

Supporting Information

Not So Inert *Mer-Tris-Chelate* Cobalt(III) complex of Hydroxypyridine Functionalized NHC ligand for cyclic carbonates synthesis

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Experimental Details

Materials and methods:

Glasswares were dried in the oven at 100 °C before use. The chemicals CoBr₂, K₂CO₃, 2-chloro-3-hydroxypyridine, 1-methyl imidazole, allyl glycidyl ether, neopentyl glycol diglycidyl ether, 2,3-epoxypropyl phenyl ether (Sigma Aldrich), epichlorohydrin (ECH), styrene oxide, 1,2-epoxy hexane, and 1,2-epoxy cyclohexane (TCI) were purchased. **1** was prepared according to the already reported procedure.^[1] ¹H NMR and ¹³C NMR spectra were recorded on JOEL-DELTA 400 MHz and 500 MHz spectrometers, and the chemical shifts were referenced to tetramethylsilane (TMS). ESI-MS (+) spectra were recorded on the Agilent 6546 LC/Q-TOF instrument. Elemental analysis for the compounds was done using a Perkin Elmer series-II CHNS/O analyser 2400. For single crystal X-ray crystallography, the crystal data were collected on a Bruker D8 QUEST CCD diffractometer using graphite-monochromated MoK_α radiation ($\lambda = 0.71073 \text{ \AA}$) at 293 K. The data integration and reduction were processed with SAINT software², and the data were corrected for absorption by using the SADABS program. The structure was solved by direct methods using the SHELXS program of the SHELXTL package and refined by full-matrix least-squares methods with SHELXL-2014. All the hydrogen atoms were included in idealized positions, and a riding model was used. Non-hydrogen atoms were refined with anisotropic displacement parameters. All the cycloaddition reactions were performed in a Schlenk tube attached to CO₂-filled balloons (Table 1, entry 1-13). The other small-scale reactions were performed in the Parr reactor with small autoclave vessels (Table 1, entry 14-19), whereas large-scale reactions were performed using a stir tank autoclave reactor (Table 1, entry 20-25). Microbalance sartorius CPA225D was used for weighing.

Preparation of [Co(κ CN-IMepyO)₃] (2)

[Co(κ CN-IMepyO)₃] (2): **1** (0.317 g, 1.5 mmol), CoBr₂ (0.109 g, 0.5 mmol), and K₂CO₃ (0.552 g, 4 mmol) were taken in a dry round-bottomed flask and methanol (20 mL) was added to it. The reaction mixture was refluxed for 10 h under open air to provide a yellow-brown coloured suspension. The volatiles were removed under vacuum, and the residue was extracted with dry dichloromethane five times (5 x 50 mL) and filtered using Whatman filter paper, leaving a brown residue. Bright, yellow-colored crystals were obtained upon slow evaporation of concentrated DCM in the air. Yield: 0.155 g, 53%. Anal. Calcd. for C₂₇H₃₅CoN₉O_{8.5}: C, 47.65; H, 5.18; N, 18.52; Found: C, 47.93; H, 5.01; N, 18.53. ESI-MS calcd. for C₂₇H₂₅CoN₉O₃ m/z 582.1412; Found 582.1437 (M+H)⁺. ¹H NMR (CD₃OD, 400 MHz): δ 3.06 (s, 9H, N-CH₃), 6.06 (d, *J* = 4.8 Hz, 3H, Im-H), 7.03 (dd, *J* = 8.4, 5.6 Hz, 3H, py-H), 7.25 (d, *J* = 8.4 Hz, 3H, py-H), 7.39 (d, *J* = 2.4 Hz, 3H, Im-H), 9.13 (d, *J* = 1.6 Hz, 3H, py-H), ¹³C NMR (CD₃OD, 100 MHz): δ 35.3, 122.2, 125.9, 126.5, 128.3, 133.0, 142.7, 158.3. IR (KBr): $\tilde{\nu}$ 3176 (w), 2920 (w), 2853 (w), 1652 (w), 1583 (w), 1557 (m), 1475 (s), 1443 (s), 1340 (s), 1304 (m), 1280 (m), 1237 (w), 1110 (w), 1082 (w), 960 (w), 880 (w), 790 (w), 733 (w), 661 (m), 592 (m), 470 (w) cm⁻¹.

The procedure of cycloaddition of CO₂ into epoxides: All catalytic cycloaddition reactions (table 1, entry 1-13) were performed in the Schlenk tube (10 mL). The catalyst (**2**) and cocatalyst (TBAB) were placed in the Schlenk tube and evacuated for 15 min. Epoxide (10 mmol; 0.78 mL) was added to the reaction mixture and stirred for 5 min. The Schlenk tube was sealed with a septum, and carbon dioxide gas was purged using a balloon into the mixture for an appropriate time specified in Table 1 or Figure 2. Upon completion of the reaction, the reaction mixture was cooled to RT. Before purification (isolation) of the final product, the completion of the reaction was monitored by the ¹H NMR spectroscopy. Subsequently, the

ethyl acetate (5 mL) was added to the product, and the solution was filtered using a small silica pad to obtain the pure products of **4a**, **4d**, and **4h** (Figure S4-S19). For all the other compounds, a slurry of crude reaction mixture made using SiO₂ was transferred to column chromatography, and the desired COC was separated using the eluent (see characterization of COC).

Large-scale reactions (entry 20-25): The procedure which is described is for entry 24 and it is applicable to all the other entries from 20-25 except the catalyst **2** concentration was taken as mentioned in the Table 1 and appropriate quantities of TBAB was calculated. In a parr reactor autoclave (100 mL), catalyst **2** (0.408 mg, 0.0006 mmol), TBAB (257.8 mg, 0.8 mmol), and ECH (31.3 mL, 400 mmol) were taken. The reactor was charged and vented with CO₂ three times. The reaction was stirred for 24 h at 100 °C and 1 atm pressure. After completion of the reaction, it was cooled down to room temperature. The ¹H NMR spectrum of crude sample was recorded and the conversion to COC was calculated.

Reusability of the catalyst: ECH (0.78 mL, 10 mmol) was placed in a Schlenk tube with **2** (2.9 mg, 0.0043 mmol) and TBAB (6.44 mg, 0.02 mmol) at 100 °C and 1 atm pressure (Table 1, entry 11). After the reaction was completed in 3 h, fresh ECH (10 mmol) was added to the same mixture, and the reaction continued for a further 3 h. Likewise, the process was repeated five times.

Crystallographic Tables

Table S1: Crystal data and structure refinement for Co(III)-NHC complex, **2·5.5 H₂O**

Identification code	2368776 (3sepb_0m)
Empirical formula	C ₂₇ H ₃₅ CoN ₉ O _{8.5} (2·5.5 H ₂ O)
Formula weight	679.56
Temperature/K	273.15
Crystal system	monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> /Å	8.5150(6)
<i>b</i> /Å	17.8418(12)
<i>c</i> /Å	19.7536(14)
α /°	90
β /°	96.895(2)
γ /°	90
Volume /Å ³	2979.3(4)
<i>Z</i>	4
ρ_{calc} g/cm ³	1.517
μ /mm ⁻¹	0.644
<i>F</i> (000)	1420.0
Crystal size/mm ³	0.2 × 0.18 × 0.16
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection /°	5.014 to 50.1
Index ranges	-10 ≤ <i>h</i> ≤ 10, -21 ≤ <i>k</i> ≤ 21, -23 ≤ <i>l</i> ≤ 23
Reflections collected	21547
Independent reflections	5267 [<i>R</i> _{int} = 0.0995, <i>R</i> _{sigma} = 0.1123]
Data/restraints/parameters	5267/0/434
Goodness-of-fit on <i>F</i> ²	1.028
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0718, <i>wR</i> ₂ = 0.1377
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.1351, <i>wR</i> ₂ = 0.1592

Table S2: Bond Lengths for 2·5.5 H₂O

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Co1	N6	1.959(4)		N8	C19	1.344(6)
Co1	N9	1.987(4)		N8	C27	1.455(6)
Co1	N3	1.953(4)		N4	C10	1.344(6)
Co1	C19	1.940(5)		N4	C18	1.448(6)
Co1	C1	1.931(5)		N4	C11	1.380(7)
Co1	C10	1.886(5)		C22	C23	1.425(7)
O2	C23	1.280(5)		N2	C1	1.337(6)
O1	C5	1.307(6)		N2	C2	1.392(6)
O3	C14	1.281(6)		N2	C9	1.469(6)
N6	C17	1.351(6)		C16	C17	1.369(7)
N6	C13	1.337(6)		C16	C15	1.368(7)
N9	C22	1.332(6)		C23	C24	1.404(7)
N9	C26	1.353(6)		C21	C20	1.347(7)
N3	C4	1.348(6)		C4	C5	1.401(7)
N3	C8	1.345(6)		C26	C25	1.380(7)
N7	C22	1.406(6)		C13	C14	1.417(7)
N7	C21	1.396(6)		C15	C14	1.418(7)
N7	C19	1.352(6)		C24	C25	1.364(7)
N1	C4	1.417(6)		C12	C11	1.335(7)
N1	C1	1.376(6)		C5	C6	1.397(7)
N1	C3	1.384(6)		C8	C7	1.360(7)
N5	C13	1.407(6)		C3	C2	1.337(7)
N5	C10	1.351(6)		C6	C7	1.335(7)
N5	C12	1.379(6)		O5	O5 ¹	1.39(3)
N8	C20	1.389(6)				

¹-X,-Y,1-Z

Table S3: Bond Angles (°) for 2·5.5 H₂O

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N6	Co1	N9	93.86(16)	C1	N2	C2	110.6(4)
N3	Co1	N6	175.99(16)	C1	N2	C9	126.8(5)
N3	Co1	N9	89.11(16)	C2	N2	C9	122.6(4)
C19	Co1	N6	89.25(18)	C15	C16	C17	121.4(5)
C19	Co1	N9	81.50(19)	N6	C17	C16	120.3(5)
C19	Co1	N3	93.86(18)	O2	C23	C22	121.6(5)
C1	Co1	N6	94.97(18)	O2	C23	C24	125.7(5)
C1	Co1	N9	96.75(18)	C24	C23	C22	112.7(4)
C1	Co1	N3	81.99(18)	C20	C21	N7	105.3(4)
C1	Co1	C19	175.5(2)	N3	C4	N1	111.8(4)
C10	Co1	N6	82.35(19)	N3	C4	C5	124.5(5)
C10	Co1	N9	175.10(19)	C5	C4	N1	123.6(5)
C10	Co1	N3	94.83(19)	C21	C20	N8	108.3(4)
C10	Co1	C19	95.3(2)	N7	C19	Co1	112.2(3)
C10	Co1	C1	86.7(2)	N8	C19	Co1	141.8(4)
C17	N6	Co1	126.9(4)	N8	C19	N7	106.0(4)
C13	N6	Co1	114.8(3)	N9	C26	C25	120.1(5)
C13	N6	C17	118.3(4)	N1	C1	Co1	112.4(3)
C22	N9	Co1	114.9(3)	N2	C1	Co1	143.0(4)
C22	N9	C26	119.0(4)	N2	C1	N1	104.3(4)
C26	N9	Co1	126.0(3)	N6	C13	N5	111.6(4)
C4	N3	Co1	115.9(3)	N6	C13	C14	126.1(4)
C8	N3	Co1	126.3(4)	N5	C13	C14	122.3(5)
C8	N3	C4	117.8(4)	N5	C10	Co1	113.2(3)
C21	N7	C22	130.3(4)	N4	C10	Co1	141.2(4)
C19	N7	C22	118.8(4)	N4	C10	N5	105.6(4)
C19	N7	C21	110.8(4)	C16	C15	C14	121.0(5)
C1	N1	C4	117.2(4)	O3	C14	C13	122.3(5)
C1	N1	C3	111.3(4)	O3	C14	C15	124.8(5)
C3	N1	C4	131.3(5)	C13	C14	C15	112.8(5)
C10	N5	C13	117.9(4)	C25	C24	C23	122.5(5)
C10	N5	C12	110.8(4)	C24	C25	C26	120.2(5)
C12	N5	C13	131.2(4)	C11	C12	N5	105.9(5)
C20	N8	C27	122.5(4)	O1	C5	C4	121.0(5)
C19	N8	C20	109.6(4)	O1	C5	C6	124.7(5)
C19	N8	C27	127.7(4)	C6	C5	C4	114.3(5)
C10	N4	C18	128.6(4)	N3	C8	C7	120.7(5)
C10	N4	C11	109.4(4)	C2	C3	N1	105.7(5)
C11	N4	C18	122.0(4)	C7	C6	C5	121.2(5)
N9	C22	N7	112.2(4)	C3	C2	N2	108.0(5)
N9	C22	C23	125.3(4)	C12	C11	N4	108.4(5)
N7	C22	C23	122.5(4)	C6	C7	C8	121.5(5)

