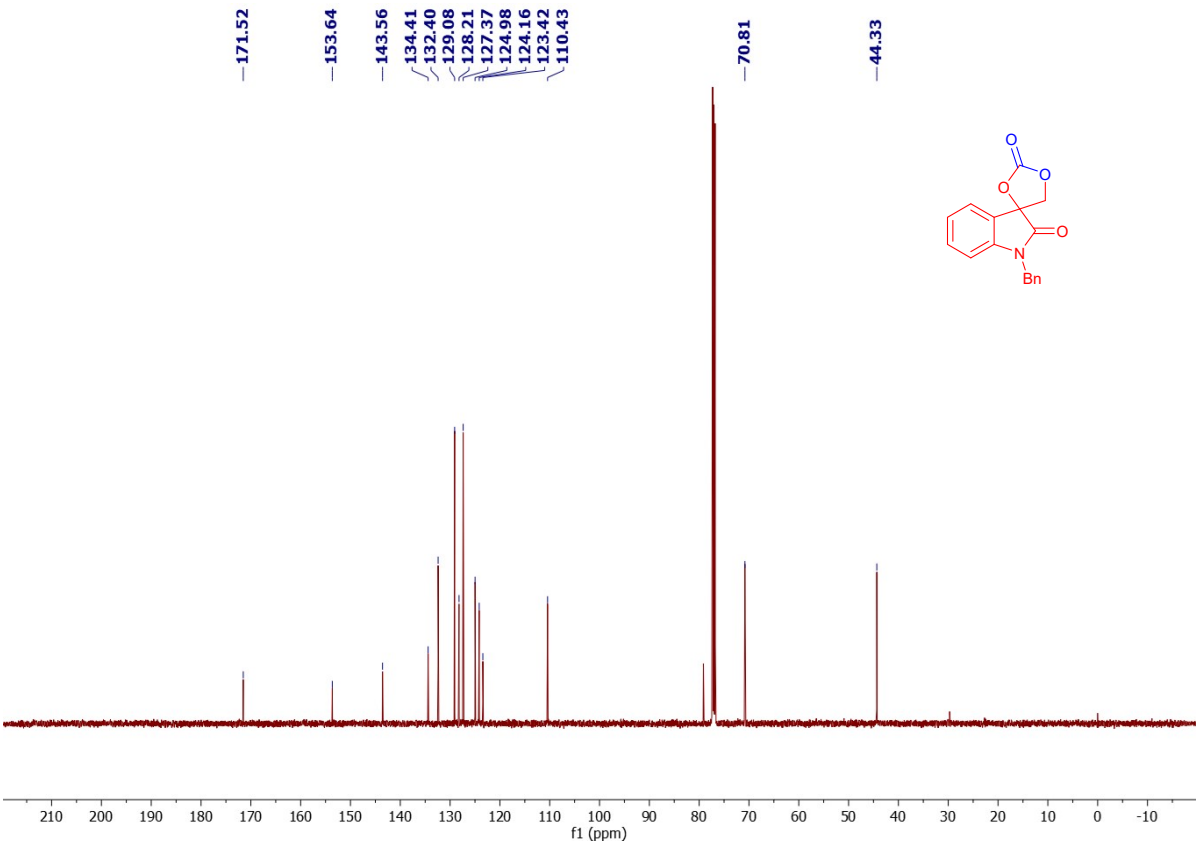


Figure S50: [13]C-NMR of 1-benzylspiro[indoline-3,4'-[1,3]dioxolane]-2,2'-dione:

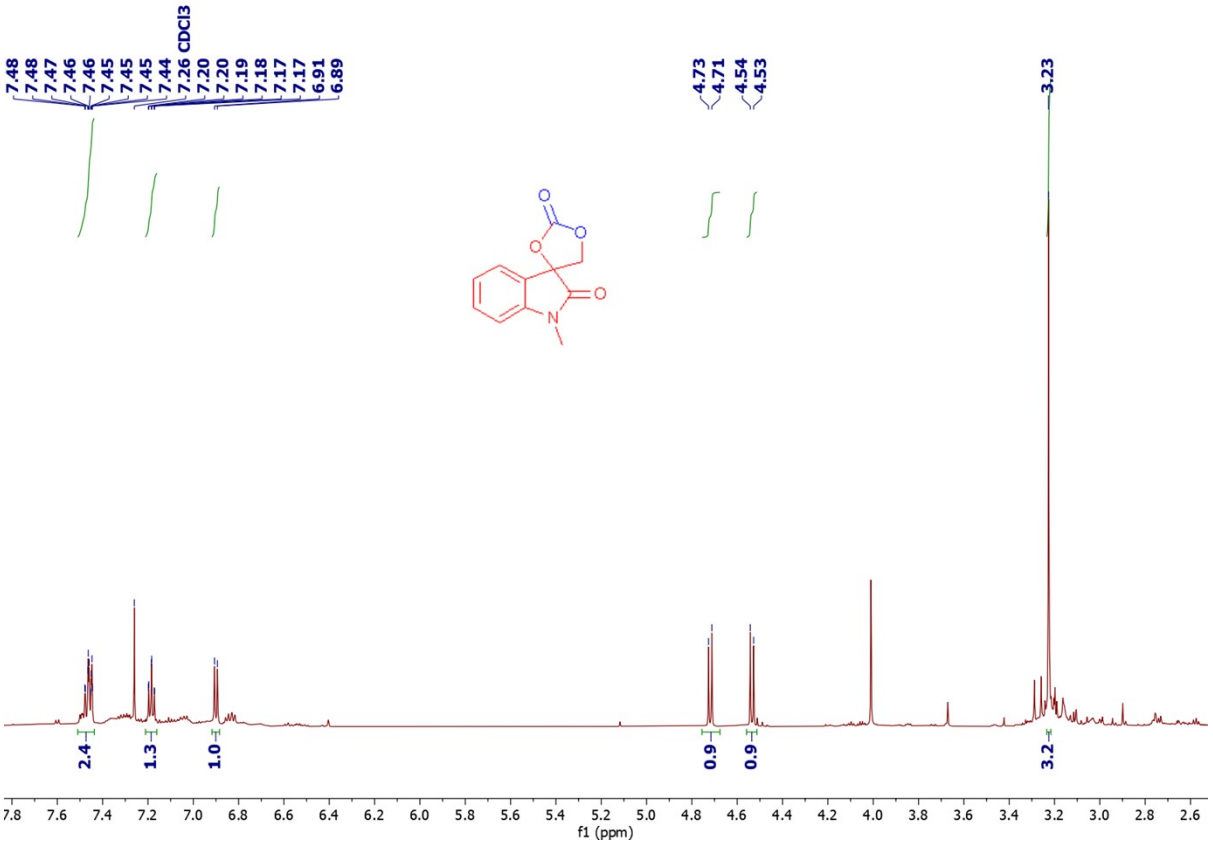


Figure S51: [1]H-NMR of 1-methylspiro[indoline-3,4'-[1,3]dioxolane]-2,2'-dione.

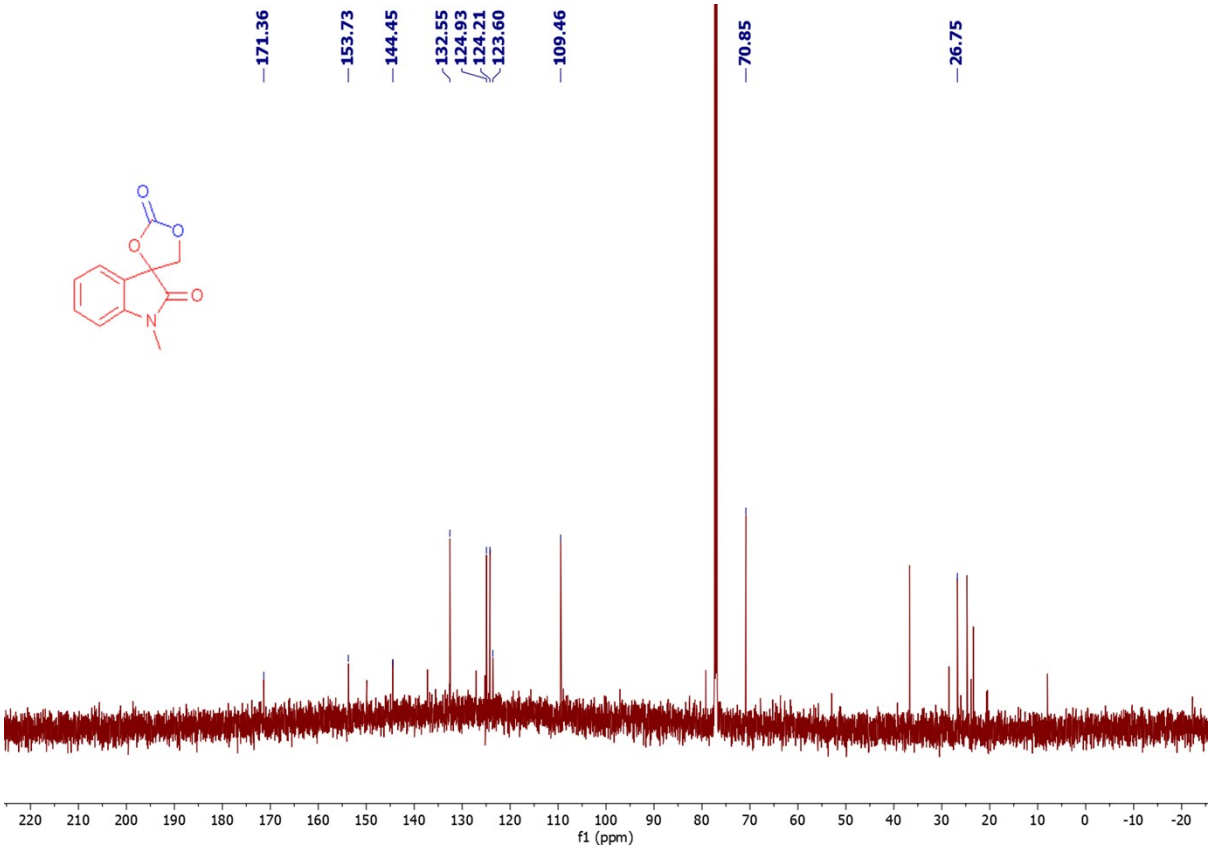


Figure S52: [13]C-NMR of 1-methylspiro[indoline-3,4'-[1,3]dioxolane]-2,2'-dione.

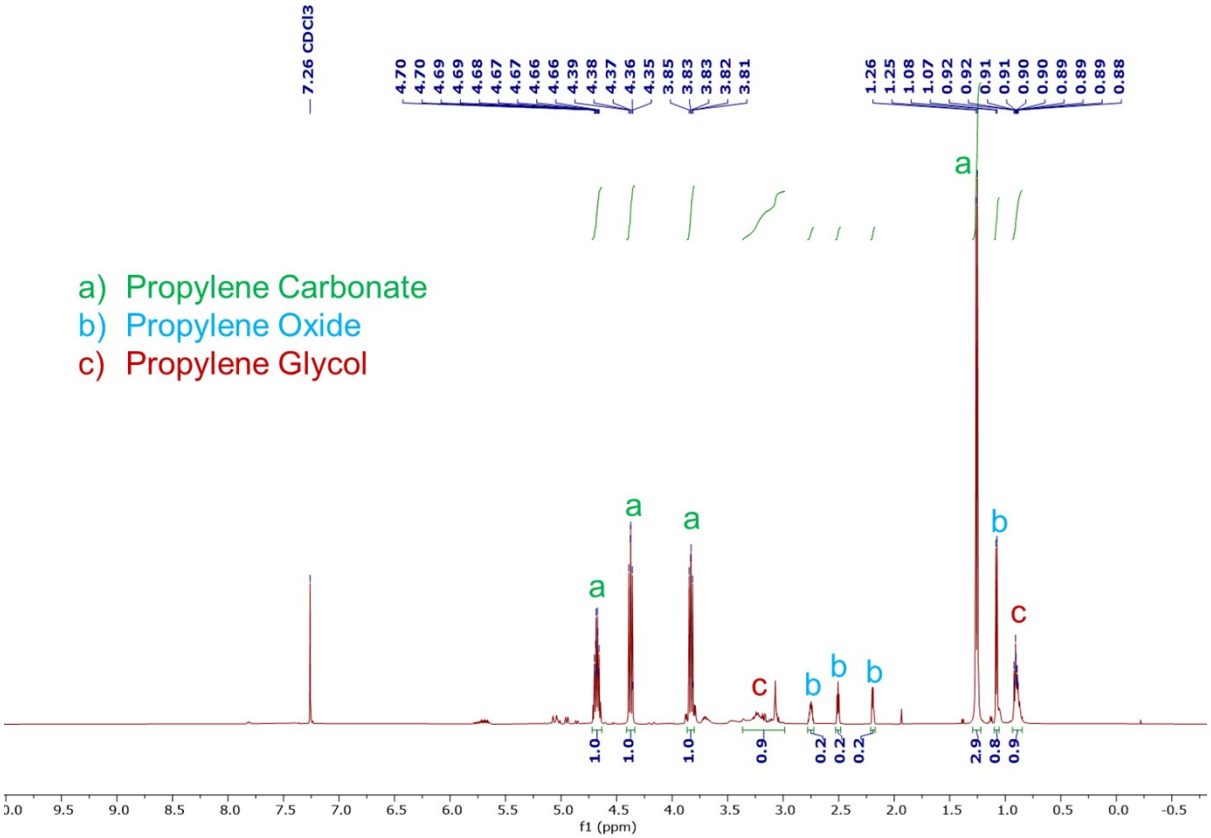
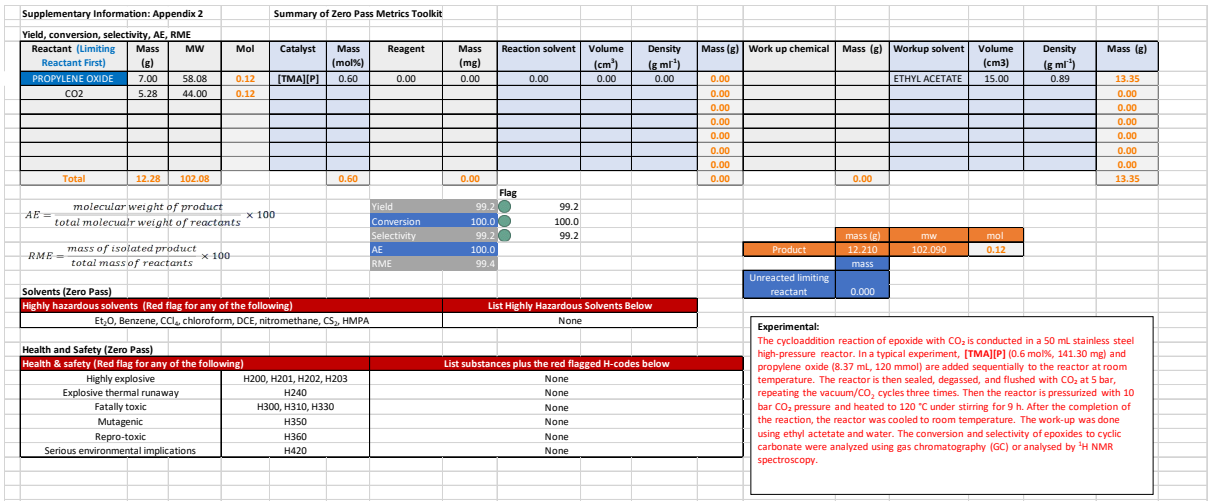


Figure S53: ^{1}H-NMR of Propylene carbonate using [TMA][Bz] as catalyst

Green Parameter

CHEM21 green metrics toolkit

[TMA][P] Zero and First Pass CHEM21 green metrics toolkit



Supplementary Information: Appendix 2 — Summary of Zero Pass Metrics Toolkit

Yield, conversion, selectivity, AE, RME

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TMA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			ETHYL ACETATE	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$AE = \frac{molecular\ weight\ of\ product}{total\ molecualr\ weight\ of\ reactants} \times 100$$

$$RME = \frac{mass\ of\ isolated\ product}{total\ mass\ of\ reactants} \times 100$$

		Flag
Yield	99.2	99.2
Conversion	100.0	100.0
Selectivity	99.2	99.2
AE	100.0	
RME	99.4	

	mass (g)	mw	mol
Product	12.210	102.090	0.12
	mass		
Unreacted limiting reactant	0.000		

Solvents (Zero Pass)

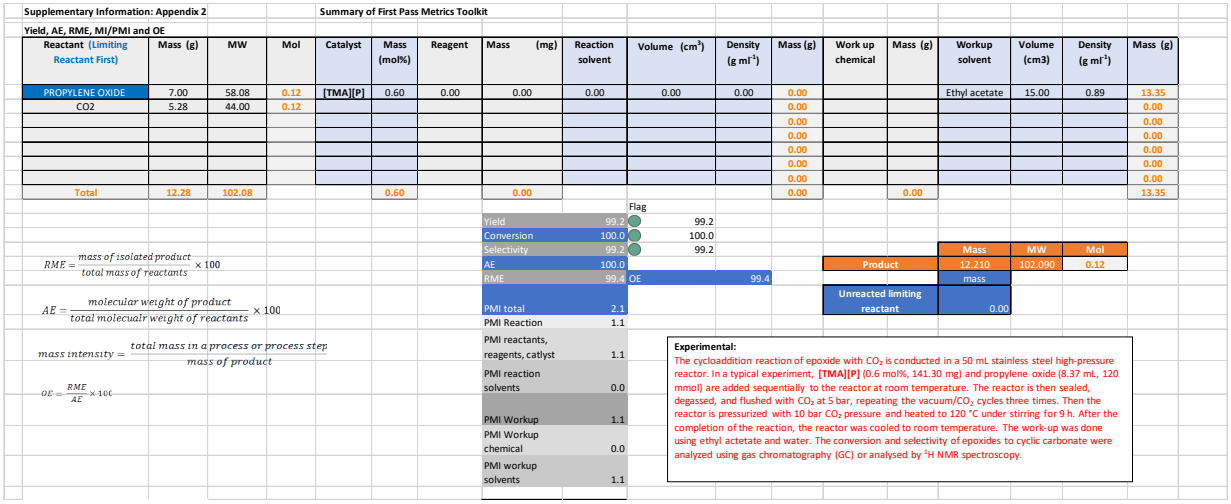
Highly hazardous solvents (Red flag for any of the following)	List Highly Hazardous Solvents Below
Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	None

Health and Safety (Zero Pass)

Health & safety (Red flag for any of the following)		List substances plus the red flagged H-codes below
Highly explosive	H200, H201, H202, H203	None
Explosive thermal runaway	H240	None
Fatally toxic	H300, H310, H330	None
Mutagenic	H350	None
Repro-toxic	H360	None
Serious environmental implications	H420	None

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TMA][P]** (0.6 mol%, 141.30 mg) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by ^{1}H NMR spectroscopy.

Figure S54. **[TMA][P]** Zero Pass CHEM21 green metrics toolkit.



Supplementary Information: Appendix 2 — Summary of First Pass Metrics Toolkit

Yield, AE, RME, MI/PMI and OE

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TMA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			Ethyl acetate	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$RME = \frac{mass\ of\ isolated\ product}{total\ mass\ of\ reactants} \times 100$$

$$AE = \frac{molecular\ weight\ of\ product}{total\ molecualr\ weight\ of\ reactants} \times 100$$

$$mass\ intensity = \frac{total\ mass\ in\ a\ process\ or\ process\ step}{mass\ of\ product}$$

$$OE = \frac{RME}{AE} \times 100$$

		Flag
Yield	99.2	99.2
Conversion	100.0	100.0
Selectivity	99.2	99.2
AE	100.0	
RME	99.4	OE 99.4
PMI total	2.1	
PMI Reaction	1.1	
PMI reactants, reagents, catlyst	1.1	
PMI reaction solvents	0.0	
PMI Workup	1.1	
PMI Workup chemical	0.0	
PMI workup solvents	1.1	

	Mass	MW	Mol
Product	12.210	102.090	0.12
	mass		
Unreacted limiting reactant	0.00		

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TMA][P]** (0.6 mol%, 141.30 mg) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by ^{1}H NMR spectroscopy.

