Supporting Information

Cycloaddition of CO_2 to epoxides "around water": A strategy to apply and recycle efficient water-soluble bio-based organocatalysts in biphasic media

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Contents

S1. General Information

L-ascorbic acid (>99%), Tributylamine, tetra-N-butyl ammonium chloride (TBAC), tetra-N-butyl ammonium iodide (TBAI), tetra-N-ethyl ammonium iodide (TEAI), Choline Iodide (ChI), Hydrochloric acid (37%), Hydrobromic acid (57%), Hydroiodic acid (57%), Epichlorohydrin, Styrene oxide, Glycidyl Phenyl Ether, Glycidyl Methacrylate, Benzyl Glycidyl Ether, Propylene oxide, 1-Dodecene oxide, Methyl ricinoleate (>75%) and Methyl linolenate (>70%) were purchased from TCI Chemicals. Tetra-N-butyl ammonium bromide (TBAB), 1-Butene oxide, Potassium Carbonate, and Triethylamine were purchased from Merck. 1-Hexene oxide was purchased from Alfa Aesar. Furfuryl Glycidyl Ether was obtained from ACROS. Methyl *cis*-9-octadecenoate (99%), Ethyl oleate (70%), and m-CPBA were purchased from Sigma Aldrich. The CO_2 (99.99%) was obtained from Bangkok Industrial Gases. All solvents and reagents were used as received without further purification. Seawater was collected from cape Mae Phim, gulf of Thailand, in September 2022. The collected seawater was filtered to remove impurities before using as a reaction medium.

NMR spectra were measured on an automated "Bruker" for ^{1}H NMR (600 MHz) and ^{13}C (150 MHz). Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26 ppm, DMSO-d_6: δ 2.50 ppm, MeOD-d_4: δ 3.31, 4.87 ppm and D_2O: 4.79 ppm). Chemical shifts for carbon are referenced to the carbon resonances of the solvent (MeOD-d_4: δ 49 ppm). High-resolution mass spectra (ESI/QTOF) were obtained using a compact™ ESI QTOF Mass Spectrometer. All mass spectra were calibrated post-run by the sodium formate cluster ions, which were used as the internal standard.

S2. Synthesis and Characterization of Catalysts.

Please refer to Scheme 1 of the manuscript for the synthetic strategy and product structures.

2.1 General Procedure for the synthesis of glycidyltrialkylammonium chlorides

Glycidyltributhylammonium chloride (3a) was synthesized by a modified version of a previously described procedure.[1] Briefly, epichlorohydrin (216 mmol, 2.5 equiv.) was dissolved in methanol (20 mL) in a two-neck round-bottom flask. Tributylamine (86.5 mmol, 1 equiv.) dissolved in 16 mL methanol was added dropwise for 30 min. The reaction mixture was heated to reflux at 50 °C for 5 hours. Then, the mixture was cooled to room temperature and the volatile compounds were evaporated

using a rotary evaporator leading to the formation of two distinct phases. The lower phase was separated from the reaction mixture using a separatory funnel and washed several times with hexane. The residue was evacuated under a high vacuum to obtain **3a** (93 % yield) as a viscous yellowish liquid. **^{1}H NMR** of compound **3a (**600 MHz, MeOD-d_4) δ 4.07 (d, J = 14.7 Hz, 1H), 3.57 – 3.48 (m, 7H), 3.26 (dd, J = 14.7, 9.2 Hz, 1H), 3.08 (t, J = 4.7 Hz, 1H), 2.88 (dd, J = 4.9, 2.2 Hz, 1H), 1.91 – 1.80 (m, 6H), 1.60 – 1.53 (m, 6H), 1.15 (t, J = 7.4 Hz, 9H). **^{13}C NMR** of compound **3a** (151 MHz, MeOD-d_4) δ 62.71, 60.48, 45.65, 45.33, 24.85, 20.67, 14.00. **HRMS** (ESI/QTOF), m/z: $[M+H]^+$ Calcd for $[C_{15}H_{33}NOCl]^+$: 242.2478; found: 242.2479.

Glycidyltriethylammonium chloride (3b) was synthesized by a modified version of a previously described procedure.[1] Triethylamine (10 g, 99 mmol, 1 equiv.), epichlorohydrin (13.74 g, 149 mmol, 1.5 equiv.), and methanol (40 mL) were added into a 250 mL round bottom flask containing a stirring bar. This mixture was stirred under reflux at 50 °C for 2.5 h. Then, the mixture was cooled to room temperature, evaporating the volatile compounds under reduced pressure and obtaining a viscous liquid. Diethyl ether (100 mL) was added to the reaction product, and the mixture was stirred for 30 min after which the diethyl ether phase was discarded by decantation. The latter step was repeated five times. Finally, the volatile compounds in the reaction product were evaporated under reduced pressure to afford **3b** (90 %yield) a colorless oil. **^{1}H NMR** of **3b** (600 MHz, MeOD-d_4) δ 4.13 (d, J = 14.8 Hz, 1H), 3.75 (m, J = 7.0 Hz, 7H), 3.38 (dd, J = 14.9, 9.1 Hz, 1H), 3.19 (t, J = 4.8 Hz, 1H), 3.05 – 3.01 (m, 1H), 1.58 (t, J = 7.7 Hz, 9H). **^{13}C NMR** of compound **3b** (151 MHz, MeOD-d_4) δ 61.08, 55.30, 54.99, 45.67, 45.39, 8.24, 8.06, 7.95. **HRMS** (ESI/QTOF), m/z: $[M+H]^+$ Calcd. for $[C_9H_{21}NOCl]^+$: 158.1539; found: 158.1532.