Characterization of **2**:

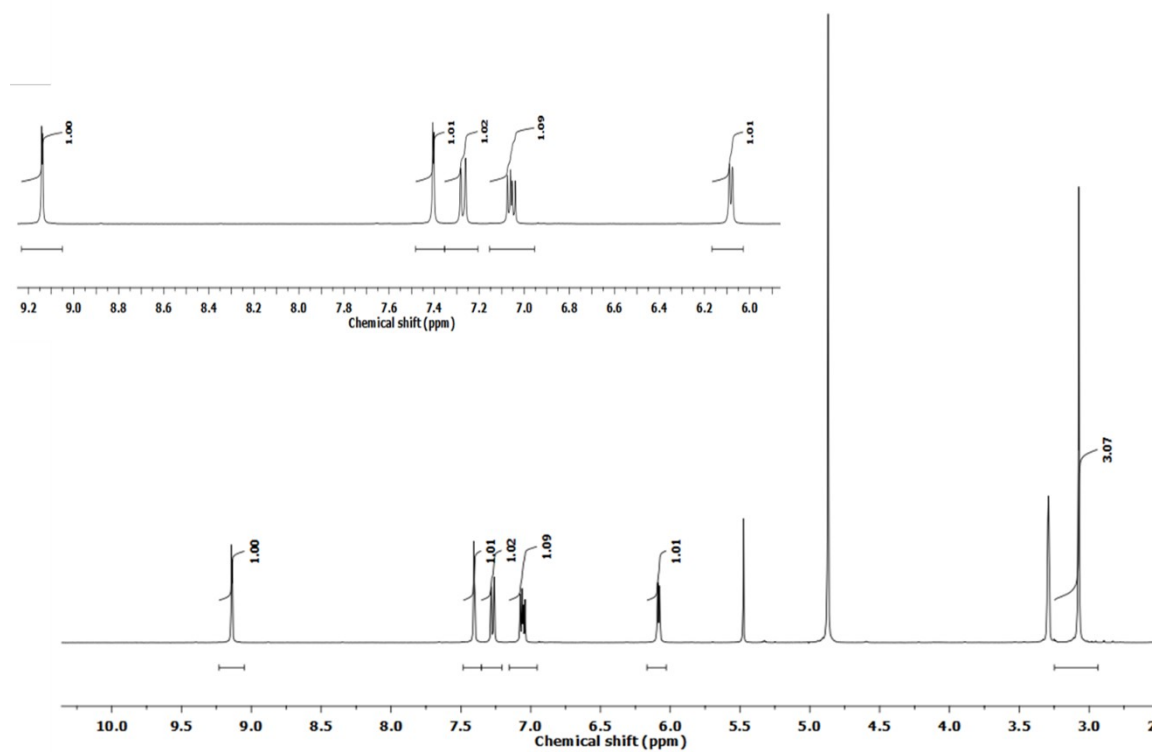


Fig. S1a. ^1H NMR spectrum of **2** (CD_3OD)

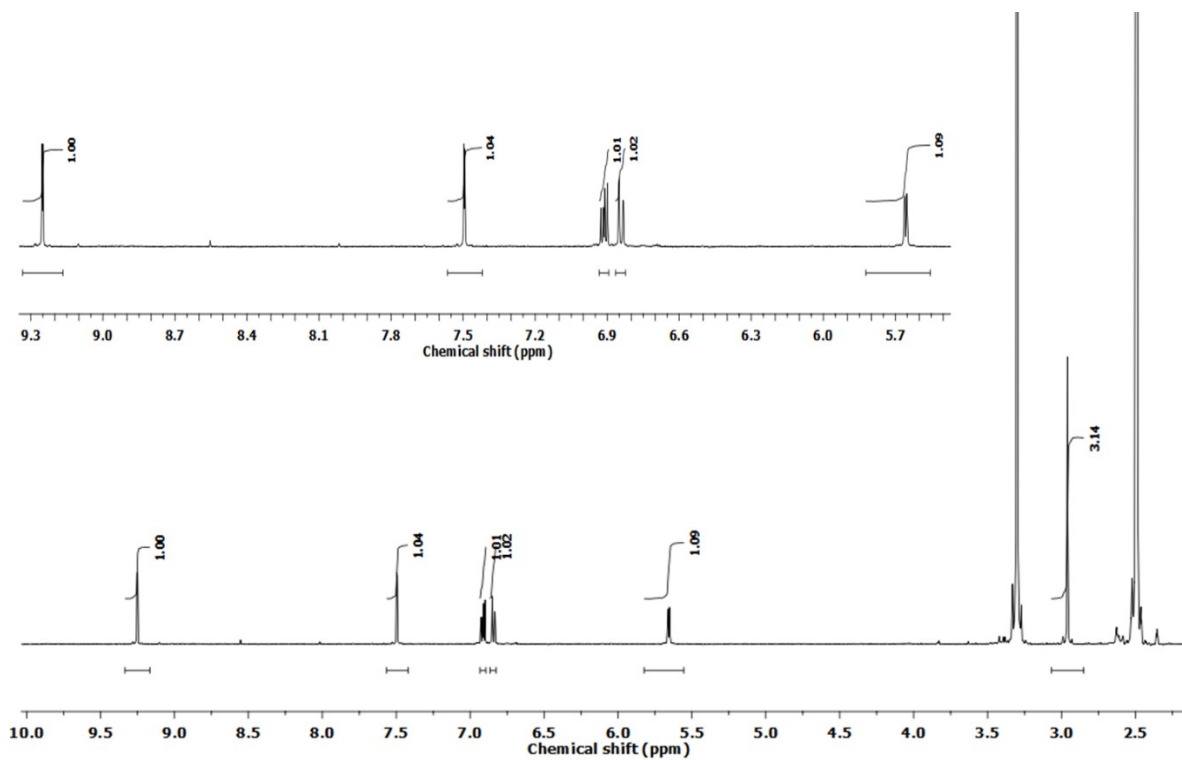


Fig. S1b. ^1H NMR spectrum of **2** ($\text{DMSO}-d_6$)

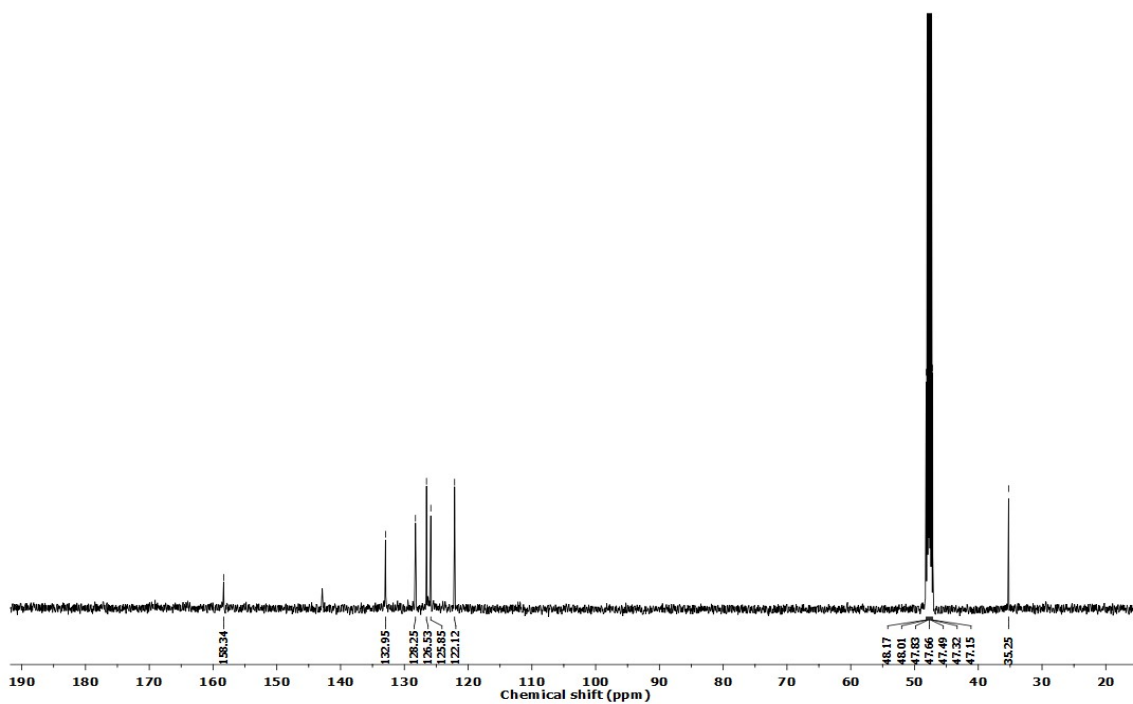


Fig. S2. ^{13}C NMR spectrum of **2** (CD_3OD)

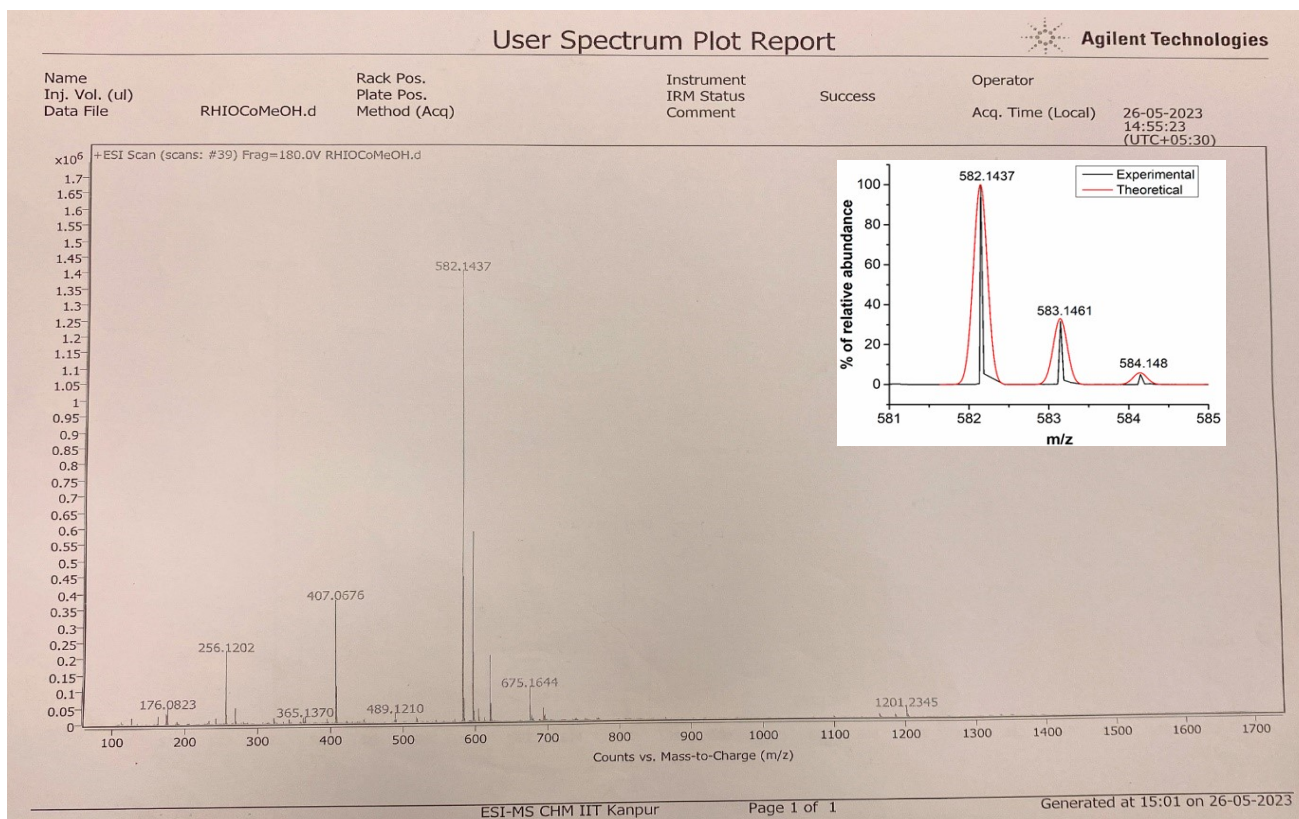


Fig. S3. ESI-MS(+) spectrum of **2**

Characterization of COC: [3-16]

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

The pale-yellow coloured liquid was obtained. ¹H NMR (CDCl₃, 400 MHz): δ 5.00 – 4.94 (m, 1H, OCH), 4.60-4.56 (t, 1H, OCH₂), 4.41-4.37 (t, 1H, OCH₂), 3.81-3.69 (m, 2H, -CH₂Cl). ¹³C NMR (CDCl₃, 100 MHz): δ 154.8, 78.9, 74.6, 44.0.