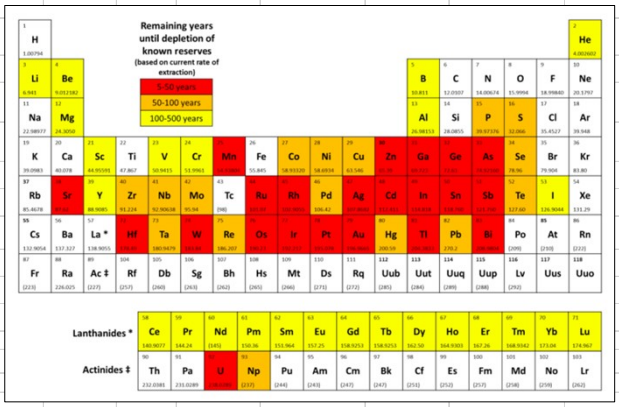
Solvents (First Pass)		List solvents below
Preferred solvents	**water,** EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, **AcOEt,** sulfolane	none
Problematic solvents: (acceptable only if substitution does not offer advantages)	DMSO, cyclohexanone, DMPU, AcOH, Ac2O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, **cyclohexane**, chlorobenzene, formic acid, pyridine, Me-THF	none
Hazardous solvents: These solvents have significant health and/or safety concerns.	dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane	none
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening	Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	none

Catalyst/enzyme (First Pass)		Tick
Catalyst or enzyme used, **or** reaction takes place without **any** catalyst/reagents.	Green Flag	X
Use of stoichiometric quantities of reagents	Amber Flag	
Use of reagents in excess	Red Flag	

		Tick
Facile recovery of catalyst/enzyme	Green Flag	X
catalyst/enzyme not recovered	Amber Flag	

Critical elements

Supply remaining	Flag colour	Note element
5-50 years	Red Flag	none
50-500 years	Amber Flag	none
+500 years	Green Flag	none



Energy (First Pass)		Tick
Reaction run between 0 to 70°C	Green Flag	
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	X
Reaction run below -20 or above 140°C	Red Flag	

		Tick
Reaction run at reflux	Red Flag	X
Reaction run 5°C or more below the solvent boiling point	Green Flag	

Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	X

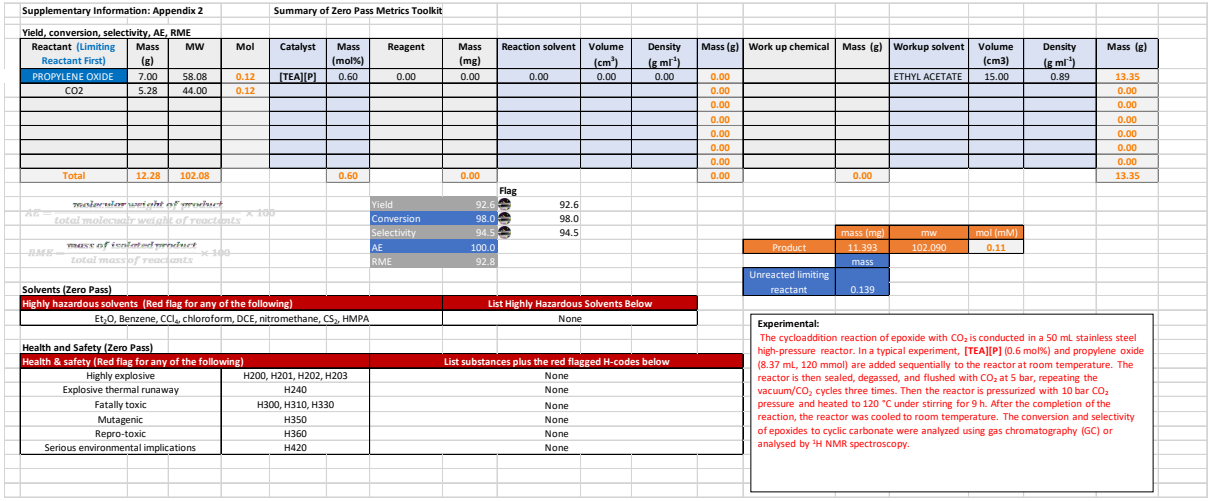
Work Up		List
quenching filtration centrifugation crystallisation Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric	Green Flag	
solvent exchange, quenching into aqueous solvent	Amber Flag	X
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	

Health & safety	Red Flag	Amber Flag	Green Flag	List substances and H-codes	List substances and H-codes	List substances and H-codes
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag			
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331,				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412				

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	NONE

Figure S55. **[TMA][P]** First Pass CHEM21 green metrics toolkit

[TEA][P] Zero and First Pass CHEM21 green metrics toolkit



Supplementary Information: Appendix 2 — **Summary of Zero Pass Metrics Toolkit**

Yield, conversion, selectivity, AE, RME

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TEA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			ETHYL ACETATE	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$AE = \frac{molecular\ weight\ of\ product}{total\ molecular\ weight\ of\ reactants} \times 100$$

$$RME = \frac{mass\ of\ isolated\ product}{total\ mass\ of\ reactants} \times 100$$

		Flag	
Yield	92.6		92.6
Conversion	98.0		98.0
Selectivity	94.5		94.5
AE	100.0		
RME	92.8		

	mass (mg)	mw	mol (mM)
Product	11.393	102.090	0.11
	mass		
Unreacted limiting reactant	0.139		

Solvents (Zero Pass)

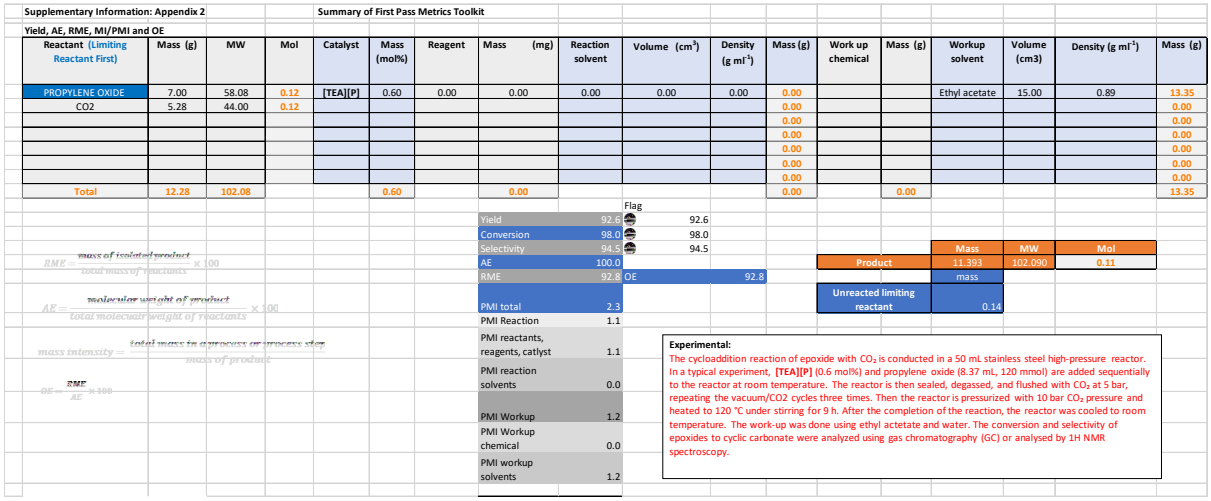
Highly hazardous solvents (Red flag for any of the following)	List Highly Hazardous Solvents Below
Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	None

Health and Safety (Zero Pass)

Health & safety (Red flag for any of the following)		List substances plus the red flagged H-codes below
Highly explosive	H200, H201, H202, H203	None
Explosive thermal runaway	H240	None
Fatally toxic	H300, H310, H330	None
Mutagenic	H350	None
Repro-toxic	H360	None
Serious environmental implications	H420	None

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TEA][P]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by ^{1}H NMR spectroscopy.

Figure S56. **[TEA][P]** Zero Pass CHEM21 green metrics toolkit.



Supplementary Information: Appendix 2 — **Summary of First Pass Metrics Toolkit**

Yield, AE, RME, MI/PMI and OE

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TEA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			Ethyl acetate	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$RME = \frac{mass\ of\ isolated\ product}{total\ mass\ of\ reactants} \times 100$$

$$AE = \frac{molecular\ weight\ of\ product}{total\ molecular\ weight\ of\ reactants} \times 100$$

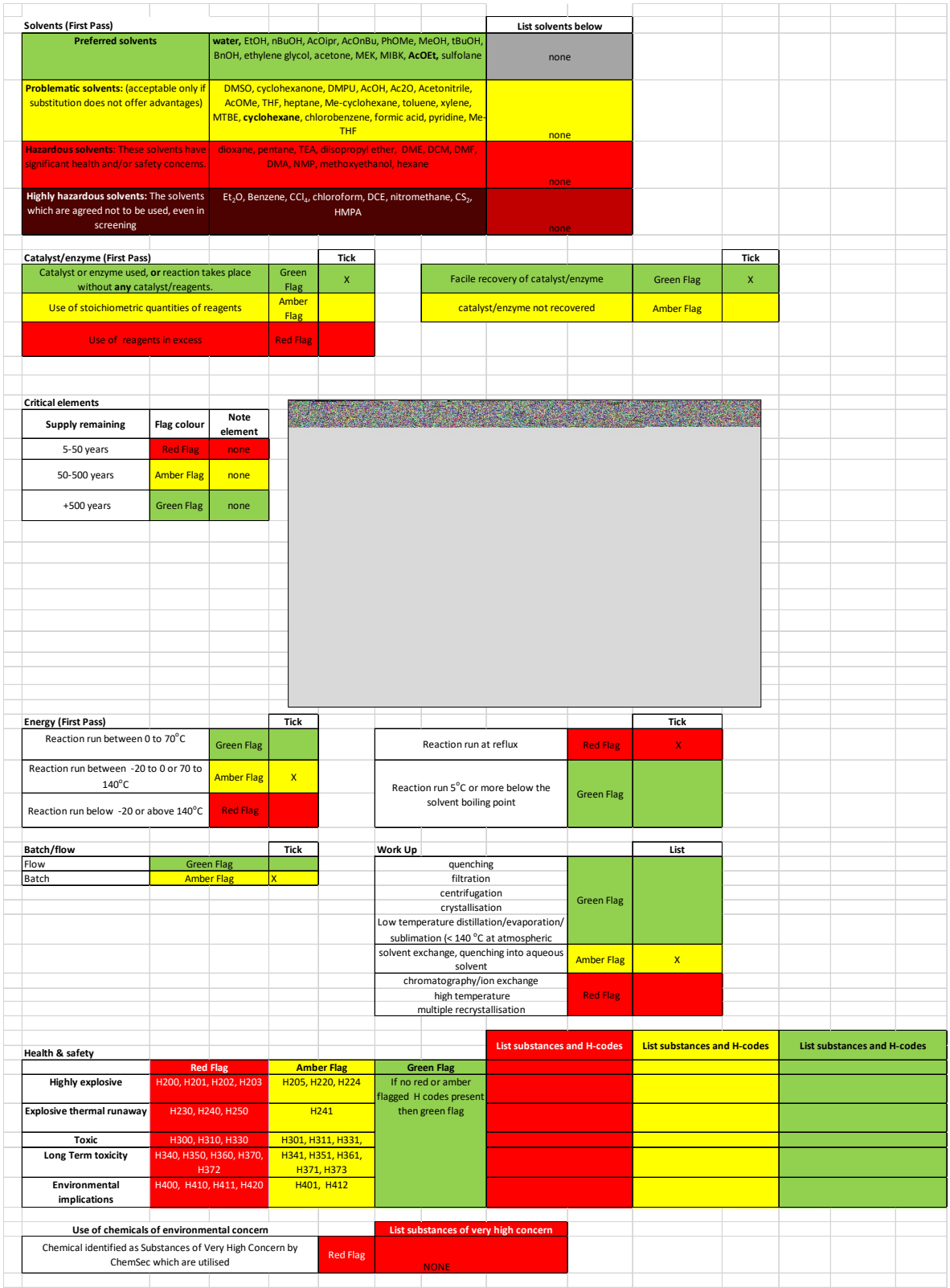
$$mass\ intensity = \frac{total\ mass\ in\ a\ process\ or\ process\ step}{mass\ of\ product}$$

$$OE = \frac{RME}{AE} \times 100$$

		Flag	
Yield	92.6		92.6
Conversion	98.0		98.0
Selectivity	94.5		94.5
AE	100.0		
RME	92.8	OE	92.8
PMI total	2.3		
PMI Reaction	1.1		
PMI reactants, reagents, catlyst	1.1		
PMI reaction solvents	0.0		
PMI Workup	1.2		
PMI Workup chemical	0.0		
PMI workup solvents	1.2		

	Mass	MW	Mol
Product	11.393	102.090	0.11
	mass		
Unreacted limiting reactant	0.14		

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TEA][P]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by 1H NMR spectroscopy.



Solvents (First Pass)		List solvents below
Preferred solvents	**water,** EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, **AcOEt,** sulfolane	none
Problematic solvents: (acceptable only if substitution does not offer advantages)	DMSO, cyclohexanone, DMPU, AcOH, Ac2O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, **cyclohexane**, chlorobenzene, formic acid, pyridine, Me-THF	none
Hazardous solvents: These solvents have significant health and/or safety concerns.	dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane	none
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening	Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	none

Catalyst/enzyme (First Pass)		Tick
Catalyst or enzyme used, **or** reaction takes place without **any** catalyst/reagents.	Green Flag	X
Use of stoichiometric quantities of reagents	Amber Flag	
Use of reagents in excess	Red Flag	

		Tick
Facile recovery of catalyst/enzyme	Green Flag	X
catalyst/enzyme not recovered	Amber Flag	

Critical elements		
Supply remaining	**Flag colour**	**Note element**
5-50 years	Red Flag	none
50-500 years	Amber Flag	none
+500 years	Green Flag	none

Energy (First Pass)		Tick
Reaction run between 0 to 70°C	Green Flag	
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	X
Reaction run below -20 or above 140°C	Red Flag	

		Tick
Reaction run at reflux	Red Flag	X
Reaction run 5°C or more below the solvent boiling point	Green Flag	

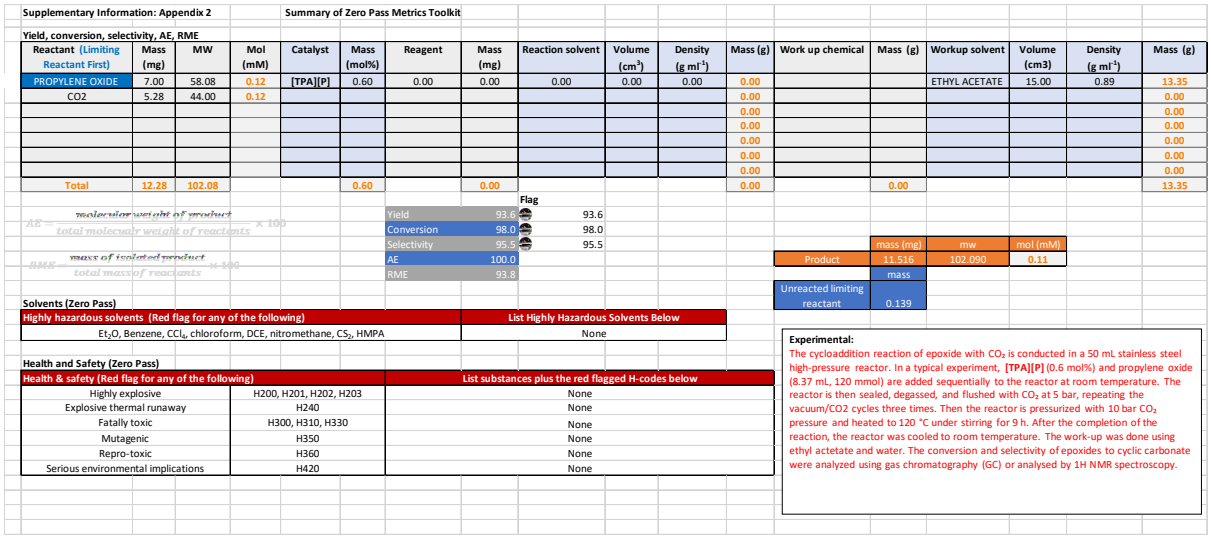
Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	X

Work Up		List
quenching filtration centrifugation crystallisation Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric	Green Flag	
solvent exchange, quenching into aqueous solvent	Amber Flag	X
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	

Health & safety	Red Flag	Amber Flag	Green Flag	List substances and H-codes	List substances and H-codes	List substances and H-codes
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag			
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331,				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412				

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	NONE

Figure S57. [TEA][P] First Pass CHEM21 green metrics toolkit



Supplementary Information: Appendix 2 — Summary of Zero Pass Metrics Toolkit

Yield, conversion, selectivity, AE, RME

Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TPA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			ETHYL ACETATE	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$$

$$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$$

		Flag
Yield	93.6	93.6
Conversion	98.0	98.0
Selectivity	95.5	95.5
AE	100.0	
RME	93.8	

	mass (mg)	mw	mol (mM)
Product	11.516	102.090	0.11
	mass		
Unreacted limiting reactant	0.139		

Solvents (Zero Pass)

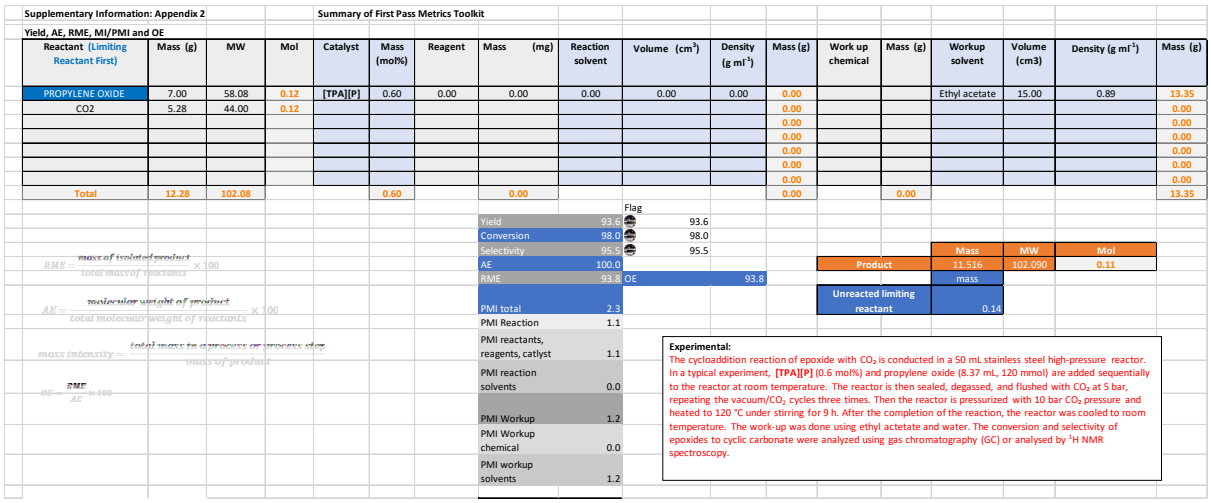
Highly hazardous solvents (Red flag for any of the following)	List Highly Hazardous Solvents Below
Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	None

Health and Safety (Zero Pass)

Health & safety (Red flag for any of the following)		List substances plus the red flagged H-codes below
Highly explosive	H200, H201, H202, H203	None
Explosive thermal runaway	H240	None
Fatally toxic	H300, H310, H330	None
Mutagenic	H350	None
Repro-toxic	H360	None
Serious environmental implications	H420	None

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TPA][P]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by 1H NMR spectroscopy.

Figure S58. [TPA][P] Zero Pass CHEM21 green metrics toolkit.