2.2 General Procedure for the synthesis of Ascorbic acid-based compounds **5a**, **5b**, **6a** and **6b**

Procedure A

Compounds **5a-b** and **6a-b** were synthesized by ring-opening of glycidyltrialkylammonium chlorides **3a** (**5a** and **6a**) and **3b** (**5b** and **6b**) with ascorbic acid (**5a** and **5b**) or 5,6-Isopropylidene-L-ascorbic acid (**4**, for **6a** and **6b**).[2] A mixture of ascorbic acid or **4** (5 g, 28.39 mmol, 1 equiv.), K_2CO_3 (4.71 g, 34.07 mmol, 1.2 equiv.), DMF (5 mL) and H_2O (5 mL) was stirred at room temperature for 30 min. Then, glycidyltrialkylammonium chloride **3a** or **3b** (34.07 mmol, 1.2 equiv.) was added, and the resulting mixture was stirred at 60 °C for 24 hours. Then, the solvent was evaporated under vacuum, and the crude product was purified by flash chromatography to afford the series of ascorbic acid derivatives **5a-b** and **6a-b**.

Procedure B

Compounds **5a-b** and **6a-b** were synthesized by ring-opening of glycidyltrialkylammonium chlorides **3a** (**5a** and **6a**) and **3b** (**5b** and **6b**) with ascorbic acid (**5a** and **5b**) or 5,6-Isopropylidene-L-ascorbic acid (**4**, for **6a** and **6b**).[2] A mixture of ascorbic acid or **4** (5 g, 28.39 mmol, 1 equiv.), K_2CO_3 (4.71 g, 34.07 mmol, 1.2 equiv.), MeOH (7 mL) and H_2O (7 mL) was stirred at room temperature for 30 min. Then, glycidyltrialkylammonium chloride **3a** or **3b** (34.07 mmol, 1.2 equiv.) was added and the resulting mixture was refluxed at 55 °C for 24 hours. Then, the solvent was evaporated under vacuum, and the crude product was purified by flash chromatography to afford the series of ascorbic acid derivatives **5a-b** and **6a-b**.

5-(1,2-dihydroxyethyl)-4-(2-hydroxy-3-(tributylammonio)propoxy)-2-oxo-2,5-dihydrofuran-3-olate (5a) The crude product was purified by flash chromatography on silica gel (EtOAc: EtOH, 80:20) affording a yellow foam (72% yield for procedure A and 55% yield for procedure B). **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.42 (dd, J = 5.7, 2.3 Hz, 1H), 4.38 – 4.25 (m, 1H), 3.96 – 3.84 (m, 2H), 3.77 – 3.63 (m, 3H), 3.58 – 3.47 (m, 4H), 3.46 – 3.37 (m, 4H), 1.33 (q, J = 6.8, 4.7 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 180.01, 179.72, 177.84, 177.69, 118.38, 118.14, 79.82, 79.79, 76.06, 75.89, 71.54, 71.49, 65.58, 65.35, 64.07, 64.05, 60.62, 60.40, 54.84, 7.87. **HRMS** (ESI/QTOF), m/z: $[M+HCOO]^-$ Calcd. for $[C_{21}H_{39}NO_7+HCOO]^-$: 462.2709; found: 462.2706.

5-(1,2-dihydroxyethyl)-4-(2-hydroxy-3-(triethylammonio)propoxy)-2-oxo-2,5-dihydrofuran-3-olate (5b) The crude product was purified by flash chromatography on silica gel (EtOAc: MeOH, 35:65) affording a pale yellow foam (89% yield for procedure A and 61% yield for procedure B). **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.42 (dd, J = 5.7, 2.3 Hz, 1H), 4.38 – 4.25 (m, 1H), 3.96 – 3.84 (m, 2H), 3.77 – 3.63 (m, 3H), 3.58 – 3.47 (m, 4H), 3.46 – 3.37 (m, 4H), 1.33 (q, J = 6.8, 4.7 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 180.01, 179.72, 177.84, 177.69, 118.38, 118.14, 79.82, 79.79, 76.06, 75.89, 71.54, 71.49, 65.58, 65.35, 64.07, 64.05, 60.62, 60.40, 54.84, 7.87. **HRMS** (ESI/QTOF), m/z: $[M+HCOO]^-$ Calcd for $[C_{15}H_{27}NO_7+HCOO]^-$: 378.1770; found: 378.1771.