4-butyl-1,3-dioxolan-2-one (4b):

The pale-yellow coloured liquid was obtained by purification through column chromatography (5:1 hexane/ethyl acetate as an eluent). ¹H NMR (CDCl₃, 400 MHz): δ 4.69-4.63 (m, 1H, CHO), 4.50-4.47 (t, 1H, OCH₂), 4.04-4.01 (t, 1H, OCH₂), 1.75- 1.64 (m, 2H, CH₂), 1.41-1.32 (m, 4H, CH₂), 0.90- 0.86 (t, 3H, CH₃). ¹³C NMR (CDCl₃, 100 MHz): δ 155.2, 77.2, 69.5, 33.2, 26.2, 22.3, 13.8.

4-(phenoxyethyl)-1,3-dioxolan-2-one (4c):

Colourless solid were obtained by column chromatography. (3:2 hexane/ethyl acetate as an eluent) ¹H NMR (CDCl₃, 400 MHz): δ 7.31-7.21 (t, 2H, *m*-Ph), 7.00 (t, 1H, *p*-Ph), 6.88 (d, 2H, *o*-Ph), 5.00-4.98 (m, 1H, OCH), 4.61-4.54 (m, 2H, OCH₂), 4.23 (dd, 1H, CH₂), 4.20 (dd, 1H, CH₂). ¹³C NMR (CDCl₃, 100 MHz): δ 158.2, 154.6, 129.6, 121.9, 115.4, 77.5, 73.9, 67.0.

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

A colourless and odourless liquid was obtained, ¹H NMR (CDCl₃, 400 MHz): δ 4.83 (d, 1H), 4.62 – 4.48 (m, 1H), 3.98 (dd, 1H), 1.47 (d, 3H). ¹³C NMR (CDCl₃, 100 MHz): δ 155.2, 73.6, 70.9, 19.5.

4-phenyl-1,3-dioxolan-2-one (4e):

Colourless solid was obtained, through column chromatography. (3:1 hexane/ethyl acetate as an eluent) ¹H NMR (CDCl₃, 400 MHz): δ 7.48- 7.16 (m, 5H, Ph), 5.64 (t, 1H, OCH), 4.78 (t, 1H, CH₂), 4.36 (t, 1H, CH₂). ¹³C NMR (CDCl₃, 100 MHz): δ 154.5, 135.8, 129.8, 128.9, 76.2, 71.4.

hexahydro-1,3-benzodioxol-2-one (4f):

Pale-yellow coloured liquid was obtained column chromatography. (3:1 hexane/ethyl acetate as an eluent) ¹H NMR (CDCl₃, 400 MHz): δ 4.65 (m, 2H, OCHCH₂), 1.91-1.84 (m, 4H, OCHCH₂), 1.53 (m, 2H, CH₂), 1.39 (m, 2H, CH₂). ¹³C NMR (CDCl₃, 100 MHz): δ 155.1, 75.5, 27.2, 19.3.

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

A pale-yellow coloured liquid was obtained in column chromatography. (3:1 hexane/ethyl acetate as an eluent) ¹H NMR (CDCl₃, 400 MHz): δ 5.85-5.76 (m, 1H, CH), 5.24- 5.20 (d, 1H, CH), 5.16-5.14 (d, 1H, CH), 4.80- 4.75 (m, 1H, CH), 4.47- 4.43 (t, 1H, CH₂), 4.35-4.31 (t, 1H, CH₂), 3.98 (s, 2H, CH), 3.66-3.53 (dd, 2H, CH₂). ¹³C NMR (CDCl₃, 100 MHz): δ 155.0, 134.2, 117.5, 75.3, 72.0, 68.9, 66.03.

4,4'-[(((2,2-dimethylpropane-1,3-diyl)bis(oxy))bis(methylene))bis(1,3-dioxolan-2-one)] (4h):

The pale green coloured liquid was obtained, ¹H NMR (CDCl₃, 400 MHz): δ 4.84 – 4.75 (m, 1H, CH), 4.50 – 4.34 (m, 2H, CH₂), 3.70-3.52 (m, 2H, CH₂), 3.34-3.17 (m, 2H, CH₂), 0.89-

0.76 (s, 3H, CH₃). ¹³C NMR (CDCl₃, 100 MHz): δ 155.2, 79.5, 78.8, 77.3, 76.9, 75.4, 70.4, 70.2, 66.3, 44.2, 43.9, 36.3, 22.0.

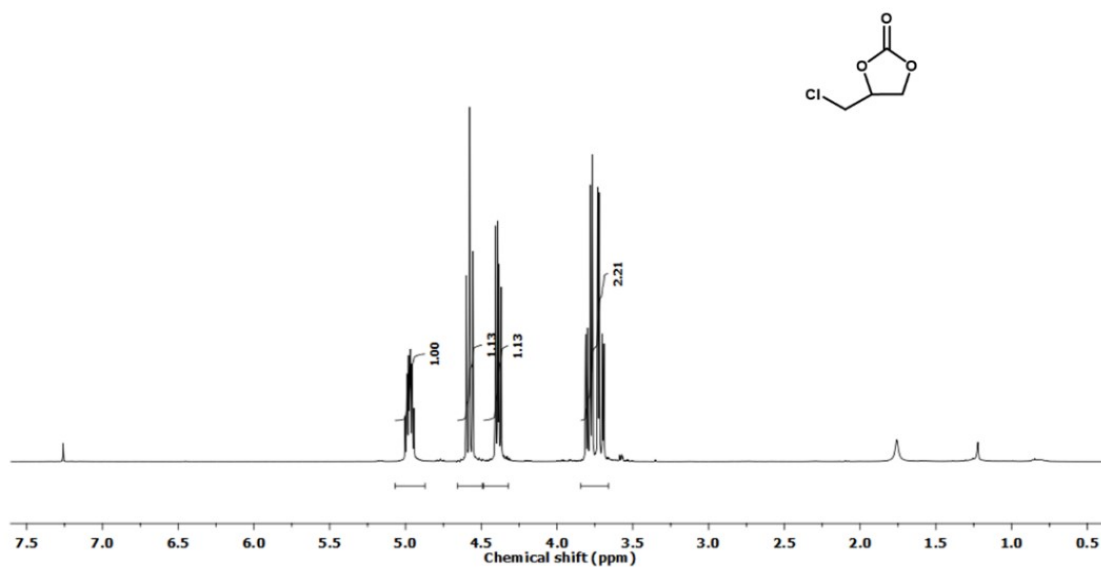


Figure S4: ¹H NMR spectrum of 4-(chloromethyl)-1,3-dioxolan-2-one (**4a**).

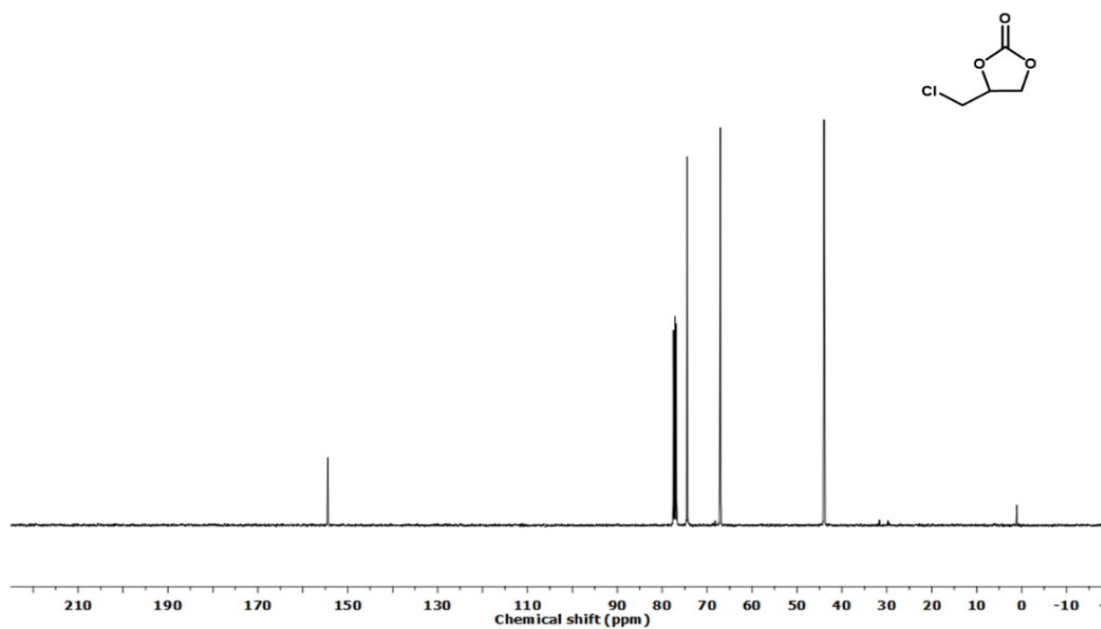


Figure S5: ¹³C NMR spectrum of 4-(chloromethyl)-1,3-dioxolan-2-one (**4a**).

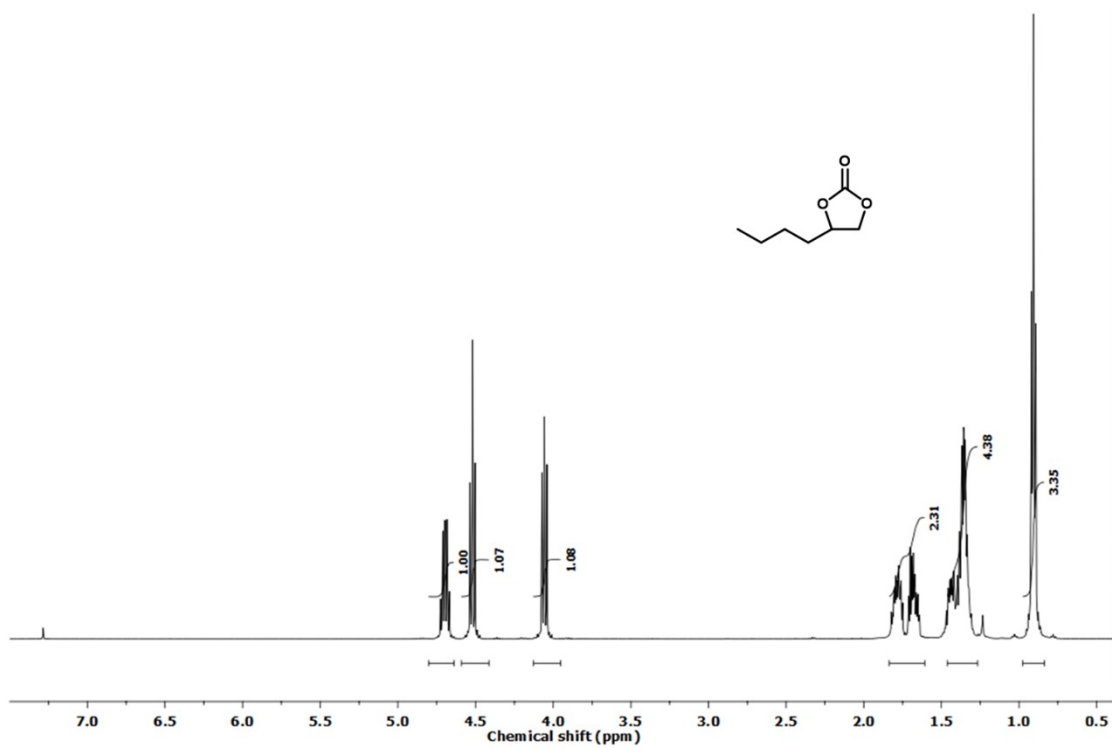


Figure S6: ^1H NMR spectrum of 4-butyl-1,3-dioxolan-2-one (**4b**).