Supplementary Information: Appendix 2 — Summary of First Pass Metrics Toolkit

Yield, AE, RME, MI/PMI and OE

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TPA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			Ethyl acetate	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$$

$$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$$

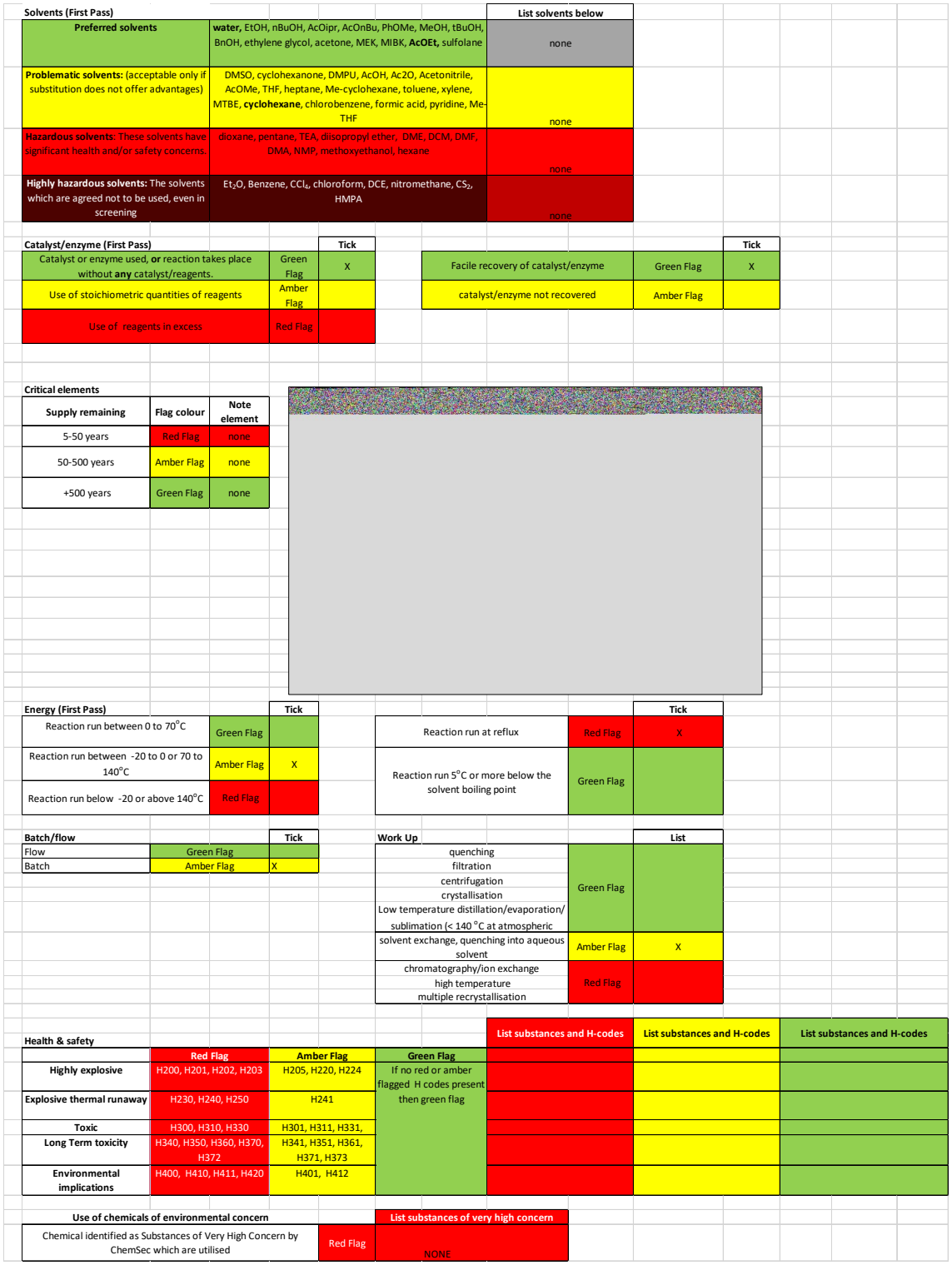
$$\text{mass intensity} = \frac{\text{total mass in a process or process step}}{\text{mass of product}}$$

$$OE = \frac{RME}{AE} \times 100$$

		Flag
Yield	93.6	93.6
Conversion	98.0	98.0
Selectivity	95.5	95.5
AE	100.0	
RME	93.8	OE 93.8
PMI total	2.3	
PMI Reaction	1.1	
PMI reactants, reagents, catlyst	1.1	
PMI reaction solvents	0.0	
PMI Workup	1.2	
PMI Workup chemical	0.0	
PMI workup solvents	1.2	

	Mass	MW	Mol
Product	11.516	102.090	0.11
	mass		
Unreacted limiting reactant	0.14		

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TPA][P]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by ^{1}H NMR spectroscopy.



Solvents (First Pass)		List solvents below
Preferred solvents	**water,** EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, **AcOEt,** sulfolane	none
Problematic solvents: (acceptable only if substitution does not offer advantages)	DMSO, cyclohexanone, DMPU, AcOH, Ac2O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, **cyclohexane**, chlorobenzene, formic acid, pyridine, Me-THF	none
Hazardous solvents: These solvents have significant health and/or safety concerns.	dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane	none
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening	Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	none

Catalyst/enzyme (First Pass)		Tick			Tick
Catalyst or enzyme used, **or** reaction takes place without **any** catalyst/reagents.	Green Flag	X	Facile recovery of catalyst/enzyme	Green Flag	X
Use of stoichiometric quantities of reagents	Amber Flag		catalyst/enzyme not recovered	Amber Flag	
Use of reagents in excess	Red Flag				

Critical elements

Supply remaining	Flag colour	Note element
5-50 years	Red Flag	none
50-500 years	Amber Flag	none
+500 years	Green Flag	none

Energy (First Pass)		Tick			Tick
Reaction run between 0 to 70°C	Green Flag		Reaction run at reflux	Red Flag	X
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	X	Reaction run 5°C or more below the solvent boiling point	Green Flag	
Reaction run below -20 or above 140°C	Red Flag				

Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	X

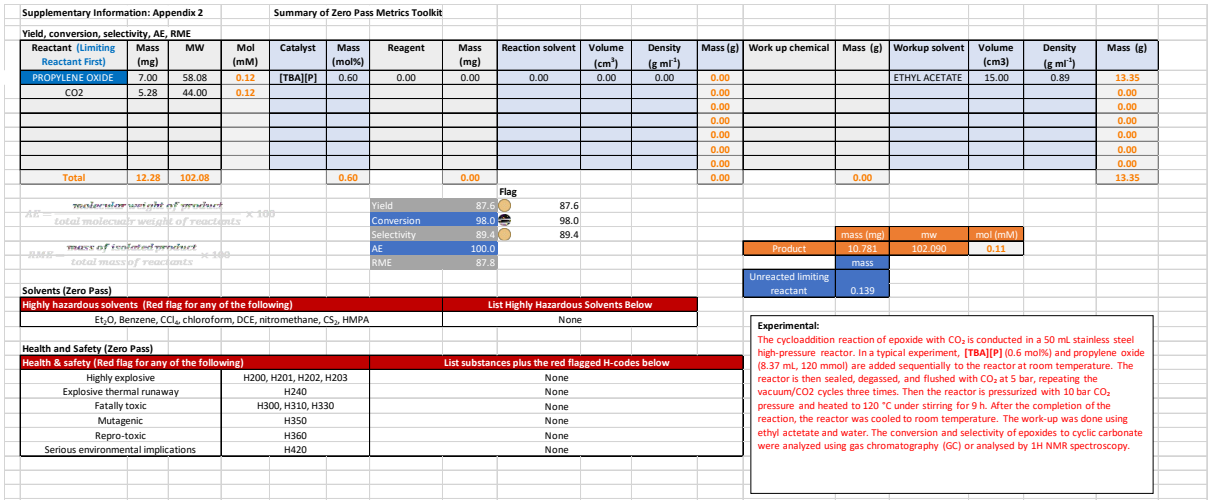
Work Up		List
quenching filtration centrifugation crystallisation Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric	Green Flag	
solvent exchange, quenching into aqueous solvent	Amber Flag	X
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	

Health & safety	Red Flag	Amber Flag	Green Flag	List substances and H-codes	List substances and H-codes	List substances and H-codes
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag			
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331,				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412				

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	NONE

Figure S59. **[TPA][P]** First Pass CHEM21 green metrics toolkit

[TBA][P] Zero and First Pass CHEM21 green metrics toolkit



Supplementary Information: Appendix 2 — Summary of Zero Pass Metrics Toolkit

Yield, conversion, selectivity, AE, RME

Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TBA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			ETHYL ACETATE	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$$

$$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$$

		Flag	
Yield	87.6		87.6
Conversion	98.0		98.0
Selectivity	89.4		89.4
AE	100.0		
RME	87.8		

	mass (mg)	mw	mol (mM)
Product	10.781	102.090	0.11
	mass		
Unreacted limiting reactant	0.139		

Solvents (Zero Pass)

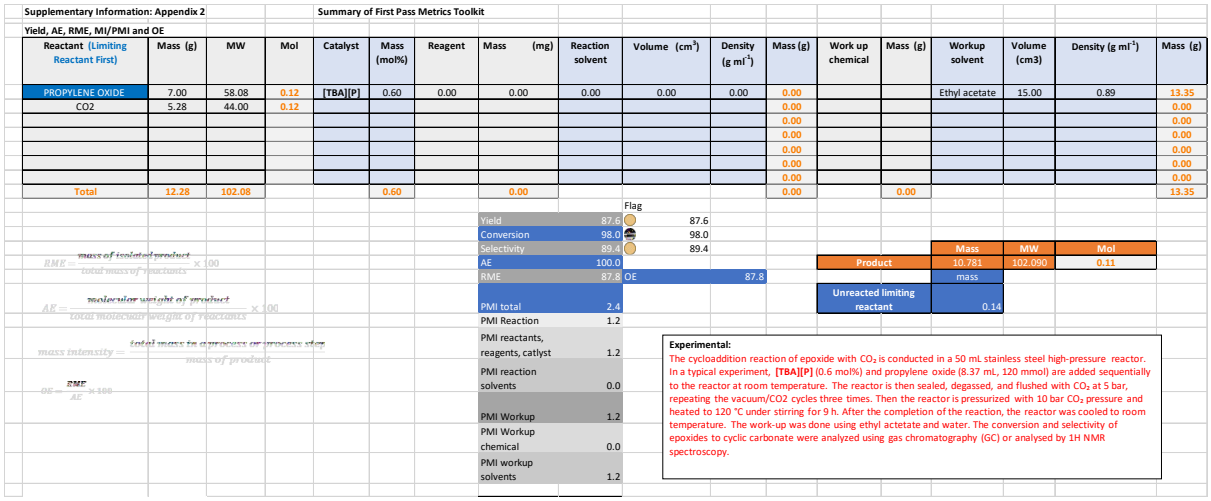
Highly hazardous solvents (Red flag for any of the following)	List Highly Hazardous Solvents Below
Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	None

Health and Safety (Zero Pass)

Health & safety (Red flag for any of the following)		List substances plus the red flagged H-codes below
Highly explosive	H200, H201, H202, H203	None
Explosive thermal runaway	H240	None
Fatally toxic	H300, H310, H330	None
Mutagenic	H350	None
Repro-toxic	H360	None
Serious environmental implications	H420	None

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TBA][P]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by 1H NMR spectroscopy.

Figure S60. [TBA][P] Zero Pass CHEM21 green metrics toolkit.



Supplementary Information: Appendix 2 — Summary of First Pass Metrics Toolkit

Yield, AE, RME, MI/PMI and OE

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TBA][P]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			Ethyl acetate	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$$

$$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$$

$$\text{mass intensity} = \frac{\text{total mass in a process or process step}}{\text{mass of product}}$$

$$OE = \frac{RME}{AE} \times 100$$

		Flag	
Yield	87.6		87.6
Conversion	98.0		98.0
Selectivity	89.4		89.4
AE	100.0		
RME	87.8	OE	87.8
PMI total	2.4		
PMI Reaction	1.2		
PMI reactants, reagents, catlyst	1.2		
PMI reaction solvents	0.0		
PMI Workup	1.2		
PMI Workup chemical	0.0		
PMI workup solvents	1.2		

	Mass	MW	Mol
Product	10.781	102.090	0.11
	mass		
Unreacted limiting reactant	0.14		

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TBA][P]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by 1H NMR spectroscopy.

Solvents (First Pass)		List solvents below
Preferred solvents	**water,** EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, **AcOEt,** sulfolane	none
Problematic solvents: (acceptable only if substitution does not offer advantages)	DMSO, cyclohexanone, DMPU, AcOH, Ac2O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, **cyclohexane**, chlorobenzene, formic acid, pyridine, Me-THF	none
Hazardous solvents: These solvents have significant health and/or safety concerns.	dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane	none
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening	Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	none

Catalyst/enzyme (First Pass)		Tick
Catalyst or enzyme used, **or** reaction takes place without **any** catalyst/reagents.	Green Flag	X
Use of stoichiometric quantities of reagents	Amber Flag	
Use of reagents in excess	Red Flag	

		Tick
Facile recovery of catalyst/enzyme	Green Flag	X
catalyst/enzyme not recovered	Amber Flag	

Critical elements

Supply remaining	Flag colour	Note element
5-50 years	Red Flag	none
50-500 years	Amber Flag	none
+500 years	Green Flag	none

Energy (First Pass)		Tick
Reaction run between 0 to 70°C	Green Flag	
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	X
Reaction run below -20 or above 140°C	Red Flag	

		Tick
Reaction run at reflux	Red Flag	X
Reaction run 5°C or more below the solvent boiling point	Green Flag	

Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	X

Work Up		List
quenching filtration centrifugation crystallisation Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric	Green Flag	
solvent exchange, quenching into aqueous solvent	Amber Flag	X
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	

Health & safety	Red Flag	Amber Flag	Green Flag	List substances and H-codes	List substances and H-codes	List substances and H-codes
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag			
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331,				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412				

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	NONE

Figure S61. [TBA][P] First Pass CHEM21 green metrics toolkit

[TMA][Bz] Zero and First Pass CHEM21 green metrics toolkit

Supplementary Information: Appendix 2 — **Summary of Zero Pass Metrics Toolkit**

Yield, conversion, selectivity, AE, RME

Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TMA][Bz]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			ETHYL ACETATE	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$$

$$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$$

		Flag
Yield	62.7	62.7
Conversion	82.7	82.7
Selectivity	75.9	75.9
AE	100.0	
RME	62.9	

	mass (mg)	mw	mol (mM)
Product	7.718	102.090	0.08
	mass		
Unreacted limiting reactant	1.212		

Solvents (Zero Pass)

Highly hazardous solvents (Red flag for any of the following)	List Highly Hazardous Solvents Below
Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	None

Health and Safety (Zero Pass)

Health & safety (Red flag for any of the following)		List substances plus the red flagged H-codes below
Highly explosive	H200, H201, H202, H203	None
Explosive thermal runaway	H240	None
Fatally toxic	H300, H310, H330	None
Mutagenic	H350	None
Repro-toxic	H360	None
Serious environmental implications	H420	None

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TMA][Bz]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by 1H NMR spectroscopy.

Figure S62. **[TMA][Bz]** Zero Pass CHEM21 green metrics toolkit.

Supplementary Information: Appendix 2 — **Summary of First Pass Metrics Toolkit**

Yield, AE, RME, MI/PMI and OE

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[TMA][Bz]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			Ethyl acetate	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$$

$$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$$

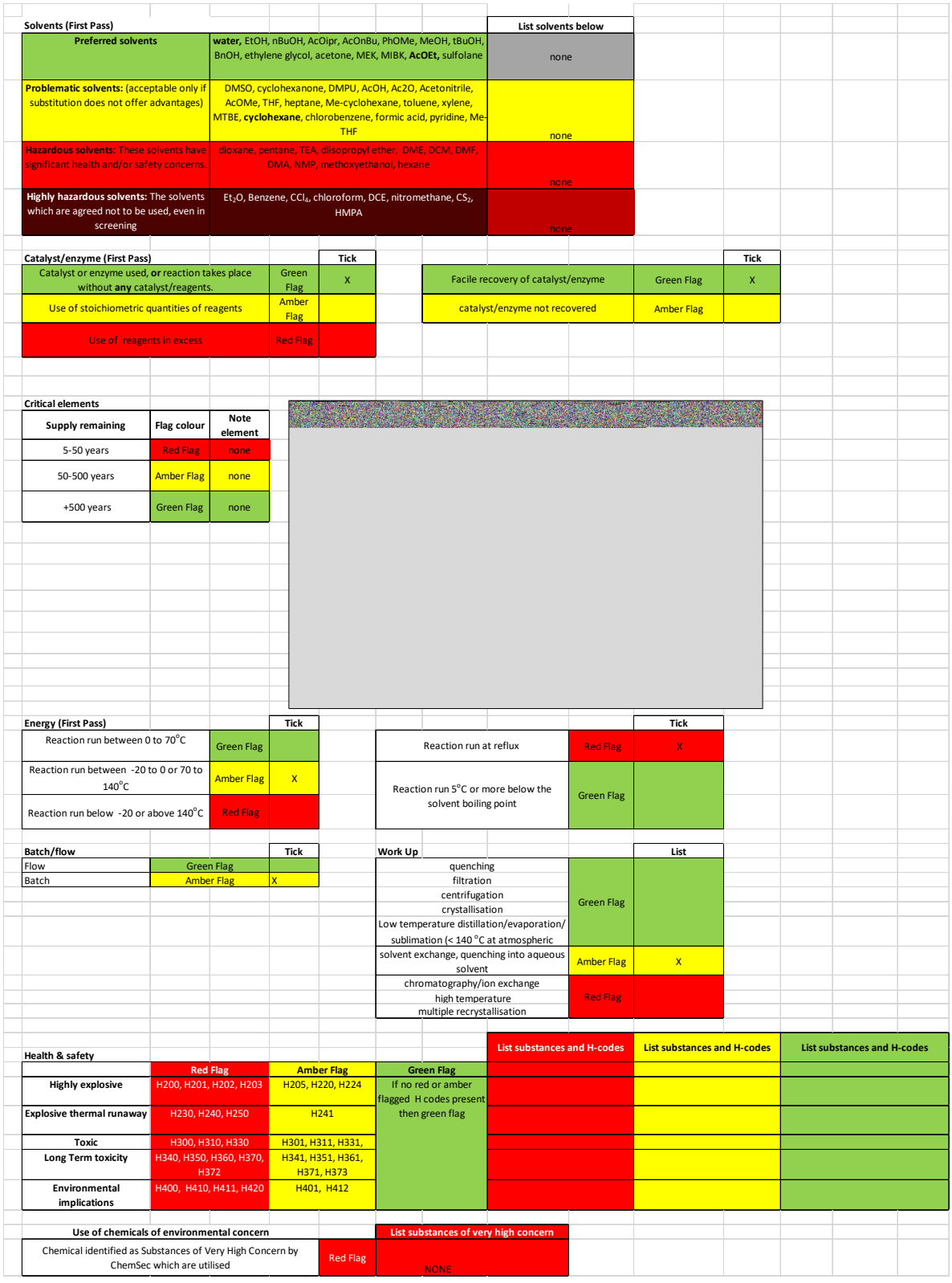
$$\text{mass intensity} = \frac{\text{total mass in a process or process step}}{\text{mass of product}}$$

$$OE = \frac{RME}{AE} \times 100$$

		Flag
Yield	62.7	62.7
Conversion	82.7	82.7
Selectivity	75.9	75.9
AE	100.0	
RME	62.9	OE 62.8
PMI total	3.4	
PMI Reaction	1.7	
PMI reactants, reagents, catlyst	1.7	
PMI reaction solvents	0.0	
PMI Workup	1.7	
PMI Workup chemical	0.0	
PMI workup solvents	1.7	

	Mass	MW	Mol
Product	7.718	102.090	0.08
	mass		
Unreacted limiting reactant	1.21		

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[TMA][Bz]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by ^1H NMR spectroscopy.