5-(2,2-dimethyl-1,3-dioxolan-4-yl)-4-(2-hydroxy-3-(tributylammonio)propoxy)-2-oxo-2,5 dihydrofuran-3-olate (6a) The crude product was purified by flash chromatography on silica gel (EtOAc: EtOH, 90:10) to afford a light yellow foam in 67% yield (procedure A) and 53% yield (procedure B). **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.39 – 4.25 (m, 3H), 4.16 (t, J = 7.8 Hz, 1H), 4.08 (t, J = 7.7 Hz, 1H), 3.96 – 3.89 (m, 1H), 3.75 – 3.68 (m, 1H), 3.65 (d, J = 14.4 Hz, 1H), 3.53 – 3.42 (m, 4H), 3.39 – 3.31 (m, 3H), 1.84 – 1.75 (m, 3H), 1.75 – 1.66 (m, 3H), 1.47 – 1.40 (m, 6H), 1.37 (s, 3H), 1.34 (s, 3H), 1.04 (t, J = 7.5 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 177.90, 177.84, 177.26, 177.23, 118.60, 118.49, 110.57, 76.13, 76.09, 76.05, 75.93, 66.53, 65.71, 65.65, 62.39, 62.32, 60.51, 26.51, 26.49, 25.99, 25.97, 24.81, 20.66, 13.99. **HRMS** (ESI/QTOF), m/z: $[M+HCOO]^-$ Calcd for $[C_{24}H_{43}NO_7+HCOO]^-$: 502.3022; found: 502.3022.

5-(2,2-dimethyl-1,3-dioxolan-4-yl)-4-(2-hydroxy-3-(triethylammonio)propoxy)-2-oxo-2,5-dihydrofuran-3-olate (6b) The crude product was purified by column chromatography (EtOAc: MeOH, 65:35) to afford **6b** as a light brown foam in 85% yield (procedure A) and 71% yield (procedure B). **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.41 – 4.32 (m, 2H), 4.30 (d, J = 3.3 Hz, 1H), 4.17 (t, J = 7.7 Hz, 1H), 4.10 (t, J = 7.7 Hz, 1H), 3.97 – 3.88 (m, 1H), 3.77 – 3.67 (m, 1H), 3.65 – 3.51 (m, 4H), 3.51 – 3.41 (m, 4H), 1.42 – 1.32 (m, 15H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 179.02, 178.90, 177.47, 118.21, 110.56, 110.54, 78.98, 78.97, 76.05, 76.03, 66.48, 65.57, 65.54, 60.72, 60.57, 54.88, 26.48, 25.93, 7.90. **HRMS** (ESI/QTOF), m/z: $[M+HCOO]^-$ Calcd for $[C_{18}H_{31}NO_7+HCOO]^-$: 418.2083; found: 418.2083.

2.3 General Procedure for the protonation of compounds **5a-b** and **6a-b**

The ascorbic acid-based catalysts **7a-X**, **7b-X** (X= Cl, Br, I), **8a-I,** and **8b-I** were synthesized according to a method reported in the literature. In a representative experiment, 2M hydrohalic acid (HCl, HBr, or HI) was added to a solution of **5a** (3g) dissolved in water (5 mL) until reaching pH 2 at room temperature. Afterward, the mixture was frozen and freeze-dried overnight to afford **7a-X** (X= Cl, Br, I).

***N,N*-dibutyl-N-(3-((2-(1,2-dihydroxyethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-2-hydroxypropyl)butan-1-ammonium chloride (7a-Cl)** A light-brown foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.84 (s, 1H), 4.37 (q, J = 6.8 Hz, 1H), 4.04 – 3.96 (m, 1H), 3.91 (t, J = 7.5 Hz, 1H), 3.88 – 3.82 (m, 1H), 3.67 – 3.59 (m, 2H), 3.54 (d, J = 14.6 Hz, 1H), 3.46 (dd, J = 14.5, 9.3 Hz, 1H), 3.41 – 3.35 (m, 3H), 3.32 – 3.26 (m, 3H), 1.77 – 1.68 (m, 3H), 1.67 – 1.57 (m, 3H), 1.36 (h, J = 7.4 Hz, 6H), 0.96 (t, J = 7.4 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.70, 172.66, 162.29, 162.20, 121.73, 121.67, 76.99, 75.10, 75.01, 70.37, 70.34, 65.40, 65.35, 63.37, 61.95, 60.55, 24.77, 20.58, 13.93. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{21}H_{39}ClNO_7]^-$: 452.2421; found: 452.2427.

***N,N*-dibutyl-N-(3-((2-(1,2-dihydroxyethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-2-hydroxypropyl)butan-1-ammonium bromide (7a-Br)** A light-brown foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.94 (s, 1H), 4.47 (q, J = 6.9 Hz, 1H), 4.12 – 4.06 (m, 1H), 3.98 (t, J = 7.8 Hz, 1H), 3.97 – 3.90 (m, 1H), 3.74 – 3.68 (m, 2H), 3.63 (d, J = 14.1 Hz, 1H), 3.55 (dd, J = 15.0, 9.2 Hz, 1H), 3.50 – 3.44 (m, 3H), 3.42 – 3.35 (m, 3H), 1.86 – 1.78 (m, 3H), 1.76 – 1.67 (m, 3H), 1.46 (h, J = 7.3 Hz, 6H), 1.05 (t, J = 7.4 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.55, 172.51, 162.12, 162.04, 121.60, 121.53, 76.84, 74.96, 74.87, 70.23, 70.19, 65.26, 65.21, 63.22, 61.81, 60.41, 24.63, 20.44, 13.79. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{21}H_{39}BrNO_7]^-$: 496.1915; found: 496.1915.