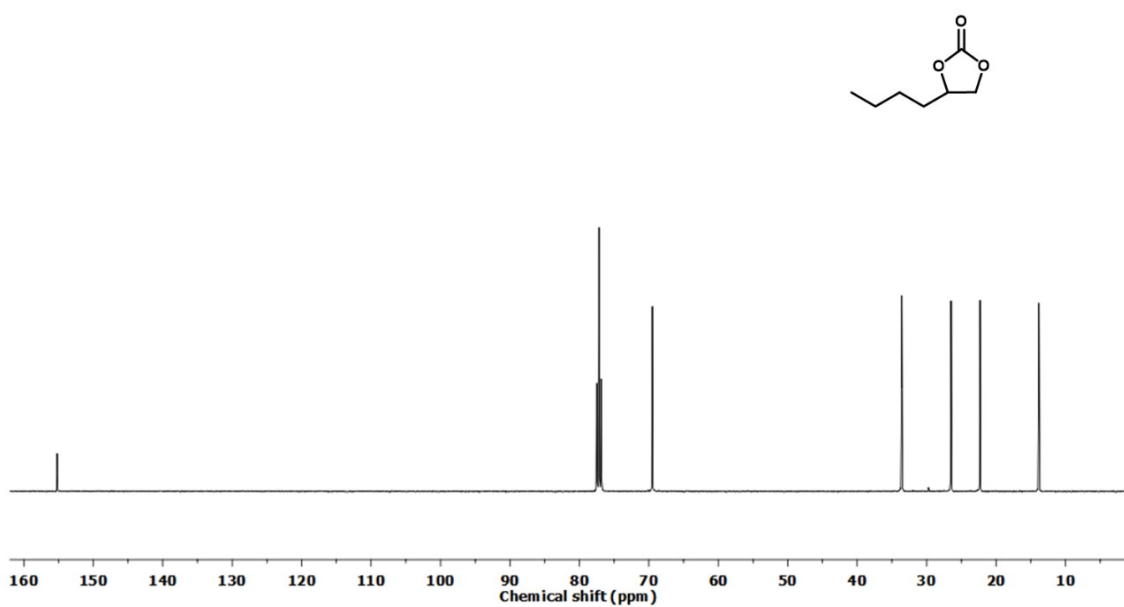


Figure S7: ^{13}C NMR spectrum of 4-butyl-1,3-dioxolan-2-one (**4b**).

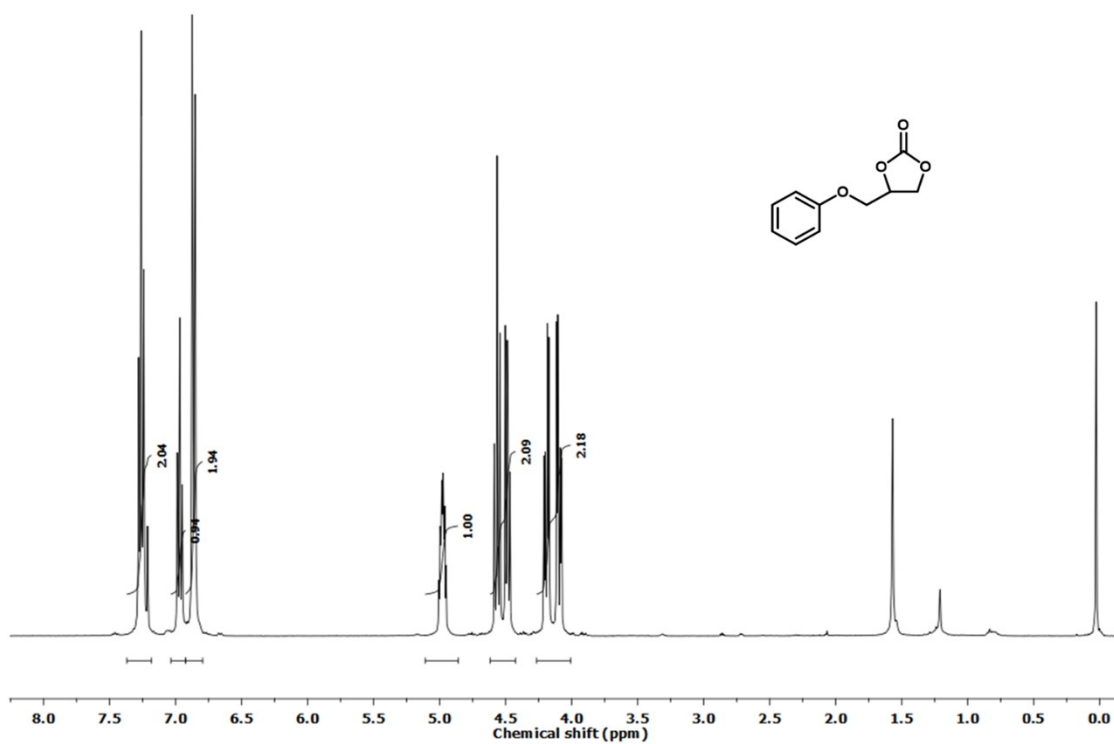


Figure S8: $^1\text{H NMR}$ spectrum of 4-(phenoxyethyl)-1,3-dioxolan-2-one (4c).

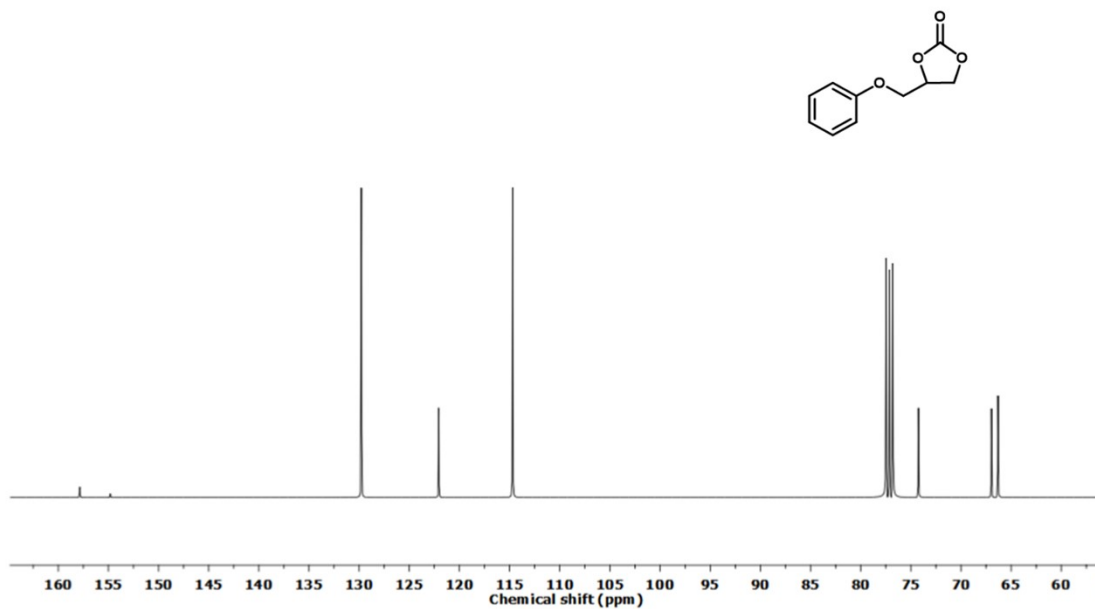


Figure S9: $^{13}\text{C NMR}$ spectrum of pure 4-(phenoxyethyl)-1,3-dioxolan-2-one (4c).

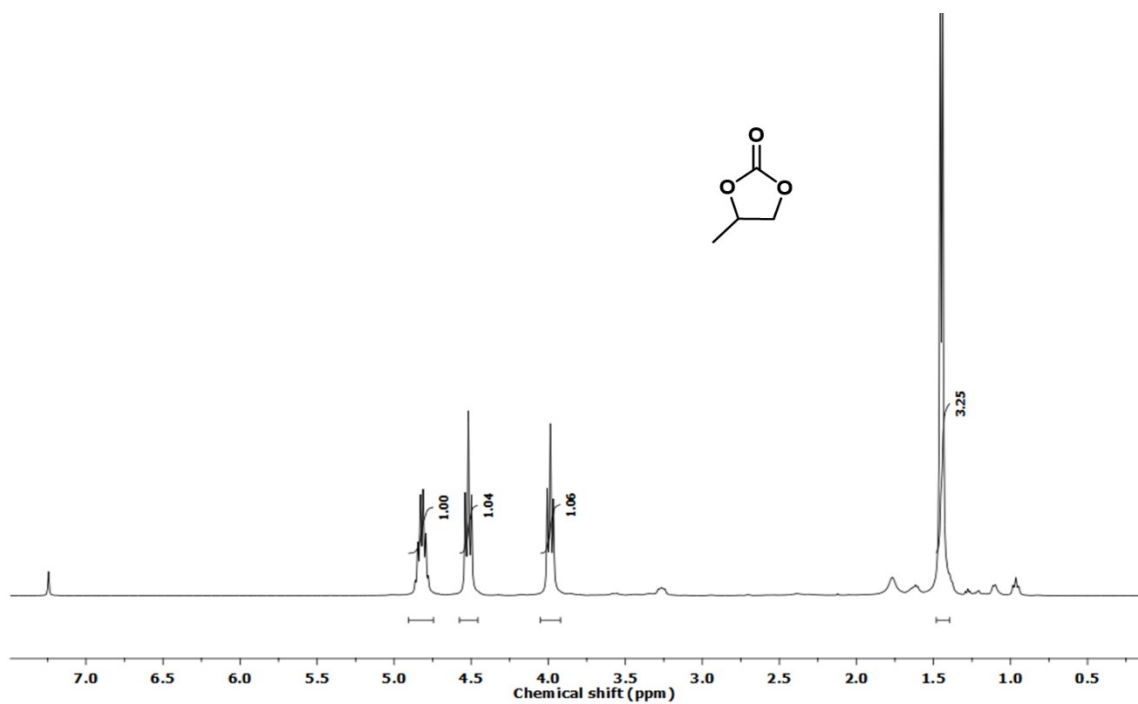


Figure S10: ^1H NMR spectrum of 4-methyl-1,3-dioxolan-2-one (**4d**).

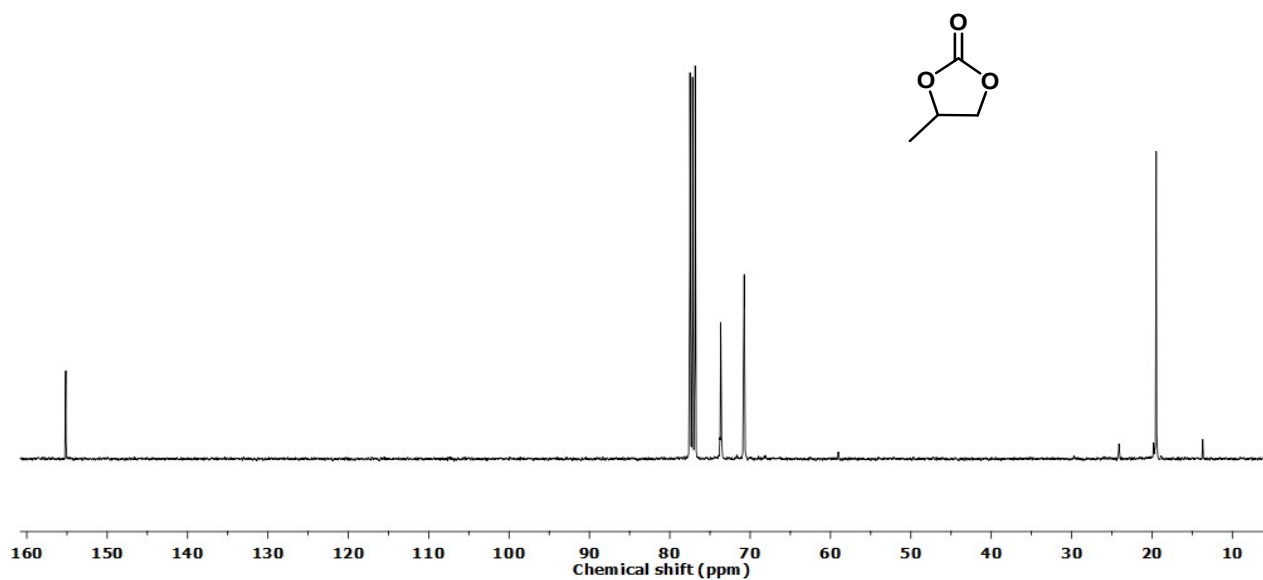


Figure S11: ^{13}C NMR spectrum of 4-methyl-1,3-dioxolan-2-one (**4d**).

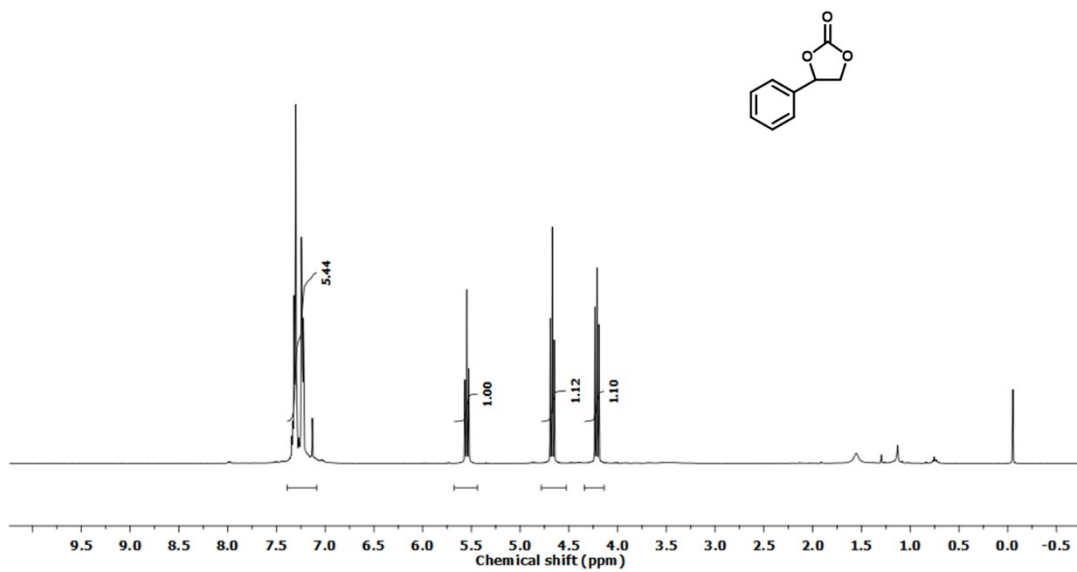


Figure S12: ^1H NMR spectrum of 4-phenyl-1,3-dioxolan-2-one (4e).