Solvents (First Pass)		List solvents below
Preferred solvents	**water,** EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, **AcOEt,** sulfolane	none
Problematic solvents: (acceptable only if substitution does not offer advantages)	DMSO, cyclohexanone, DMPU, AcOH, Ac2O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, **cyclohexane**, chlorobenzene, formic acid, pyridine, Me-THF	none
Hazardous solvents: These solvents have significant health and/or safety concerns.	dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane	none
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening	Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	none

Catalyst/enzyme (First Pass)		Tick
Catalyst or enzyme used, **or** reaction takes place without **any** catalyst/reagents.	Green Flag	X
Use of stoichiometric quantities of reagents	Amber Flag	
Use of reagents in excess	Red Flag	

		Tick
Facile recovery of catalyst/enzyme	Green Flag	X
catalyst/enzyme not recovered	Amber Flag	

Critical elements		
Supply remaining	**Flag colour**	**Note element**
5-50 years	Red Flag	none
50-500 years	Amber Flag	none
+500 years	Green Flag	none

Energy (First Pass)		Tick
Reaction run between 0 to 70°C	Green Flag	
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	X
Reaction run below -20 or above 140°C	Red Flag	

		Tick
Reaction run at reflux	Red Flag	X
Reaction run 5°C or more below the solvent boiling point	Green Flag	

Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	X

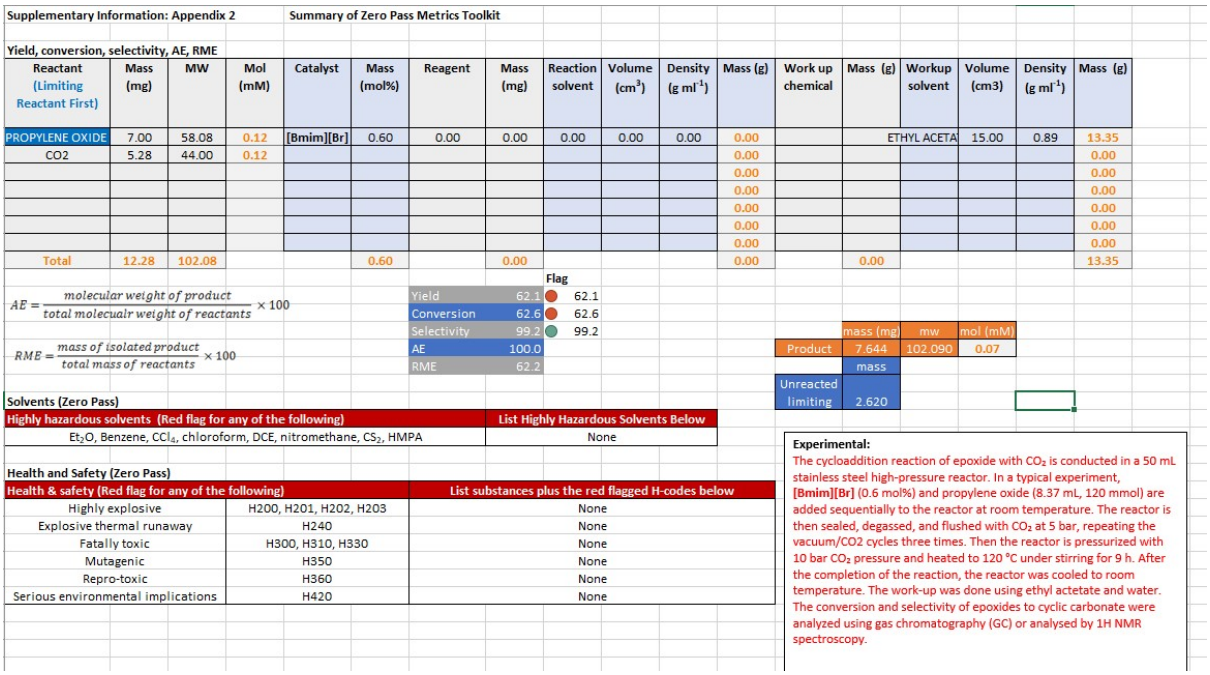
Work Up		List
quenching filtration centrifugation crystallisation Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric	Green Flag	
solvent exchange, quenching into aqueous solvent	Amber Flag	X
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	

Health & safety	Red Flag	Amber Flag	Green Flag	List substances and H-codes	List substances and H-codes	List substances and H-codes
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag			
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331,				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412				

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	NONE

Figure S63. **[TMA][Bz]** First Pass CHEM21 green metrics toolkit

[Bmim][Br] Zero and First Pass CHEM21 green metrics toolkit



Supplementary Information: Appendix 2 — Summary of Zero Pass Metrics Toolkit

Yield, conversion, selectivity, AE, RME

Reactant (Limiting Reactant First)	Mass (mg)	MW	Mol (mM)	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[Bmim][Br]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			ETHYL ACETA	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$AE = \frac{molecular\ weight\ of\ product}{total\ molecualr\ weight\ of\ reactants} \times 100$$

$$RME = \frac{mass\ of\ isolated\ product}{total\ mass\ of\ reactants} \times 100$$

		Flag
Yield	62.1	62.1
Conversion	62.6	62.6
Selectivity	99.2	99.2
AE	100.0	
RME	62.2	

	mass (mg)	mw	mol (mM)
Product	7.644	102.090	0.07
	mass		
Unreacted limiting	2.620		

Solvents (Zero Pass)

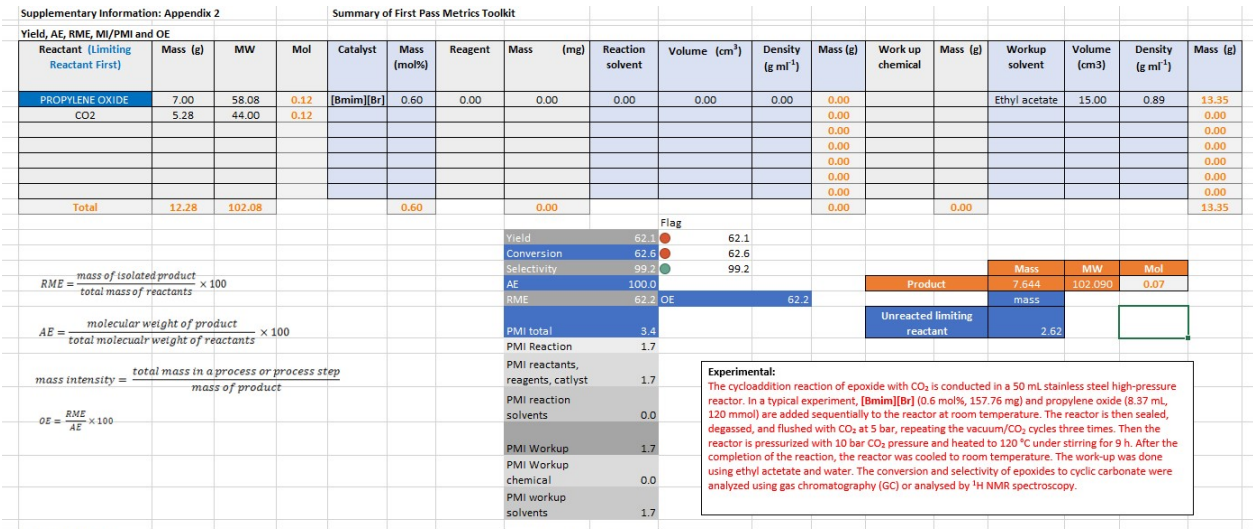
Highly hazardous solvents (Red flag for any of the following)	List Highly Hazardous Solvents Below
Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	None

Health and Safety (Zero Pass)

Health & safety (Red flag for any of the following)		List substances plus the red flagged H-codes below
Highly explosive	H200, H201, H202, H203	None
Explosive thermal runaway	H240	None
Fatally toxic	H300, H310, H330	None
Mutagenic	H350	None
Repro-toxic	H360	None
Serious environmental implications	H420	None

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[Bmim][Br]** (0.6 mol%) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by 1H NMR spectroscopy.

Figure S64. **[Bmim][Br]** Zero Pass CHEM21 green metrics toolkit.



Supplementary Information: Appendix 2 — Summary of First Pass Metrics Toolkit

Yield, AE, RME, MI/PMI and OE

Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (mol%)	Reagent	Mass (mg)	Reaction solvent	Volume (cm^3)	Density ($g\ ml^{-1}$)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density ($g\ ml^{-1}$)	Mass (g)
PROPYLENE OXIDE	7.00	58.08	0.12	[Bmim][Br]	0.60	0.00	0.00	0.00	0.00	0.00	0.00			Ethyl acetate	15.00	0.89	13.35
CO2	5.28	44.00	0.12								0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
											0.00						0.00
Total	12.28	102.08			0.60		0.00				0.00		0.00				13.35

$$RME = \frac{mass\ of\ isolated\ product}{total\ mass\ of\ reactants} \times 100$$

$$AE = \frac{molecular\ weight\ of\ product}{total\ molecualr\ weight\ of\ reactants} \times 100$$

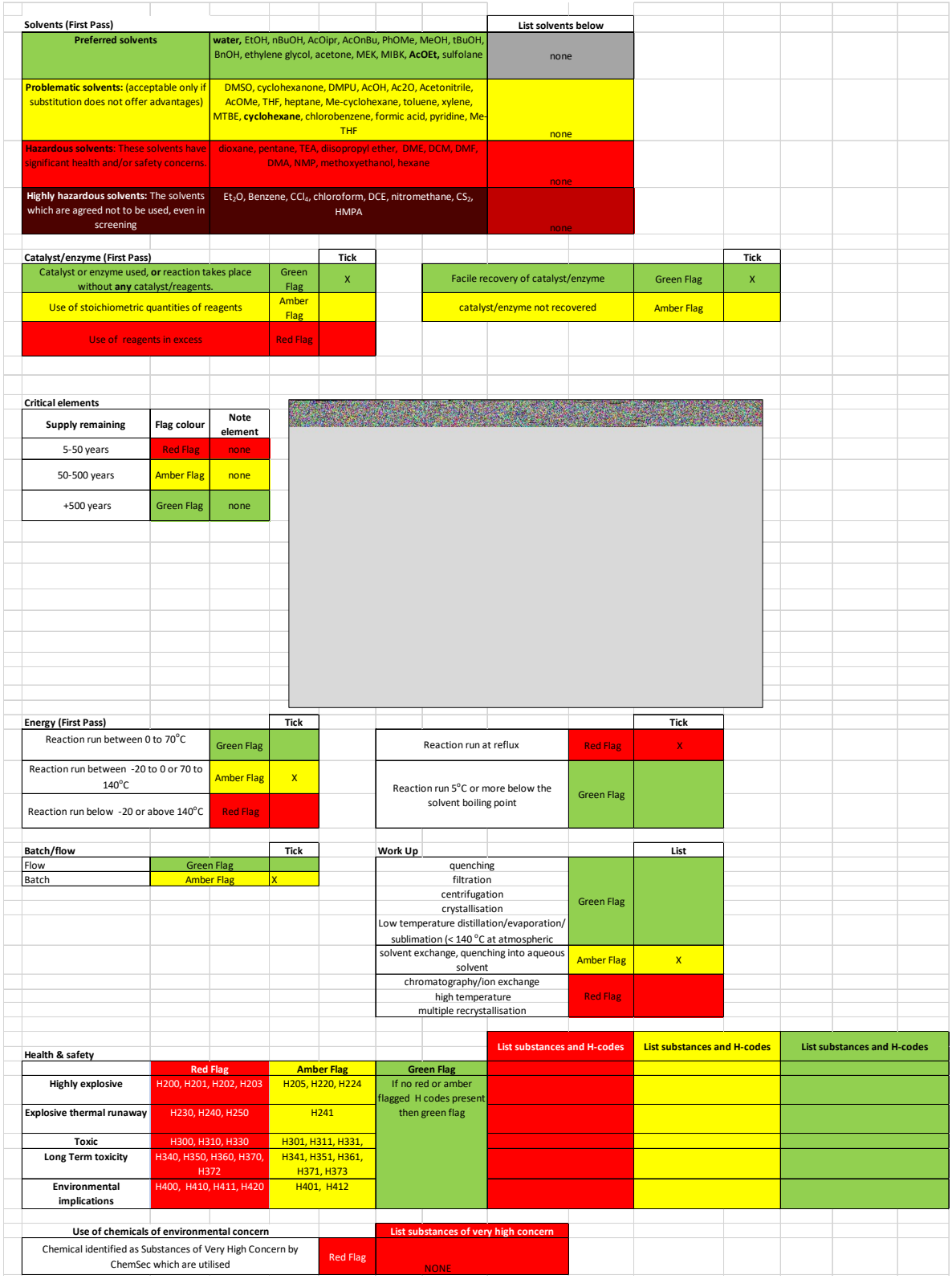
$$mass\ intensity = \frac{total\ mass\ in\ a\ process\ or\ process\ step}{mass\ of\ product}$$

$$OE = \frac{RME}{AE} \times 100$$

		Flag
Yield	62.1	62.1
Conversion	62.6	62.6
Selectivity	99.2	99.2
AE	100.0	
RME	62.2	OE 62.2
PMI total	3.4	
PMI Reaction	1.7	
PMI reactants, reagents, catlyst	1.7	
PMI reaction solvents	0.0	
PMI Workup	1.7	
PMI Workup chemical	0.0	
PMI workup solvents	1.7	

	Mass	MW	Mol
Product	7.644	102.090	0.07
	mass		
Unreacted limiting reactant	2.62		

Experimental:
The cycloaddition reaction of epoxide with CO_2 is conducted in a 50 mL stainless steel high-pressure reactor. In a typical experiment, **[Bmim][Br]** (0.6 mol%, 157.76 mg) and propylene oxide (8.37 mL, 120 mmol) are added sequentially to the reactor at room temperature. The reactor is then sealed, degassed, and flushed with CO_2 at 5 bar, repeating the vacuum/CO_2 cycles three times. Then the reactor is pressurized with 10 bar CO_2 pressure and heated to 120 °C under stirring for 9 h. After the completion of the reaction, the reactor was cooled to room temperature. The work-up was done using ethyl acetate and water. The conversion and selectivity of epoxides to cyclic carbonate were analyzed using gas chromatography (GC) or analysed by ^{1}H NMR spectroscopy.



Solvents (First Pass)		List solvents below
Preferred solvents	**water,** EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, **AcOEt,** sulfolane	none
Problematic solvents: (acceptable only if substitution does not offer advantages)	DMSO, cyclohexanone, DMPU, AcOH, Ac2O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, **cyclohexane**, chlorobenzene, formic acid, pyridine, Me-THF	none
Hazardous solvents: These solvents have significant health and/or safety concerns.	dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane	none
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening	Et_2O, Benzene, CCl_4, chloroform, DCE, nitromethane, CS_2, HMPA	none

Catalyst/enzyme (First Pass)		Tick
Catalyst or enzyme used, **or** reaction takes place without **any** catalyst/reagents.	Green Flag	X
Use of stoichiometric quantities of reagents	Amber Flag	
Use of reagents in excess	Red Flag	

		Tick
Facile recovery of catalyst/enzyme	Green Flag	X
catalyst/enzyme not recovered	Amber Flag	

Critical elements		
Supply remaining	**Flag colour**	**Note element**
5-50 years	Red Flag	none
50-500 years	Amber Flag	none
+500 years	Green Flag	none

Energy (First Pass)		Tick
Reaction run between 0 to 70°C	Green Flag	
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	X
Reaction run below -20 or above 140°C	Red Flag	

		Tick
Reaction run at reflux	Red Flag	X
Reaction run 5°C or more below the solvent boiling point	Green Flag	

Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	X

Work Up		List
quenching filtration centrifugation crystallisation Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric	Green Flag	
solvent exchange, quenching into aqueous solvent	Amber Flag	X
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	

Health & safety				List substances and H-codes	List substances and H-codes	List substances and H-codes
	Red Flag	**Amber Flag**	**Green Flag**			
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag			
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331,				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412				

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	NONE

Figure S65. **[Bmim][Br]** Zero Pass CHEM21 green metrics toolkit.

EcoScale Calculation

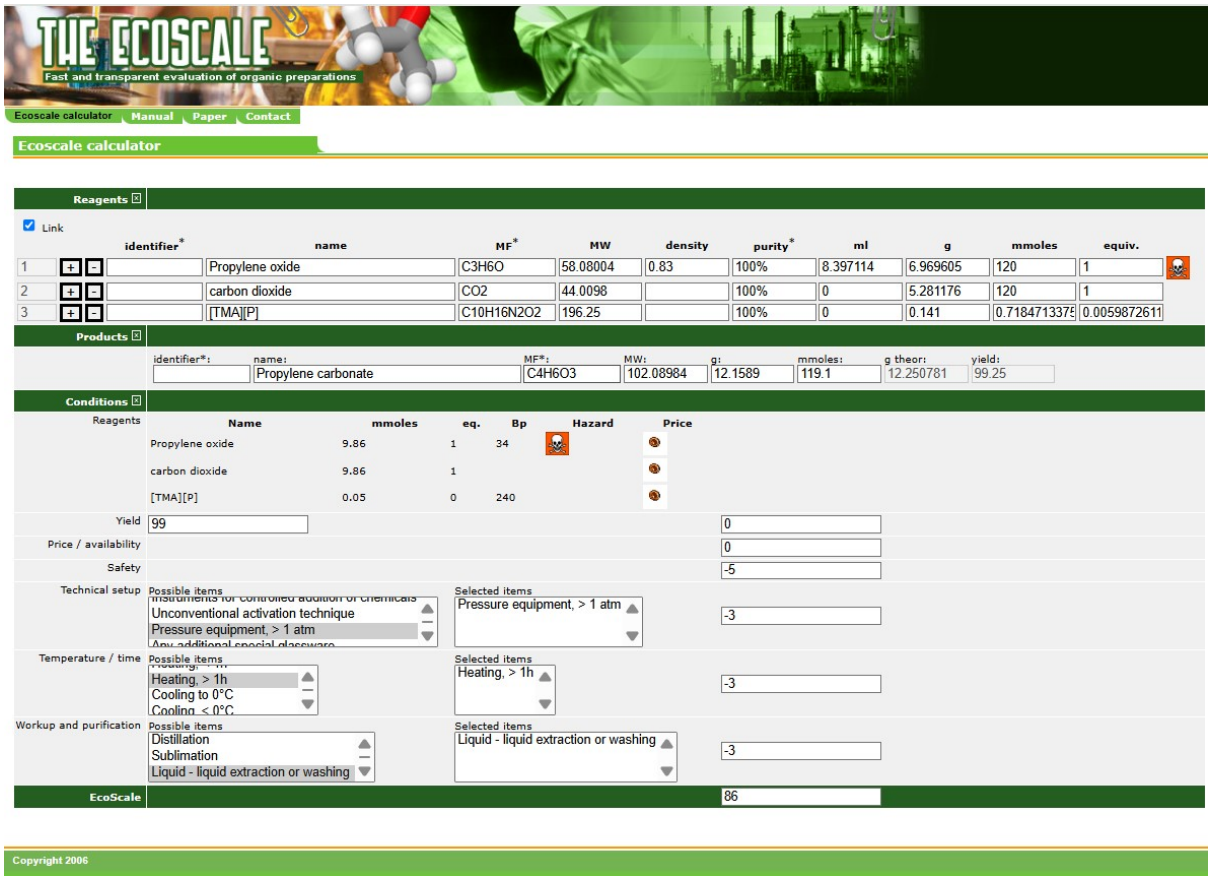


Figure S66. EcoScale calculation of overall reaction.

Cartesian coordinates for the optimized geometries

M

SCF Energy =-808.176875

Thermal correction to Gibbs Free Energy = 0.321737

Charge = 0, Multiplicity = 1

C	-4.94700500	-1.19887700	-0.15472900
C	-5.71855700	-0.03566600	-0.14137700
C	-5.05395200	1.19040800	-0.13607000
C	-3.66277900	1.19343600	-0.14402100
C	-2.97564700	-0.02814000	-0.15828800
N	-3.61064300	-1.21163100	-0.16397000
H	-5.61132000	2.12417800	-0.12594900
H	-5.43282900	-2.17492900	-0.15878600
H	-6.80343100	-0.09402700	-0.13550200
H	-3.08095500	2.10705600	-0.13942200
C	-1.44242700	-0.02133500	-0.16767600
O	-0.85945100	-1.13380900	-0.19751700
O	-0.90854900	1.12865800	-0.13136300
N	2.72092800	-0.00154000	0.12102100
C	2.04956600	1.21261400	-0.51952200
H	2.26186000	1.12846700	-1.58697800
H	0.95972700	1.09080900	-0.38307500
C	2.50248200	2.56068800	0.01601600
H	1.94826000	3.32407100	-0.53853200
H	2.24930200	2.69480600	1.07139900
H	3.57065800	2.76289100	-0.12163400
C	2.49256000	-0.02181000	1.62780200
H	3.03749900	-0.89510800	1.99295100
H	3.00651200	0.86202200	2.01208000
C	1.04360400	-0.05174000	2.08142300
H	0.50567100	-0.92870200	1.71655000
H	1.04970600	-0.06441400	3.17714000
H	0.47652700	0.81507600	1.73614600

C	2.08671700	-1.22163200	-0.54716800
H	2.31676200	-1.11931800	-1.60931300
H	0.99273000	-1.11764700	-0.42784800
C	2.55622900	-2.56732300	-0.02052000
H	2.28010300	-2.72311000	1.02597600
H	2.03210200	-3.33366700	-0.59965100
H	3.63165200	-2.74472700	-0.13512800
C	4.22519000	0.02298800	-0.07340600
H	4.59007700	0.89514200	0.47201000
H	4.61263100	-0.86274700	0.43301500
C	4.71010000	0.06170800	-1.51502900
H	4.37897400	0.95895100	-2.04356300
H	5.80466500	0.07327200	-1.49961200
H	4.39863400	-0.81684600	-2.08519800

N

SCF Energy =-193.177740

Thermal correction to Gibbs Free Energy = 0.059620

Charge = 0, Multiplicity = 1

C	1.04247600	0.61619900	-0.05928900
C	-0.15181500	-0.04016400	0.49063100
O	0.82667000	-0.78846000	-0.24475400
H	0.95028400	1.22472600	-0.95981600
H	1.87347000	0.88026300	0.59553600
H	-0.15499000	-0.26035300	1.56081200
C	-1.50895400	0.10059500	-0.14863800
H	-2.07739200	-0.83214500	-0.05921200
H	-2.08571100	0.89687700	0.33686800
H	-1.40926200	0.33853900	-1.21238200

CO_2

SCF Energy = -188.648279

Thermal correction to Gibbs Free Energy = -0.009126

Charge = 0, Multiplicity = 1

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16912200
O	0.00000000	0.00000000	-1.16912200

int1a

SCF Energy =-1190.033130

Thermal correction to Gibbs Free Energy = 0.406472

Charge = 0, Multiplicity = 1

C	0.81606800	1.82057000	-0.57248300
C	0.89679400	1.65217800	0.88038500
O	-0.39174500	1.84816500	0.24131700
H	1.07839400	2.78999500	-0.99509500
H	0.92504300	0.95255900	-1.21741800
H	1.03405100	0.63616500	1.24971400
C	1.35760700	2.75701700	1.79230400
H	0.83337700	2.71493200	2.75460200
H	2.43094800	2.65369100	1.98983400
H	1.17391100	3.73632700	1.34092100
C	4.69979100	0.39970700	-1.17651700
C	5.63642000	0.03689000	-0.20789600
C	5.23750300	-0.85401000	0.78869800
C	3.93114000	-1.33206200	0.77116100
C	3.06778400	-0.92340000	-0.25393300
N	3.44730300	-0.06648400	-1.21664800
H	5.93156700	-1.16382000	1.56621000
H	4.97244000	1.10187000	-1.96428500
H	6.64306700	0.44407500	-0.23568800
H	3.54776600	-2.00772900	1.52628200
C	1.62326900	-1.43525000	-0.26751900
O	0.96786800	-1.28849700	-1.32919400
O	1.21981900	-1.92679700	0.82942900
N	-2.56082400	-1.36730800	0.04818600
C	-1.64330600	-1.02740500	1.22203400

