SUPPLEMENTARY INFORMATION for

The coupling of CO_2 with diols promoted by organic dual systems: towards products divergence via benchmarking of the performance metrics

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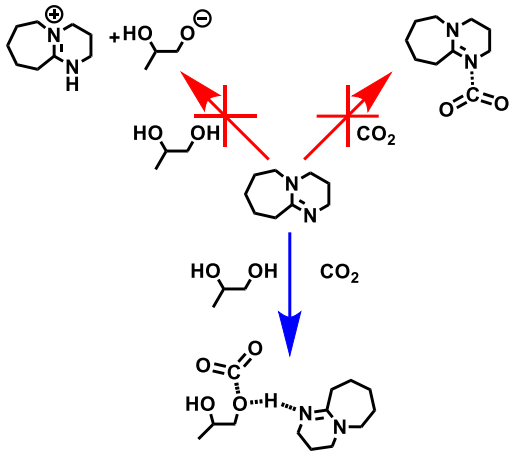
ESI 1 : Evidences of the trimolecular interaction between CO_2, DBU and PG



Scheme S1: Trimolecular reaction between PG, DBU and CO_2. No adduct or special interaction is observed with only two species at the same time.

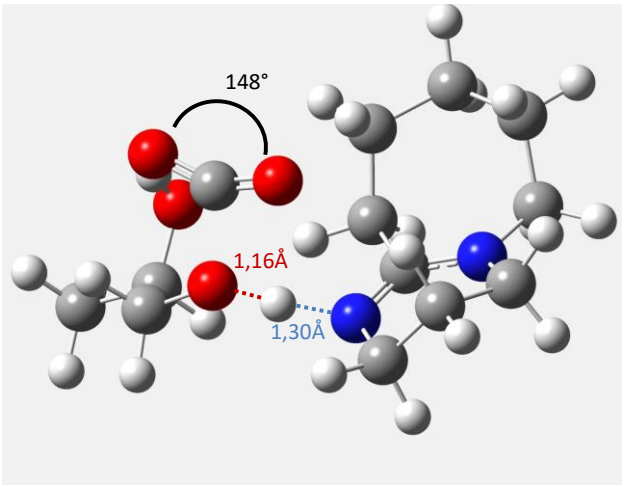


Figure S1: Molecular modelling of the transition state TS1 with trimolecular interaction between PG, DBU and CO_2. Hydrogen bonding between PG and DBU, and angular deformation of CO_2 occur at the same time.

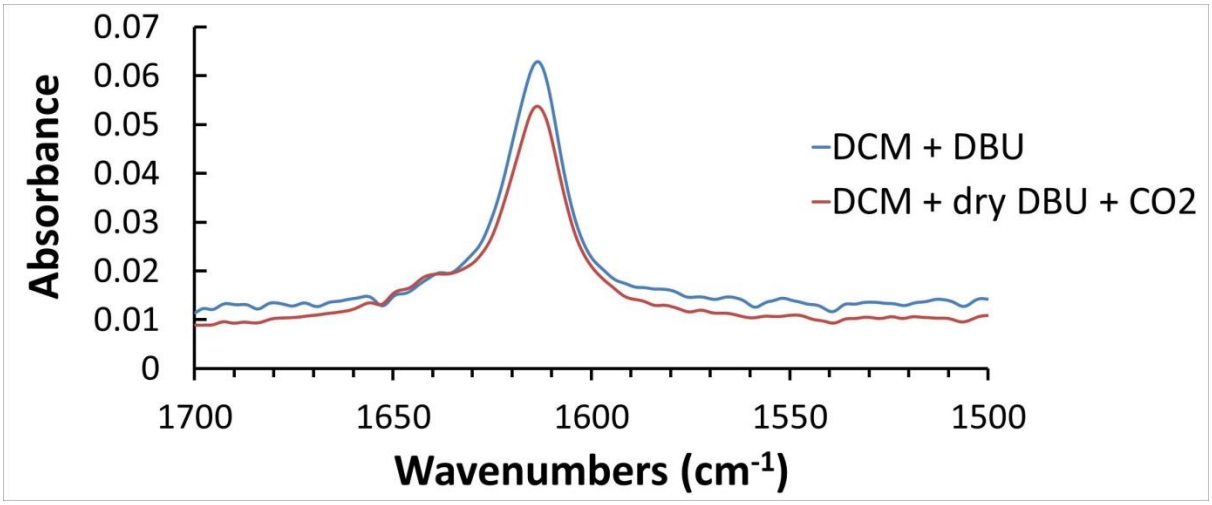


Figure S2: ATR-IR spectra of the DBU/CO_2 system in dichloromethane (DCM). A pressure of 1 MPa CO_2 was applied. When DBU was dried, no interaction or adduct between DBU and CO_2 can be observed. In the presence of water, $DBUH^+/HCO_3^-$ salts are formed.

ESI 2 : Molar attenuation coefficient determination of propylene carbonate for quantitative ATR-IR measurements

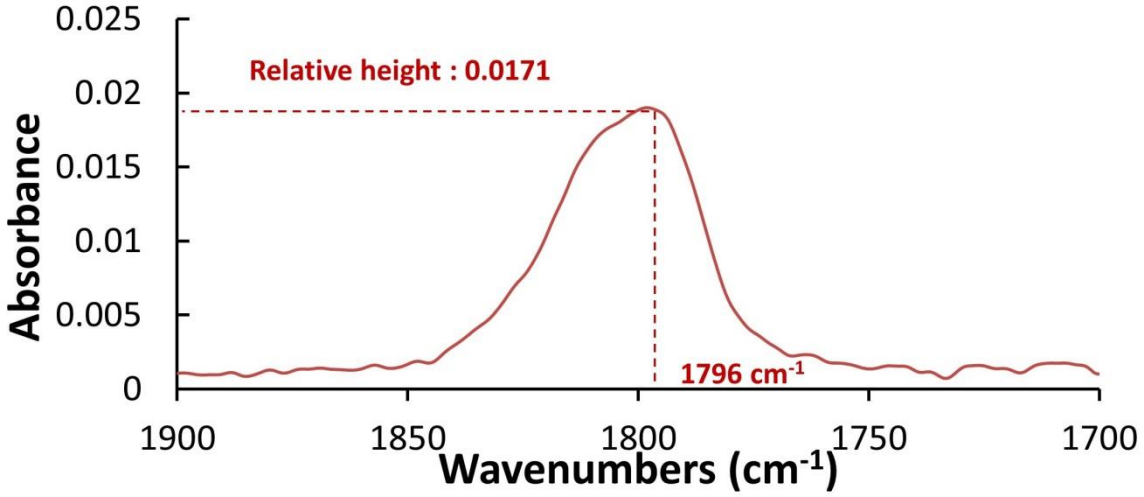


Figure S3: Experimental determination of the molar attenuation coefficient of propylene carbonate by ATR-IR : Propylene carbonate (0.5mmol ; 42.3µL) ; DBU (1mmol ; 149.2µL) ; BuBr (1.2mmol ; 130µL) ; CH_2Cl_2 : (200µL).

Table S1: Results obtained for the determination of ε*l of propylene carbonate. Concentration of propylene carbonate (PC) in all experiments was calculated through Beer-Lambert law using a value of ε*l for pure propylene carbonate (0.0192mL/mmol) since no significant difference was observed for other molecular environments.

Molecular species	Carbonate concentration	Peak height	ε*l (mL/mmol)
PC ; DBU ; BuBr ; CH_2Cl_2	0.96 mol/L	0.0171	0.0178
PC	11.85 mol/L	0.227	0.0192

ESI 3 : ^{1}H NMR characterization of the crude reaction mixture

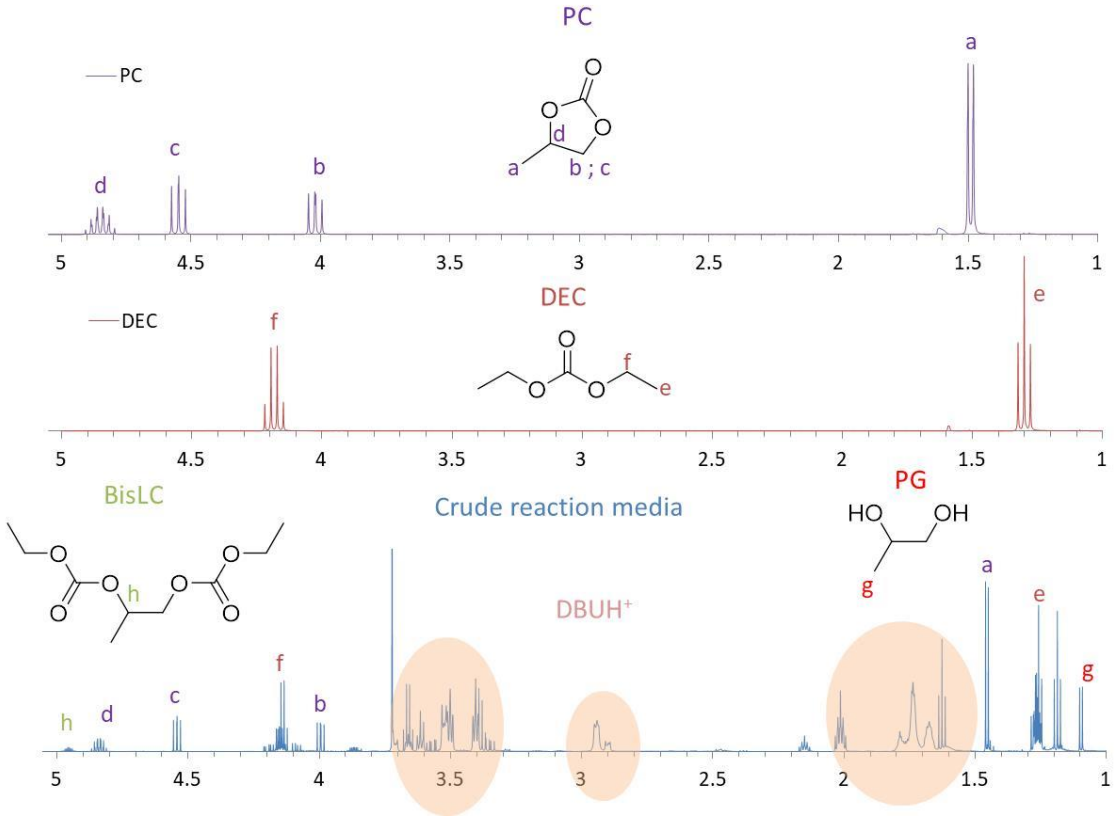


Figure S4: ^{1}H NMR (300MHz, $CDCl_3$) of (a) propylene carbonate (PC), (b) diethyl carbonate (DEC) and (c) the crude reaction mixture (sample entry 1, Table 1)

Chemical shifts ($CDCl_3$) :

PC:

a: 1.48 – 1.42 ppm (3H, d, C*H*$_3$CHO) ; b: 4.02 – 3.95 ppm (1H, dd, C*H*HO) ; c: 4.57 – 4.50 ppm (1H, dd, CH*H*O) ; d: 4.9 – 4.77 ppm (1H, m, MeC*H*O)

DEC:

e: 1.27 – 1.24 ppm (6H, t, *CH*$_3$CH$_2$); f: 4.16 – 4.12 ppm (4H, q, CH$_3$*CH*$_2$)

PG:

g: 1.11 – 1.09 ppm (3H, d, *CH*$_3$CHOH)

BisLC:

h: 4.98 – 4.93 ppm (1H, m, CH$_3$C*H*O)

ESI 4 : DFT discrimination of (R) and (S) configurations and of primary and secondary alcohol reactivities of PG.

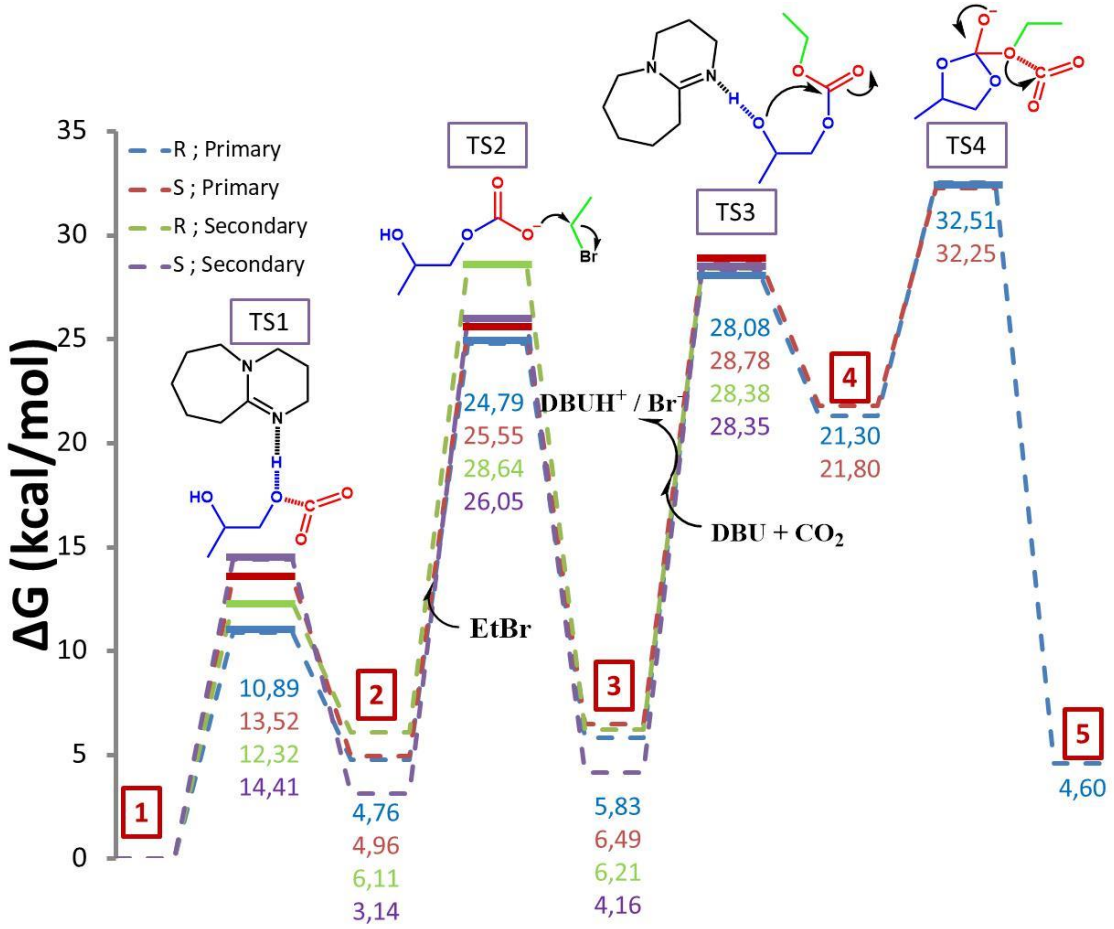


Figure S5: DFT computed pathway (*M062X/6-311g(d,p)*) of model reaction as depicted in Scheme 4. All pathways were considered for the monocarbonation of propylene glycol: carbonation on the primary or secondary alcohol moiety, with either (R) or (S) stereochemistry. Red numbers correspond to optimized reaction intermediates shown in Scheme 4 (Van Der Waals interactions were accounted). Transition states (TS) were optimized using the same molecular species as in the intermediates. The optimized structures of the intermediates and transition states for the reaction path calculated with the (R) primary alcohol are reported at the end of the ESI.