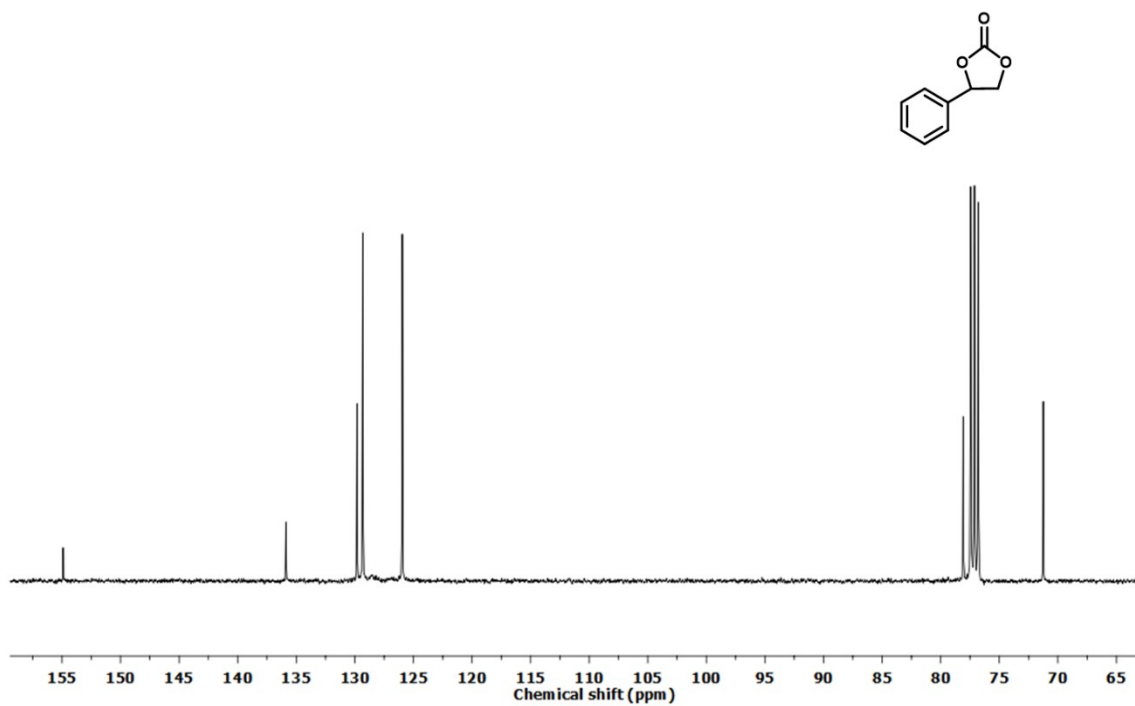


Figure S13: ^{13}C NMR spectrum of 4-phenyl-1,3-dioxolan-2-one (4e).

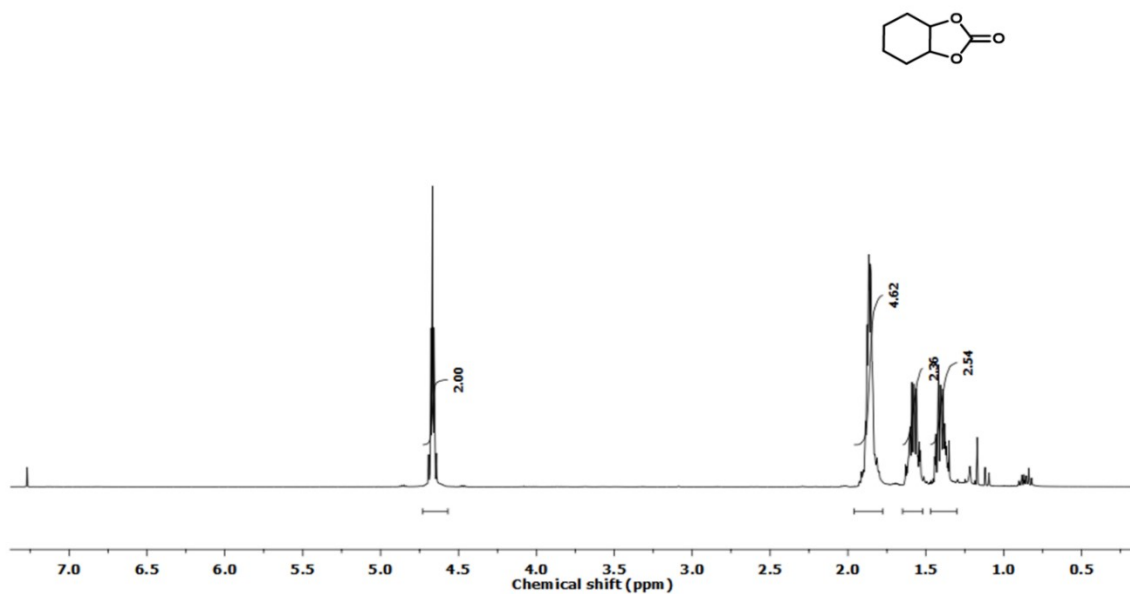


Figure S14: ¹H NMR spectrum of hexahydro-1,3-benzodioxol-2-one (4f).

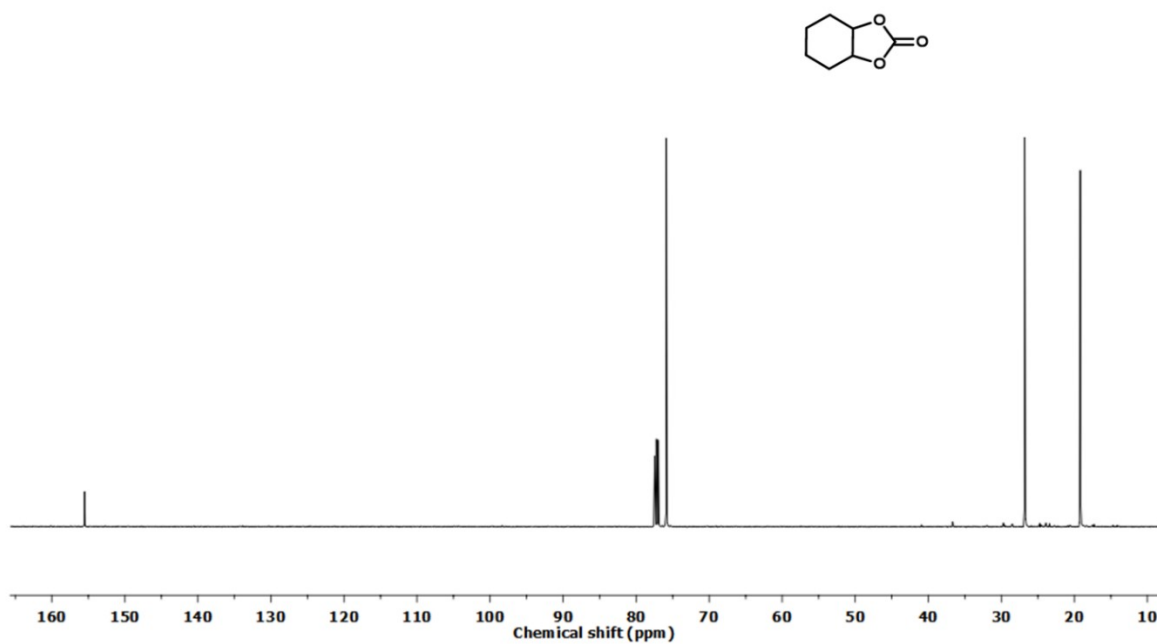


Figure S15: ¹³C NMR spectrum of hexahydro-1,3-benzodioxol-2-one (4f).

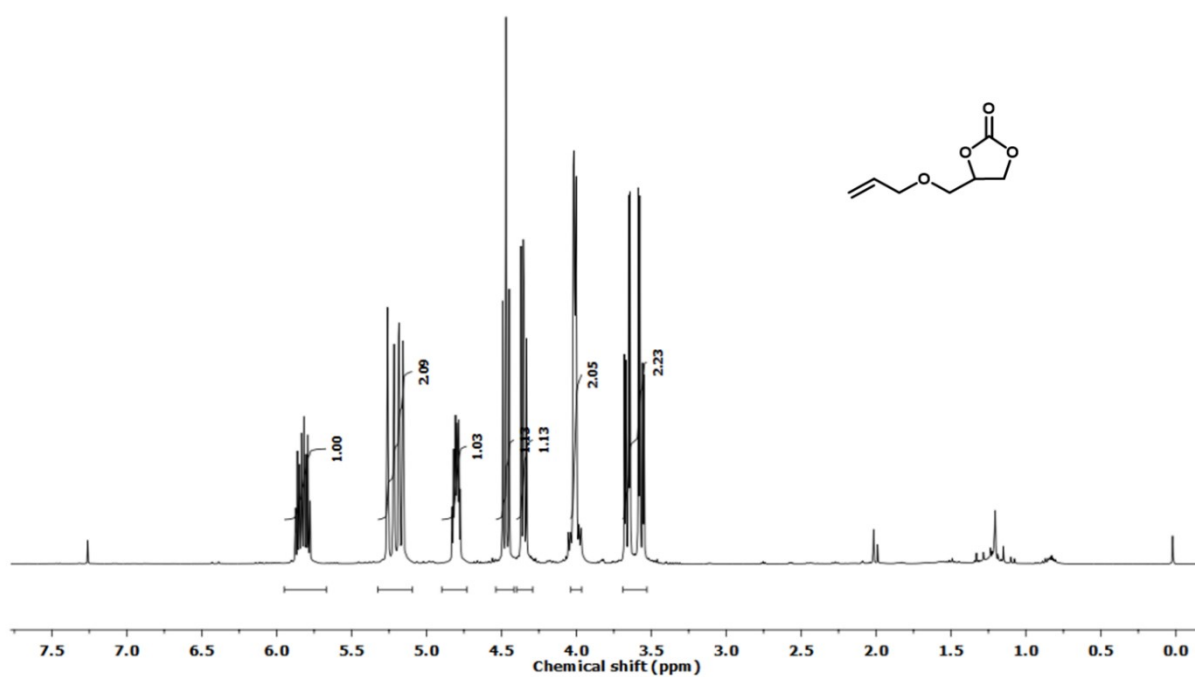


Figure S16: ¹H NMR spectrum of 4-((allyloxy)methyl)-1,3-dioxolan-2-one (**4g**).