H	-0.64502500	-1.40407800	0.96532400
H	-1.58243500	0.06029900	1.23497200
C	-2.07794600	-1.58206300	2.56869000
H	-1.31492000	-1.28098600	3.29317100
H	-3.03940700	-1.19392400	2.92158600
H	-2.11071400	-2.67547400	2.58596900
C	-3.98616200	-0.93106800	0.32061600
H	-4.56118500	-1.19234700	-0.56943800
H	-4.34749600	-1.56059400	1.13638200
C	-4.16523400	0.54083800	0.65991400
H	-3.81786700	1.20495300	-0.13271400
H	-5.23506400	0.72323200	0.80557100
H	-3.65250200	0.81814400	1.58395300
C	-1.97618100	-0.64019500	-1.16307800
H	-0.92996700	-0.96713200	-1.23445200
H	-1.95801400	0.41464100	-0.89266800
C	-2.71701400	-0.86571800	-2.47041000
H	-3.74964300	-0.50028400	-2.46309100
H	-2.17911200	-0.30333000	-3.23992400
H	-2.71512400	-1.91375500	-2.78424200
C	-2.60166700	-2.86984600	-0.18847700
H	-2.99871400	-3.30172800	0.73242400
H	-3.35227900	-3.02657500	-0.96685600
C	-1.27761500	-3.51667300	-0.56503200
H	-0.48697900	-3.33040600	0.16647200
H	-1.45552500	-4.59565400	-0.63728500
H	-0.89623500	-3.16159700	-1.52365000
C	-1.75819700	4.01814600	-0.42460500
O	-0.86028200	4.74252900	-0.23896700
O	-2.70141200	3.35949200	-0.64014200

TSa1

SCF Energy =-1190.005989

Thermal correction to Gibbs Free Energy = 0.411025

Charge = 0, Multiplicity = 1

C	1.15191000	1.23033400	-0.36949200
C	0.88148700	1.42545100	1.06183900
O	-0.35842200	1.89516600	0.62574900
H	1.47361600	2.10065300	-0.93104200
H	0.65373900	0.43983800	-0.90386900
H	0.83416600	0.47581200	1.62509600
C	1.73297000	2.43687500	1.81549600
H	1.25406400	2.68081000	2.77046700
H	2.73417200	2.03985200	2.02403500
H	1.82361600	3.36177500	1.23688500
C	4.08180200	0.74211400	-0.38887100
C	5.23985000	0.04284900	-0.07199900
C	5.14083100	-1.33639200	0.13353600
C	3.89986100	-1.95025800	0.01464500
C	2.78306700	-1.18824400	-0.34828900
N	2.89579900	0.13895200	-0.54368300
H	6.02055500	-1.91738600	0.39650100
H	4.08935000	1.82070300	-0.52558600
H	6.18588700	0.56574600	0.02227900
H	3.75992400	-3.00836000	0.20379800
C	1.40495100	-1.85324400	-0.50185800
O	0.74836700	-1.53144000	-1.52345800
O	1.09232400	-2.62519800	0.43759300
N	-2.65090900	-1.03663600	0.15474700
C	-1.53278200	-0.97179600	1.19731700
H	-0.71663000	-1.58723200	0.81577300
H	-1.20720200	0.07084200	1.18834900
C	-1.91301100	-1.42838800	2.59659300
H	-0.99525200	-1.40229900	3.19221800
H	-2.64010800	-0.77337300	3.08663000
H	-2.28195900	-2.45837000	2.63267800
C	-3.88497200	-0.30623900	0.64559400
H	-4.65173300	-0.45250700	-0.11795600

H	-4.21380100	-0.83960000	1.53949600
C	-3.68804000	1.17621100	0.93027300
H	-3.49646100	1.75293100	0.02442700
H	-4.60995300	1.55352100	1.38547300
H	-2.85883200	1.37195900	1.61272300
C	-2.08757400	-0.37809000	-1.10249300
H	-1.18580600	-0.94430800	-1.35361300
H	-1.76292700	0.61518800	-0.78916900
C	-3.05122700	-0.31088900	-2.27535400
H	-3.93479600	0.30376500	-2.07599300
H	-2.51363600	0.15674400	-3.10599900
H	-3.37701200	-1.29803400	-2.61799300
C	-3.05409000	-2.47720800	-0.11351500
H	-3.37423700	-2.87798100	0.85032200
H	-3.93895900	-2.42852800	-0.75273800
C	-1.98012400	-3.35672200	-0.73945200
H	-1.03836100	-3.36293600	-0.18294000
H	-2.37764300	-4.37735800	-0.77289300
H	-1.74162100	-3.05223700	-1.76053100
C	-0.90309800	3.89925300	-0.74271700
O	0.13858600	4.42922900	-0.66444700
O	-1.99051400	3.50480000	-0.93066100

int2

SCF Energy =-1190.052498

Thermal correction to Gibbs Free Energy = 0.422624

Charge = 0, Multiplicity = 1

C	1.88918700	1.10487900	-0.60540200
C	1.16725400	1.41967000	0.72985900
O	-0.16830800	1.81041700	0.50173200
H	2.31751400	2.00028000	-1.04613100
H	1.19855700	0.63987100	-1.30449500
H	1.08250700	0.46931200	1.27460600
C	1.93931800	2.41860200	1.59212600

H	1.40725000	2.57093500	2.53624700
H	2.94650300	2.05132300	1.83082800
H	2.00721700	3.37319800	1.06684700
C	4.25693800	0.58602200	-0.27658500
C	5.31140700	-0.25820000	-0.00763400
C	5.04837300	-1.61996000	0.19232000
C	3.74144500	-2.07292600	0.11745400
C	2.69724900	-1.19387600	-0.18325400
N	2.98507200	0.12106100	-0.37263100
H	5.85834000	-2.30771500	0.41477900
H	4.37480600	1.65199800	-0.42255400
H	6.31549100	0.14481200	0.05166900
H	3.48175700	-3.10874600	0.30008400
C	1.24938300	-1.71800700	-0.28656100
O	0.68012800	-1.50720600	-1.37661000
O	0.87051900	-2.29406400	0.75497000
N	-2.89209700	-0.70171500	0.06917700
C	-1.87758200	-0.68792200	1.20636600
H	-1.02309100	-1.27347200	0.86893800
H	-1.54625000	0.34729600	1.28858100
C	-2.38550000	-1.24181100	2.52867800
H	-1.56549800	-1.15217800	3.24787900
H	-3.23991900	-0.69138200	2.93350200
H	-2.64372400	-2.30378700	2.47351100
C	-4.13437800	0.09196200	0.44584900
H	-4.73035200	0.15585300	-0.46578300
H	-4.68864700	-0.53066200	1.15281400
C	-3.87360000	1.47742600	1.02276200
H	-3.17956400	2.07837900	0.42267800
H	-4.83513700	2.00056100	1.06710500
H	-3.48263400	1.42278900	2.04258500
C	-2.20248900	-0.06383000	-1.14324800
H	-1.24027000	-0.56951700	-1.23757700
H	-2.01901700	0.97986300	-0.88072600

C	-2.97937800	-0.14419400	-2.44790100
H	-3.96022800	0.33937800	-2.40136100
H	-2.39328500	0.40777400	-3.18908600
H	-3.10295300	-1.16524200	-2.82191200
C	-3.33381700	-2.11834200	-0.24029800
H	-3.82815100	-2.48696400	0.66062400
H	-4.09827400	-2.03140500	-1.01534700
C	-2.22201000	-3.06528500	-0.66995000
H	-1.45604800	-3.19735000	0.09726700
H	-2.68000700	-4.03879500	-0.87664300
H	-1.70534800	-2.72712000	-1.56968700
C	-0.42335100	2.90596500	-0.45680700
O	0.57803300	3.48820600	-0.88799200
O	-1.63950600	3.01442900	-0.67731400

TSc

SCF Energy =-1190.025405

Thermal correction to Gibbs Free Energy = 0.421308

Charge = 0, Multiplicity = 1

C	1.78048100	1.53090300	-0.68711100
C	1.19394000	1.58810900	0.71975600
O	-0.19416200	1.91373600	0.64143300
H	2.56488800	2.20843300	-0.98914300
H	1.29146500	0.92562100	-1.43361600
H	1.21627500	0.59229900	1.16813200
C	1.92968600	2.58244700	1.61252400
H	1.44720000	2.63275300	2.59275600
H	2.97360900	2.28041200	1.75592900
H	1.90588100	3.57659600	1.15644000
C	4.37896400	0.48678300	-0.24411900
C	5.38937600	-0.42304700	0.03117600
C	5.03630200	-1.76241400	0.22315100
C	3.69987300	-2.12914800	0.13330400
C	2.73454900	-1.16612900	-0.18230800

N	3.09526500	0.11794700	-0.35716600
H	5.79708600	-2.50350400	0.45104900
H	4.58534900	1.54512700	-0.38067100
H	6.41878000	-0.08908200	0.10252700
H	3.36688100	-3.14512400	0.31023900
C	1.25509800	-1.56333900	-0.30714100
O	0.65426800	-1.12789800	-1.31757900
O	0.83833600	-2.27491700	0.63767200
N	-2.89925000	-0.75171400	0.07831700
C	-1.86043000	-0.73147800	1.19497900
H	-0.98685700	-1.26783600	0.82267600
H	-1.57619000	0.31351700	1.31184600
C	-2.31403400	-1.34964600	2.50831300
H	-1.48083400	-1.24809000	3.21046200
H	-3.18247800	-0.85349700	2.95252500
H	-2.52382600	-2.41991900	2.42210500
C	-4.16724000	-0.03147200	0.50616500
H	-4.78992100	0.02924500	-0.38777900
H	-4.67366100	-0.69596200	1.21051500
C	-3.95825200	1.34928100	1.11733800
H	-3.32033600	2.00592300	0.51679500
H	-4.94250300	1.82070700	1.21048200
H	-3.52773300	1.28678700	2.12024800
C	-2.26801100	-0.04142600	-1.12311300
H	-1.27268600	-0.47823600	-1.23973000
H	-2.15234100	0.99939700	-0.82797300
C	-3.05931900	-0.12418700	-2.41909200
H	-4.06717300	0.29700900	-2.34476800
H	-2.51679600	0.48219400	-3.15089400
H	-3.12776900	-1.13879500	-2.82204800
C	-3.27635900	-2.17732400	-0.27571600
H	-3.70967900	-2.60920800	0.62841500
H	-4.07814200	-2.10059400	-1.01368700
C	-2.13238300	-3.03898200	-0.79259700

H	-1.30377400	-3.12176500	-0.08514500
H	-2.53560700	-4.03951200	-0.98401200
H	-1.70996500	-2.65442000	-1.72272400
C	-0.48803200	2.77048300	-0.44048300
O	0.52859900	3.03580000	-1.15571700
O	-1.66535400	3.10195700	-0.56320400

int3

SCF Energy =-1190.065931

Thermal correction to Gibbs Free Energy = 0.416528

Charge = 0, Multiplicity = 1

C	4.78966400	-0.11325800	0.33416000
C	5.55138200	-1.23848100	0.02132500
C	4.87804100	-2.40691500	-0.33613500
C	3.48739600	-2.39471200	-0.36173400
C	2.80599300	-1.22138700	-0.01405800
N	3.45168600	-0.09235100	0.32774400
H	5.42968000	-3.30768800	-0.59332300
H	5.28038000	0.82107900	0.60601700
H	6.63603300	-1.19480000	0.05378500
H	2.89989600	-3.25979700	-0.64404900
C	1.27170500	-1.22164300	-0.01989300
O	0.69155200	-0.24328200	0.52236400
O	0.73161200	-2.22299100	-0.56239200
N	-2.94736600	-0.88374000	0.22458900
C	-2.11179500	-0.97793100	-1.05620600
H	-2.05715400	0.04030000	-1.44088000
H	-1.10456700	-1.27844800	-0.75584700
C	-2.64363000	-1.94328800	-2.10261100
H	-1.94993900	-1.89920400	-2.94768500
H	-2.64788500	-2.98111100	-1.75678600
H	-3.63991700	-1.68904700	-2.47914800
C	-2.98505800	-2.21958900	0.94818100
H	-3.71028900	-2.09868500	1.75696500

H	-3.40962300	-2.93100700	0.23760800
C	-1.64812000	-2.71695300	1.47528500
H	-1.25861100	-2.07876800	2.27199400
H	-1.81439900	-3.71522500	1.89549000
H	-0.87844400	-2.78160900	0.69869000
C	-2.28028000	0.18433500	1.09227300
H	-2.35552800	1.10965300	0.52576900
H	-1.21759900	-0.07799600	1.11467800
C	-2.86835500	0.35527200	2.48354900
H	-2.76190200	-0.53450800	3.11064600
H	-2.30405200	1.16055500	2.96436600
H	-3.92086400	0.65836500	2.48078500
C	-4.38472400	-0.51256400	-0.08572300
H	-4.82674100	-1.38469400	-0.57264400
H	-4.88143100	-0.39418100	0.87897800
C	-4.57279900	0.73070200	-0.94386700
H	-4.19133100	0.59444200	-1.95781200
H	-5.64792600	0.92740500	-1.01223600
H	-4.08807900	1.61465900	-0.52683200
C	1.74060200	2.43036200	-0.91486800
C	1.29448500	2.61553000	0.54373800
O	0.51283400	2.20969800	-1.63815700
H	2.22188000	3.32142300	-1.33410600
H	2.37823600	1.55518500	-1.02237300
H	1.45595200	1.68342100	1.08489100
C	1.87555900	3.82485000	1.24373400
H	1.45755500	3.93195800	2.24936900
H	2.96037400	3.70144200	1.33902700
H	1.67589400	4.74407400	0.68139100
C	-0.53504400	2.43424600	-0.83092400
O	-0.15139600	2.77387400	0.40953500
O	-1.69084800	2.34819800	-1.18515100

int1

SCF Energy =-1001.376050

Thermal correction to Gibbs Free Energy = 0.402094

Charge = 0, Multiplicity = 1

C	0.94011900	1.86942500	-1.20344100
C	1.05189100	2.05744400	0.24375700
O	-0.16595200	2.43267400	-0.44862500
H	1.43414200	2.58233800	-1.86363400
H	0.79264200	0.86692500	-1.59757200
H	0.94225300	1.16934700	0.86573200
C	1.85144200	3.18099100	0.84625000
H	1.39537000	3.53499800	1.77847100
H	2.86477100	2.83140300	1.07659200
H	1.91957200	4.02569100	0.15319500
C	4.48157700	-0.15256200	-1.22648000
C	5.32599100	-0.23659700	-0.11860100
C	4.78880500	-0.70485600	1.08066400
C	3.44343100	-1.05779500	1.11522300
C	2.67732300	-0.94784500	-0.05298800
N	3.19097500	-0.50106400	-1.21122200
H	5.40744100	-0.78756400	1.97103100
H	4.86473900	0.21488100	-2.17845900
H	6.36865900	0.05773600	-0.19723000
H	2.95567200	-1.40850500	2.01668700
C	1.18460200	-1.29652200	-0.00696600
O	0.57830400	-1.39600300	-1.10185000
O	0.69719300	-1.40067500	1.15978600
N	-2.86889800	-0.31496700	0.08439400
C	-1.89259200	0.15900800	1.16159300
H	-1.01439400	-0.49622800	1.10083200
H	-1.57363400	1.15158400	0.84431300
C	-2.44122300	0.17418100	2.57894800
H	-1.62127000	0.49652400	3.22824600
H	-3.27144700	0.87299900	2.72729000
H	-2.74670200	-0.81631900	2.92927800

C	-4.15043000	0.49083700	0.11484400
H	-4.78871100	0.08378300	-0.67140600
H	-4.63011000	0.26801300	1.06999600
C	-3.97757700	1.99243600	-0.06215500
H	-3.53285800	2.24931100	-1.02599800
H	-4.96941100	2.45367100	-0.01655000
H	-3.36366600	2.43752000	0.72375500
C	-2.13737200	-0.14666400	-1.24602900
H	-1.20423800	-0.72028100	-1.15674000
H	-1.85390500	0.90449000	-1.29228100
C	-2.92746900	-0.56816800	-2.47343700
H	-3.83173600	0.02612800	-2.64477300
H	-2.27216100	-0.42235300	-3.33772000
H	-3.20028000	-1.62758100	-2.45792900
C	-3.25466900	-1.76974300	0.30962100
H	-3.71342500	-1.80197300	1.29988700
H	-4.04191600	-1.98504100	-0.41702300
C	-2.11882600	-2.77645300	0.20065900
H	-1.26959600	-2.53981500	0.84770000
H	-2.52614300	-3.75416100	0.48189500
H	-1.72070800	-2.84596800	-0.81306000

TSa

SCF Energy =-1001.345206

Thermal correction to Gibbs Free Energy = 0.405789

Charge = 0, Multiplicity = 1

C	1.19653500	1.37783600	-0.95625300
C	0.89777600	2.04437900	0.32544700
O	-0.27207000	2.47529400	-0.27692500
H	1.58668500	2.00604500	-1.75072800
H	0.60841900	0.52526600	-1.24862500
H	0.77093200	1.32105600	1.15682500
C	1.84358500	3.15532800	0.76917200
H	1.37928100	3.72915200	1.57909900

H	2.79972100	2.75698200	1.13207900
H	2.03218700	3.84354900	-0.06311700
C	4.02107100	0.73013800	-0.72833700
C	5.12135100	0.09370700	-0.16937100
C	4.91939400	-1.13648400	0.46390200
C	3.63784700	-1.67100600	0.50911500
C	2.58162600	-0.99437200	-0.11238300
N	2.79489700	0.18943800	-0.71822700
H	5.75179100	-1.65956800	0.92653200
H	4.10693800	1.70514200	-1.20119000
H	6.10242500	0.55444600	-0.21838500
H	3.41939700	-2.60045600	1.02229900
C	1.16114800	-1.58385800	-0.08971100
O	0.55179800	-1.59092600	-1.18732600
O	0.77850500	-1.96860500	1.04220200
N	-2.79296300	-0.24649100	0.12444700
C	-1.67552700	0.08180500	1.11887900
H	-0.92754900	-0.70489200	1.01263800
H	-1.24507800	1.01738000	0.74982700
C	-2.10111200	0.19971700	2.57345500
H	-1.18289800	0.33582300	3.15320100
H	-2.74146200	1.06499800	2.77138200
H	-2.58893500	-0.69999900	2.96267600
C	-3.93637200	0.73825800	0.26643200
H	-4.74055600	0.37335600	-0.37629000
H	-4.28226600	0.64860900	1.29735100
C	-3.58531000	2.18179800	-0.07676100
H	-3.50174500	2.32873700	-1.15645700
H	-4.39480800	2.82346600	0.28641900
H	-2.64192800	2.51493700	0.36317200
C	-2.15972900	-0.14866600	-1.25999600
H	-1.31738000	-0.84723900	-1.25592800
H	-1.73507400	0.85598800	-1.30983500
C	-3.10817100	-0.42811900	-2.41413600

H	-3.93969500	0.28151700	-2.47666300
H	-2.52925100	-0.33376500	-3.33810500
H	-3.51517300	-1.44384700	-2.39315100
C	-3.34738100	-1.63736800	0.37846700
H	-3.70790000	-1.62811400	1.40904900
H	-4.22209000	-1.73886400	-0.26857200
C	-2.36992100	-2.78327900	0.15090700
H	-1.42740500	-2.67275900	0.69521500
H	-2.86425600	-3.70295600	0.48325700
H	-2.11259500	-2.89959400	-0.90408300

int2a

SCF Energy =-1001.373451

Thermal correction to Gibbs Free Energy = 0.409480

Charge = 0, Multiplicity = 1

C	1.60943700	1.14986800	-1.05129600
C	0.88573700	1.82882900	0.19476400
O	-0.31866000	2.26606900	-0.17985600
H	1.98821200	1.91264900	-1.73536000
H	0.90079700	0.50215700	-1.55493300
H	0.87293000	0.99674300	0.95722100
C	1.78507500	2.93888600	0.78392300
H	1.27560500	3.36998000	1.65187400
H	2.77276100	2.58627900	1.11431100
H	1.91594300	3.73980200	0.04499300
C	3.99026600	0.84686900	-0.60419700
C	5.06109800	0.18252900	-0.04983100
C	4.84876300	-1.07516100	0.53006200
C	3.56933600	-1.60776500	0.51687700
C	2.50913000	-0.92561100	-0.08463900
N	2.74420200	0.30299300	-0.63282700
H	5.67017600	-1.61672800	0.98863900
H	4.07341500	1.83524100	-1.03718600
H	6.03982600	0.64816200	-0.06323900