ESI 5 : Comparison between quantitative ATR-IR and quantitative ^{1}H NMR

All yields were determined by quantitative ^{1}H NMR using 1,3,5-trimethoxybenzene (TMB) as internal standard, except for the synthesis of propylene carbonate where the yield was determined by both ^{1}H quantitative NMR and ATR-IR. A known mass of TMB (0.333 equivalent) was added to the reaction mixture before the introduction of CO_2. Here are presented ^{1}H NMR spectrum and ATR-IR spectrum of the same sample at the end of reaction time to compare the yields obtained and confirm both methods work as quantitative methods. Attribution of peaks is detailed in ESI 3.

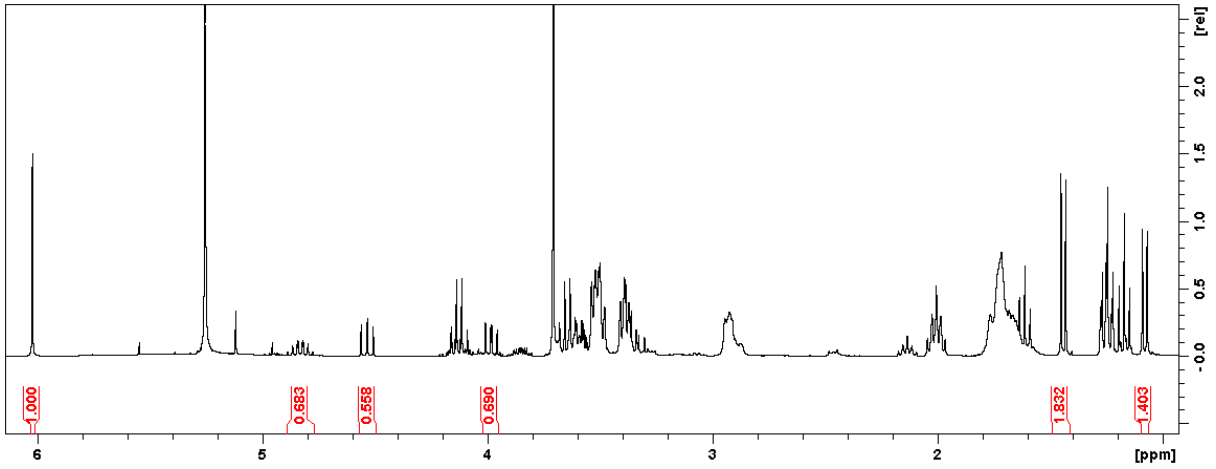


Figure S9: ^{1}H NMR spectrum of model reaction in $CDCl_3$ (Scheme 2) after 20h for the synthesis of Propylene carbonate. Propylene glycol (0.5mmol ; 36.7µL) ; DBU (1mmol ; 149.2µL) ; EtBr (1.2mmol ; 89.4µL) ; CH_2Cl_2 (200µL) ; 1,3,5-trimethoxybenzene (0.162mmol ; 27.22mg) as internal standard. 50µL of the reaction mixture are mixed with 600µL $CDCl_3$ to perform ^{1}H NMR analysis.

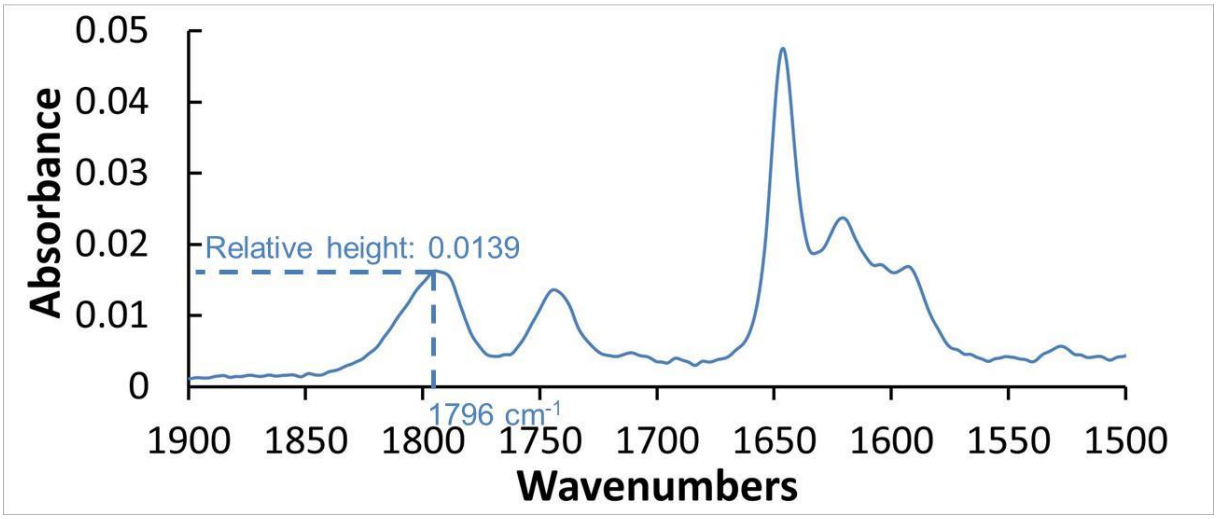


Figure S10: ATR-IR spectra of model reaction (same sample that for ^{1}H NMR spectrum, Fig. S9).

- Yield obtained from ^{1}H NMR analysis :

Propylene carbonate: δ: 4.9 – 4.77 (1 H, m, MeC*H*O), 4.57 – 4.50 (1 H, dd, CH*H*O), 4.02 – 3.95 (1 H, dd, C*H*HO), 1.48 – 1.42 (3 H, d, C*H*$_3$CHO).

Propylene glycol: δ: 3.91 – 3.8 (1H, m, MeC*H*OH), 3.63 – 3.55 (1H, m, CH*H*OH), 3.42 – 3.2 (1H, m, C*H*HOH), 1.10 – 1.06 (3H, d, C*H*$_3$CHOH)

TMB: δ: 6.02 (3H, Ar*H*), 3.71 (9H, OC*H*$_3$)

Proton signals of propylene carbonate were integrated with aromatic protons signal of TMB (3H) as reference (integration value of 1). As TMB was introduced with a known mass (0.333 equivalent of propylene glycol), one can calculate the exact mole number of propylene carbonate.

$$n(PC) = \frac{\sum_i \frac{\int_i PC}{N_H^i}}{i} * 3 * n_{TMB}$$

$n(PC)$: $Mole\ number\ of\ propylene\ carbonate$

$\int_i PC$: $integration\ value\ of\ signal$ "i" $relative\ to\ propylene\ carbonate$

N_H^i : $number\ of\ hydrogen\ taken\ into\ account\ for\ signal$ "i"

n_{TMB} : $mole\ number\ of\ TMB\ initially\ introduced\ in\ the\ reaction\ media$

Yield obtained from Fig. 12 is of **62 %**.

- Yield obtained from ATR-IR analysis :

Propylene carbonate: ν(C=O) : 1796cm^{-1}

As we calculated the value of ε*l for propylene carbonate (see ESI 5), one can calculate the concentration of propylene carbonate in the reaction media using Beer-Lambert law with the absorbance at 1796cm^{-1}.

Yield obtained from Fig. 13 is of **69 %**.

Both methods lead to the same yield with only small differences attributed to experimental factors.

ESI 6 : Evidence of the $DBUH^+/RCO_3^-$ salt precipitation at 4 MPa

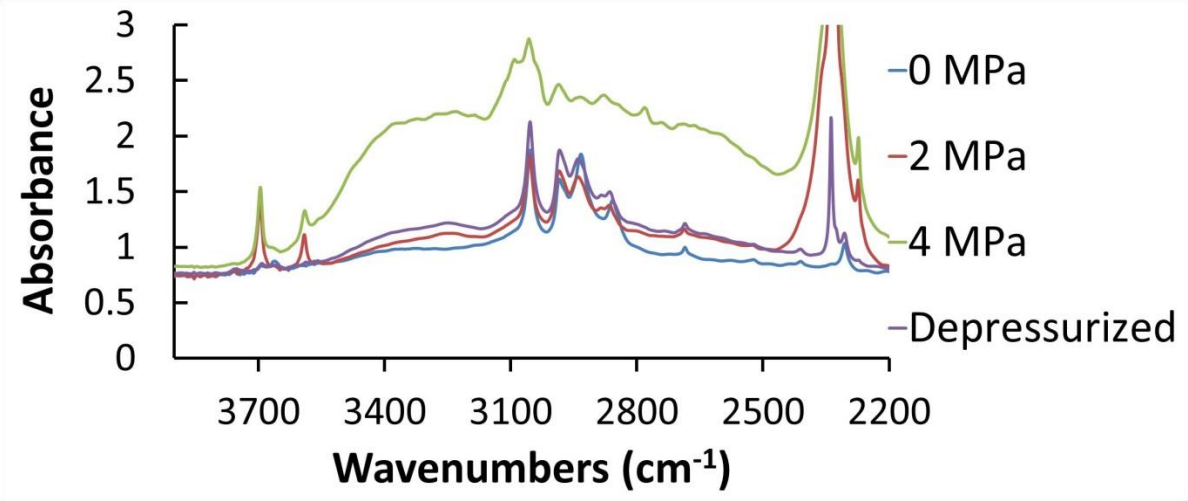
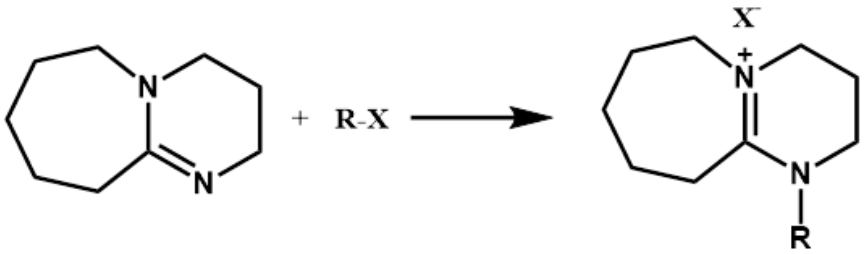


Figure S6: FT-IR (transmission) spectra collected at the equilibrium over different pressure. Purple curve was collected after depressurizing the cell at 4 MPa. Conditions: PG (0.67 mmol ; 49.2 µL), DBU (0.67 mmol ; 100 µL), CH_2Cl_2 (850 µL)

As the system is under pressure, carbonation of the alcohol moiety occurs. Around 4 MPa, large absorption band between 2400cm^{-1} and 3500cm^{-1} appears, characteristic of the formation of solid organic salts (here $RCO_3^-/DBUH^+$) that interferes with the infrared beam as it deposits on the FT-IR cell window. When the system is depressurized, FT-IR profile is nearly fully recovered from the initial state, indicating organic salts are well solubilized in dichloromethane.

ESI 7 : Evidences of the DBU quaternization with alkylating agents R-X



Scheme S2: Side reaction between DBU and alkyl halide (R-X): formation of ionic liquid.

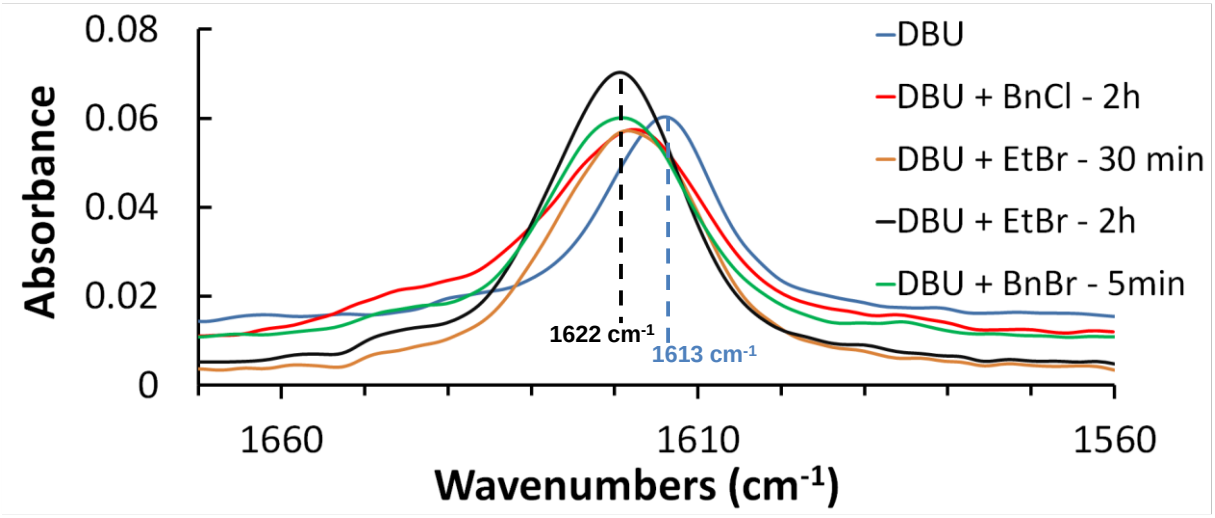


Figure S7 : ATR-IR spectra of the DBU/BnCl, DBU/BnBr and DBU/EtBr systems over time. DBU absorption band is shifted from 1613cm^{-1} to 1622cm^{-1} while alkylation occurs. Depending on the reactivity of R-X, reaction time varies greatly (5min for BnBr, several hours for BnCl).