***N,N*-dibutyl-N-(3-((2-(1,2-dihydroxyethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-2-hydroxypropyl)butan-1-ammonium iodide (7a-I)** A pale-yellow foam was obtained. **^{1}H NMR**

(600 MHz, MeOD-d_4) δ 4.95 (s, 1H), 4.49 (q, J = 6.8 Hz, 1H), 4.14 – 4.07 (m, 1H), 4.01 (t, J = 8.0 Hz, 1H), 4.01 – 3.92 (m, 1H), 3.76 – 3.70 (m, 2H), 3.65 (d, J = 14.4 Hz, 1H), 3.57 (dd, J = 14.8, 9.2 Hz, 1H), 3.54 – 3.45 (m, 3H), 3.45 – 3.35 (m, 3H), 1.88 – 1.79 (m, 3H), 1.79 – 1.70 (m, 3H), 1.69 (s, 0H), 1.48 (h, J = 7.3 Hz, 6H), 1.07 (t, J = 7.4 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.58, 172.54, 161.79, 161.76, 121.90, 121.87, 76.95, 75.17, 75.11, 70.38, 70.35, 65.45, 65.43, 63.34, 61.98, 60.68, 24.90, 20.65, 13.96 **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{21}H_{39}INO_7]^-$: 544.1777; found: 544.1781.

3-((2-(1,2-dihydroxyethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-*N,N,N*-triethyl-2-hydroxypropan-1-ammonium chloride (7b-Cl) A light-brown foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.58 (s, 2H), 4.09 (q, J = 6.6 Hz, 1H), 3.77 – 3.69 (m, 1H), 3.64 (t, J = 7.0 Hz, 1H), 3.63 – 3.55 (m, 1H), 3.38 – 3.27 (m, 2H), 3.25 – 3.14 (m, 4H), 3.17 – 3.05 (m, 4H), 0.99 (t, J = 7.4 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.34, 172.30, 161.34, 161.30, 121.73, 121.69, 76.81, 75.00, 74.94, 70.20, 70.17, 65.25, 65.22, 63.33, 60.19, 54.92, 7.93. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{15}H_{27}ClNO_7]^-$: 368.1482; found: 368.1489.

3-((2-(1,2-dihydroxyethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-*N,N,N*-triethyl-2-hydroxypropan-1-ammonium bromide (7b-Br) A pale-yellow foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.72 (s, 1H), 4.29 (q, J = 6.7 Hz, 1H), 3.93 – 3.86 (m, 1H), 3.86 – 3.81 (m, 1H), 3.81 – 3.73 (m, 1H), 3.58 – 3.48 (m, 2H), 3.42 – 3.34 (m, 4H), 3.34 – 3.26 (m, 4H), 1.19 (t, J = 7.4 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 173.17, 164.35, 164.13, 121.16, 121.05, 77.24, 77.22, 75.17, 75.10, 70.32, 70.30, 65.25, 65.20, 63.37, 60.15, 54.94, 8.00. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{15}H_{27}BrNO_7]^-$: 412.0976; found: 412.0981.

3-((2-(1,2-dihydroxyethyl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-*N,N,N*-triethyl-2-hydroxypropan-1-ammonium iodide (7b-I) A pale-yellow foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.79 (s, 1H), 4.36 (q, J = 5.7 Hz, 1H), 4.01 – 3.92 (m, 1H), 3.90 (t, J = 6.9 Hz, 1H), 3.87 – 3.80 (m, 1H), 3.66 – 3.57 (m, 2H), 3.50 – 3.42 (m, 4H), 3.44 – 3.33 (m, 4H), 1.28 (t, J = 7.2 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.89, 163.11, 162.99, 121.51, 121.43, 77.09, 75.19, 75.13, 70.32, 70.30, 65.32, 65.29, 63.33, 60.27, 55.08, 8.10. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{15}H_{27}INO_7]^-$: 460.0838; found: 460.0838.

***N,N*-dibutyl-*N*-(3-((2-(2,2-dimethyl-1,3-dioxolan-4-yl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-2-hydroxypropyl)butan-1-ammonium iodide (8a-I)** A light yellow foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.72 (s, 1H), 4.47 – 4.38 (m, 2H), 4.20 (t, J = 7.8 Hz, 1H), 4.11 – 3.98 (m, 2H), 3.86 (dd, J = 10.2, 6.8 Hz, 1H), 3.62 (dd, J = 14.5, 8.4 Hz, 1H), 3.56 – 3.48 (m, 1H), 3.49 – 3.41 (m, 3H), 3.39 – 3.32 (m, 3H), 1.84 – 1.74 (m, 3H), 1.76 – 1.65 (m, 3H), 1.48 – 1.39 (m, 6H), 1.34 (s,

3H), 1.33 (s, 3H), 1.02 (t, J = 7.4 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 173.13, 173.09, 164.26, 164.19, 121.43, 121.35, 111.12, 111.11, 76.84, 76.82, 75.37, 75.27, 75.01, 66.46, 65.54, 65.48, 62.11, 60.60, 26.29, 25.71, 25.69, 24.82, 20.65, 13.94. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{24}H_{44}INO_7]^-$: 584.2090; found: 584.2090.