H	3.33719000	-2.56123600	0.97569300
C	1.12336600	-1.60796300	-0.15684300
O	0.59083400	-1.62543100	-1.28758100
O	0.74578800	-2.08189300	0.93665600
N	-2.78794100	-0.19319500	0.12443500
C	-1.70446500	0.01933000	1.18836200
H	-0.99250900	-0.79517600	1.06241100
H	-1.21138800	0.95430900	0.88602100
C	-2.19486400	0.07070700	2.62619400
H	-1.30037800	0.11905300	3.25521300
H	-2.79267800	0.96039200	2.84774100
H	-2.75429900	-0.81793600	2.93907400
C	-3.88390000	0.84310000	0.27731200
H	-4.68173800	0.55116100	-0.40957600
H	-4.27173000	0.71935200	1.28976200
C	-3.44586000	2.28150500	0.02013300
H	-3.36397500	2.48568600	-1.05041000
H	-4.20998700	2.94887000	0.43280000
H	-2.47163800	2.52440500	0.45419000
C	-2.08842000	-0.04458000	-1.22476700
H	-1.30920300	-0.80917100	-1.24593900
H	-1.56857100	0.92047700	-1.17142000
C	-3.00694800	-0.17028700	-2.42898600
H	-3.77121300	0.61218000	-2.47632600
H	-2.38277000	-0.06783200	-3.32234000
H	-3.50169400	-1.14544700	-2.49388900
C	-3.42323900	-1.56284000	0.26760400
H	-3.82352900	-1.60255300	1.28272900
H	-4.27533100	-1.58000300	-0.41627700
C	-2.49711700	-2.74269100	-0.00166600
H	-1.56590100	-2.70932600	0.57003700
H	-3.04030800	-3.65550100	0.26695100
H	-2.21991600	-2.81289300	-1.05579600

int2b

SCF Energy =-1190.033431

Thermal correction to Gibbs Free Energy = 0.414741

Charge = 0, Multiplicity = 1

C	1.39988700	-0.60851000	1.23793100
C	0.58205600	-1.93199000	0.90289900
O	-0.59767000	-1.86744800	1.52568300
H	1.76952200	-0.64147700	2.26486900
H	0.73106500	0.23204900	1.10315200
H	0.52833600	-1.91571900	-0.22348700
C	1.41272300	-3.17759500	1.28122400
H	0.83094900	-4.06939700	1.02666100
H	2.37848800	-3.24497500	0.75991400
H	1.58477000	-3.19285800	2.36515600
C	3.76688400	-0.87414800	0.71803900
C	4.84467700	-0.87520500	-0.13840500
C	4.66956300	-0.40262100	-1.44518000
C	3.41917000	0.05938900	-1.82528900
C	2.35572000	0.08228000	-0.92157400
N	2.55084600	-0.40096700	0.33871600
H	5.49671700	-0.40443100	-2.14794800
H	3.82040700	-1.25409800	1.72980600
H	5.80042700	-1.24810100	0.21118400
H	3.21885600	0.41419600	-2.82909100
C	1.01145300	0.69458100	-1.36310100
O	0.56445900	1.60904000	-0.62832800
O	0.55953500	0.21658500	-2.42124600
N	-2.97368400	-0.03216700	-0.27951900
C	-2.04710100	-1.06053200	-0.93836600
H	-1.28317500	-0.48760800	-1.46143300
H	-1.56640000	-1.57442900	-0.09269700
C	-2.71841200	-2.03171700	-1.89539700
H	-1.91659600	-2.62582200	-2.34500100
H	-3.39662500	-2.73125500	-1.39677400

H	-3.25362000	-1.54636400	-2.71901000
C	-4.12071900	-0.73002300	0.42472600
H	-4.80856000	0.05657900	0.74398600
H	-4.63250300	-1.31191900	-0.34360700
C	-3.71247600	-1.60540800	1.60496800
H	-3.48375100	-1.00206900	2.48698500
H	-4.55781800	-2.25648500	1.85221000
H	-2.82501400	-2.21363700	1.40909500
C	-2.11040500	0.73175400	0.72301400
H	-1.30958700	1.18707700	0.13893400
H	-1.64499100	-0.04474300	1.34261500
C	-2.84936900	1.78370200	1.53255700
H	-3.62114200	1.36531100	2.18666100
H	-2.10560200	2.27445500	2.16701900
H	-3.30191700	2.56440200	0.91178100
C	-3.56965600	0.90125500	-1.31525500
H	-4.13153000	0.26668200	-2.00391500
H	-4.29440200	1.52412100	-0.78597600
C	-2.56712300	1.76834900	-2.06643800
H	-1.77134800	1.19630100	-2.54912700
H	-3.11988100	2.31622400	-2.83757400
H	-2.08094300	2.49670200	-1.41429100
C	1.49126100	2.84162800	1.47050300
O	2.60885200	2.54550000	1.28661000
O	0.40944200	3.18533400	1.75157800

TSb

SCF Energy =-1190.027846

Thermal correction to Gibbs Free Energy = 0.415664

Charge = 0, Multiplicity = 1

C	1.66469900	0.97696800	0.52272800
C	0.86556700	0.41648000	1.77780900
O	-0.30294100	1.05643300	1.86120700
H	2.12375400	1.93835500	0.75794700

H	0.96348400	1.06686700	-0.29863300
H	0.78935000	-0.68825600	1.55359000
C	1.73053700	0.53763300	3.05193900
H	1.16783200	0.12110000	3.89379300
H	2.68990500	0.00345600	2.99058400
H	1.92036200	1.59622100	3.27051200
C	3.98508400	0.22744000	0.56326600
C	4.98427100	-0.69018800	0.32831000
C	4.68419100	-1.84014500	-0.41345000
C	3.39331900	-2.00880500	-0.88959700
C	2.40848800	-1.04460100	-0.66373300
N	2.72866100	0.06126400	0.07062300
H	5.44722400	-2.58845000	-0.60345100
H	4.13558000	1.12253500	1.15262900
H	5.97579500	-0.50959600	0.72728800
H	3.09261100	-2.89022700	-1.44270100
C	1.00839300	-1.24255400	-1.29333500
O	0.53154500	-0.25295900	-1.88971300
O	0.56120100	-2.40013200	-1.13814200
N	-2.88250600	-0.56864200	0.06576200
C	-1.76882000	-1.30286900	0.81923700
H	-1.10513400	-1.70855200	0.05748500
H	-1.23698100	-0.50365900	1.35566400
C	-2.22570600	-2.40548100	1.76095500
H	-1.31743800	-2.89987900	2.11966500
H	-2.75557400	-2.02776500	2.64093600
H	-2.83955800	-3.17766100	1.28349600
C	-3.93633200	-0.07725500	1.03825700
H	-4.75842400	0.31091300	0.43273000
H	-4.30709700	-0.96695900	1.54980300
C	-3.44756800	0.97442900	2.02973900
H	-3.38804100	1.96064200	1.56204100
H	-4.17284300	1.03423900	2.84826100
H	-2.45265500	0.76341800	2.43471000

C	-2.21418900	0.60797300	-0.64320900
H	-1.44752800	0.17705700	-1.29044200
H	-1.67542000	1.14943200	0.14101900
C	-3.17422000	1.48633600	-1.42852600
H	-3.91698000	1.98447200	-0.79701100
H	-2.57823100	2.26779200	-1.90501500
H	-3.69968700	0.94403000	-2.22180200
C	-3.55875600	-1.49613300	-0.92576200
H	-3.90194300	-2.35456600	-0.34494400
H	-4.44774500	-0.97177000	-1.28436900
C	-2.69010200	-1.94063700	-2.09673700
H	-1.71989900	-2.34618200	-1.79565700
H	-3.23960100	-2.71795700	-2.63910400
H	-2.49639600	-1.12069500	-2.79240300
C	0.62130700	3.64123700	-1.18808100
O	1.76992400	3.83342700	-1.08472800
O	-0.52882800	3.47127100	-1.29989600

P1

SCF Energy = -381.851661

Thermal correction to Gibbs Free Energy = 0.073262

Charge = 0, Multiplicity = 1

C	-0.57522700	1.31247100	0.18674100
C	-1.09020200	-0.10247000	0.50314700
O	0.13977700	-0.85132700	0.60186300
H	-1.18251800	1.83803100	-0.55323300
H	-0.46727500	1.93320800	1.08259600
H	-1.57487700	-0.15310000	1.48111700
C	-1.97389600	-0.70026400	-0.57988900
H	-2.16402400	-1.75763700	-0.37642500
H	-2.93383600	-0.17318000	-0.61900000
H	-1.48989800	-0.61536300	-1.55900400
C	1.14351300	-0.17390200	-0.01967800
O	0.72151500	1.07315300	-0.37342300

O	2.23712100	-0.60769700	-0.22818700

TSa2

SCF Energy =-1001.322335

Thermal correction to Gibbs Free Energy = 0.402454

Charge = 0, Multiplicity = 1

C	1.16531800	1.81203900	0.69278600
C	1.35591100	2.34767600	-0.70474100
O	1.57304000	3.61646800	-0.33957700
H	0.29825800	2.24989800	1.18159100
H	2.06603700	1.84427000	1.29036500
H	2.21815000	1.80154500	-1.18317900
C	0.14612000	2.13316400	-1.64325400
H	0.33544900	2.65896600	-2.58610300
H	-0.04802200	1.07300100	-1.86707500
H	-0.74680400	2.58967300	-1.19241000
C	4.83219300	-0.05816200	0.97552700
C	5.55405500	-0.71347200	-0.02355300
C	4.84673900	-1.42234400	-0.99437000
C	3.45790000	-1.43983000	-0.92818000
C	2.82587900	-0.72921800	0.09937700
N	3.49882000	-0.05769900	1.04625000
H	5.36926500	-1.95009100	-1.78742500
H	5.35057900	0.49553700	1.75613700
H	6.63873300	-0.66827700	-0.03483400
H	2.85112300	-1.98096800	-1.64419900
C	1.32113500	-0.75452900	0.17427500
O	0.70275500	0.18480500	0.83636600
O	0.71272200	-1.68855700	-0.37631800
N	-3.02018700	-0.42736400	0.15601400
C	-2.20159600	-0.86603200	-1.05923900
H	-2.15191800	0.00804000	-1.70889900
H	-1.18550000	-1.06405700	-0.70442400
C	-2.74013100	-2.07432800	-1.80683200

H	-2.04657300	-2.26927700	-2.63033600
H	-2.75837500	-2.97795700	-1.19102100
H	-3.73292600	-1.91966200	-2.24150600
C	-3.06344200	-1.52690400	1.20832400
H	-3.74256400	-1.16670300	1.98409600
H	-3.54579800	-2.37885700	0.72580400
C	-1.72066900	-1.92569000	1.80011100
H	-1.25118700	-1.11124500	2.35531700
H	-1.90615900	-2.74963800	2.49743000
H	-1.00369400	-2.25834200	1.04653700
C	-2.32217300	0.81683300	0.70056500
H	-2.32994400	1.54151900	-0.11228800
H	-1.27990800	0.52738100	0.84791900
C	-2.92666700	1.40957600	1.96191100
H	-2.88060200	0.72772400	2.81567100
H	-2.32568800	2.28741800	2.21874100
H	-3.95966800	1.74914800	1.83493300
C	-4.45870000	-0.13165400	-0.22373500
H	-4.89375600	-1.08381900	-0.53273000
H	-4.96011600	0.17179500	0.69668300
C	-4.64892700	0.92022300	-1.30654200
H	-4.19950200	0.62738400	-2.25832600
H	-5.72437700	1.03906200	-1.47172500
H	-4.25074800	1.89615900	-1.01892700

int2c

SCF Energy =-1001.325695

Thermal correction to Gibbs Free Energy = 0.404277

Charge = 0, Multiplicity = 1

C	1.17983900	1.72355300	0.74692600
C	1.37384500	2.29216200	-0.68075600
O	1.87265400	3.49996000	-0.57641700
H	0.38788100	2.25811600	1.28152900
H	2.11624400	1.78404100	1.29345800

H	2.04484000	1.49140500	-1.16778300
C	0.05343900	2.21936600	-1.51052600
H	0.25284600	2.65555800	-2.49474300
H	-0.33335800	1.19867300	-1.65392900
H	-0.71404800	2.84311600	-1.02712500
C	4.84649700	-0.14102600	1.02804500
C	5.57346900	-0.82080000	0.05030200
C	4.86771500	-1.47610100	-0.96222700
C	3.48153500	-1.41015700	-0.96146600
C	2.84530400	-0.66920000	0.04678600
N	3.51382300	-0.06449800	1.04344100
H	5.39316300	-2.02651500	-1.73771000
H	5.36010200	0.36546700	1.84320700
H	6.65812800	-0.84033400	0.08736500
H	2.87964100	-1.90288500	-1.71560400
C	1.35136500	-0.64013400	0.07032400
O	0.71096700	0.30741600	0.75919000
O	0.70081800	-1.55053800	-0.45895300
N	-3.05453600	-0.43003900	0.17350900
C	-2.28006400	-0.90784000	-1.05587300
H	-2.30331300	-0.07336000	-1.75708800
H	-1.23912000	-1.03915900	-0.74549300
C	-2.80176800	-2.18008000	-1.70267300
H	-2.15038100	-2.38905900	-2.55659500
H	-2.73872700	-3.04727300	-1.03940500
H	-3.82511600	-2.09548900	-2.08226600
C	-3.02358400	-1.47791000	1.27797300
H	-3.67273800	-1.09434400	2.06787100
H	-3.50906700	-2.36156200	0.86024200
C	-1.64612000	-1.82086100	1.82333200
H	-1.17274200	-0.97447300	2.32474000
H	-1.77920800	-2.61943600	2.56079000
H	-0.95600400	-2.16962500	1.05246300
C	-2.36676600	0.85581600	0.62655300

H	-2.40998100	1.53497200	-0.22348100
H	-1.31678400	0.59525900	0.75831900
C	-2.94252400	1.50491500	1.87361200
H	-2.86148300	0.86923100	2.75986400
H	-2.34688100	2.40249000	2.06630400
H	-3.98359000	1.82339300	1.75978400
C	-4.51602300	-0.18782100	-0.15440500
H	-4.93764700	-1.16341700	-0.40280700
H	-4.98483400	0.14241200	0.77388500
C	-4.78208400	0.81079700	-1.27107100
H	-4.37251900	0.48590800	-2.23045200
H	-5.86669000	0.89915800	-1.38842300
H	-4.39357000	1.80670300	-1.04526100

TSa3

SCF Energy =-1189.985792

Thermal correction to Gibbs Free Energy = 0.409042

Charge = 0, Multiplicity = 1

C	1.18895200	1.23008100	0.66219100
C	1.50071400	1.50819600	-0.75125300
O	2.05700400	2.70711000	-0.31200200
H	0.41768100	1.84301100	1.11046400
H	2.00710600	0.90544000	1.28505700
H	2.24550500	0.80941000	-1.15761600
C	0.33637300	1.68370600	-1.71683600
H	0.70038000	2.10012900	-2.66213800
H	-0.15975800	0.72628800	-1.92306600
H	-0.39326000	2.39017800	-1.30150600
C	4.08910800	-1.51705500	0.83809800
C	4.56530000	-2.42235400	-0.11199700
C	3.64375800	-3.06112800	-0.93915000
C	2.29230700	-2.76190200	-0.79080200
C	1.91594200	-1.82559200	0.17778700
N	2.79618400	-1.22413700	0.99133200

H	3.97276700	-3.77412800	-1.69024700
H	4.77807200	-0.99232700	1.49496100
H	5.63053600	-2.61137000	-0.20042100
H	1.52564900	-3.22624900	-1.39936500
C	0.45221700	-1.46253500	0.30887900
O	0.13359900	-0.35376700	0.88987900
O	-0.38899600	-2.25670600	-0.15990200
N	-3.57415000	0.04884300	0.13526500
C	-2.91938800	-0.73536800	-1.00232800
H	-2.63205800	0.01298800	-1.74239500
H	-1.99985500	-1.17526400	-0.60006200
C	-3.78159400	-1.81781200	-1.63017700
H	-3.17533400	-2.29227300	-2.40766100
H	-4.05087400	-2.60449500	-0.91996100
H	-4.69229000	-1.43977100	-2.10578800
C	-3.92079400	-0.86992700	1.30089500
H	-4.46603400	-0.24700400	2.01329900
H	-4.62829700	-1.59805600	0.90014800
C	-2.74469800	-1.56468000	1.96821800
H	-2.05655700	-0.86146100	2.44095800
H	-3.15553400	-2.21665100	2.74660200
H	-2.15630800	-2.16950500	1.27477500
C	-2.55021000	1.09906300	0.55817800
H	-2.37258500	1.70957800	-0.32691900
H	-1.62628600	0.54693800	0.75533200
C	-2.95056900	1.96665400	1.73970900
H	-3.07665800	1.39223600	2.66141900
H	-2.13118200	2.67173900	1.91143700
H	-3.85482300	2.55820800	1.56380900
C	-4.87509100	0.69069000	-0.30989200
H	-5.56180300	-0.13064800	-0.52208600
H	-5.26429400	1.22393900	0.55884700
C	-4.77407200	1.62462000	-1.50676700
H	-4.43028700	1.11360800	-2.40927700

H	-5.77592900	2.01522100	-1.71082500
H	-4.12127700	2.48045500	-1.31858700
C	4.01776100	2.62861900	-0.04437700
O	4.31834400	1.49817500	-0.29245800
O	4.25920500	3.74359300	0.28603100

int2d

SCF Energy =-1190.009424

Thermal correction to Gibbs Free Energy = 0.415803

Charge = 0, Multiplicity = 1

C	1.01533000	0.97430200	0.79121500
C	1.31701400	1.64253400	-0.55200800
O	2.15086200	2.73016300	-0.28969200
H	0.40433000	1.62291200	1.42550700
H	1.94444900	0.71647500	1.28883500
H	1.83905700	0.90203200	-1.17501900
C	0.06908400	2.14680000	-1.27417600
H	0.36618000	2.66427000	-2.19091900
H	-0.60464000	1.32223500	-1.54287400
H	-0.47505800	2.86670100	-0.64772800
C	4.10594500	-1.54584800	1.17980400
C	4.81340400	-2.01122200	0.06954700
C	4.11118900	-2.31032900	-1.09299800
C	2.73212700	-2.11849600	-1.10827900
C	2.13106700	-1.60821000	0.04215400
N	2.78870200	-1.34734300	1.17944900
H	4.62706900	-2.67525800	-1.97607400
H	4.62428300	-1.31153800	2.10596300
H	5.89169300	-2.12055400	0.11902800
H	2.13118200	-2.33352500	-1.98471200
C	0.66060300	-1.33939000	0.02969700
O	0.18687700	-0.23898800	0.63478600
O	-0.13647000	-2.10656000	-0.50100500
N	-3.61430400	-0.11777300	0.13729700

C	-2.88819400	-0.67062300	-1.09023400
H	-2.71680100	0.18928600	-1.73862900
H	-1.91341100	-1.02579300	-0.74938700
C	-3.61312200	-1.77857800	-1.83585100
H	-2.96843400	-2.07211600	-2.66963200
H	-3.75972900	-2.67223500	-1.22325300
H	-4.57563000	-1.47049200	-2.25562400
C	-3.83096100	-1.20935700	1.17879400
H	-4.42398700	-0.74789400	1.97074000
H	-4.46153800	-1.95718900	0.69528500
C	-2.56964200	-1.84545600	1.74114400
H	-1.94967300	-1.13345900	2.28991500
H	-2.88544200	-2.62404100	2.44318800
H	-1.94573600	-2.30714900	0.97356400
C	-2.72234700	0.99097000	0.69113100
H	-2.61203500	1.71584800	-0.11444400
H	-1.74537600	0.53202000	0.83377200
C	-3.21794000	1.66259000	1.96088000
H	-3.28273700	0.97398700	2.80766200
H	-2.48266500	2.42884700	2.22531200
H	-4.18143400	2.16658600	1.83850600
C	-4.99014500	0.41247900	-0.22731100
H	-5.57115000	-0.45245600	-0.55138700
H	-5.43287300	0.77162200	0.70292000
C	-5.01608800	1.50313500	-1.28766500
H	-4.62362500	1.16388600	-2.24927800
H	-6.06043000	1.79123800	-1.44274200
H	-4.47162800	2.40029300	-0.98318500
C	3.62153500	2.37325800	-0.11052300
O	3.85616500	1.15701800	-0.22896000
O	4.28279700	3.37335700	0.12556400