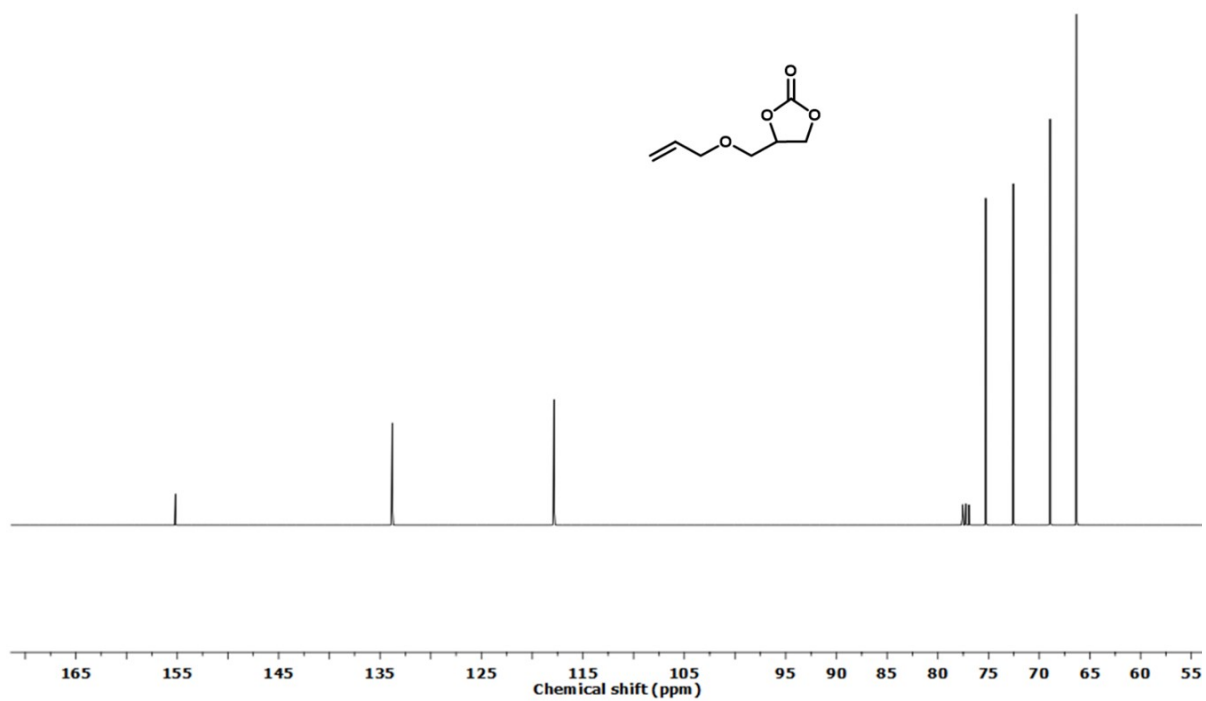


Figure S17: ¹³C NMR spectra of 4-((allyloxy)methyl)-1,3-dioxolan-2-one (**4g**).

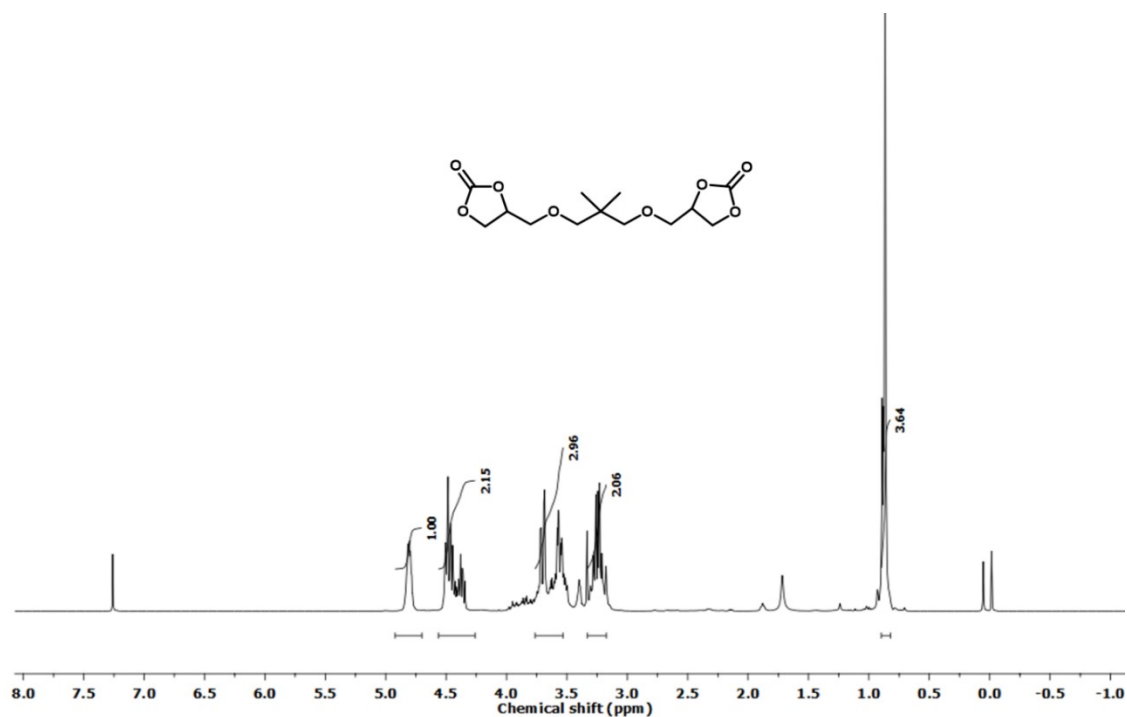


Figure S18: ^1H NMR spectrum of 4,4'-(((2,2-dimethylpropane-1,3-diyl)bis(oxy))bis(methylene))bis(1,3-dioxolan-2-one) (**4h**).

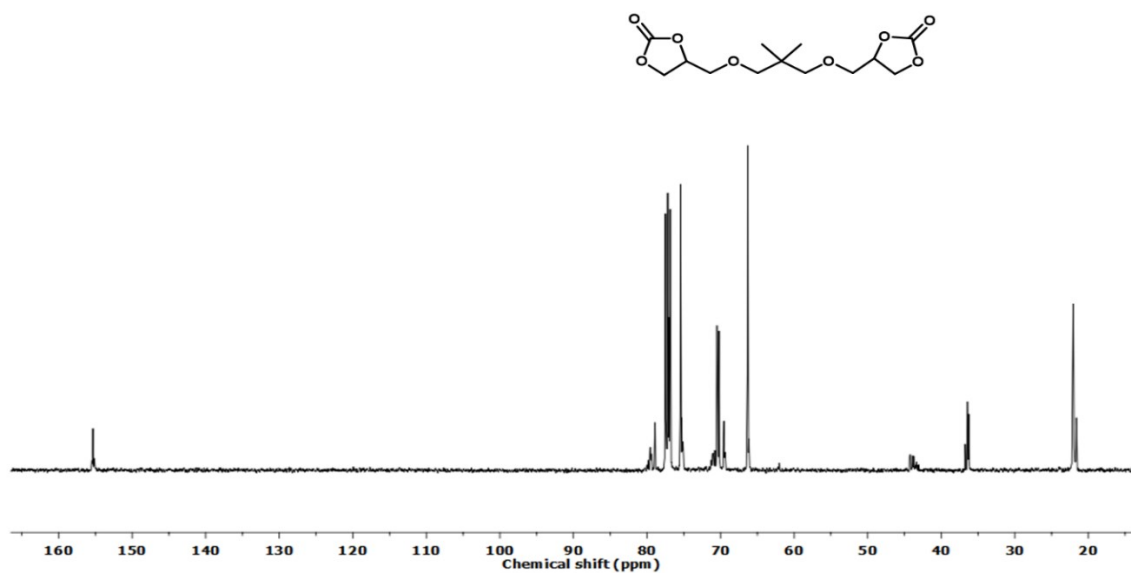


Figure S19: ^{13}C NMR spectra of 4,4'-(((2,2-dimethylpropane-1,3-diyl)bis(oxy))bis(methylene)) bis(1,3-dioxolan-2-one) (**4h**).

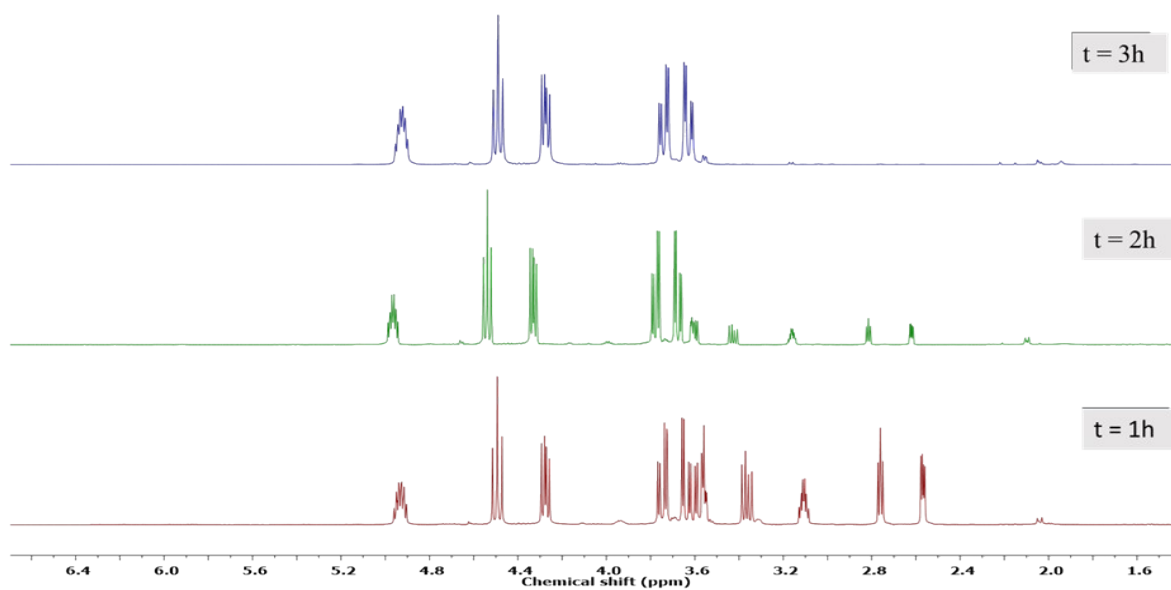


Figure S20: Time-dependant NMR spectra of the conversion of ECH to corresponding **4a** in the presence of **2** at 120 °C and 4 bar pressure.