3-((2-(2,2-dimethyl-1,3-dioxolan-4-yl)-4-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)oxy)-*N,N,N*-triethyl-2-hydroxypropan-1-ammonium iodide (8b-I) A light brown foam was obtained. **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.67 (d, J = 2.5 Hz, 1H), 4.33 – 4.26 (m, 2H), 4.06 (t, J = 7.9 Hz, 1H), 3.96 – 3.88 (m, 2H), 3.81 – 3.72 (m, 1H), 3.45 – 3.38 (m, 4H), 3.39 – 3.32 (m, 1H), 3.35 – 3.26 (m, 3H), 1.20 (t, J = 7.3 Hz, 9H), 1.18 (s, 3H), 1.17 (s, 3H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.12, 172.09, 161.38, 161.36, 121.79, 121.73, 111.09, 76.46, 75.11, 75.01, 74.70, 66.39, 65.32, 65.27, 60.32, 54.98, 26.27, 25.60, 7.96. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{18}H_{31}INO_7]^-$:500.1150; found: 500.1153.

2-(1,2-dihydroxyethyl)-4-(2-hydroxy-3-(triethylammonio)propoxy)-5-oxo-2,5-dihydrofuran-3-olate (9b)

Ascorbic acid (5 g, 28.39 mmol, 1 equiv.) and NaOH (1.7 g, 42.58 mmol 1.5 equiv.) were dissolved in a mixture of DMF (7 mL) and water (5 mL) at room temperature for 30 minutes. Afterward, **3b** (42.58 mmol, 1.5 equiv.) was added and stirred at 60 °C for 24 hours. The solvent was concentrated under vacuum, and the crude product was purified by flash chromatography ($CHCl_3$: MeOH, 40:60). **^{1}H NMR** (600 MHz, MeOD-d_4) δ 4.42 (dd, 1H), 4.36 – 4.26 (m, 1H), 3.97 – 3.81 (m, 2H), 3.77 – 3.63 (m, 3H), 3.58 – 3.46 (m, 4H), 3.46 – 3.36 (m, 4H), 1.33 (q, J = 6.5 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 179.97, 179.70, 177.80, 177.65, 118.33, 118.10, 79.77, 79.73, 76.05, 75.87, 71.45, 71.41, 65.54, 65.32, 64.02, 63.99, 60.54, 60.33, 54.82, 7.87. **HRMS** (ESI/QTOF), m/z: $[M+HCOO]^-$ Calcd for $[C_{15}H_{27}NO_7+HCOO]^-$: 378.1770; found: 378.1772.

3-((5-(1,2-dihydroxyethyl)-4-hydroxy-2-oxo-2,5-dihydrofuran-3-yl)oxy)-N,N,N-triethyl-2-hydroxypropan-1-ammonium (9b-I) was obtained as a pale yellow foam from **9b** following the procedure listed above for the synthesis of **7a-X** from **5a** (89 %yield). **^{1}H NMR** of (600 MHz, MeOD-d_4) δ 5.00 (d, J = 1.7 Hz, 1H), 4.58 – 4.51 (m, 1H), 4.19 – 4.11 (m, 1H), 4.07 – 3.98 (m, 2H), 3.80 – 3.72 (m, 2H), 3.69 – 3.59 (m, 4H), 3.58 – 3.50 (m, 4H), 1.43 (t, J = 7.2 Hz, 9H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 172.46, 172.41, 161.45, 161.40, 121.85, 121.82, 76.88, 76.87, 75.12, 75.06, 70.27, 70.25, 65.34, 65.32, 63.30, 55.14, 8.09. **HRMS** (ESI/QTOF), m/z: $[M-H]^-$ Calcd for $[C_{15}H_{27}INO_7]^-$: 460.0838; found: 460.0838.