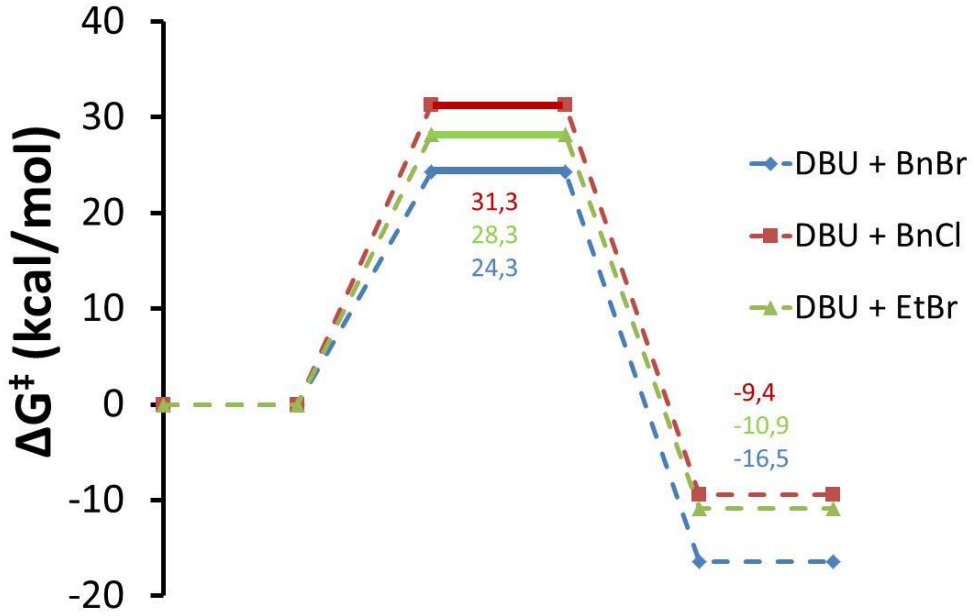


Figure S8 : DFT computed pathway (*M062X/6-311g(d,p)*) of side reaction depicted in Scheme S2.

ESI 8: *In-situ* ATR-IR monitoring of the carbonation reaction of PG to afford PC

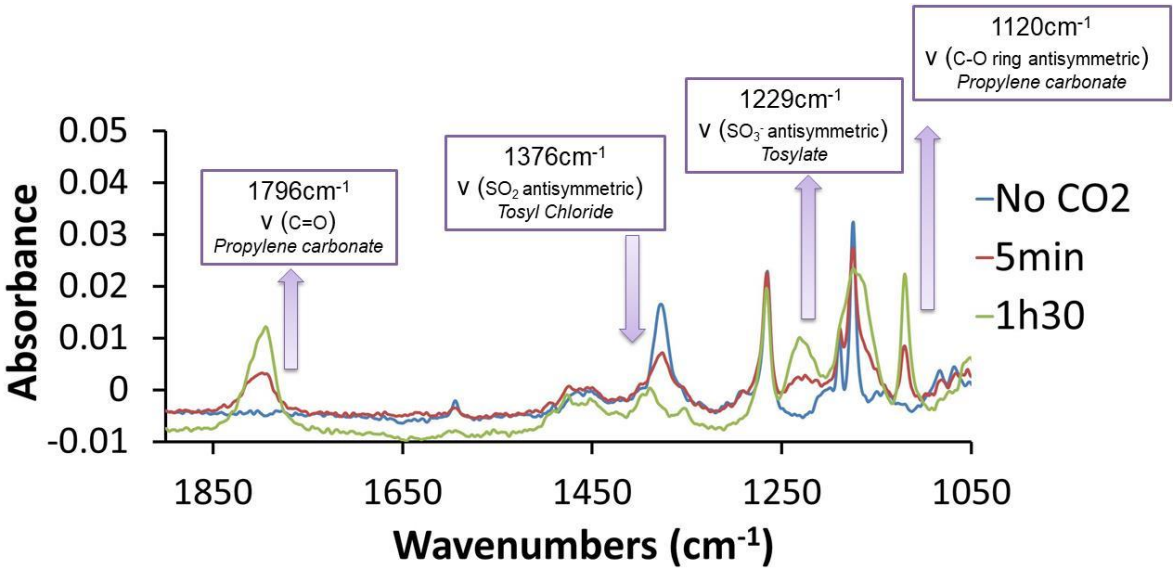
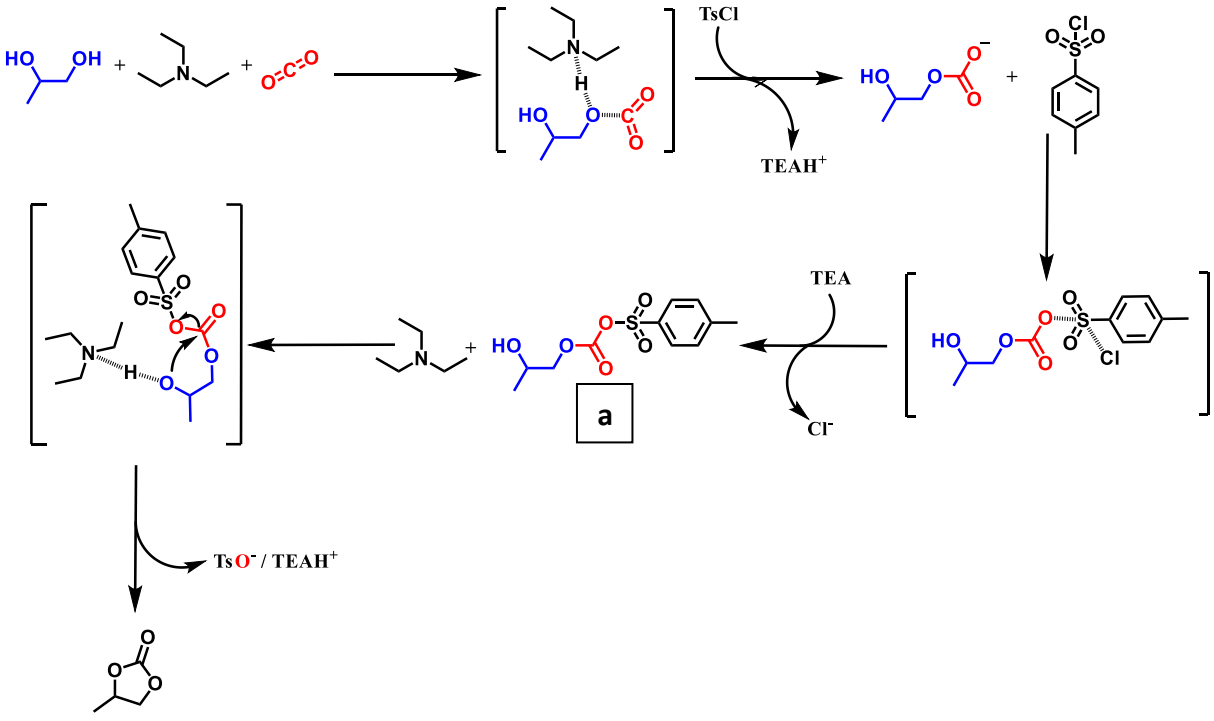


Figure S11: Monitoring of the model reaction between PG and CO2 promoted by a dual TEA/TsCl system using ATR-IR spectroscopy. Conditions: PG (0.5 mmol) ; TEA (1 mmol) ; TsCl (0.5 mmol) ; CH_2Cl_2 (200 µL) ; 1 MPa ; 25°C

Identification of product formation and reactant consumption could confirm the mechanism already proposed in the literature[1]

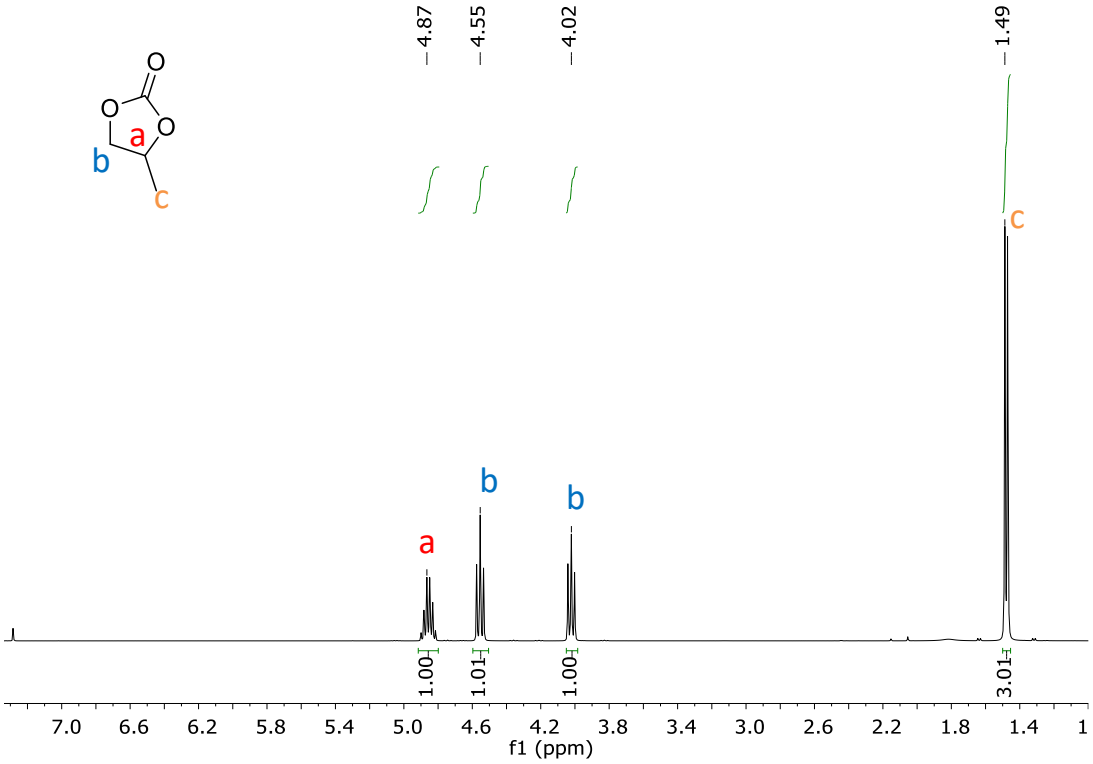


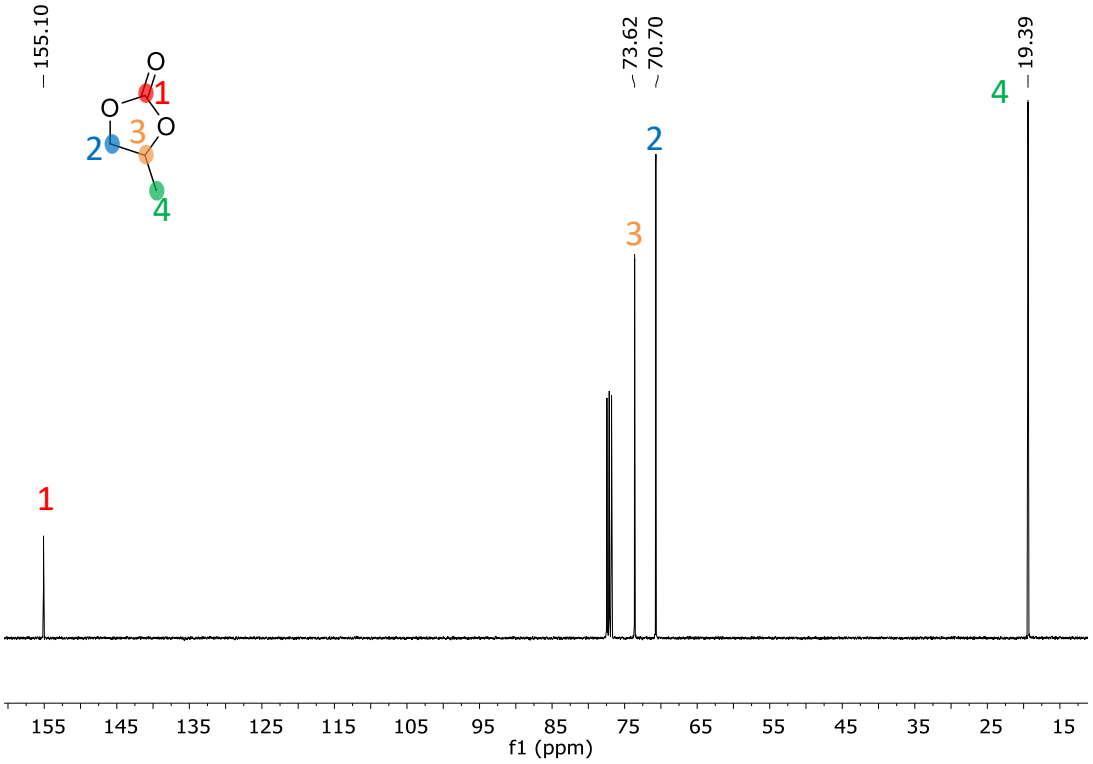
Scheme S3 : Mechanism proposal for the formation of propylene carbonate from PG, inspired from Buchard *et al* [1]. The presence of **a** was not shown by ATR-IR experiments but was proposed regarding preliminaries DFT calculations.