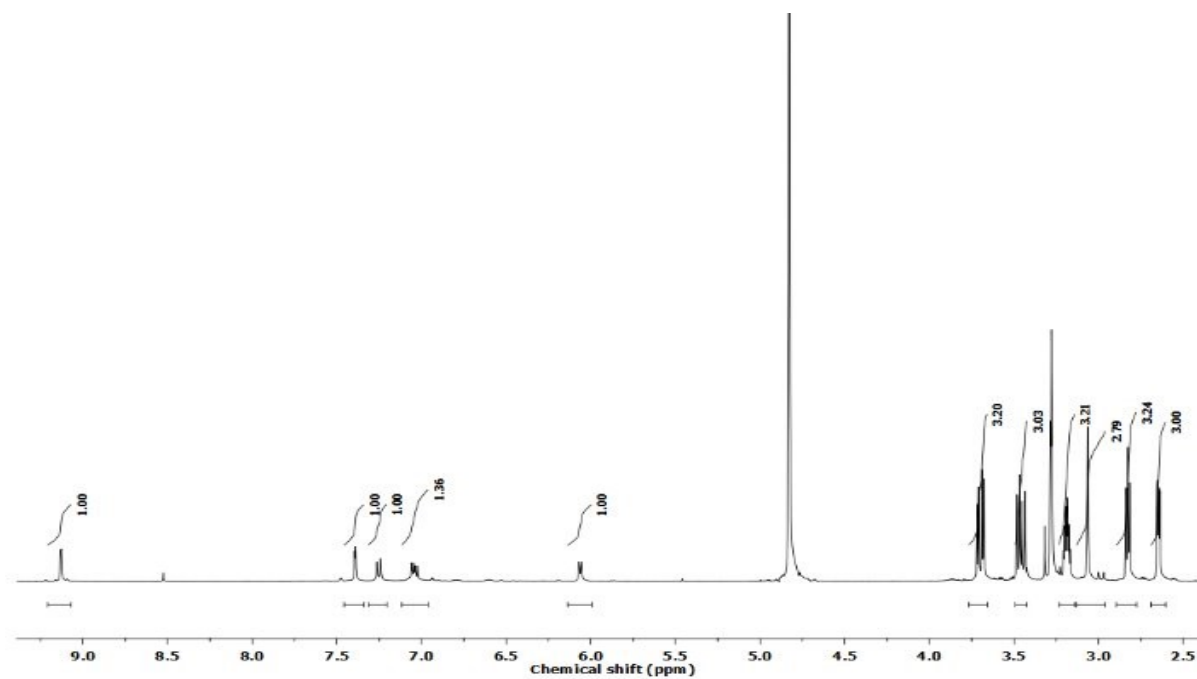


Figure S21: ¹H NMR spectrum of **2** and ECH

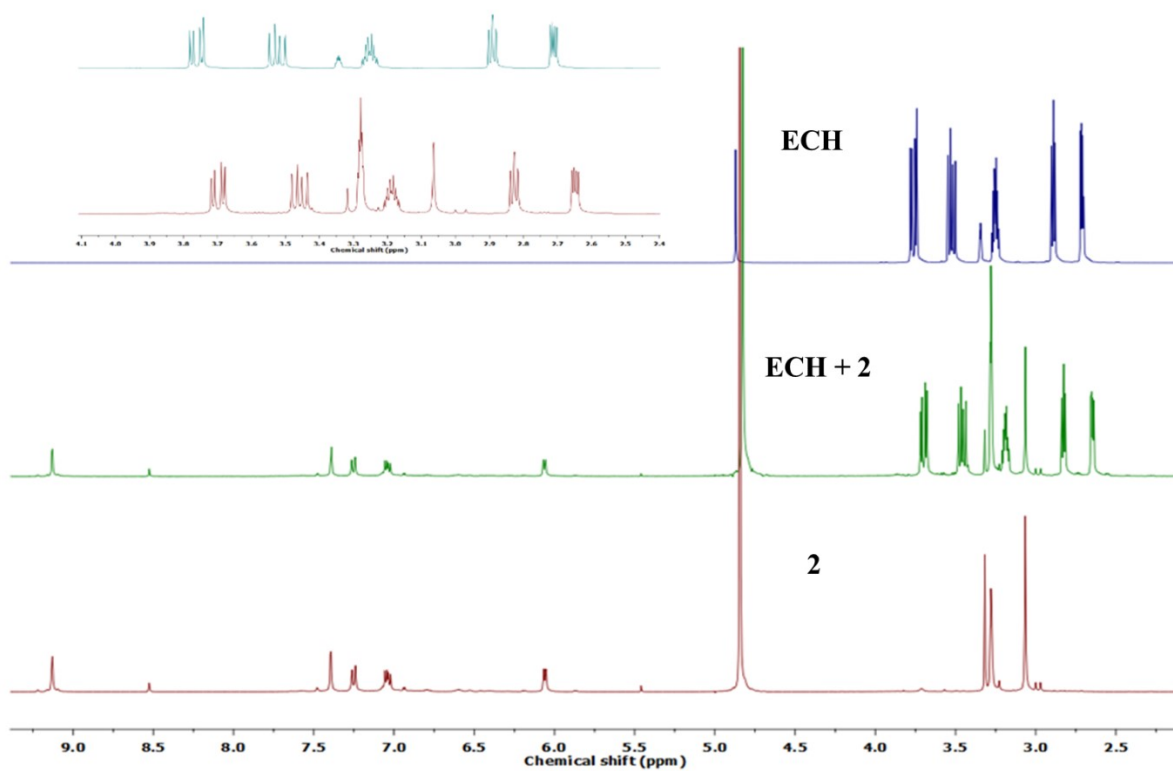


Figure S22: Stacked ^1H NMR spectra of ECH, ECH+2 and 2 recorded in CD_3OD

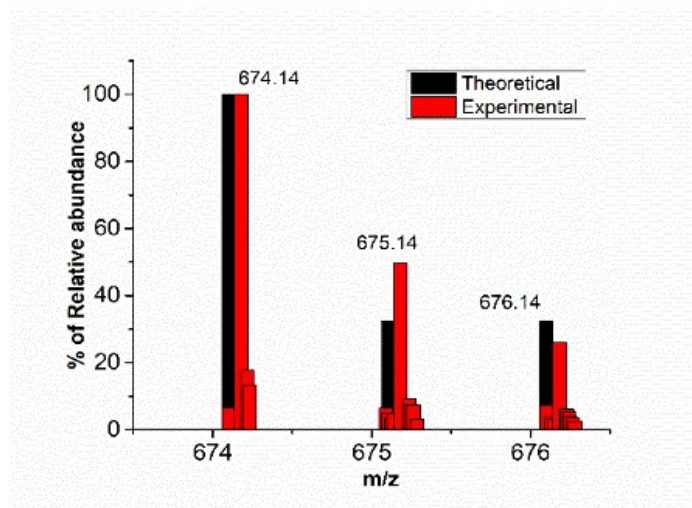


Figure S23: ESI-MS spectra of 2/ECH

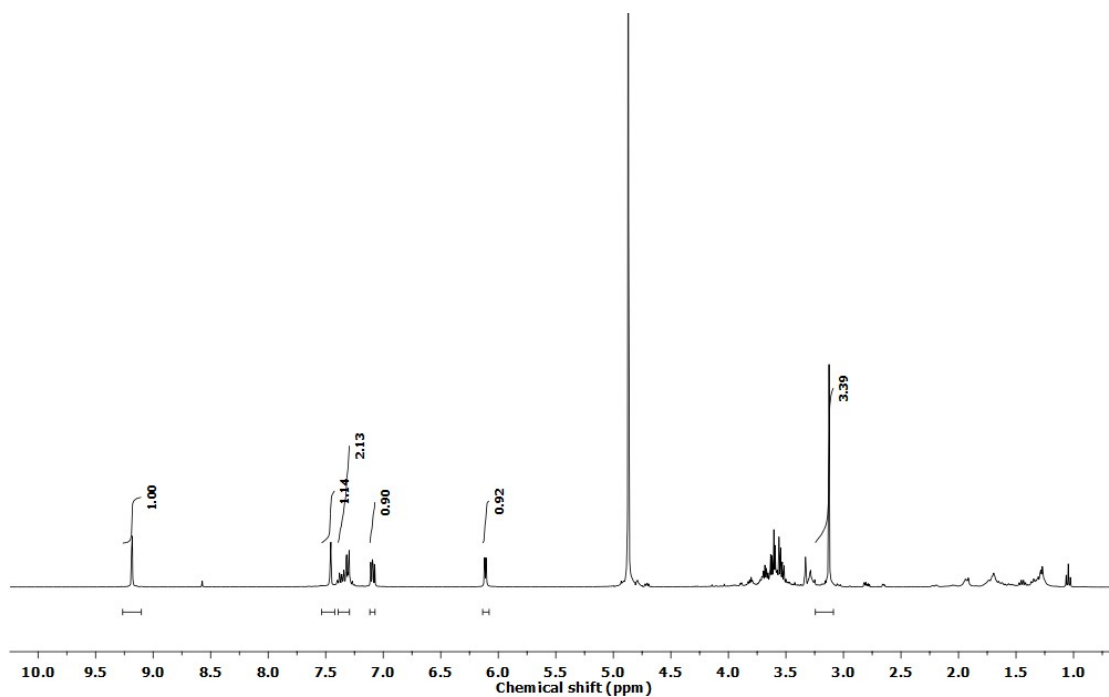


Figure S24: ^1H NMR spectrum of **2** after the reaction with CO_2

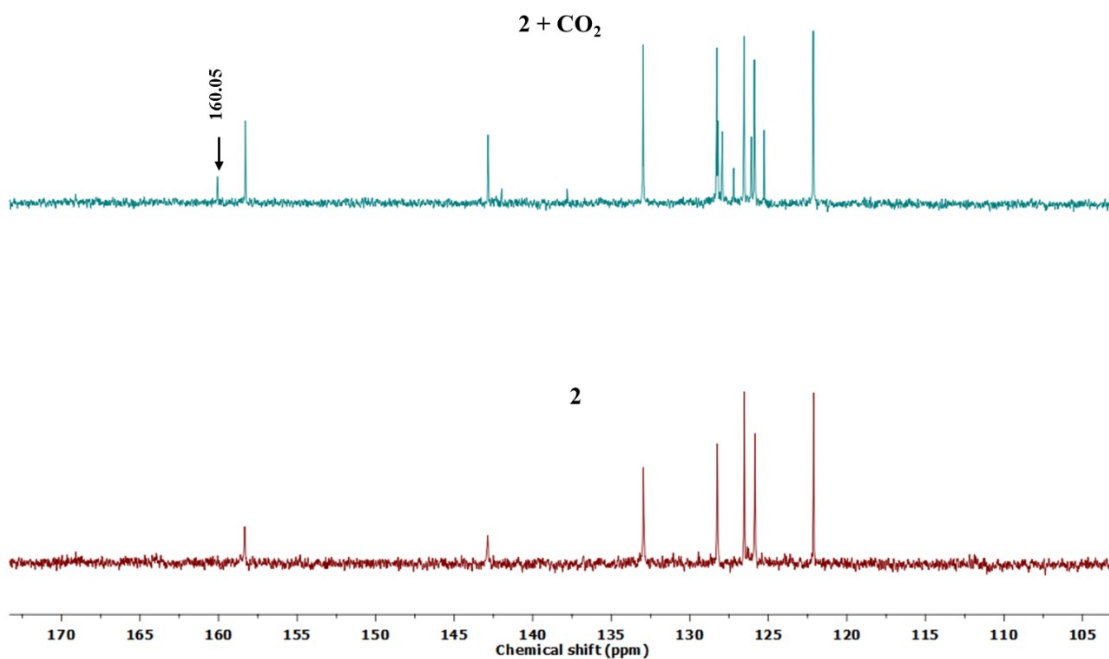


Figure S25: ^{13}C NMR spectrum of **2** and after the reaction with CO_2 (Note: only the range between 100-175 is shown here)