S3. ^{1}H NMR and ^{13}C NMR Spectra of Catalysts

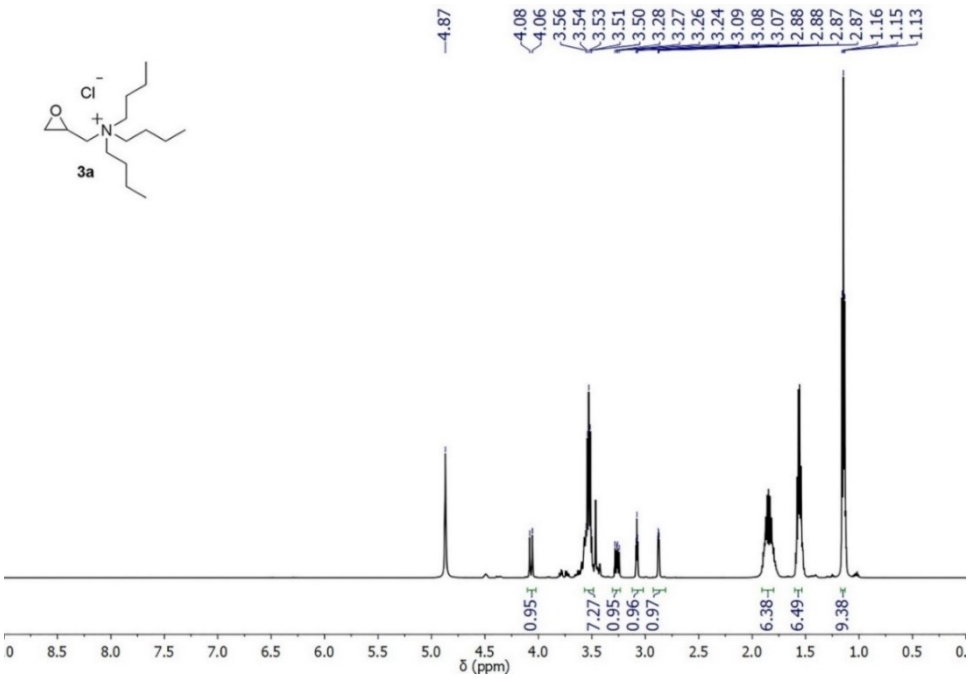


Figure S1. ^{1}H NMR (MeOD-d_4) spectrum of compound **3a**.

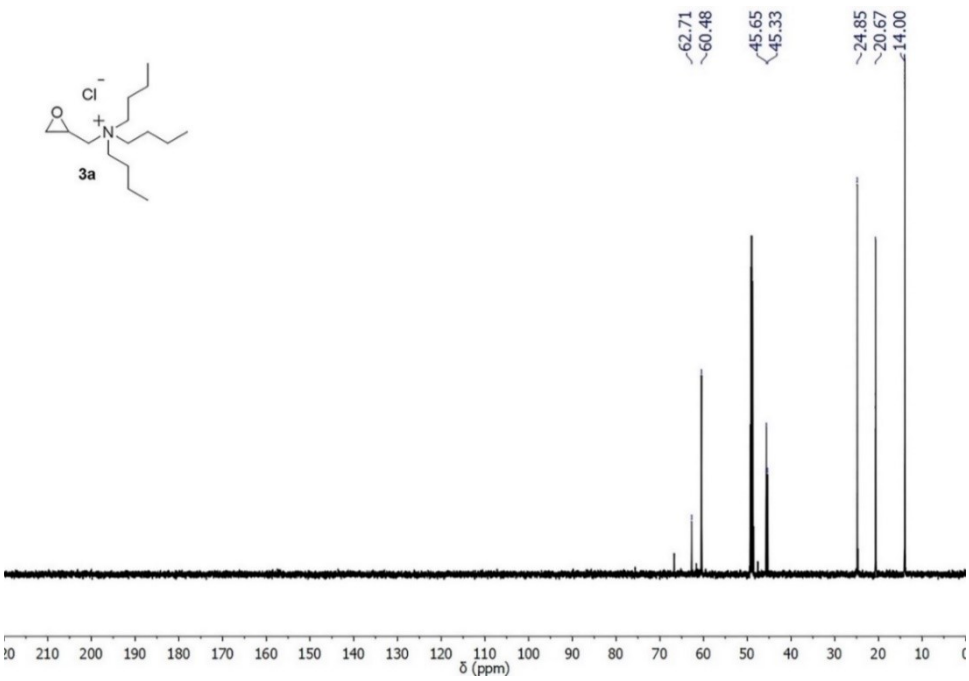


Figure S2. ^{13}C NMR (MeOD-d_4) spectrum of compound **3a**.