Characterization of organic carbonates

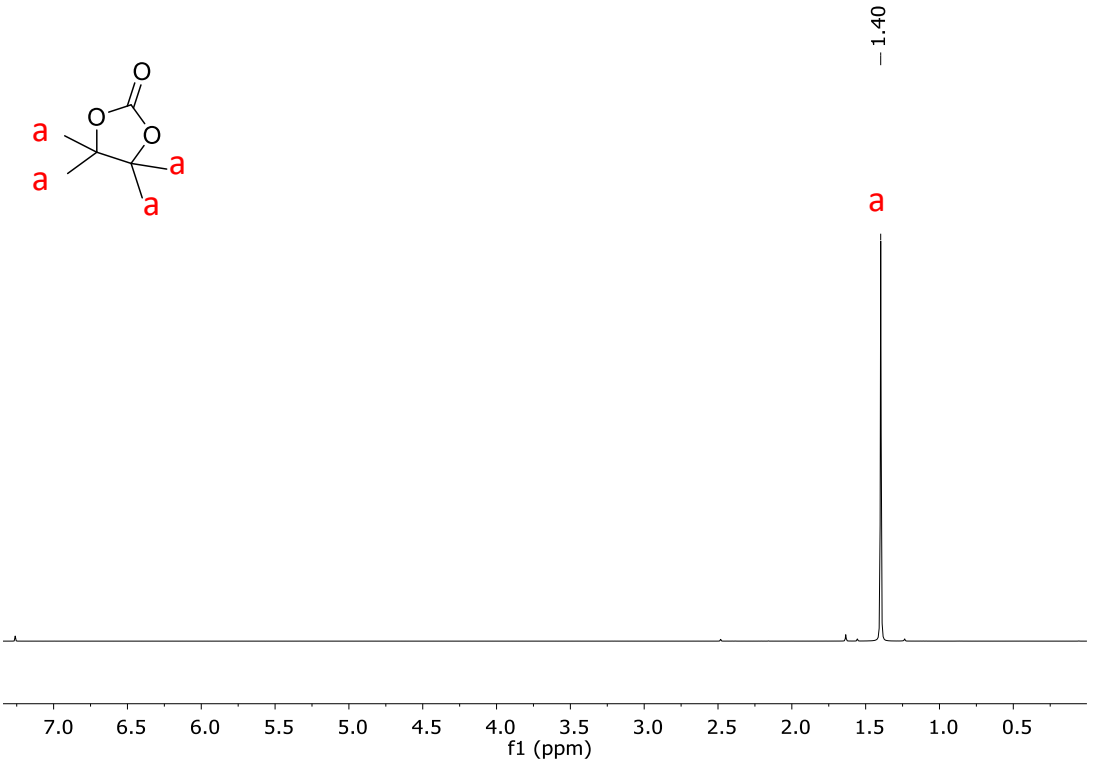
4-Methyl-1,3-dioxolan-2-one : The product was isolated as a colourless oil, 2.136 g (isolated yield 55 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 4.82-4.90 (m, 1 H), 4.55 (dd, *J* = 7.8 Hz, *J* = 8.3 Hz, 1 H), 4.02 (dd, *J* = 7.4 Hz, *J* = 8.3 Hz, 1 H), 1.49 (d, *J* = 6.2 Hz, 3 H).

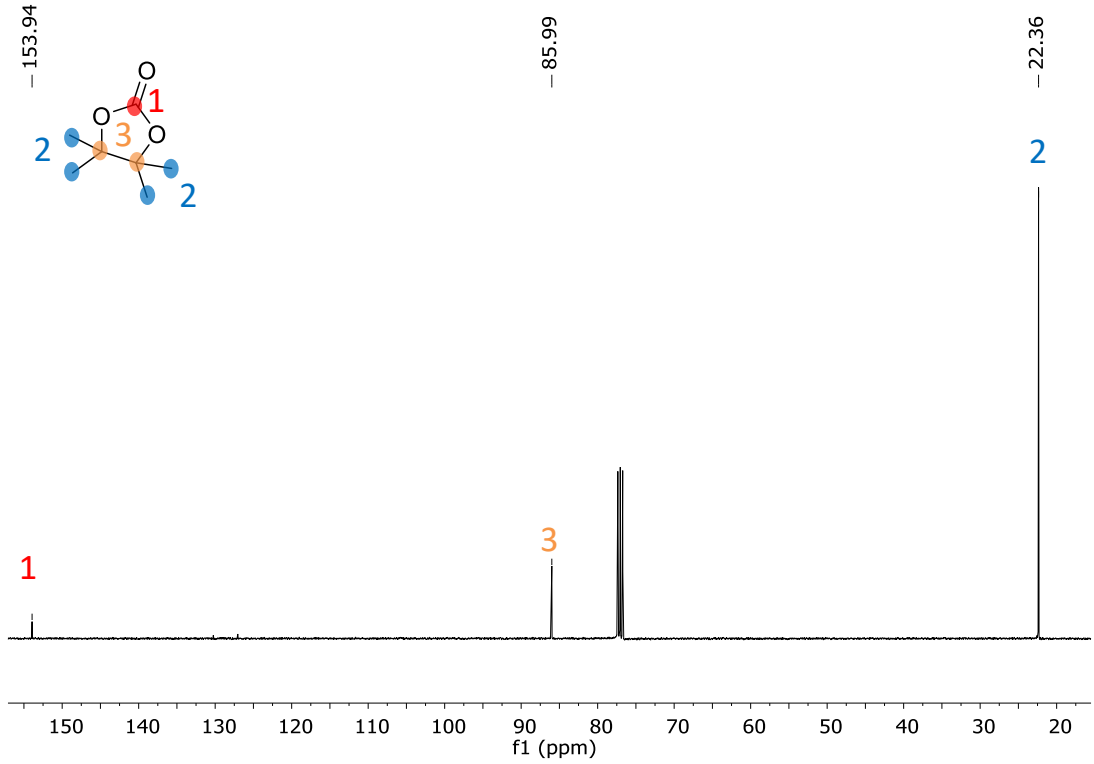
^{13}C NMR (400 MHz, $CDCl_3$) δ (ppm): 155.0, 73. 5, 70.6, 19.2





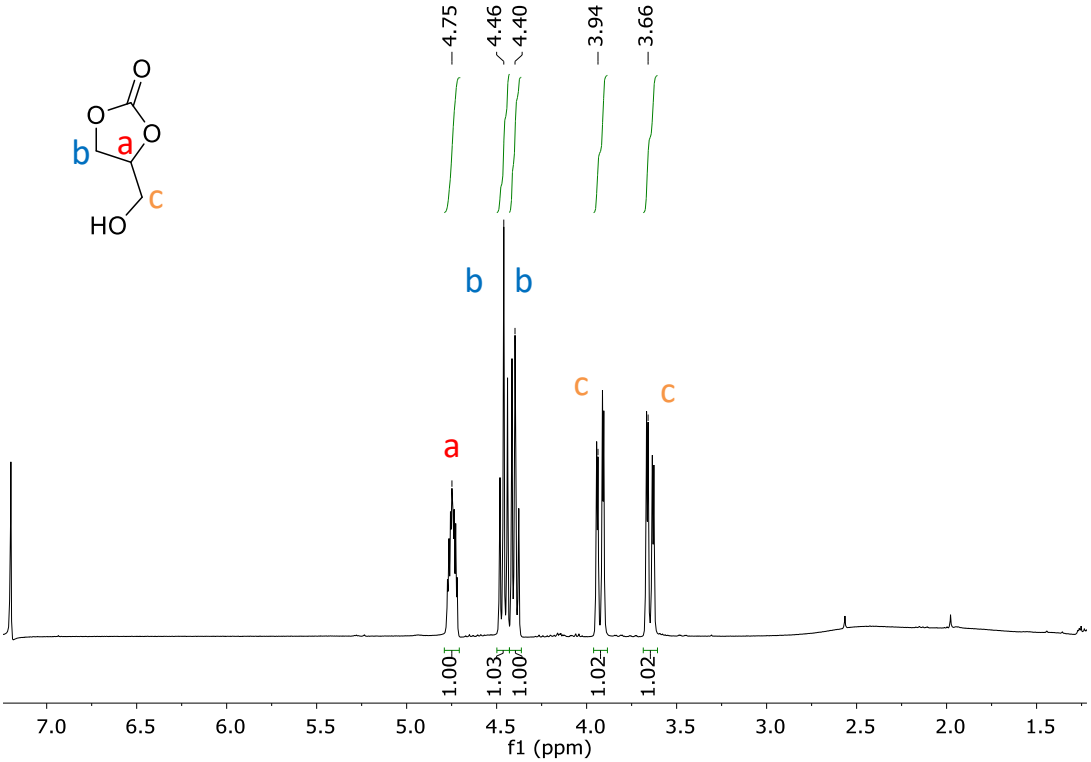
4,4,5,5-Tetramethyl-1,3-Dioxolan-2-one : The product was isolated as a white solid, 1.2976 g (isolated yield 50 %). ^{1}H NMR (400 MHz, CDCl3) δ (ppm): 1.40 (s, 12 H).
^{13}C NMR (400 MHz, CDCl3) δ (ppm): 153.9, 88.99, 22.36

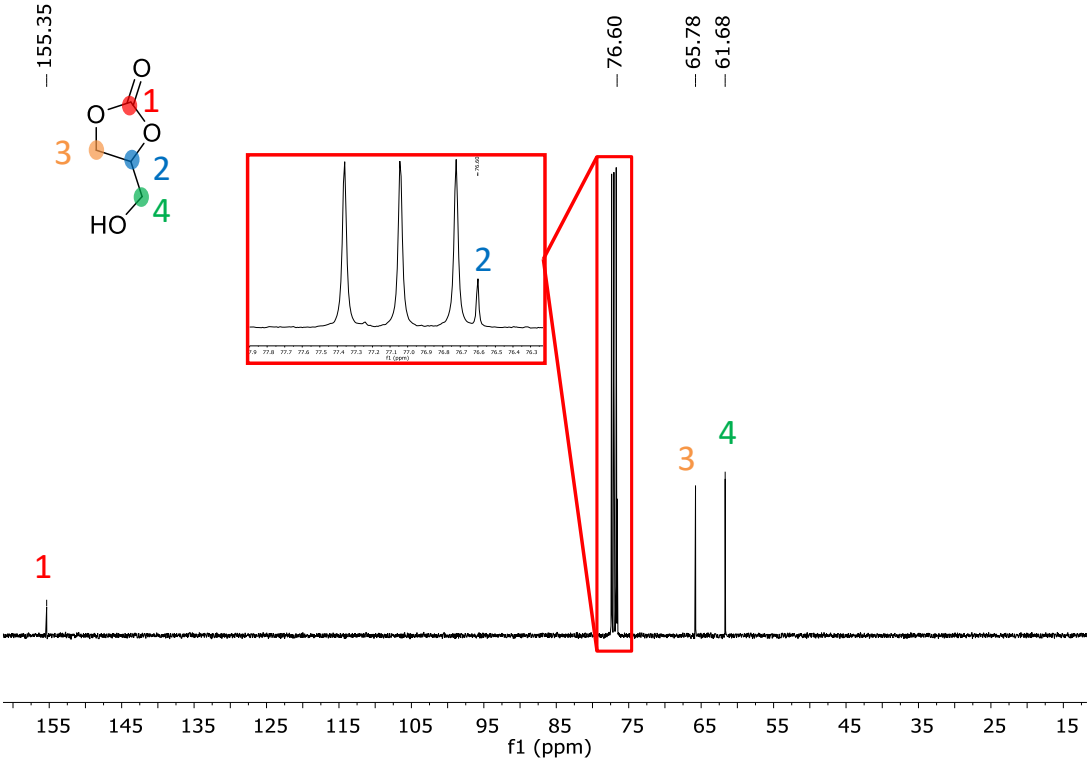




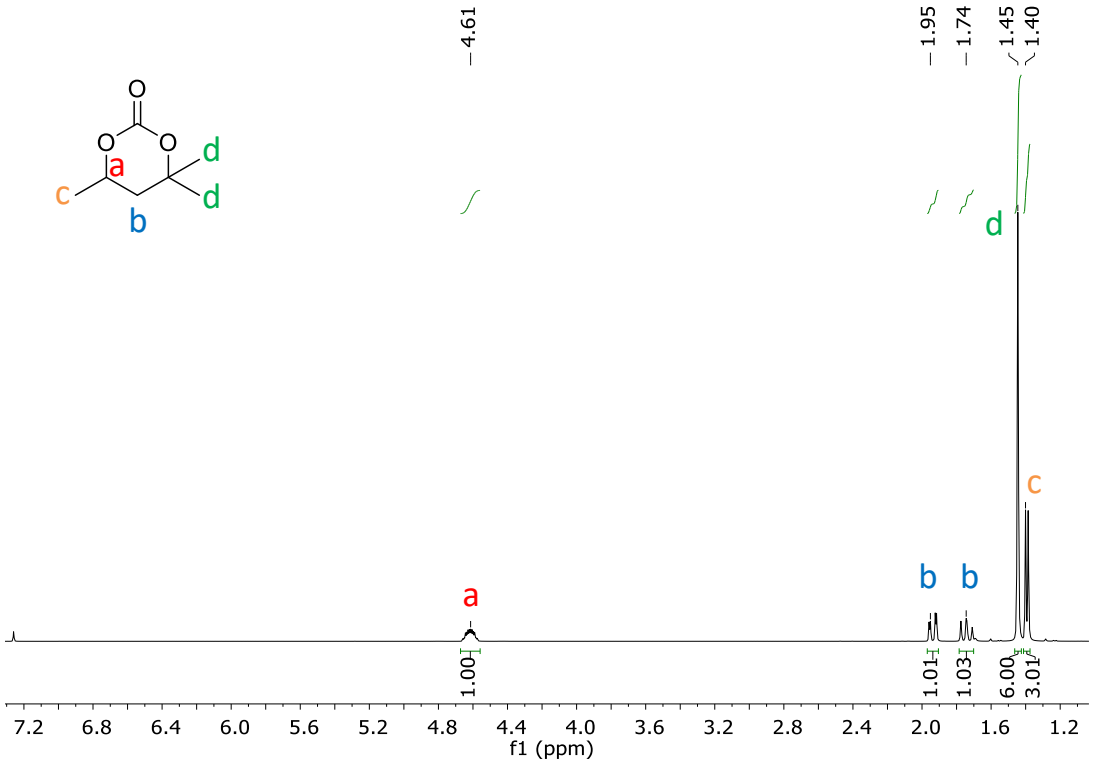
4-(Hydroxymethyl)-1,3-Dioxolan-2-one : The product was isolated as a colourless oil, 0.215 g (isolated yield 60 %). ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 4.75 (m, 1 H), 4.46 (dd, *J* = 8.30 Hz, *J* = 8.46 Hz, 1 H); 4.40 (dd, *J* = 6.74 Hz, *J* = 8.23 Hz, 1 H); 3.94 (dd, *J* = 2.99 Hz, *J* = 9.91 Hz, 1 H); 3.66 (dd, *J* = 3.14 Hz, *J* = 9.38 Hz, 1 H).