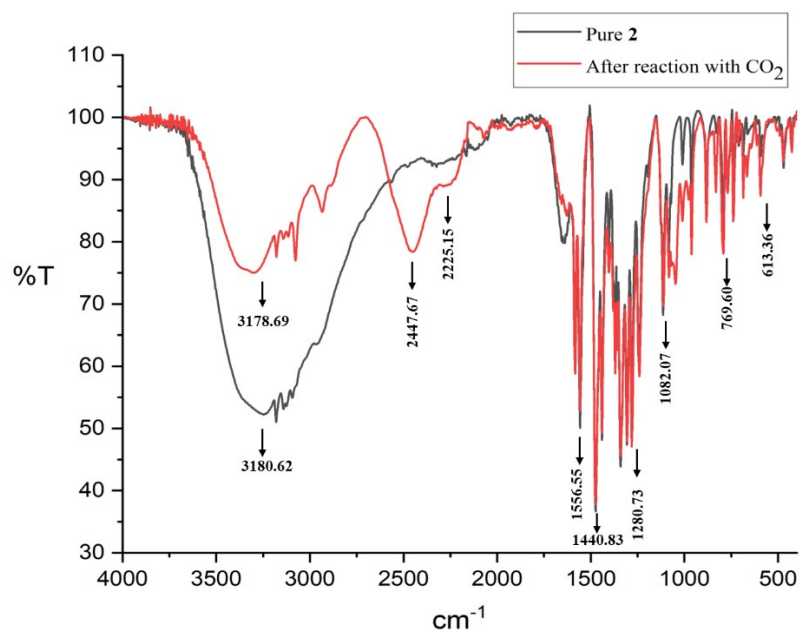


Figure S26: FT-IR spectra of **2** and after the reaction with CO₂

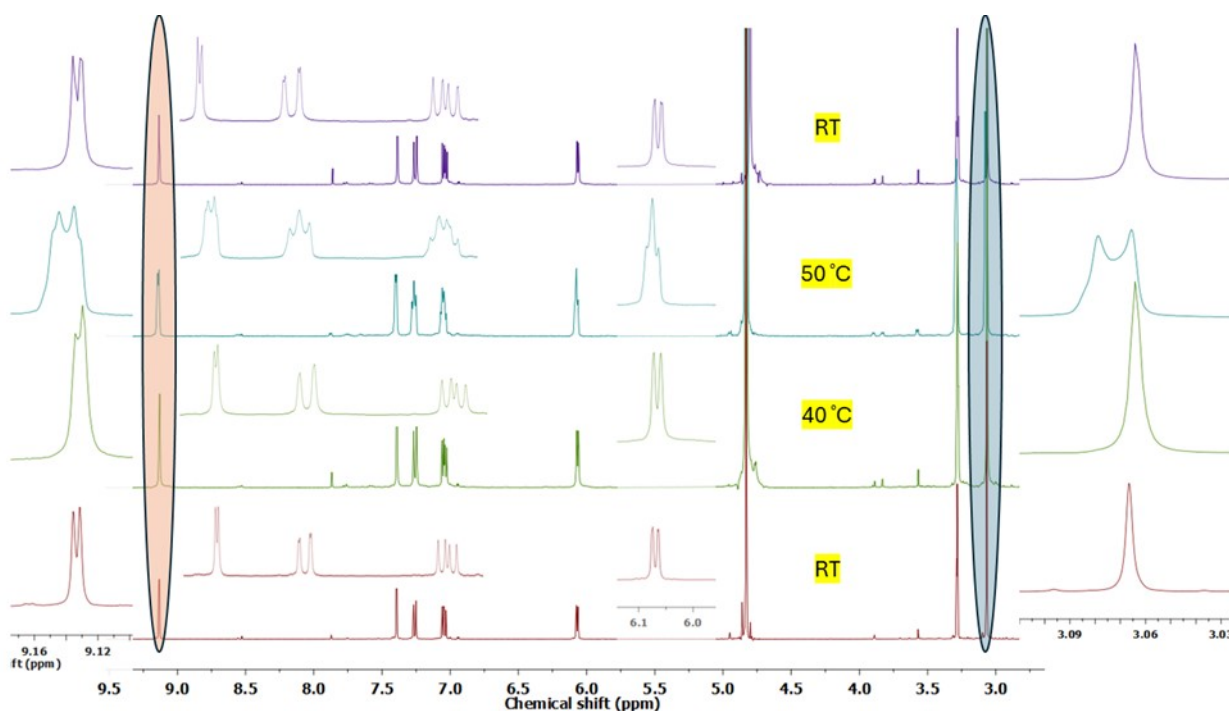
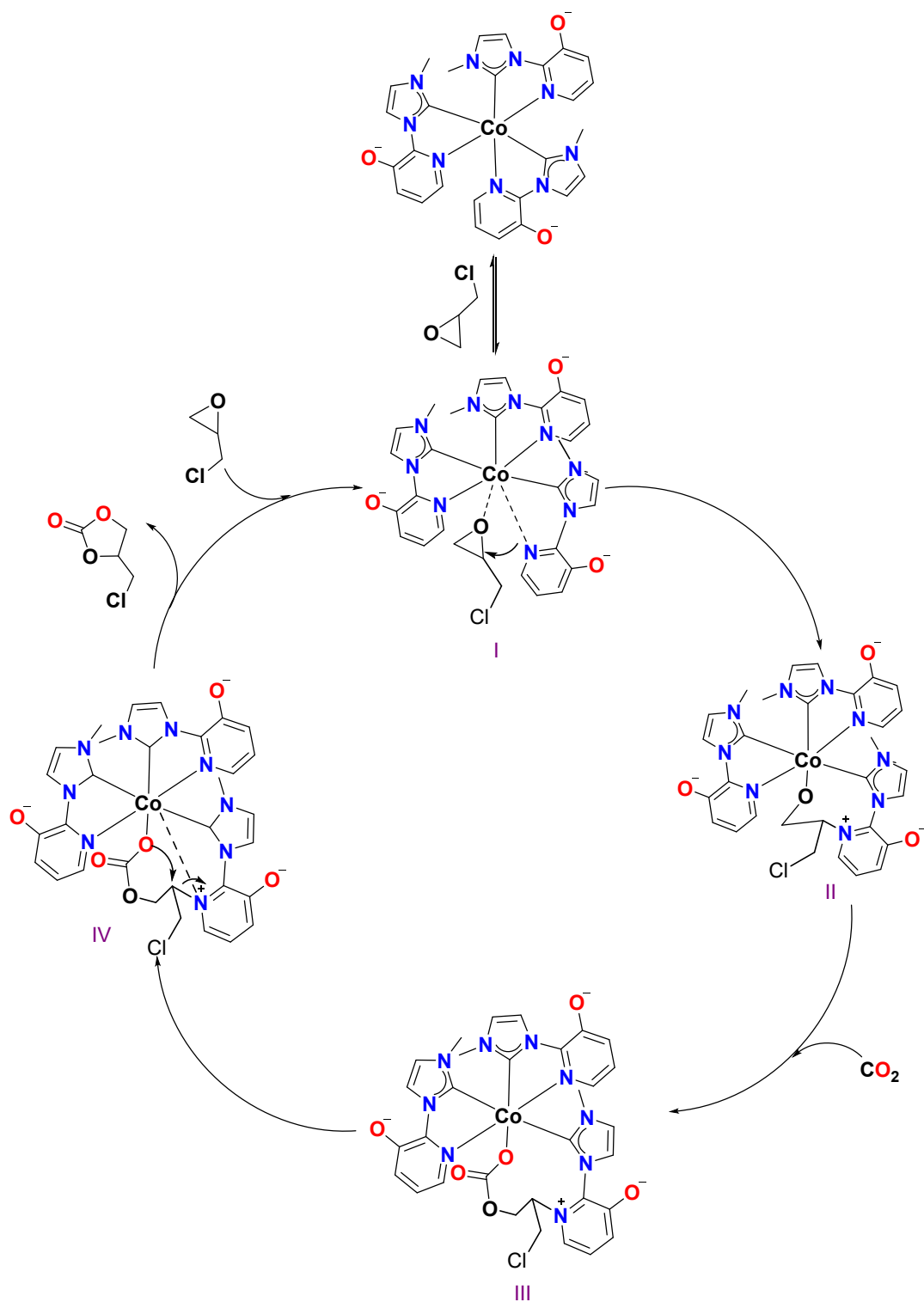


Figure S27: Variable temperature NMR of **2** recorded in CD₃OD with the enlarged portion of spectra indicating the changes in peaks between the regions 3.0 – 9.5 ppm. Note: In the inset, the expanded regions are shown within the full spectrum.



Scheme S1: The proposed mechanism of conversion ECH with CO_2 in the presence of only catalyst **2**. Note: Here, in the case of ECH, an electronegative chloride is present, so methine carbon is more electrophilic also due to interaction with the Lewis acidic Co(III) center, the electrophilicity of that carbon is increasing, and pyridine lone pair helps in epoxide ring opening, and generating a secondary carbocation which the pyridine lone-pair can stabilize.[8]

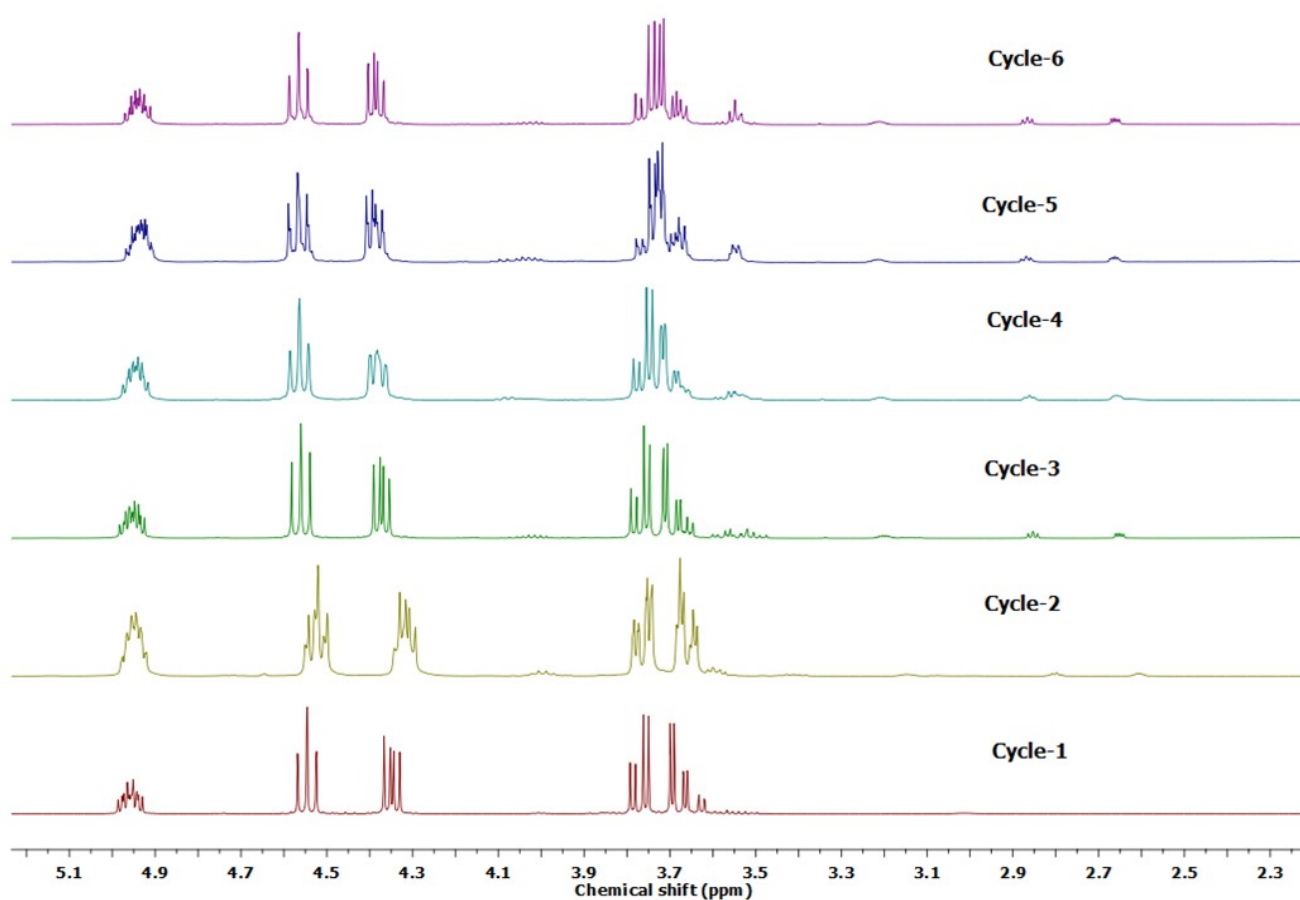


Figure S28: ¹H NMR spectra of the conversion of ECH to **4a** in the presence of catalyst **2** up to six cycles.

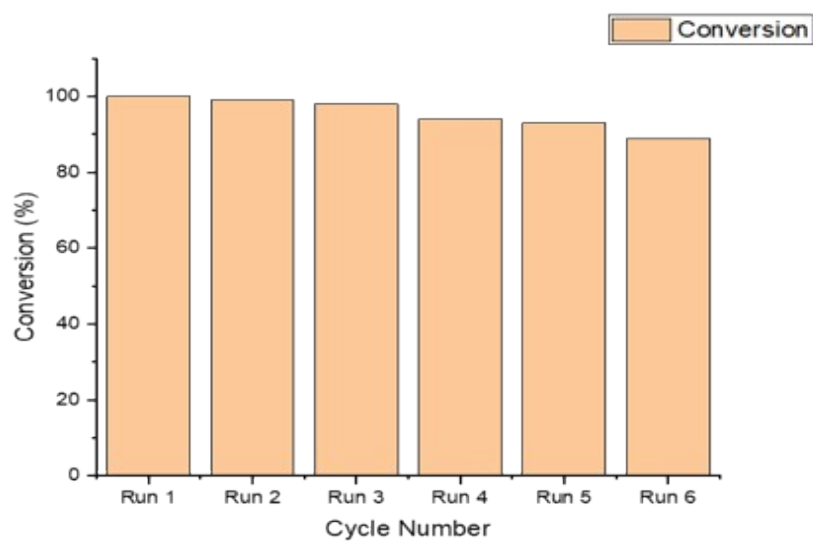


Figure S29: Reusability of catalyst **2** for the conversion of CO₂ with ECH.

Table S4: Comparison of **2** with other cobalt catalysts

Entry	Substrate	Catalyst	Cocatalyst	Time (h)	Temp (°C)	CO ₂ Pressure (atm)	Conv. (%)	TON	TOF (h ⁻¹)	Ref
1	ECH	Cobalt	KBr	5	100	6	85	42.5	8.5	11
2	ECH	Cobalt	TBAB	72	120	0.987	84.3	168600	2342	7
3	ECH	Cobalt	TBAB	1	90	9.86	99	3960	3960	6
5	ECH	Cobalt	TBAB	24	20	1	48	960	40	5
6	ECH	Cobalt	DMAP	2	100	15.7	71.6	716	358	3
7	ECH	Cobalt	TBAB	4	100	9.869	96	757	189	10
8	ECH	Cobalt	DMAP	48	120	0.987	99	200000	4166	8
9	ECH	Cobalt	DMAP	2	100	15.7	97.9	979	490	15
10	ECH	Cobalt	-----	6	120	20	99	990	165	4
11	ECH	Cobalt	TBAC	48	120	0.987	85	85000	1770	9
13	ECH	Cobalt	TBAB	6	100	30	99	1414	235	14
14	ECH	Cobalt	TBAI	24	65	1	91	91	3.8	13
15	ECH	Cobalt	TBAB	24	30	3	86	430	17.9	12
16	ECH	Cobalt	PPNCl	1	120	20	41	41000	41000	16
17	ECH	2	TBAB	3	100	1	68	158139	52713	This work
18	ECH	2	TBAB	24	100	1	100	666667	27778	This work

Table S5: Comparison of **2** with other earth-abundant metal catalysts

Entry	Substrate	Catalyst	Co-catalyst	Time (h)	Temp (°C)	CO ₂ Pressure (atm)	Conv. (%)	TON	TOF (h ⁻¹)	Ref
1	1,2 epoxy-hexane	Zn	-----	120	120	17	92	310000	2583	17
2	1,2 epoxy-hexane	Zn	-----	1	160	17	79	40000	40000	17
3	ECH	Zn	TBAB	3	120	17	80	800000	266667	18
4	ECH	Zn	TBAB	3	120	10	84	1120000	373000	19
5	1,2 epoxy-hexane	Mg	-----	72	120	17	67	220000	3056	17
6	1,2 epoxy-hexane	Mg	-----	1	160	17	91	46000	46000	17
7	PO	Al	PPNCl	0.5	120	30	46.3	92500	185000	20
8	ECH	2	TBAB	3	100	1	68	158139	52713	This work
9	ECH	2	TBAB	24	100	1	100	666667	27778	This work

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