TSa4

SCF Energy = -1001.343723

Thermal correction to Gibbs Free Energy = 0.406104

Charge = 0, Multiplicity = 1

C	4.09004700	0.89352500	0.08491500
C	5.13436300	0.07842900	-0.33345000
C	4.87555600	-1.28259800	-0.51611400
C	3.59435400	-1.76281500	-0.27519200
C	2.59940500	-0.89003100	0.18106500
N	2.86664000	0.41871900	0.35468500
H	5.66182100	-1.95211800	-0.85390400
H	4.22721200	1.96292400	0.21799900
H	6.11578300	0.50186700	-0.52010500
H	3.32580100	-2.80004300	-0.43785800
C	1.18781400	-1.42913100	0.47104000
O	0.75379600	-2.22878600	-0.39453900
O	0.63562300	-1.00526300	1.51593000
N	-2.78908800	-0.29805300	-0.09550900
C	-2.11892900	0.29614700	1.13951300
H	-1.27263100	-0.35854300	1.36791000
H	-1.69379300	1.24541300	0.80527000
C	-3.03565700	0.46188700	2.34031300
H	-2.43110600	0.87456300	3.15406200
H	-3.86276700	1.15752600	2.16425700
H	-3.44740700	-0.48762200	2.69680600
C	-3.94851500	0.56551000	-0.54906500
H	-4.32490200	0.10518200	-1.46399700
H	-4.72804700	0.45980000	0.20864600
C	-3.60598700	2.03486200	-0.76791600
H	-2.67885900	2.18486600	-1.32655300
H	-4.43381400	2.49882900	-1.31426900
H	-3.49185100	2.56531200	0.18064600
C	-1.70387200	-0.35175600	-1.17633100
H	-0.95173900	-1.05692600	-0.82050600
H	-1.26505700	0.65135600	-1.17320200
C	-2.17767200	-0.75025000	-2.56479200

H	-2.82110000	-0.00092000	-3.03640800
H	-1.27920400	-0.84169100	-3.18304600
H	-2.68226300	-1.72171500	-2.59653900
C	-3.33214600	-1.68763600	0.18890200
H	-4.20178600	-1.54876100	0.83599100
H	-3.69904900	-2.06344000	-0.76830700
C	-2.34206900	-2.66112200	0.81571500
H	-2.09427500	-2.38622600	1.84348100
H	-2.82167500	-3.64611600	0.83581900
H	-1.39675100	-2.74035300	0.27003700
C	0.85120500	1.80053700	-1.07107600
C	1.25063300	1.70284400	0.34878500
O	-0.34750200	2.36948200	-0.69652900
H	1.52241100	2.44913000	-1.67032200
H	0.79754700	0.81554400	-1.57934900
H	0.71409900	0.97627700	0.93949300
C	1.78515100	2.90870000	1.06280300
H	0.94845600	3.56530500	1.31370400
H	2.28852100	2.61862900	1.98933100
H	2.47613500	3.48121300	0.43309800

int2e

SCF Energy =-1001.371406

Thermal correction to Gibbs Free Energy = 0.409710

Charge = 0, Multiplicity = 1

C	-3.93089600	0.98807700	0.09997900
C	-4.97550000	0.18536500	0.50802400
C	-4.77793900	-1.19649700	0.58553600
C	-3.53061900	-1.70858300	0.25823000
C	-2.49873700	-0.87567900	-0.17429900
N	-2.72585900	0.47122400	-0.26063700
H	-5.57931900	-1.85298200	0.90979500
H	-4.01828900	2.06211900	0.03818900
H	-5.92314800	0.64298200	0.76824700

H	-3.30329400	-2.76431600	0.34182100
C	-1.13920700	-1.51514000	-0.54821300
O	-0.71690300	-2.29929100	0.33030400
O	-0.66011900	-1.19439100	-1.65733600
N	2.76890000	-0.21653400	0.10895800
C	2.01338600	0.37043300	-1.08054500
H	1.23059900	-0.35024300	-1.32636300
H	1.50874600	1.26045400	-0.68367100
C	2.87604200	0.66224300	-2.29722700
H	2.21311600	1.05238500	-3.07598800
H	3.64328200	1.42110800	-2.11358400
H	3.35903800	-0.23162900	-2.70619200
C	3.88355900	0.71236700	0.54942500
H	4.31347300	0.25794600	1.44354700
H	4.64666800	0.66881800	-0.23117500
C	3.45623600	2.15299200	0.80887300
H	2.51970500	2.23481800	1.36660700
H	4.25938100	2.64953800	1.36383900
H	3.30615000	2.69858600	-0.12596900
C	1.73299500	-0.37311400	1.22903600
H	0.99899800	-1.09022300	0.86307800
H	1.24975500	0.61222400	1.28928100
C	2.28114400	-0.82387400	2.57312600
H	2.91931100	-0.07576500	3.05375400
H	1.41485200	-0.97405700	3.22504600
H	2.81929600	-1.77734700	2.53619900
C	3.39622400	-1.55265500	-0.24209300
H	4.21368500	-1.33445000	-0.93358000
H	3.84559100	-1.92358800	0.68135800
C	2.44787300	-2.58293900	-0.84216100
H	2.11088200	-2.29856500	-1.84138000
H	2.99867000	-3.52642500	-0.92566700
H	1.54876800	-2.75396500	-0.24439700
C	-0.86727000	1.63968900	0.91382500

C	-1.57874800	1.38462400	-0.48487300
O	0.31713300	2.22294300	0.75344600
H	-1.62485400	2.22706800	1.50717000
H	-0.85122000	0.62637400	1.40302600
H	-0.89687200	0.82061400	-1.11198200
C	-1.92551400	2.69591500	-1.16429500
H	-0.97238300	3.21845700	-1.27938100
H	-2.39099700	2.55881500	-2.14661800
H	-2.55994100	3.34498700	-0.54866400

TSb1

SCF Energy = -1190.031236

Thermal correction to Gibbs Free Energy = 0.416424

Charge = 0, Multiplicity = 1

C	3.92324900	0.93667400	-0.00644800
C	5.07735300	0.30813900	-0.42152700
C	5.07238100	-1.08303400	-0.57301100
C	3.90120000	-1.77822600	-0.31541200
C	2.75420800	-1.11588600	0.12659600
N	2.79600400	0.23878800	0.28950200
H	5.96470000	-1.60515000	-0.90401800
H	3.85536400	2.00846600	0.10667500
H	5.95882000	0.90277000	-0.63169600
H	3.82619900	-2.84879600	-0.46308100
C	1.47007900	-1.93588300	0.39797700
O	1.12728000	-2.62401600	-0.58801400
O	0.96721300	-1.81453500	1.53457500
N	-2.60060400	-1.03178300	-0.10506200
C	-1.88538900	-0.44885900	1.11298800
H	-1.02745600	-1.09908500	1.29440100
H	-1.49192000	0.51673700	0.77795600
C	-2.74359200	-0.32774800	2.36099900
H	-2.10120700	0.07029600	3.15260600
H	-3.57856100	0.36967700	2.24399400

H	-3.13200800	-1.28903300	2.71387700
C	-3.82929400	-0.21232600	-0.45095500
H	-4.26226100	-0.68136400	-1.33658900
H	-4.53482100	-0.36048700	0.36943900
C	-3.57521700	1.27132400	-0.68155600
H	-2.77869500	1.45945200	-1.40353600
H	-4.50570100	1.71419800	-1.05286800
H	-3.29163300	1.79080500	0.23539500
C	-1.58625000	-0.98995500	-1.25283700
H	-0.75906100	-1.63237800	-0.95166400
H	-1.22388700	0.04504500	-1.26205300
C	-2.11683100	-1.41925500	-2.61110900
H	-2.87052400	-0.73712100	-3.01650900
H	-1.26444400	-1.40295600	-3.29750300
H	-2.51673700	-2.43862400	-2.62623000
C	-3.06252400	-2.45316900	0.15946500
H	-3.86687200	-2.37998400	0.89517800
H	-3.50992700	-2.80069500	-0.77389200
C	-1.98274800	-3.41497500	0.63840500
H	-1.61894800	-3.16516800	1.63712400
H	-2.42960000	-4.41446900	0.67937300
H	-1.10761900	-3.45058400	-0.01500200
C	0.83123800	1.34937000	-0.79889800
C	1.53217200	0.97719100	0.56654500
O	-0.45007800	1.71328600	-0.57896500
H	1.46089900	2.14013900	-1.27571600
H	0.93885800	0.44684500	-1.44695600
H	0.90176400	0.25367100	1.06990700
C	1.64431500	2.20952000	1.44957900
H	0.66128700	2.65290800	1.28407500
H	1.80302900	1.97990300	2.50627800
H	2.38947300	2.93938900	1.11367600
C	-1.00855300	3.83613700	-0.12282200
O	-1.55722100	3.65493600	0.91006600

O	-0.55607900	4.35937100	-1.07535900

int3a

SCF Energy =-1190.048403

Thermal correction to Gibbs Free Energy = 0.421815

Charge = 0, Multiplicity = 1

C	4.32338200	0.50523400	-0.10474800
C	5.30386000	-0.40637800	-0.43153500
C	4.96793500	-1.76341700	-0.49942000
C	3.65900300	-2.14181500	-0.25090100
C	2.69296300	-1.19465900	0.09948300
N	3.05406000	0.11565100	0.17552100
H	5.71770800	-2.50418000	-0.75941800
H	4.51441500	1.56652100	-0.05266400
H	6.30799400	-0.05461800	-0.63746700
H	3.33261600	-3.17112800	-0.33546300
C	1.24363800	-1.66889600	0.35936300
O	0.79703100	-2.34143300	-0.59448400
O	0.74280900	-1.34704000	1.45553100
N	-2.92552000	-0.72317000	0.00923600
C	-2.21121900	0.07258000	1.10974300
H	-1.23854000	-0.40575300	1.23297800
H	-2.04707900	1.07726100	0.71135500
C	-2.94734000	0.14156200	2.43841400
H	-2.34141200	0.77411000	3.09453700
H	-3.93109900	0.61608800	2.36709900
H	-3.05573600	-0.82968000	2.93115700
C	-4.20787900	-0.01989800	-0.41118200
H	-4.76917700	-0.74538200	-1.00556300
H	-4.76822600	0.14546700	0.51015700
C	-4.02021200	1.28394700	-1.17465300
H	-3.67879100	1.10609200	-2.19829100
H	-4.99824700	1.77369800	-1.23554000
H	-3.31532800	1.97283000	-0.69485400

C	-1.95127700	-0.81728200	-1.15924300
H	-1.06577500	-1.33105400	-0.78691700
H	-1.65462600	0.20787600	-1.37781800
C	-2.48471100	-1.54360600	-2.38437600
H	-3.37686000	-1.07964300	-2.81548200
H	-1.69694100	-1.51019400	-3.14328600
H	-2.69435500	-2.60024000	-2.19207300
C	-3.31352300	-2.10434700	0.50133400
H	-4.06298000	-1.94453100	1.27959600
H	-3.81675000	-2.59393900	-0.33466800
C	-2.16492500	-2.96130600	1.01327400
H	-1.64873900	-2.51011700	1.86219200
H	-2.58791700	-3.91996000	1.33344700
H	-1.40461900	-3.15164200	0.25277200
C	1.23232200	1.44964800	-0.86546600
C	1.99393400	1.15465700	0.45921800
O	-0.12790300	1.66511500	-0.61994800
H	1.68389400	2.31450700	-1.36549100
H	1.30026000	0.56779400	-1.51489100
H	1.30396700	0.64020100	1.12487300
C	2.55697500	2.38581200	1.15386800
H	1.71265400	3.02432700	1.41572600
H	3.11757800	2.11709300	2.05649200
H	3.18391600	2.99851300	0.49761400
C	-0.53535900	3.03359800	-0.22043200
O	-1.73242500	3.04425500	0.11011300
O	0.35211500	3.88781500	-0.26494300

TSa5

SCF Energy = -1190.005098

Thermal correction to Gibbs Free Energy = 0.411269

Charge = 0, Multiplicity = 1

C	-4.17747000	0.69281500	-0.27342600
C	-5.27536200	0.03720400	0.27174600

C	-5.11456700	-1.29034900	0.67693400
C	-3.87392600	-1.89736900	0.52253300
C	-2.82494600	-1.18532800	-0.07067500
N	-2.99591800	0.09164600	-0.45987900
H	-5.94430000	-1.83506500	1.11904900
H	-4.23694200	1.73489000	-0.57808700
H	-6.22129200	0.55652300	0.38546800
H	-3.68101900	-2.91012000	0.85682100
C	-1.45332800	-1.85295900	-0.26073200
O	-0.88192700	-1.64497700	-1.36027000
O	-1.05766000	-2.51861700	0.72866300
N	2.65699400	-1.09763100	0.06717000
C	1.63615300	-0.90347800	1.19047500
H	1.32916600	0.14112400	1.10641500
H	0.77674200	-1.52915300	0.94084300
C	2.13227700	-1.23340100	2.58922900
H	1.28003300	-1.09874200	3.26257800
H	2.45950300	-2.27192700	2.70006200
H	2.93129300	-0.57116600	2.93706000
C	3.02770900	-2.56436600	-0.07605100
H	3.86785600	-2.59713900	-0.77406300
H	3.40829900	-2.86993000	0.90036800
C	1.90313600	-3.48292900	-0.53555300
H	1.62245500	-3.29975300	-1.57497400
H	2.27228500	-4.51185000	-0.46049200
H	0.99075200	-3.39072100	0.06142000
C	1.98827400	-0.57607800	-1.20291000
H	1.67354800	0.44246900	-0.96897100
H	1.07241600	-1.16294600	-1.32049100
C	2.85212900	-0.63559400	-2.45170100
H	3.17756600	-1.65080200	-2.70031900
H	2.23519100	-0.28458900	-3.28487500
H	3.73182700	0.01433800	-2.40402500
C	3.93303200	-0.33504100	0.36328400

H	4.36364700	-0.79952400	1.25290600
H	4.61033400	-0.54065900	-0.46787000
C	3.76110100	1.16420300	0.55856500
H	3.09028600	1.40830600	1.38363900
H	4.74622100	1.58675600	0.78255500
H	3.37145400	1.66722000	-0.32706600
C	-0.80951800	1.44988900	0.73597800
C	-1.20791600	1.25676200	-0.66514500
O	0.43730200	1.84371300	0.25117600
H	-1.36367000	2.24385000	1.26093500
H	-0.81188900	0.53317700	1.34769000
H	-0.79999900	0.39146800	-1.16668600
C	-1.66073900	2.40963400	-1.50747100
H	-0.81099100	2.81012000	-2.06858400
H	-2.39967500	2.06636500	-2.23754800
H	-2.08089800	3.21886300	-0.90365000
C	0.91623400	4.06552500	0.34069800
O	-0.10615700	4.45597700	0.77425500
O	2.00827000	3.96836300	-0.08705000

int4

SCF Energy =-1190.056400

Thermal correction to Gibbs Free Energy = 0.421448

Charge = 0, Multiplicity = 1

C	3.86505400	0.11074900	-0.49049200
C	4.38276900	-0.78328200	-1.40102000
C	3.72168300	-1.99845300	-1.59562900
C	2.57044500	-2.25297300	-0.86969200
C	2.08469100	-1.33592900	0.06764500
N	2.75543000	-0.16476600	0.23868000
H	4.09551400	-2.72284300	-2.31272700
H	4.31442400	1.07704500	-0.32133800
H	5.27508200	-0.51854000	-1.95601300
H	1.98455900	-3.15360200	-0.99791600

C	0.79591600	-1.73120700	0.85117500
O	0.64510700	-1.26176000	1.99408300
O	0.07277300	-2.50756900	0.18222300
N	-2.97187000	-0.20019300	-0.10872500
C	-1.93569100	-0.50373900	-1.19411100
H	-1.31683600	0.39145200	-1.29348600
H	-1.31156700	-1.30594100	-0.79977500
C	-2.50047900	-0.87158900	-2.55708100
H	-1.63942500	-1.03015100	-3.21358300
H	-3.08653500	-1.79637700	-2.56010300
H	-3.09526200	-0.07008500	-3.00504500
C	-3.83857700	-1.41559300	0.17013700
H	-4.68351200	-1.05874900	0.76380800
H	-4.23452800	-1.72792100	-0.79719600
C	-3.13788000	-2.56969400	0.87705400
H	-2.98824200	-2.35947200	1.93924400
H	-3.78289200	-3.45155800	0.79989000
H	-2.15844800	-2.81063200	0.45576800
C	-2.18443500	0.20159900	1.13639700
H	-1.52440200	1.01871300	0.83065500
H	-1.55346600	-0.64994000	1.38882500
C	-3.03671500	0.61191000	2.32643900
H	-3.74296200	-0.16131900	2.64755800
H	-2.34993600	0.79082400	3.15932300
H	-3.58637100	1.54232900	2.15513200
C	-3.89793300	0.91750300	-0.55501800
H	-4.46343300	0.51546400	-1.39886500
H	-4.60435300	1.06533800	0.26433700
C	-3.21292600	2.22472800	-0.92403600
H	-2.49030100	2.11876300	-1.73607600
H	-3.99510200	2.92720800	-1.23305500
H	-2.65922000	2.65731100	-0.08900400
C	2.35440700	2.28695700	0.56452700
C	2.29302400	0.89768300	1.21269800

O	1.81618100	2.26597500	-0.73499400
H	1.78875900	2.95341600	1.22251800
H	3.38116000	2.66864300	0.48777200
H	1.25249900	0.66678000	1.40766900
C	3.08707600	0.77296500	2.50601300
H	2.75858900	1.55187900	3.20170600
H	2.89364200	-0.19922100	2.96475400
H	4.16436200	0.89668600	2.33976000
C	0.37387500	2.18500100	-0.78233700
O	-0.21019800	2.38486300	0.30781800
O	-0.05293100	1.89966300	-1.90915800

TSc1

SCF Energy = -1190.020339

Thermal correction to Gibbs Free Energy = 0.418821

Charge = 0, Multiplicity = 1

C	4.53961100	0.21719900	0.11008800
C	5.40160500	-0.82483700	-0.20336200
C	4.85497600	-2.09320000	-0.41372800
C	3.48124600	-2.25876500	-0.30086800
C	2.67232800	-1.17158000	0.05399700
N	3.21702500	0.04439700	0.24833000
H	5.49366300	-2.93299200	-0.67240100
H	4.91107000	1.22577500	0.25844800
H	6.46710300	-0.64055100	-0.29013700
H	2.99321300	-3.20753500	-0.48817600
C	1.15798200	-1.40034500	0.21748900
O	0.60786000	-0.81049400	1.18033400
O	0.66746300	-2.18224600	-0.62904500
N	-3.05176000	-0.66786400	0.08070300
C	-2.09069000	-0.57718800	-1.10864500
H	-1.91546500	0.48874200	-1.25890500
H	-1.15606200	-1.03406800	-0.78327400
C	-2.57308400	-1.24919100	-2.38335500

H	-1.78294600	-1.10663800	-3.12673900
H	-2.71370700	-2.32892600	-2.27341700
H	-3.48928500	-0.80991200	-2.79081100
C	-3.27685800	-2.11146600	0.49718600
H	-4.06488400	-2.08343700	1.25371800
H	-3.69053100	-2.61228900	-0.38019100
C	-2.05325600	-2.85282500	1.01243500
H	-1.66956400	-2.42363600	1.94031000
H	-2.36236100	-3.88443100	1.21628000
H	-1.22569800	-2.86482700	0.29790900
C	-2.39690500	0.13474100	1.20665500
H	-2.29274800	1.14873300	0.81956200
H	-1.38891900	-0.27654600	1.31017500
C	-3.14639600	0.12196400	2.52912200
H	-3.23374800	-0.87732400	2.96658500
H	-2.56527900	0.73160300	3.22808300
H	-4.14439500	0.56819800	2.46746900
C	-4.41666700	-0.10649800	-0.27306600
H	-4.84684200	-0.80031200	-0.99893300
H	-5.01584900	-0.18004200	0.63659900
C	-4.43392000	1.31490400	-0.81376900
H	-3.89705600	1.40883200	-1.75884900
H	-5.48164400	1.58607800	-0.98427900
H	-3.99231800	2.03813500	-0.12794900
C	1.70965300	1.88698700	-1.04568100
C	1.96882200	1.67271100	0.43642800
O	0.32987100	1.79646900	-1.34116200
H	2.10139600	2.87478300	-1.32834900
H	2.19827400	1.13138700	-1.66281000
H	1.30956600	1.01174300	0.98001800
C	2.89252700	2.57333900	1.20115300
H	2.29788400	3.40572400	1.58179100
H	3.34580400	2.05180400	2.04751800
H	3.68121900	2.99323000	0.56634800