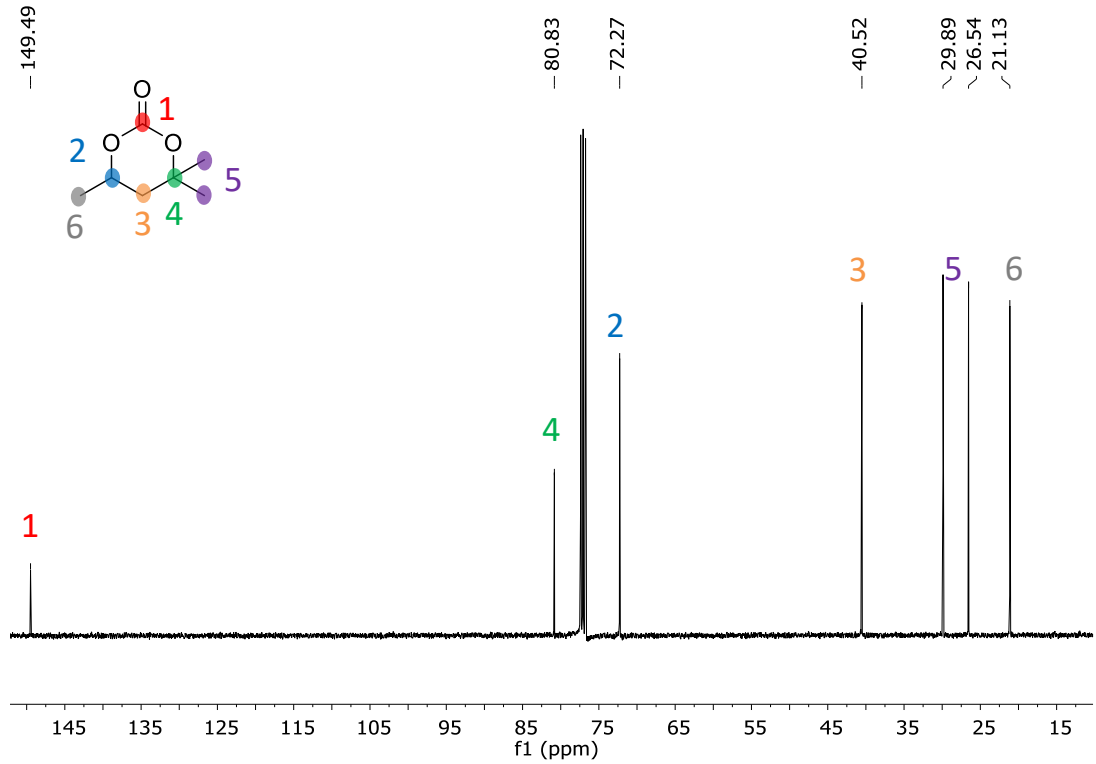
^{13}C NMR (400 MHz, $CDCl_3$) δ (ppm): 155.3, 76.6, 65.8, 61.7





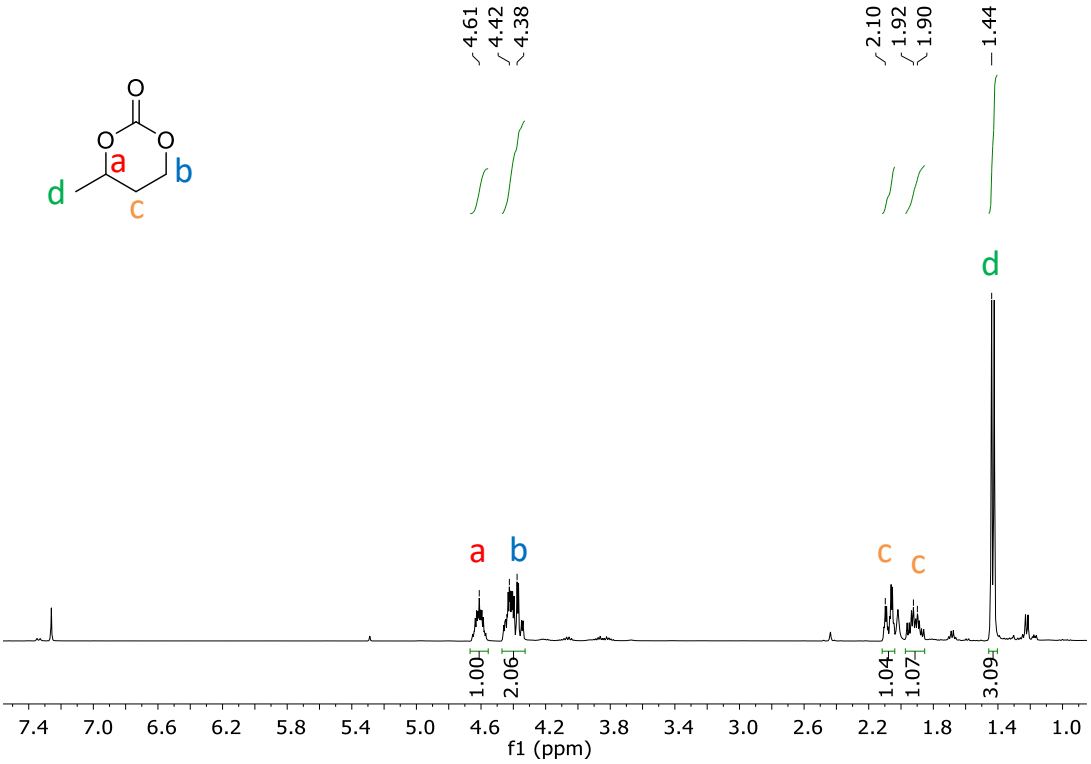
4,4,6-Trimethyl-1,3-Dioxan-2-one : The product was isolated as a white solid, 0.850 g (isolated yield 59 %). ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 4.63 (m, 1 H), 1.95 (dd, *J* =3.0 Hz, *J* = 11.1 Hz, 1 H); 1.74 (dd, *J* = 12.2 Hz, *J* = 13.8 Hz, 2 H); 1.45 (s, 6H); 1.40 (d, *J* = 6.2 Hz, 3 H).
^{13}C NMR (CDCl3, 100 MHz) δ (ppm): 149.5, 80.9, 72.3, 40.5, 29.9, 26.5, 21.1.

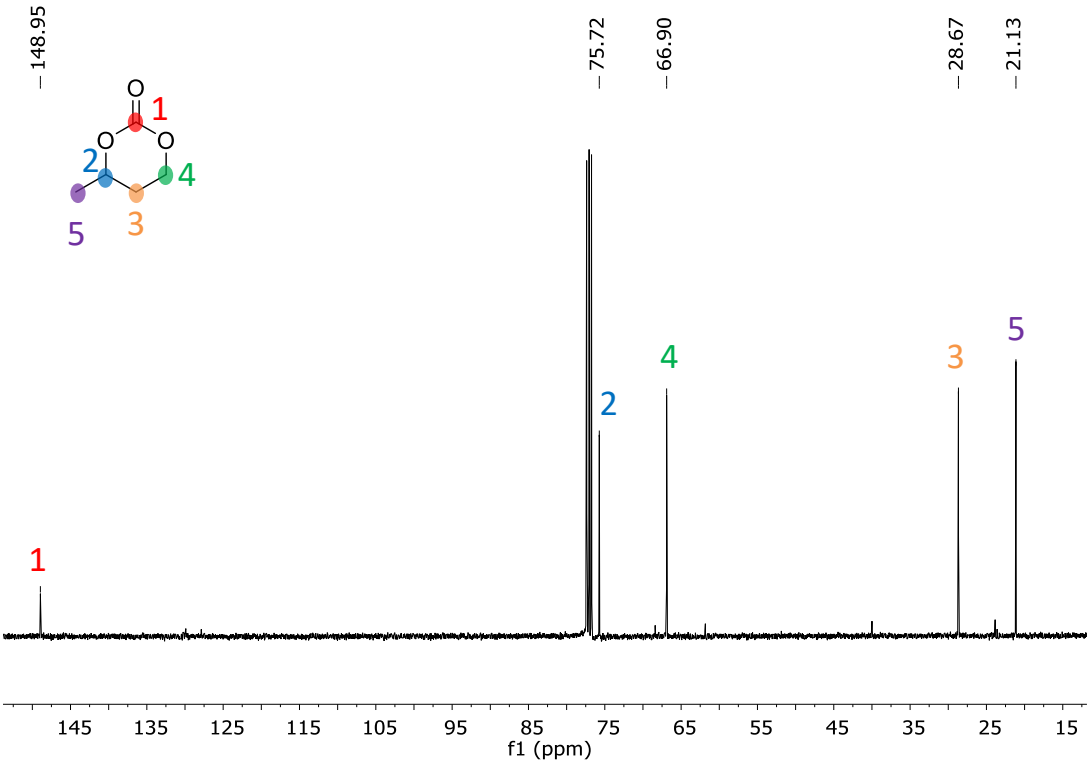




4-Methyl-[1,3]-dioxan-2-one : The product was isolated as a colourless oil, 0.452 g (isolated yield 39 %). ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 4.57-4.65 (m, 1 H), 4.34-4.46 (m, 2 H), 2.04-2.11 (m, 1 H), 1.86-1.96 (m, 1 H), 1.44 (d, J = 6.3, 3 H.

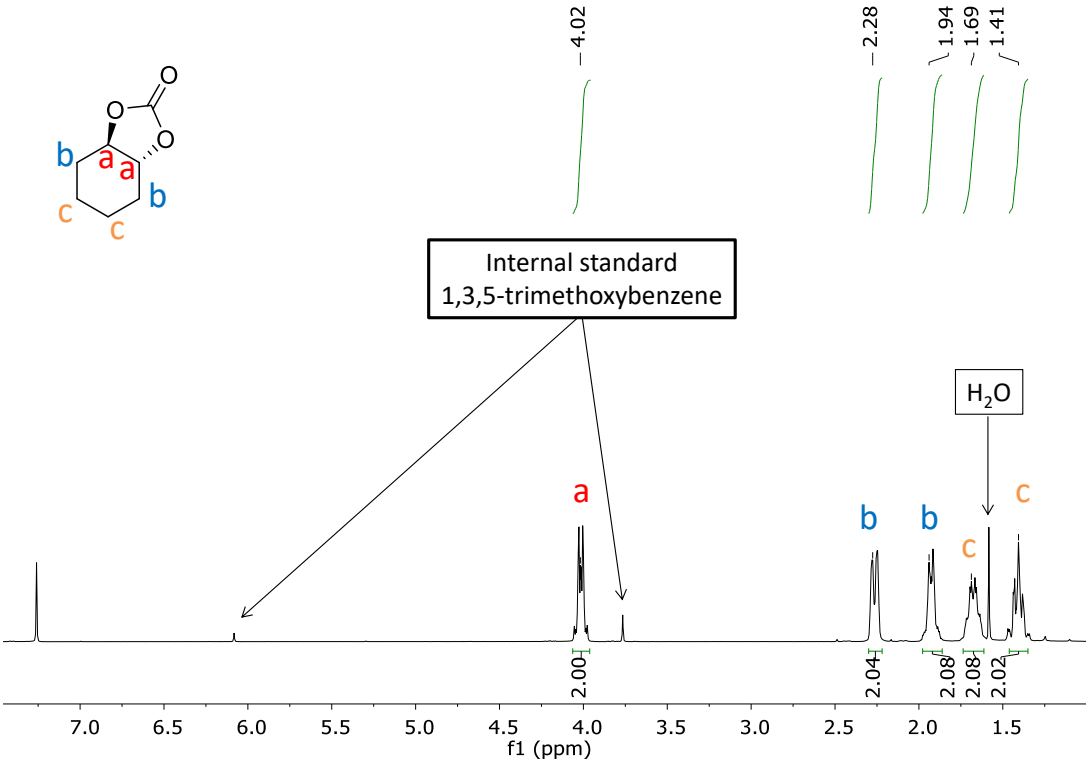
^{13}C NMR ($CDCl_3$, 400 MHz) δ (ppm): 148.9, 75.7, 66.9, 28.7, 21.1