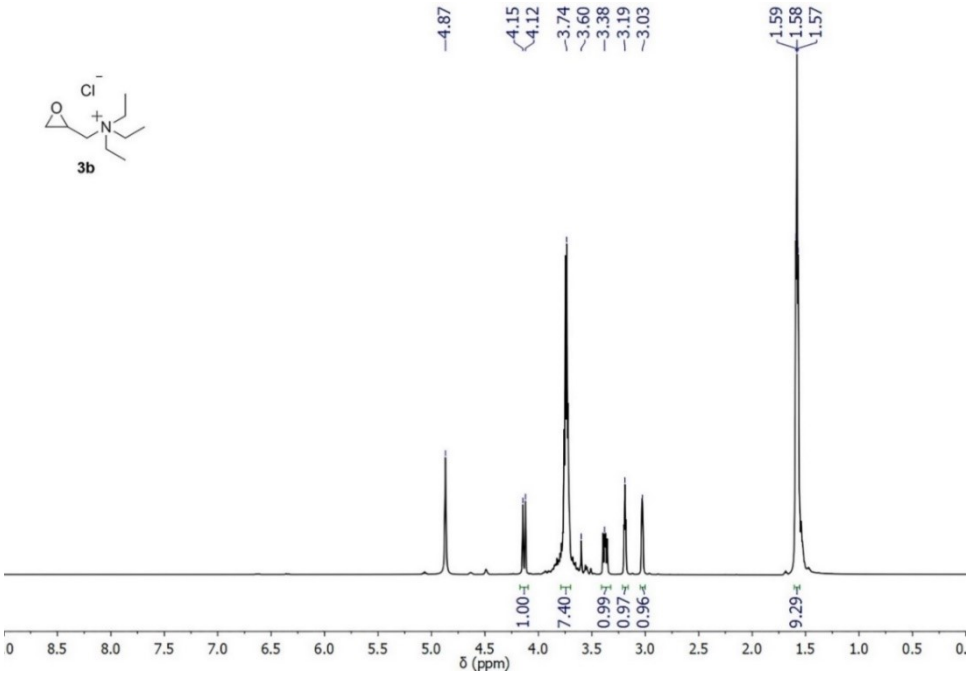


Figure S3. ^{1}H NMR (MeOD-d_4) spectrum of compound **3b**.

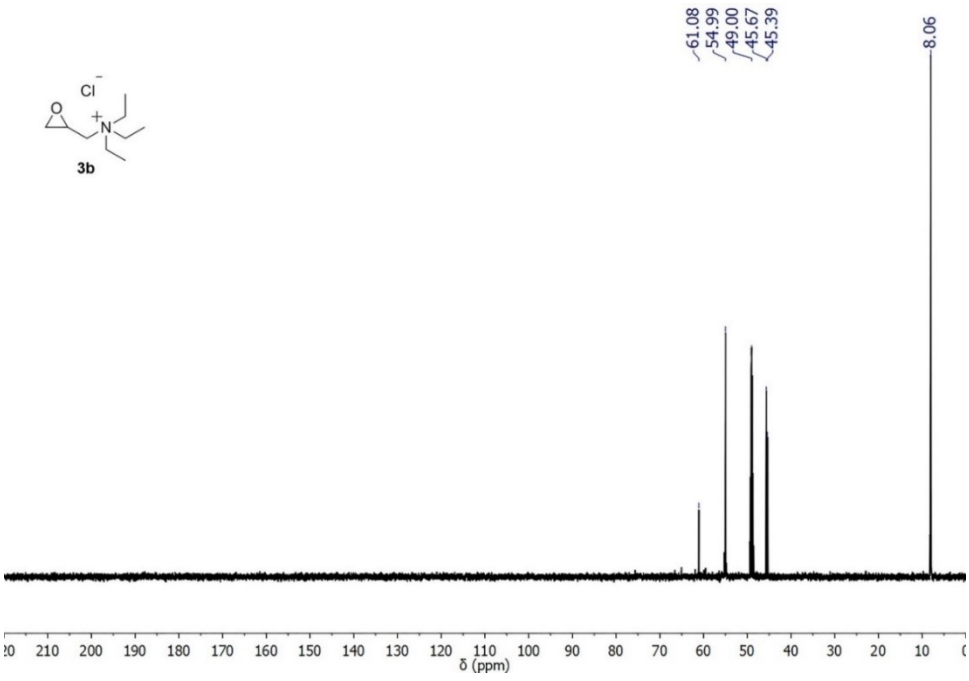


Figure S4. ^{13}C NMR (MeOD-d_4) spectrum of compound **3b**.

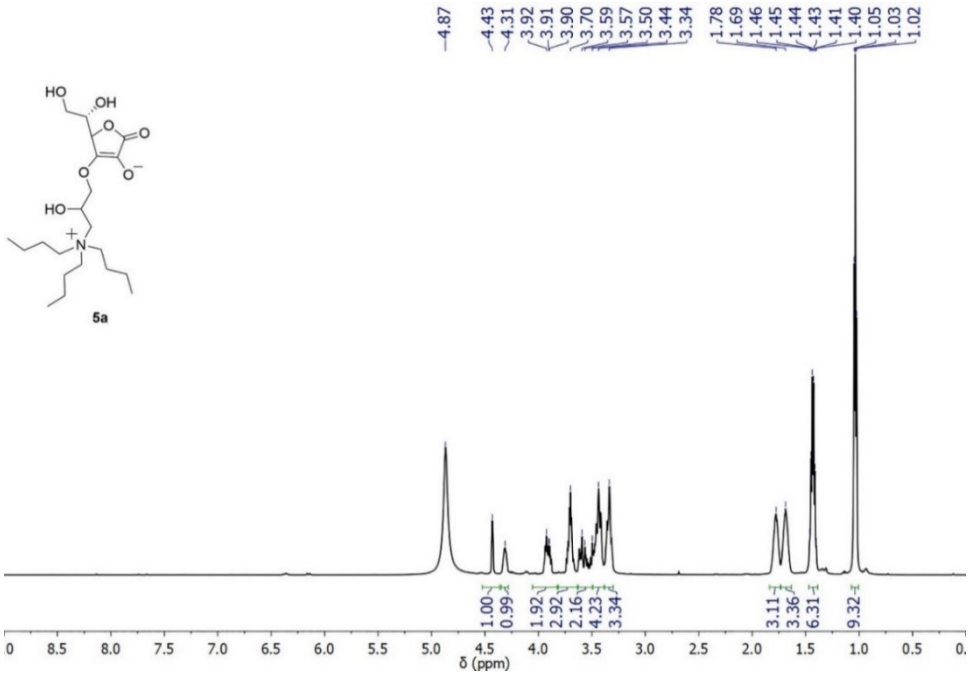


Figure S5. ^{1}H NMR (MeOD-d_4) spectrum of compound **5a**.