C	-0.42713000	2.52630100	-0.40262600
O	0.25838600	2.97794400	0.56073700
O	-1.63980600	2.58701000	-0.62905800

M_0

SCF Energy = -436.454154

Thermal correction to Gibbs Free Energy = 0.057567

Charge = -1, Multiplicity = 1

C	-1.73947200	-1.19687700	0.00019200
C	-2.50631900	-0.03212800	-0.00001700
C	-1.82713100	1.18944100	-0.00019100
C	-0.43828700	1.17673500	-0.00013900
C	0.25460600	-0.04776100	-0.00000500
N	-0.40144300	-1.22469900	0.00016900
H	-2.37832600	2.12955900	-0.00035200
H	-2.23637800	-2.17053200	0.00036000
H	-3.59322400	-0.08326200	-0.00003300
H	0.16911000	2.07452600	-0.00017900
C	1.81871700	-0.01841600	-0.00000500
O	2.39213900	-1.12583300	-0.00038800
O	2.29239100	1.15041300	0.00038900

int $1a_0$

SCF Energy = -629.649087

Thermal correction to Gibbs Free Energy = 0.133831

Charge = -1, Multiplicity = 1

C	-2.16656800	-0.34606100	-0.75143200
C	-2.09605800	0.14224800	0.62390000
O	-3.32827800	-0.40223300	0.11691300
H	-2.24108900	0.38724700	-1.55616300
H	-1.66858100	-1.28476600	-0.99305300
H	-1.59211400	-0.50435300	1.34473800
C	-2.08536100	1.61211000	0.95671300

H	-2.59984800	1.80987200	1.90667100
H	-1.05268400	1.96893700	1.04207100
H	-2.58903500	2.18465400	0.16978400
C	0.96476700	1.52738600	-1.37477500
C	1.53710600	2.31539600	-0.37698300
C	1.94907100	1.67702700	0.79650800
C	1.77337400	0.30302500	0.90251700
C	1.16798800	-0.40970200	-0.14771100
N	0.76869600	0.20745700	-1.27609400
H	2.40142800	2.24655000	1.60729100
H	0.63733000	1.98897100	-2.30887100
H	1.65445400	3.38756500	-0.51641800
H	2.08881500	-0.27157000	1.76564900
C	0.95539200	-1.94421300	0.02455400
O	0.13465600	-2.48580300	-0.75124300
O	1.64139600	-2.44054000	0.95323200

TSa_0

SCF Energy = -629.613937

Thermal correction to Gibbs Free Energy = 0.137085

Charge = -1, Multiplicity = 1

C	1.55494600	0.50069900	-0.68038100
C	2.41655900	0.30816100	0.53093000
O	3.42695800	0.96482100	-0.08320000
H	1.90742300	-0.03792900	-1.55473300
H	1.17287800	1.49921800	-0.84177000
H	1.95877400	0.81432700	1.41624100
C	2.73006500	-1.14353400	0.93305500
H	3.53821600	-1.13528700	1.67560400
H	1.86764300	-1.67093700	1.36564000
H	3.09384600	-1.70194300	0.05974400
C	-0.05262700	-1.68363000	-0.72171200
C	-1.07341100	-2.54058200	-0.34425500

C	-2.21766000	-1.98255800	0.23722500
C	-2.28360100	-0.60619000	0.39189400
C	-1.23313600	0.21468600	-0.04945800
N	-0.13110700	-0.34890500	-0.58741100
H	-3.03717100	-2.61937300	0.56346700
H	0.87741700	-2.05741100	-1.14061200
H	-0.96867900	-3.61134800	-0.49196000
H	-3.12491300	-0.09504400	0.84465200
C	-1.42544000	1.76599800	0.03585900
O	-0.70648100	2.44489100	-0.72659400
O	-2.32820800	2.09775900	0.83687600

M_1

SCF Energy = -650.857355

Thermal correction to Gibbs Free Energy = 0.213749

Charge = 0, Multiplicity = 1

C	-3.92568500	-1.30203300	0.00035800
C	-4.78664600	-0.20331100	0.00082600
C	-4.22173300	1.07180500	0.00066700
C	-2.83523000	1.18549000	0.00004300
C	-2.05438500	0.02170900	-0.00040900
N	-2.59240000	-1.20864900	-0.00023800
H	-4.85146300	1.95828800	0.00102800
H	-4.33247800	-2.31346700	0.00044100
H	-5.86345400	-0.34739900	0.00130600
H	-2.32810300	2.14263200	-0.00012700
C	-0.52867200	0.15143500	-0.00101500
O	0.14429800	-0.91828600	-0.00134800
O	-0.08077200	1.33048300	-0.00106200
N	3.38752400	-0.04133500	0.00036800
C	2.89267200	1.38375100	-0.00059900
H	3.28661700	1.87266400	-0.89449200
H	1.78355900	1.38014300	-0.00107700
C	2.85607400	-0.74514900	1.22454400

H	3.28977600	-1.74711600	1.25366300
H	3.16100700	-0.17577000	2.10439900
C	2.85759600	-0.74627800	-1.22382400
H	3.16381900	-0.17783100	-2.10383300
H	1.76567200	-0.80085100	-1.10939300
C	4.87997000	-0.06184700	0.00129400
H	5.24093200	0.45057600	0.89492800
H	5.22307000	-1.09804000	0.00190900
H	3.29115300	-1.74835200	-1.25134600
H	3.28571500	1.87354500	0.89321100
H	1.76431000	-0.80002100	1.10873800
H	5.24202900	0.44988200	-0.89229300

int1b

SCF Energy = -844.053612

Thermal correction to Gibbs Free Energy = 0.293213

Charge = 0, Multiplicity = 1

C	-0.23206300	2.16181900	1.06151300
C	-0.39541800	2.12082800	-0.39180700
O	0.88562700	2.46646600	0.18233600
H	-0.61385400	3.02667400	1.60456800
H	-0.16547300	1.22469900	1.60960000
H	-0.41179900	1.13452700	-0.85643700
C	-1.10149600	3.20812700	-1.15668900
H	-0.65787600	3.34562700	-2.15008600
H	-2.15742300	2.94529700	-1.29097600
H	-1.04215100	4.15964300	-0.61868500
C	-3.83019500	0.05230200	0.85404600
C	-4.54805400	-0.46489100	-0.22554800
C	-3.87996500	-1.30704000	-1.11424500
C	-2.53568600	-1.58470500	-0.88630400
C	-1.90303100	-1.02583700	0.23197200
N	-2.54310400	-0.21754700	1.09330000
H	-4.39749400	-1.73385500	-1.96987700

H	-4.31779200	0.71816900	1.56585100
H	-5.59569400	-0.21226100	-0.36163700
H	-1.95085400	-2.21436800	-1.54588400
C	-0.41536000	-1.30307400	0.47002700
O	0.07011800	-0.97431500	1.57779800
O	0.20254100	-1.81093500	-0.51750300
N	3.33221800	-0.44949600	-0.15532800
C	2.45002200	0.08121900	-1.25936600
H	1.48107300	-0.41965300	-1.16521700
H	2.35255000	1.15868200	-1.13351000
C	4.73517200	0.01191300	-0.37150200
H	5.36666000	-0.38467300	0.42542900
H	5.08646100	-0.34953200	-1.33974600
C	2.83921900	0.04897800	1.18258600
H	1.85251200	-0.39931900	1.38326400
H	2.75626700	1.13429600	1.13046900
C	3.26017000	-1.95384800	-0.16748100
H	3.68981100	-2.30945100	-1.10683500
H	3.83682200	-2.33252000	0.67854400
H	2.92035700	-0.17212700	-2.21220000
H	3.56959900	-0.25650600	1.93532500
H	4.75115800	1.10298600	-0.35148200
H	2.19715400	-2.22152500	-0.10053700

TSb

SCF Energy = -844.019951

Thermal correction to Gibbs Free Energy = 0.298039

Charge = 0, Multiplicity = 1

C	0.60778100	1.40219100	-0.95293700
C	0.25583300	2.04643200	0.32870400
O	-0.87733400	2.52034500	-0.30139400
H	1.06178200	2.03864400	-1.70653100
H	-0.00155900	0.59383800	-1.31521100
H	0.08587100	1.31002600	1.14057400

C	1.20806500	3.12593900	0.83766100
H	0.72133200	3.69221300	1.63961000
H	2.13896800	2.69895900	1.23274500
H	1.44671600	3.82781000	0.02998500
C	3.36168700	0.62704100	-0.50987300
C	4.37082200	-0.07822500	0.13273000
C	4.05702600	-1.32438300	0.68292900
C	2.75959700	-1.80816500	0.56443000
C	1.80336200	-1.06270800	-0.13375500
N	2.12260600	0.13806100	-0.65568600
H	4.81449300	-1.90032600	1.20722800
H	3.53359200	1.61697100	-0.92409700
H	5.36763900	0.34311800	0.20959900
H	2.45555200	-2.75112200	1.00439500
C	0.37265300	-1.59507400	-0.30870400
O	-0.08831900	-1.55413700	-1.47256500
O	-0.17735700	-1.98918500	0.75256100
N	-3.26706900	-0.28775300	0.14950200
C	-2.34378500	0.25563100	1.21514100
H	-1.44731300	-0.36777500	1.21874400
H	-2.10053400	1.28898100	0.94637100
C	-4.59748500	0.37806200	0.27449200
H	-5.27077600	-0.02395200	-0.48471000
H	-5.00133500	0.18720900	1.27044200
C	-2.69584700	0.00535900	-1.22042300
H	-1.85701100	-0.67782600	-1.39533200
H	-2.34055700	1.03952500	-1.22080400
C	-3.39162800	-1.77469400	0.32465100
H	-3.87286900	-1.97073300	1.28555200
H	-4.00041400	-2.17142600	-0.49039600
H	-2.86027700	0.17720600	2.17454400
H	-3.48787300	-0.16260100	-1.95363200
H	-4.45997800	1.45007100	0.12463800
H	-2.37860900	-2.19157600	0.31048500

int2b

SCF Energy = -844.048013

Thermal correction to Gibbs Free Energy = 0.301510

Charge = 0, Multiplicity = 1

C	-1.01176400	1.16102400	1.05000500
C	-0.25299000	1.86369000	-0.17186600
O	0.92531300	2.33474000	0.23310900
H	-1.47640500	1.90966400	1.69554700
H	-0.30189000	0.56692000	1.61380300
H	-0.20062100	1.03325000	-0.93452800
C	-1.16444700	2.95145900	-0.78723600
H	-0.64233200	3.39438800	-1.64152500
H	-2.13386400	2.57545200	-1.14459300
H	-1.33441100	3.74866500	-0.05257800
C	-3.32810500	0.72161700	0.41965700
C	-4.30935000	-0.00726000	-0.21472700
C	-3.98388100	-1.26311600	-0.74286200
C	-2.68775800	-1.73286300	-0.59404900
C	-1.72451200	-0.98723800	0.08763300
N	-2.06500400	0.24326600	0.57571900
H	-4.73140900	-1.85335600	-1.26343100
H	-3.49969100	1.71279800	0.81870700
H	-5.30656200	0.40847500	-0.30188200
H	-2.37226000	-2.68668300	-0.99982800
C	-0.33396400	-1.60450200	0.34705600
O	0.02436200	-1.60991900	1.54246800
O	0.23390200	-2.04707800	-0.67823200
N	3.25726500	-0.20608900	-0.16266700
C	2.33208200	0.24147600	-1.27434400
H	1.49279400	-0.45415900	-1.29910100
H	1.98589700	1.25428400	-1.01297200
C	4.51284400	0.59748200	-0.24205100
H	5.19610000	0.27442400	0.54565300

H	4.97290300	0.44815400	-1.22077400
C	2.61130900	0.04047600	1.18615300
H	1.86192500	-0.73492200	1.36109900
H	2.11597300	1.02295500	1.13518900
C	3.54176500	-1.66850600	-0.31811100
H	4.05641900	-1.82802500	-1.26869800
H	4.17228900	-1.99498300	0.51190900
H	2.89553800	0.19399700	-2.20952200
H	3.39833800	-0.01421100	1.94223600
H	4.24927100	1.64734200	-0.10590800
H	2.58018600	-2.18904500	-0.31046200

M'

SCF Energy = -634.823925

Thermal correction to Gibbs Free Energy = 0.226213

Charge = 0, Multiplicity = 1

C	-4.03922400	-1.31275600	-0.00043800
C	-4.82909400	-0.16058900	-0.00099700
C	-4.22179100	1.09772100	-0.00081500
C	-2.83161800	1.20140900	-0.00008800
C	-2.03487000	0.05137600	0.00047800
H	-4.83439600	1.99619600	-0.00125200
H	-4.50931700	-2.29338700	-0.00056200
H	-5.91332300	-0.24273800	-0.00157100
H	-2.33403900	2.16541100	0.00005600
C	-0.52125900	0.16941200	0.00125400
O	0.13427300	-0.92195100	0.00150600
O	-0.03574400	1.33095600	0.00140700
N	3.39846300	-0.04213300	-0.00044700
C	2.92482600	1.39026400	0.00088200
H	3.32451300	1.87438400	-0.89302300
H	1.81547200	1.39753700	0.00148600
C	2.85755200	-0.73890600	1.22345400

H	3.28118100	-1.74521300	1.25441300
H	3.16657500	-0.17205400	2.10344800
C	2.85507400	-0.73744300	-1.22411300
H	3.16166800	-0.16908400	-2.10398500
H	1.76307500	-0.78344600	-1.10425500
C	4.89041300	-0.08537900	-0.00196900
H	5.26039500	0.42093600	0.89144100
H	5.21801500	-1.12660400	-0.00277200
C	-2.64895900	-1.20550900	0.00030300
H	-2.01246400	-2.08396600	0.00075700
H	3.32560600	1.87311200	0.89498900
H	5.25859800	0.42170400	-0.89569000
H	3.27934500	-1.74340500	-1.25757200
H	1.76532400	-0.78409100	1.10621300

Int1c

SCF Energy = -828.013806

Thermal correction to Gibbs Free Energy = 0.30471

Charge = 0, Multiplicity = 1

C	-0.52157800	2.18650200	-1.00789900
C	-1.21615500	2.26399900	0.27848800
O	-0.98413600	3.45074200	-0.50679900
H	0.56017400	2.05335400	-1.02335200
H	-1.03872700	1.79507900	-1.88136200
H	-2.25846500	1.94395600	0.29730700
C	-0.48069600	2.15781400	1.58886600
H	-1.00037400	2.71193300	2.37911800
H	-0.39496100	1.10692700	1.88417700
H	0.52585000	2.58022900	1.48635000
C	-3.97332400	-0.83819300	-1.13797800
C	-4.58352100	-0.97466100	0.11183500
C	-3.79697200	-1.13622900	1.25472900
C	-2.40654700	-1.15327100	1.14796300

C	-1.78958700	-1.00443400	-0.09851100
H	-4.26903600	-1.24738400	2.22781300
H	-4.58332500	-0.71594200	-2.02954900
H	-5.66734900	-0.95703500	0.19394500
H	-1.77400000	-1.27569300	2.02058900
C	-0.27731500	-0.96555700	-0.21018800
O	0.20977200	-0.80557800	-1.36115900
O	0.37825300	-1.06421500	0.87598900
N	3.61613100	-0.41589400	0.00967000
C	2.85859700	0.65228100	0.75798400
H	2.99311800	1.60039800	0.23503700
H	1.80971200	0.33479700	0.79138000
C	3.29973300	-1.75114900	0.63590500
H	3.77398700	-2.53046400	0.03679300
H	3.70630100	-1.75449400	1.64957100
C	3.15683300	-0.42805000	-1.42709200
H	3.40047000	0.54277100	-1.86430500
H	2.06481200	-0.60962900	-1.44532100
C	5.08358700	-0.14854900	0.07361900
H	5.40139000	-0.14805700	1.11779300
H	5.61045100	-0.93056500	-0.47605700
C	-2.58359100	-0.85560000	-1.24090900
H	-2.08440400	-0.74842200	-2.19797600
H	3.70404200	-1.21747700	-1.94687200
H	5.28601800	0.82429800	-0.37791700
H	2.20483900	-1.84045600	0.66192800
H	3.26866900	0.71611600	1.76809400

TSa5

SCF Energy = -827.960095

Thermal correction to Gibbs Free Energy = 0.306477

Charge = 0, Multiplicity = 1

C	-0.54672700	1.86212200	-0.89021900

C	-0.55500400	2.47485100	0.49870700
O	-0.93187100	3.70504200	0.15012100
H	0.19764700	2.32900300	-1.53154500
H	-1.53720700	1.88264800	-1.33024100
H	-1.27303300	1.87836800	1.13504200
C	0.81256000	2.39681400	1.21895100
H	0.75265800	2.99426300	2.13548500
H	1.10229300	1.37073200	1.49129200
H	1.58915200	2.84724900	0.58402800
C	-4.27503900	-0.51505100	-0.97374900
C	-4.78492100	-1.10067800	0.18583800
C	-3.91402800	-1.53737400	1.18801200
C	-2.54028300	-1.38546100	1.03106200
C	-2.02371700	-0.77064300	-0.11754700
H	-4.30897500	-1.99745200	2.08949600
H	-4.94840500	-0.18662000	-1.76020300
H	-5.85787100	-1.22080100	0.30751000
H	-1.84759100	-1.72963100	1.79139700
C	-0.54512200	-0.65192900	-0.26859600
O	-0.05536300	0.29457200	-1.03972800
O	0.20429500	-1.47445800	0.28981400
N	3.55636200	-0.72052200	-0.05937600
C	3.00524100	-0.72393000	1.34446100
H	3.27591900	0.21648100	1.82485400
H	1.92096800	-0.83375500	1.26960900
C	3.09458500	-1.97115400	-0.76019300
H	3.44259400	-1.93564200	-1.79386900
H	3.52565700	-2.83254400	-0.24633200
C	3.02985700	0.48032900	-0.80573500
H	3.30307900	1.37853100	-0.25211900
H	1.94064400	0.39827900	-0.88062200
C	5.04998100	-0.67125600	-0.01764300

H	5.42008500	-1.53962300	0.52988400
H	5.43365300	-0.68196400	-1.03913600
C	-2.90017100	-0.34684700	-1.12476100
H	-2.50005200	0.09368100	-2.03089200
H	3.48922600	0.48698800	-1.79619300
H	5.35717500	0.24677800	0.48571200
H	2.00321100	-1.99209800	-0.69855800
H	3.44488300	-1.56922600	1.87785000

Int2f

SCF Energy = -827.961763

Thermal correction to Gibbs Free Energy = 0.307317

Charge = 0, Multiplicity = 1

C	-0.56423400	1.80641700	-0.94799200
C	-0.55429600	2.44627800	0.45709100
O	-1.08423800	3.64105400	0.31050700
H	0.10916000	2.33220200	-1.62843100
H	-1.58154600	1.83859100	-1.33168600
H	-1.13350800	1.69035300	1.09625200
C	0.87685900	2.45723000	1.07371200
H	0.82604600	3.00665000	2.01950800
H	1.28185100	1.45436700	1.27665900
H	1.56308400	3.00456900	0.41010900
C	-4.27776200	-0.58147400	-0.99158900
C	-4.78268300	-1.17334600	0.16652500
C	-3.90944600	-1.56001000	1.18822300
C	-2.54264600	-1.34850400	1.05362700
C	-2.03185500	-0.72088400	-0.09288700
H	-4.29838100	-2.02744800	2.08847400
H	-4.95005600	-0.29506800	-1.79520800
H	-5.85120300	-1.33863200	0.27196200
H	-1.85050000	-1.65112100	1.83181600
C	-0.56046900	-0.57008500	-0.22290900

O	-0.05862700	0.38199800	-1.01213300
O	0.21153600	-1.38574200	0.30616200
N	3.57548300	-0.73400200	-0.05536500
C	3.03516900	-0.70346200	1.35284800
H	3.32993400	0.23795100	1.81666200
H	1.94832300	-0.78831200	1.28880600
C	3.08889400	-1.98926900	-0.73032600
H	3.43705200	-1.98211100	-1.76457000
H	3.50265900	-2.84857100	-0.19918400
C	3.06597700	0.46145700	-0.82211900
H	3.35743900	1.36629300	-0.28903000
H	1.97652800	0.40071700	-0.88509900
C	5.07029400	-0.70948300	-0.02418000
H	5.42900400	-1.57402600	0.53671300
H	5.44700400	-0.74515400	-1.04769100
C	-2.90948600	-0.35462200	-1.12345100
H	-2.51842500	0.08437200	-2.03405000
H	3.51730300	0.43869300	-1.81601900
H	5.39619000	0.21202000	0.46064600
H	1.99775300	-1.98792600	-0.66998900
H	3.46064500	-1.55033000	1.89517400

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