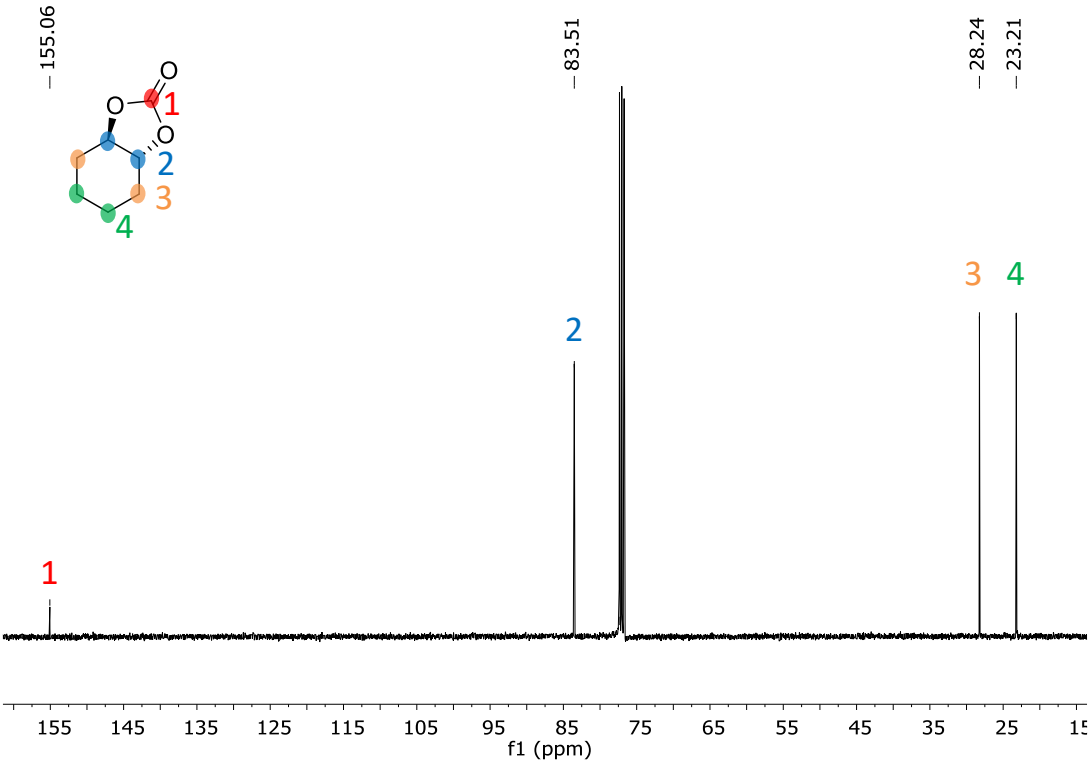




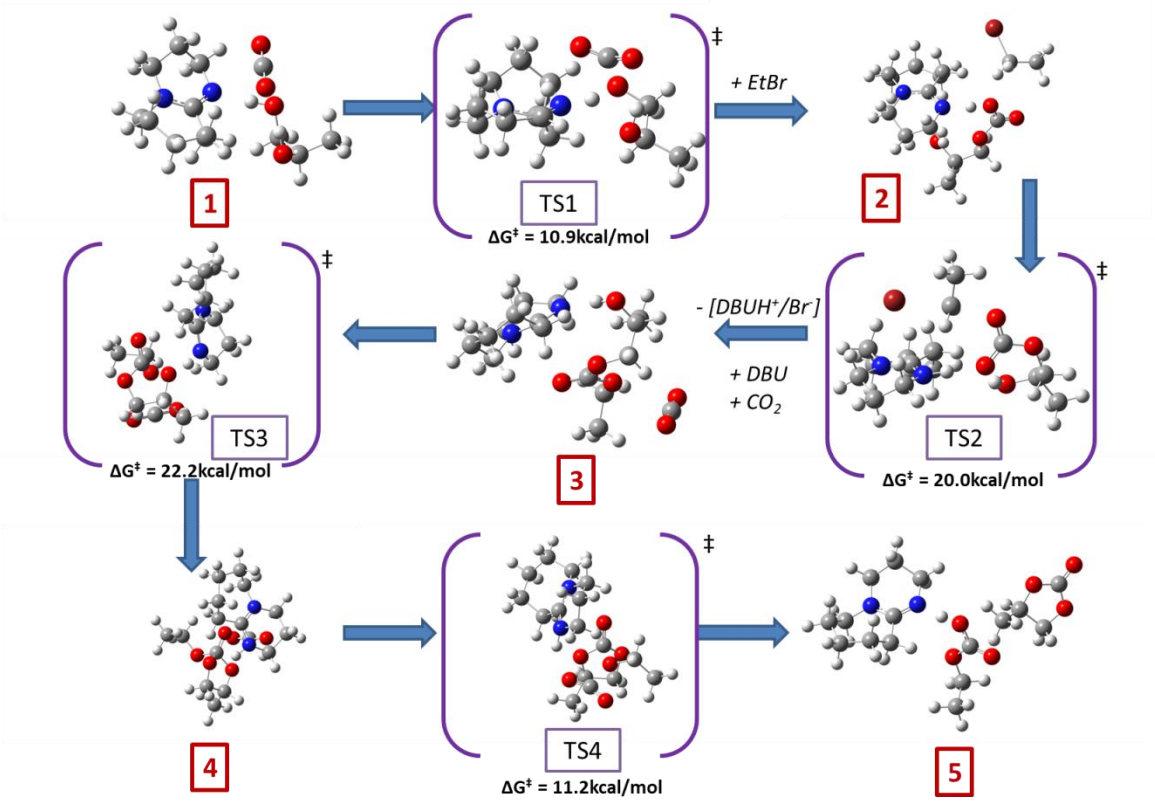
Hexahydro-,(3aR,7aR)-1,3-benzodioxol-2-one : The product was isolated as a white solid, 0.255 g (isolated yield 60 %). ^{1}H NMR (400 MHz, CDCl3) δ (ppm): 3.98-4.05 (m, 2 H), 2.23-2.30 (m, 2 H), 1.88-1.98 (m, 2 H), 1.63-1.73 (m, 2 H), 1.37-1.44 (m, 2 H).

13C NMR (400 MHz, CDCl3) δ (ppm): 155.0, 83.5, 28.2, 23.2





Optimized structures at the *M062X/6-311g(d,p)* level of the intermediates and transition states for the reaction path of the model reaction with PG, DBU (2eq), EtBr (2eq), CO_2 (2eq) calculated with the (R) primary alcohol



TS1:

0 1	X	Y	Z
C	2.131972	2.698591	0.561076
C	0.782169	1.984667	0.481838
C	0.541781	1.216272	-0.829914
C	3.345475	1.769619	0.505221
C	1.15716	-0.156586	-0.819161
C	3.379772	0.906746	-0.758819
H	2.20289	3.415736	-0.266263
H	0.670566	1.290371	1.320702
H	-0.530051	1.093669	-0.965639
H	4.259698	2.369188	0.542358
H	4.385729	0.517461	-0.926521
C	3.132229	-1.523168	-0.306941
H	3.87726	-1.294355	0.460566

N	2.498979	-0.259608	-0.699927
N	0.362704	-1.181172	-0.875277
H	3.130596	1.509612	-1.636259
H	3.358062	1.108922	1.379163
H	2.173047	3.283835	1.483312
H	-0.020046	2.719926	0.574655
H	0.918097	1.790429	-1.683401
H	3.659529	-1.947433	-1.169278
C	2.097072	-2.495229	0.231218
H	2.542476	-3.484619	0.344494
C	0.916804	-2.521114	-0.730691
H	1.225831	-2.904408	-1.710414
H	0.116935	-3.160955	-0.355121
H	1.733431	-2.155891	1.203923
C	-3.077203	-0.884805	-0.325922
C	-3.119033	0.477034	-1.013414
O	-2.616829	1.497644	-0.165286
H	-2.820106	1.260354	0.749464
O	-1.822015	-1.183555	0.236565
H	-0.854198	-1.106923	-0.408683
C	-1.454922	-0.578585	1.862149
O	-2.436452	-0.035301	2.262553
O	-0.327381	-0.898716	2.049309
H	-3.352522	-1.667483	-1.041387
H	-3.810681	-0.89677	0.487984
C	-4.530072	0.803158	-1.48287
H	-4.544155	1.785059	-1.956278
H	-4.893028	0.061776	-2.199415
H	-5.212556	0.825563	-0.62911
H	-2.446406	0.452219	-1.880181

TS2:

0 1	X	Y	Z
C	-1.191798	-3.372695	-1.77191
C	-0.044413	-2.732394	-0.992781
C	-0.223771	-1.22361	-0.756683
C	-2.547553	-3.30416	-1.069561
C	-1.093386	-0.891681	0.420131
C	-2.997998	-1.883584	-0.728372
H	-1.274761	-2.873759	-2.744455
H	0.095199	-3.234067	-0.029666
H	0.750408	-0.767309	-0.59035
H	-3.306682	-3.749059	-1.718749
H	-4.065809	-1.875245	-0.510709
C	-3.235212	-0.941706	1.567959

H	-3.940383	-1.760491	1.721915
N	-2.345186	-1.329502	0.467637
N	-0.553778	-0.205981	1.404724
H	-2.847194	-1.193071	-1.563889
H	-2.52956	-3.894883	-0.147544
H	-0.948403	-4.418088	-1.977661
H	0.891805	-2.86323	-1.537757
H	-0.66589	-0.739169	-1.635065
H	-3.785707	-0.048606	1.253362
C	-2.444847	-0.671267	2.83811
H	-3.109522	-0.261544	3.599
C	-1.326004	0.309269	2.526558
H	-1.738328	1.284739	2.247606
H	-0.649721	0.4329	3.371897
H	-2.021177	-1.603476	3.220157
C	4.570644	0.245832	0.498269
H	4.284749	0.085738	1.542232
H	5.620421	0.536557	0.454507
C	4.371512	-1.037392	-0.302589
O	3.868629	1.365384	-0.043208
H	0.409249	0.145826	1.266274
O	3.104534	-1.636201	-0.063259
H	2.591566	-0.999923	0.456793
C	2.55058	1.505023	0.234454
O	2.031733	2.523689	-0.261793
O	1.984931	0.624136	0.930069
C	-0.063206	3.806582	-1.169093
H	-0.413953	3.696377	-2.193163
H	0.929264	4.257975	-1.172603
H	-0.75487	4.452823	-0.632352
C	0.02985	2.470683	-0.498742
H	0.201953	1.573898	-1.067401
H	-0.070264	2.380349	0.569241
Br	-2.39103	1.871764	-0.682047
H	4.443627	-0.771081	-1.364781
C	5.45089	-2.05147	0.046046
H	5.239966	-2.991326	-0.4646
H	6.44115	-1.702178	-0.254328
H	5.451302	-2.244691	1.121983

TS3:

0 1	X	Y	Z
C	-1.191798	-3.372695	-1.77191
C	-0.044413	-2.732394	-0.992781
C	-0.223771	-1.22361	-0.756683

C	-2.547553	-3.30416	-1.069561
C	-1.093386	-0.891681	0.420131
C	-2.997998	-1.883584	-0.728372
H	-1.274761	-2.873759	-2.744455
H	0.095199	-3.234067	-0.029666
H	0.750408	-0.767309	-0.59035
H	-3.306682	-3.749059	-1.718749
H	-4.065809	-1.875245	-0.510709
C	-3.235212	-0.941706	1.567959
H	-3.940383	-1.760491	1.721915
N	-2.345186	-1.329502	0.467637
N	-0.553778	-0.205981	1.404724
H	-2.847194	-1.193071	-1.563889
H	-2.52956	-3.894883	-0.147544
H	-0.948403	-4.418088	-1.977661
H	0.891805	-2.86323	-1.537757
H	-0.66589	-0.739169	-1.635065
H	-3.785707	-0.048606	1.253362
C	-2.444847	-0.671267	2.83811
H	-3.109522	-0.261544	3.599
C	-1.326004	0.309269	2.526558
H	-1.738328	1.284739	2.247606
H	-0.649721	0.4329	3.371897
H	-2.021177	-1.603476	3.220157
C	4.570644	0.245832	0.498269
H	4.284749	0.085738	1.542232
H	5.620421	0.536557	0.454507
C	4.371512	-1.037392	-0.302589
O	3.868629	1.365384	-0.043208
H	0.409249	0.145826	1.266274
O	3.104534	-1.636201	-0.063259
H	2.591566	-0.999923	0.456793
C	2.55058	1.505023	0.234454
O	2.031733	2.523689	-0.261793
O	1.984931	0.624136	0.930069
C	-0.063206	3.806582	-1.169093
H	-0.413953	3.696377	-2.193163
H	0.929264	4.257975	-1.172603
H	-0.75487	4.452823	-0.632352
C	0.02985	2.470683	-0.498742
H	0.201953	1.573898	-1.067401
H	-0.070264	2.380349	0.569241
Br	-2.39103	1.871764	-0.682047
H	4.443627	-0.771081	-1.364781
C	5.45089	-2.05147	0.046046
H	5.239966	-2.991326	-0.4646

H	6.44115	-1.702178	-0.254328
H	5.451302	-2.244691	1.121983

TS4:

0 1	X	Y	Z
C	-1.191798	-3.372695	-1.77191
C	-0.044413	-2.732394	-0.992781
C	-0.223771	-1.22361	-0.756683
C	-2.547553	-3.30416	-1.069561
C	-1.093386	-0.891681	0.420131
C	-2.997998	-1.883584	-0.728372
H	-1.274761	-2.873759	-2.744455
H	0.095199	-3.234067	-0.029666
H	0.750408	-0.767309	-0.59035
H	-3.306682	-3.749059	-1.718749
H	-4.065809	-1.875245	-0.510709
C	-3.235212	-0.941706	1.567959
H	-3.940383	-1.760491	1.721915
N	-2.345186	-1.329502	0.467637
N	-0.553778	-0.205981	1.404724
H	-2.847194	-1.193071	-1.563889
H	-2.52956	-3.894883	-0.147544
H	-0.948403	-4.418088	-1.977661
H	0.891805	-2.86323	-1.537757
H	-0.66589	-0.739169	-1.635065
H	-3.785707	-0.048606	1.253362
C	-2.444847	-0.671267	2.83811
H	-3.109522	-0.261544	3.599
C	-1.326004	0.309269	2.526558
H	-1.738328	1.284739	2.247606
H	-0.649721	0.4329	3.371897
H	-2.021177	-1.603476	3.220157
C	4.570644	0.245832	0.498269
H	4.284749	0.085738	1.542232
H	5.620421	0.536557	0.454507
C	4.371512	-1.037392	-0.302589
O	3.868629	1.365384	-0.043208
H	0.409249	0.145826	1.266274
O	3.104534	-1.636201	-0.063259
H	2.591566	-0.999923	0.456793
C	2.55058	1.505023	0.234454
O	2.031733	2.523689	-0.261793
O	1.984931	0.624136	0.930069
C	-0.063206	3.806582	-1.169093

H	-0.413953	3.696377	-2.193163
H	0.929264	4.257975	-1.172603
H	-0.75487	4.452823	-0.632352
C	0.02985	2.470683	-0.498742
H	0.201953	1.573898	-1.067401
H	-0.070264	2.380349	0.569241
Br	-2.39103	1.871764	-0.682047
H	4.443627	-0.771081	-1.364781
C	5.45089	-2.05147	0.046046
H	5.239966	-2.991326	-0.4646
H	6.44115	-1.702178	-0.254328
H	5.451302	-2.244691	1.121983

XYZ coordinates of the optimized structures at the *M062X/6-311g(d,p)* level of the transition states for comparison between biscarbonation or alkylation

- Propylene glycol as substrate

TS ALKYLATION

0 1	X	Y	Z
C	-1.191798	-3.372695	-1.77191
C	-0.044413	-2.732394	-0.992781
C	-0.223771	-1.22361	-0.756683
C	-2.547553	-3.30416	-1.069561
C	-1.093386	-0.891681	0.420131
C	-2.997998	-1.883584	-0.728372
H	-1.274761	-2.873759	-2.744455
H	0.095199	-3.234067	-0.029666
H	0.750408	-0.767309	-0.59035
H	-3.306682	-3.749059	-1.718749
H	-4.065809	-1.875245	-0.510709
C	-3.235212	-0.941706	1.567959
H	-3.940383	-1.760491	1.721915
N	-2.345186	-1.329502	0.467637
N	-0.553778	-0.205981	1.404724
H	-2.847194	-1.193071	-1.563889
H	-2.52956	-3.894883	-0.147544
H	-0.948403	-4.418088	-1.977661
H	0.891805	-2.86323	-1.537757
H	-0.66589	-0.739169	-1.635065

H	-3.785707	-0.048606	1.253362
C	-2.444847	-0.671267	2.83811
H	-3.109522	-0.261544	3.599
C	-1.326004	0.309269	2.526558
H	-1.738328	1.284739	2.247606
H	-0.649721	0.4329	3.371897
H	-2.021177	-1.603476	3.220157
C	4.570644	0.245832	0.498269
H	4.284749	0.085738	1.542232
H	5.620421	0.536557	0.454507
C	4.371512	-1.037392	-0.302589
O	3.868629	1.365384	-0.043208
H	0.409249	0.145826	1.266274
O	3.104534	-1.636201	-0.063259
H	2.591566	-0.999923	0.456793
C	2.55058	1.505023	0.234454
O	2.031733	2.523689	-0.261793
O	1.984931	0.624136	0.930069
C	-0.063206	3.806582	-1.169093
H	-0.413953	3.696377	-2.193163
H	0.929264	4.257975	-1.172603
H	-0.75487	4.452823	-0.632352
C	0.02985	2.470683	-0.498742
H	0.201953	1.573898	-1.067401
H	-0.070264	2.380349	0.569241
Br	-2.39103	1.871764	-0.682047
H	4.443627	-0.771081	-1.364781
C	5.45089	-2.05147	0.046046
H	5.239966	-2.991326	-0.4646
H	6.44115	-1.702178	-0.254328
H	5.451302	-2.244691	1.121983

TS BISCARBONATION

0 1	X	Y	Z
C	5.896744	1.359414	-1.903946
C	5.024955	2.004856	-0.829043
C	3.688607	1.284353	-0.597751
C	6.358428	-0.053251	-1.557666
C	3.760553	0.08221	0.294017
C	5.215029	-1.028819	-1.290168
H	5.328612	1.32664	-2.840262
H	5.577257	2.075755	0.113981
H	2.958881	1.970261	-0.166499
H	6.944597	-0.449664	-2.391289
H	5.591697	-2.049927	-1.340484

C	4.495979	-2.165692	0.78889
H	5.480564	-2.635499	0.790064
N	4.614807	-0.899063	0.050304
N	2.964974	0.062173	1.351386
H	4.407006	-0.95379	-2.024184
H	7.01813	-0.035031	-0.683815
H	6.770471	1.990207	-2.086803
H	4.794102	3.02824	-1.131903
H	3.238466	0.929614	-1.531684
H	3.785867	-2.78449	0.230736
C	4.01142	-1.930887	2.208776
H	3.839216	-2.891332	2.695156
C	2.721877	-1.130748	2.163204
H	1.909698	-1.705114	1.704843
H	2.417671	-0.801266	3.156752
H	4.76878	-1.388223	2.780524
C	-5.298428	0.529742	-2.402024
C	-4.171841	1.11781	-1.55056
C	-4.371047	0.965437	-0.031171
C	-5.496946	-0.978921	-2.250731
C	-3.929269	-0.385877	0.463336
C	-5.772205	-1.406317	-0.807146
H	-6.235879	1.033186	-2.135955
H	-3.212075	0.670785	-1.833
H	-3.794358	1.71619	0.509356
H	-6.340402	-1.291637	-2.873106
H	-6.220196	-2.400978	-0.785455
C	-4.018381	-2.828531	0.248242
H	-4.154602	-3.400846	-0.673422
N	-4.567612	-1.486535	0.018716
N	-2.907218	-0.430579	1.262175
H	-6.494646	-0.729949	-0.341934
H	-4.614337	-1.519004	-2.610851
H	-5.109661	0.761246	-3.453531
H	-4.089372	2.184864	-1.769565
H	-5.421059	1.132234	0.229858
H	-4.597547	-3.322226	1.037384
C	-2.545644	-2.754172	0.611999
H	-2.196297	-3.730297	0.95088
C	-2.346352	-1.706251	1.694993
H	-2.821613	-2.009813	2.634696
H	-1.280509	-1.557714	1.865918
H	-1.935412	-2.46759	-0.247162
C	-0.19774	1.13551	0.964638
H	0.177181	0.248929	1.493437
H	0.514016	1.967457	1.082967

C	-0.322104	0.791649	-0.52256
H	-1.119333	0.050039	-0.631825
C	-0.622878	2.023628	-1.355642
H	0.180004	2.757701	-1.253214
H	-0.724534	1.755042	-2.409
H	-1.549601	2.491378	-1.015065
O	-1.424447	1.527791	1.509109
H	-2.253652	0.57373	1.441913
O	0.896338	0.233458	-0.995253
H	2.289821	0.812114	1.409946
C	1.143527	-1.128694	-0.69968
C	-1.764537	3.272339	1.650742
O	2.229516	-1.516098	-1.152518
O	0.300543	-1.718982	-0.009215
O	-2.936498	3.327547	1.842114
O	-0.730463	3.835544	1.503142

- Ethylene glycol as substrate

TS ALKYLATION

0 1	X	Y	Z
C	-1.69809	-3.190549	-1.743564
C	-0.439784	-2.811879	-0.964656
C	-0.280289	-1.298278	-0.744921
C	-3.006964	-2.814481	-1.049823
C	-1.058394	-0.76918	0.423807
C	-3.131658	-1.325515	-0.726048
H	-1.66494	-2.697384	-2.722013
H	-0.418232	-3.320969	0.004435
H	0.770118	-1.067675	-0.576675
H	-3.843979	-3.087187	-1.698434
H	-4.171679	-1.077793	-0.514762
C	-3.16146	-0.327583	1.558696
H	-4.03311	-0.965497	1.715637
N	-2.376278	-0.916906	0.468131
N	-0.382915	-0.211116	1.405368
H	-2.828317	-0.695355	-1.567777
H	-3.123437	-3.38362	-0.12142
H	-1.692106	-4.266295	-1.936313
H	0.445795	-3.154044	-1.502497
H	-0.600402	-0.736965	-1.63039
H	-3.49586	0.662829	1.231718
C	-2.336171	-0.228312	2.83149
H	-2.895317	0.327613	3.584441
C	-1.024589	0.473485	2.518979

H	-1.20665	1.514258	2.230852
H	-0.341325	0.449447	3.367433
H	-2.134083	-1.227885	3.224542
C	4.717277	-0.902138	0.504683
H	4.428592	-0.995488	1.554981
H	5.804386	-0.865654	0.434121
C	4.203295	-2.087375	-0.299111
O	4.291155	0.360101	-0.013711
H	0.634177	-0.081899	1.26704
O	2.867351	-2.453586	-0.006299
H	2.493896	-1.713749	0.494351
C	3.030718	0.77638	0.252013
O	2.751229	1.89307	-0.225873
O	2.276988	0.02456	0.920124
C	0.992474	3.586829	-1.172658
H	0.639607	3.545694	-2.201109
H	2.058712	3.814488	-1.164049
H	0.448798	4.371125	-0.649757
C	0.787426	2.267981	-0.493504
H	0.769295	1.349993	-1.054127
H	0.657004	2.210798	0.57347
Br	-1.702824	2.202563	-0.707916
H	4.308537	-1.845174	-1.363375
H	4.847171	-2.946622	-0.083987

TS BISCARBONATION

0 1	X	Y	Z
C	-5.89962	1.565235	1.828121
C	-4.987354	2.151637	0.753075
C	-3.670255	1.383194	0.569735
C	-6.399029	0.158017	1.513298
C	-3.76419	0.15907	-0.289447
C	-5.282406	-0.860236	1.296546
H	-5.350967	1.542434	2.776251
H	-5.51895	2.212201	-0.202523
H	-2.910536	2.03359	0.135699
H	-7.012988	-0.195485	2.346221
H	-5.692209	-1.86719	1.368234
C	-4.557025	-2.078599	-0.734465
H	-5.553168	-2.523216	-0.73605
N	-4.653113	-0.788082	-0.035046
N	-2.950746	0.084414	-1.330935
H	-4.486269	-0.789058	2.043839
H	-7.041331	0.171224	0.626473
H	-6.756449	2.227811	1.975169

H	-4.729643	3.175613	1.031111
H	-3.251629	1.041102	1.522792
H	-3.870766	-2.69878	-0.148428
C	-4.04802	-1.896919	-2.153653
H	-3.897914	-2.874735	-2.611931
C	-2.735873	-1.134211	-2.112305
H	-1.946102	-1.72097	-1.631426
H	-2.412124	-0.837302	-3.110018
H	-4.78248	-1.34842	-2.749249
C	5.534567	0.860639	2.113606
C	4.437112	1.401058	1.194898
C	4.581097	0.972617	-0.275051
C	5.626539	-0.665671	2.183659
C	4.016003	-0.397929	-0.521109
C	5.850779	-1.327408	0.820127
H	6.499722	1.249802	1.766906
H	3.449219	1.096943	1.558459
H	4.048907	1.672277	-0.917073
H	6.455562	-0.939968	2.842479
H	6.241467	-2.337636	0.949945
C	3.988849	-2.789195	0.040375
H	4.150357	-3.225239	1.029834
N	4.625117	-1.464839	0.032199
N	2.92904	-0.480428	-1.228644
H	6.600917	-0.775904	0.2472
H	4.715088	-1.083915	2.625326
H	5.386314	1.254483	3.122459
H	4.453101	2.492714	1.222633
H	5.633465	0.999004	-0.574566
H	4.491586	-3.429864	-0.693085
C	2.502833	-2.680091	-0.25252
H	2.082061	-3.668838	-0.438126
C	2.287743	-1.773272	-1.453359
H	2.699556	-2.222579	-2.364287
H	1.22054	-1.606231	-1.588267
H	1.960408	-2.25549	0.594402
C	0.233754	1.08772	-0.948069
H	-0.10212	0.198834	-1.499087
H	-0.492166	1.901006	-1.088468
C	0.31726	0.748253	0.537897
H	1.113308	0.015579	0.695569
O	1.473385	1.513757	-1.441167
H	2.287241	0.536541	-1.411508
O	-0.912688	0.261721	1.040605
H	-2.248737	0.808844	-1.393862
C	-1.215557	-1.095671	0.780311

C	1.802656	3.275844	-1.267954
O	-2.312887	-1.429815	1.24692
O	-0.398971	-1.732947	0.100054
O	2.954461	3.39591	-1.532914
O	0.777736	3.774934	-0.94126
H	0.54816	1.660396	1.093749

- 1,3-propanediol as substrate

TS ALKYLATION

0 1	X	Y	Z
C	-2.54722	-3.465127	-1.273719
C	-1.023686	-3.3707	-1.379176
C	-0.486416	-1.928639	-1.38996
C	-3.144041	-2.862643	-0.000718
C	-0.38421	-1.355706	-0.006558
C	-2.81679	-1.381868	0.185226
H	-2.986321	-2.95432	-2.138305
H	-0.55076	-3.931008	-0.5653
H	0.503015	-1.86942	-1.843063
H	-4.23156	-2.963445	-0.039561
H	-3.49543	-0.898892	0.885548
C	-1.385939	-0.687497	2.12103
H	-2.167506	-1.211502	2.674332
N	-1.462671	-1.16054	0.725058
N	0.829905	-1.126188	0.475905
H	-2.92497	-0.826463	-0.748988
H	-2.805504	-3.415996	0.88242
H	-2.844372	-4.514106	-1.348266
H	-0.707779	-3.847672	-2.309175
H	-1.119648	-1.274917	-1.994284
H	-1.628506	0.379113	2.122344
C	-0.021621	-0.97525	2.72438
H	0.062774	-0.461487	3.681932
C	1.066238	-0.502301	1.775081
H	1.062051	0.586725	1.657972
H	2.055012	-0.807607	2.116698
H	0.096538	-2.047505	2.901638
C	3.849702	0.280894	-1.332413
H	4.077968	1.334671	-1.505519
O	2.490714	0.02731	-1.687138
H	1.588291	-1.143191	-0.200152
C	1.570481	1.015795	-1.320401
O	0.446325	0.804947	-1.855489
O	1.906346	1.881743	-0.528411

C	4.143258	-0.083953	0.114564
C	5.613775	0.081397	0.471755
H	3.86271	-1.12719	0.304287
H	3.539986	0.564954	0.755792
H	6.227798	-0.598528	-0.122805
H	5.941255	1.104382	0.246682
H	4.443515	-0.330616	-2.01473
O	5.86618	-0.249297	1.825287
H	5.445009	0.418877	2.370962
C	-1.022346	1.744117	-0.890129
C	-0.883765	3.125617	-1.455703
H	-1.653088	1.01816	-1.370848
H	-0.516193	1.48484	0.023496
H	-1.822644	3.445173	-1.903924
H	-0.605768	3.827398	-0.672419
H	-0.102773	3.115998	-2.216065
Br	-3.004423	2.155092	0.567686

TS BISCARBONATION

0 1	X	Y	Z
C	4.490922	-2.074216	1.331298
C	3.512593	-0.924629	1.573395
C	3.594576	0.216584	0.542402
C	4.273414	-2.820393	0.016395
C	2.830198	-0.055889	-0.727286
C	4.385177	-1.906821	-1.204854
H	5.515431	-1.682209	1.346711
H	2.486914	-1.30392	1.60929
H	3.184355	1.13592	0.959927
H	5.02013	-3.614247	-0.074175
H	4.56304	-2.497594	-2.104617
C	2.340666	-1.602796	-2.579702
H	2.261295	-2.689529	-2.483212
N	3.178797	-1.122425	-1.473016
N	1.858522	0.743894	-1.048569
H	5.24398	-1.237127	-1.09986
H	3.288302	-3.299052	0.008
H	4.415381	-2.780495	2.161713
H	3.725575	-0.495772	2.5559
H	4.64025	0.428086	0.293354
H	2.850555	-1.385899	-3.52507
C	0.966636	-0.95742	-2.54512
H	0.456271	-1.138595	-3.492464
C	1.136002	0.533576	-2.300198
H	1.693193	1.011572	-3.112821

H	0.187279	1.058025	-2.228472
H	0.354297	-1.391341	-1.749313
C	0.728443	0.794553	2.49328
H	0.923729	0.48704	1.468263
C	0.752578	4.00457	-0.968499
O	0.642177	3.424527	-2.003133
O	0.779668	5.02789	-0.375768
C	0.311314	2.253006	2.51095
C	1.200279	3.054092	1.562388
H	0.354368	2.659547	3.524769
H	-0.719794	2.337783	2.1579
H	0.988509	4.122017	1.655529
H	2.259832	2.917351	1.834445
H	1.634529	0.638578	3.086749
O	0.968336	2.678826	0.227958
H	1.502029	1.671284	-0.364586
C	-3.480345	2.212756	-0.762782
C	-2.21569	1.455364	-1.164163
C	-1.752482	0.40402	-0.143624
C	-4.724844	1.339838	-0.621583
C	-2.443599	-0.938019	-0.24223
C	-4.546513	0.195967	0.376927
H	-3.291384	2.715241	0.193659
H	-2.356991	0.975091	-2.139947
H	-0.685533	0.220527	-0.268719
H	-5.562236	1.960648	-0.28937
H	-5.523544	-0.194166	0.666383
C	-4.548802	-2.193702	-0.27753
H	-5.481616	-1.971704	-0.804024
N	-3.797119	-0.946771	-0.150407
N	-1.697787	-1.986371	-0.415469
H	-4.072944	0.553771	1.296944
H	-5.004807	0.912521	-1.590659
H	-3.670325	3.002267	-1.494273
H	-1.404682	2.178328	-1.279178
H	-1.883209	0.79722	0.872294
H	-4.804738	-2.567113	0.721463
C	-3.733799	-3.226775	-1.034437
H	-4.234164	-4.195934	-0.994579
C	-2.346671	-3.291641	-0.411035
H	-2.419362	-3.642255	0.62668
H	-1.708949	-3.992751	-0.952953
H	-3.645962	-2.931482	-2.083831
O	-0.30834	-0.028354	3.04585
H	-0.506469	-1.864046	0.642088
C	-0.750146	-1.094726	2.361228

O	-1.818673	-1.584318	2.611586
O	0.080724	-1.517279	1.41238

➢ 1,4-butanediol as substrate

TS ALKYLATION

0 1	X	Y	Z
C	-4.58571300	-2.17616200	-1.52771300
C	-3.21198100	-2.59302500	-1.00423400
C	-2.22412300	-1.42871100	-0.82044500
C	-5.36229800	-1.25251100	-0.59174600
C	-2.40092900	-0.66653000	0.46144300
C	-4.62069700	0.04040900	-0.25671500
H	-4.45348900	-1.66976700	-2.49080000
H	-3.31365000	-3.13481600	-0.05818200
H	-1.19975500	-1.80330800	-0.82616500
H	-6.31073300	-0.98363500	-1.06482000
H	-5.31741000	0.77352000	0.14956500
C	-3.73075100	0.69344400	1.97424400
H	-4.76020400	0.57753200	2.31862500
N	-3.57679600	-0.12411600	0.76568500
N	-1.36718600	-0.60246700	1.26718600
H	-4.17458500	0.49724000	-1.14561000
H	-5.60531900	-1.77054100	0.34199000
H	-5.18119500	-3.07136700	-1.72446900
H	-2.76376100	-3.29168500	-1.71351200
H	-2.31518000	-0.70590800	-1.64024100
H	-3.56321200	1.73953600	1.69530800
C	-2.75280400	0.25897100	3.05383800
H	-2.79938100	0.95800500	3.88929100
C	-1.35213500	0.22447900	2.46423100

H	-1.03134600	1.23544400	2.18966700
H	-0.62955500	-0.20299100	3.15892500
H	-3.02013500	-0.73413400	3.42362300
C	4.20654200	-1.62565300	-0.69044800
H	4.04714100	-1.03695300	-1.59605200
O	2.95360500	-2.07676000	-0.17877800
H	-0.46439800	-1.01184900	0.92374200
C	1.92378700	-1.19539400	-0.16234300
O	0.85515100	-1.64749100	0.28231100
O	2.14501600	-0.03456500	-0.59961300
C	4.98265100	-0.81933500	0.33798100
C	6.35911200	-0.42193300	-0.18663300
H	5.08216500	-1.42021700	1.24797400
H	4.40159200	0.07217900	0.58861300
C	7.15055000	0.38118000	0.82618600
H	6.94151100	-1.31099000	-0.44904600
H	6.26111300	0.17707300	-1.09732000
H	6.59552000	1.29306400	1.08469600
H	7.27745300	-0.20867000	1.74426700
H	4.74749600	-2.53822000	-0.94711100
C	1.22158900	2.22081900	-1.57818200
H	2.25860800	1.91393300	-1.71560200
H	1.19252800	3.18288500	-1.07043500
H	0.74422700	2.32872100	-2.55020200
C	0.52148200	1.17594000	-0.76303600
H	0.52801900	1.21844400	0.31199700
H	0.02969300	0.33926500	-1.22816500
Br	-1.68918100	2.28798900	-0.68785000
O	8.40488600	0.69501800	0.24579400
H	8.91048400	1.20913400	0.87782800

TS BISCARBONATION

0 1	X	Y	Z
C	7.06411800	1.05617700	-1.74019600
C	5.87277100	1.84333100	-1.19916300
C	4.62293400	0.98532400	-0.95197000
C	7.59333000	-0.00136800	-0.77579600
C	4.61582900	0.23487000	0.34557200
C	6.55048000	-1.03584900	-0.35991900
H	6.76324400	0.56600200	-2.67270900
H	6.15223700	2.36791200	-0.27923400
H	3.72876200	1.60838400	-0.97537300
H	8.41832900	-0.53620600	-1.25429900
H	7.05221600	-1.90037300	0.07335100
C	5.44481100	-1.48622400	1.81280100
H	6.43953600	-1.75359000	2.17098000
N	5.61763000	-0.56354800	0.68019900
N	3.58994500	0.43816700	1.15767100
H	5.95236600	-1.40384900	-1.19916900
H	7.99938800	0.47262300	0.12396400
H	7.86996500	1.74998100	-1.99337700
H	5.60131300	2.61210800	-1.92569800
H	4.47415900	0.22784700	-1.72966000
H	4.93721300	-2.37238200	1.41618000
C	4.63090400	-0.83996500	2.92000600
H	4.45430500	-1.56767000	3.71241100
C	3.30640700	-0.36899400	2.34707500
H	2.67480400	-1.21054700	2.04483600
H	2.76681200	0.26118500	3.05480200
H	5.18213800	0.00302000	3.34529200
C	0.75789300	-0.31003800	-1.39971100
H	0.13211300	-1.19672200	-1.26789900

O	2.12002600	-0.68491500	-1.46009200
H	2.82607200	0.97453200	0.77032900
C	2.53254900	-1.70057200	-0.55536600
O	3.72828100	-1.99631500	-0.70420900
O	1.69497200	-2.09114900	0.26227900
C	0.46866500	0.67212100	-0.27030500
C	-0.99939000	1.07615400	-0.22955200
H	1.08616800	1.57163100	-0.40543400
H	0.74297000	0.18350800	0.67108800
C	-1.33779400	2.00165000	0.93248500
H	-1.27712500	1.58588900	-1.15982800
H	-1.61611300	0.17289300	-0.14946900
H	-1.08906600	1.51855600	1.88594200
H	-0.76555700	2.92981200	0.85353600
H	0.52594900	0.15301400	-2.36318200
C	-4.58023900	-1.82541000	-2.71471400
C	-3.64647200	-0.85456500	-1.99024100
C	-4.36473700	0.29274100	-1.25754600
C	-5.54758400	-2.57878300	-1.80132800
C	-4.85217400	-0.11035900	0.10652400
C	-6.43936500	-1.65163700	-0.97322500
H	-5.16328000	-1.26423100	-3.45461000
H	-3.01630200	-1.40194500	-1.28068800
H	-3.70137400	1.14140900	-1.11650300
H	-6.18968600	-3.21894900	-2.41287700
H	-7.30527100	-2.19770400	-0.59615600
C	-6.14069400	-1.66883900	1.49969000
H	-6.23766900	-2.74919700	1.36370900
N	-5.77276500	-1.08897600	0.20421900
N	-4.32520000	0.46968000	1.14233600
H	-6.82938600	-0.84148800	-1.59526200

H	-4.99682800	-3.23586500	-1.11923000
H	-3.98076100	-2.54810100	-3.27376000
H	-2.96681000	-0.40896600	-2.72042000
H	-5.20563400	0.66731300	-1.84908900
H	-7.11892900	-1.28028500	1.80430000
C	-5.08747400	-1.35965400	2.55196800
H	-5.46005800	-1.63885700	3.53820100
C	-4.75067600	0.12300000	2.48828900
H	-5.62100100	0.72916800	2.76237900
H	-3.94072500	0.38269000	3.17061300
H	-4.18368700	-1.94079300	2.35150400
O	-2.70822200	2.33373500	0.94470500
H	-3.54587200	1.36910000	1.01629900
C	-3.19928900	3.50911200	-0.12635500
O	-4.38325800	3.35811800	-0.26722800
O	-2.25492700	4.15784300	-0.47306700

- 1,5-pentanediol as substrate

TS ALKYLATION

0 1	X	Y	Z
C	-5.085124	-2.134001	-1.262159
C	-3.709531	-2.573967	-0.762948
C	-2.667874	-1.444367	-0.69886
C	-5.784564	-1.115602	-0.364469
C	-2.761204	-0.591072	0.53353
C	-4.977022	0.163001	-0.148153
H	-4.971303	-1.700801	-2.262587
H	-3.79482	-3.044603	0.221964
H	-1.660596	-1.862304	-0.718189
H	-6.739311	-0.837932	-0.819393
H	-5.625467	0.952128	0.232228
C	-3.972015	0.923676	1.998362
H	-4.991157	0.87707	2.38684
N	-3.900196	0.021945	0.843192
N	-1.694652	-0.519821	1.294946
H	-4.548946	0.538367	-1.082812

H	-6.011022	-1.557714	0.611497
H	-5.724259	-3.013677	-1.373345
H	-3.319979	-3.338737	-1.437833
H	-2.763406	-0.775243	-1.562484
H	-3.77121	1.940331	1.643042
C	-2.971856	0.517955	3.068763
H	-2.956026	1.271895	3.856223
C	-1.597956	0.382236	2.432574
H	-1.24591	1.357876	2.079666
H	-0.867539	-0.030666	3.127867
H	-3.266276	-0.435603	3.514285
C	3.769637	-1.88155	-0.750687
H	3.613243	-1.333546	-1.682234
O	2.511489	-2.256473	-0.192914
H	-0.824596	-0.9895	0.946454
C	1.516434	-1.335573	-0.203798
O	0.442968	-1.718776	0.29015
O	1.770941	-0.211038	-0.712753
C	4.597512	-1.056102	0.220574
C	5.972616	-0.721116	-0.351503
H	4.706606	-1.617023	1.154326
H	4.053468	-0.135323	0.446815
C	6.831202	0.09034	0.615089
H	6.49908	-1.648051	-0.609313
H	5.850486	-0.162905	-1.287413
C	8.194504	0.441189	0.037371
H	6.303835	1.016217	0.878153
H	6.981168	-0.464711	1.546286
H	8.740167	-0.471833	-0.211506
H	8.06943	1.012889	-0.892642
H	4.269061	-2.826858	-0.971339
O	9.011494	1.140854	0.958053
H	8.55285	1.949655	1.197002
C	0.899475	2.008577	-1.8121
H	1.919035	1.652822	-1.96168
H	0.923402	3.002432	-1.369486
H	0.393061	2.070971	-2.773347
C	0.189712	1.047863	-0.90655
H	0.234395	1.1615	0.162351
H	-0.350065	0.203225	-1.298211
Br	-1.973494	2.250266	-0.836248

TS BISCARBONATION

0 1	X	Y	Z
C	-7.496279	-0.475588	2.481507
C	-5.976871	-0.479424	2.633625
C	-5.220532	-0.639482	1.306433
C	-8.031134	0.702109	1.672015
C	-5.058029	0.621541	0.512425
C	-7.458521	0.791626	0.259718
H	-7.799708	-1.408031	1.992803
H	-5.645683	0.431549	3.143593
H	-4.224003	-1.041743	1.489521
H	-9.117009	0.607889	1.584299
H	-8.082813	1.451629	-0.341573
C	-5.938996	2.431194	-0.809854
H	-6.741806	3.153411	-0.657579
N	-6.103481	1.371157	0.196808
N	-3.826034	0.9744	0.180559
H	-7.429676	-0.173631	-0.255314
H	-7.833317	1.64423	2.193999
H	-7.957946	-0.47288	3.472394
H	-5.690897	-1.316397	3.274229
H	-5.706401	-1.351926	0.630255
H	-6.046768	1.948996	-1.787709
C	-4.581957	3.099495	-0.677364
H	-4.45706	3.828493	-1.478421
C	-3.500289	2.038803	-0.77235
H	-3.454789	1.595046	-1.771954
H	-2.522847	2.438826	-0.500921
H	-4.516512	3.625893	0.278746
C	5.736753	3.353137	0.469447
C	4.666358	2.271695	0.311318
C	4.824504	1.402133	-0.949634
C	7.167819	2.829755	0.601623
C	5.817144	0.287343	-0.746241
C	7.602668	1.971067	-0.588741
H	5.692313	4.025746	-0.396471
H	4.639911	1.611264	1.183297
H	3.873915	0.928695	-1.18936
H	7.852304	3.678507	0.688098
H	8.690721	1.900485	-0.633459
C	8.033902	-0.395544	0.042663
H	8.614298	0.105217	0.822249
N	7.108355	0.595597	-0.521543
N	5.358277	-0.928161	-0.744699

H	7.282627	2.429951	-1.52798
H	7.271998	2.236472	1.516657
H	5.498931	3.960754	1.346282
H	3.689728	2.758207	0.256537
H	5.115044	2.014169	-1.809762
H	8.730813	-0.722638	-0.737184
C	7.270829	-1.571926	0.626433
H	7.966173	-2.373498	0.878977
C	6.239914	-2.03345	-0.394892
H	6.730558	-2.415214	-1.297391
H	5.617345	-2.833927	0.008749
H	6.738136	-1.26241	1.528655
C	-2.809138	-2.439547	-1.473536
H	-2.601632	-2.446865	-2.546228
O	-4.113545	-1.944716	-1.235068

References

[1] T.M. McGuire, E.M. López-Vidal, G.L. Gregory, A. Buchard, J. CO2 Util., 27 (2018) 283-288.