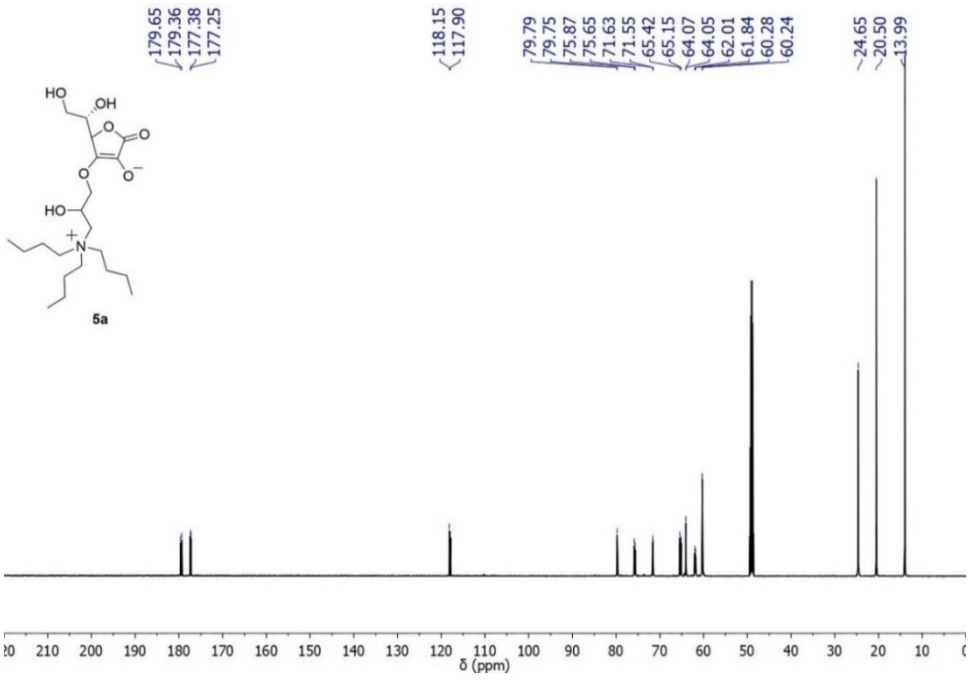


Figure S6. ^{13}C NMR (MeOD-d_4) spectrum of compound **5a**.

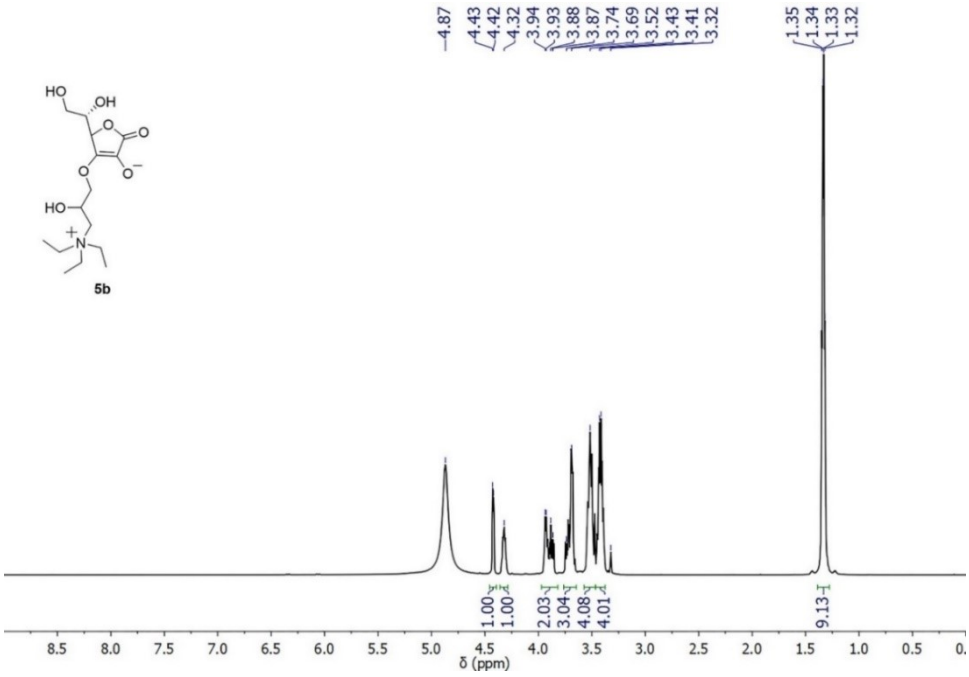


Figure S7. ^{1}H NMR (MeOD-d_4) spectrum of compound **5b**.

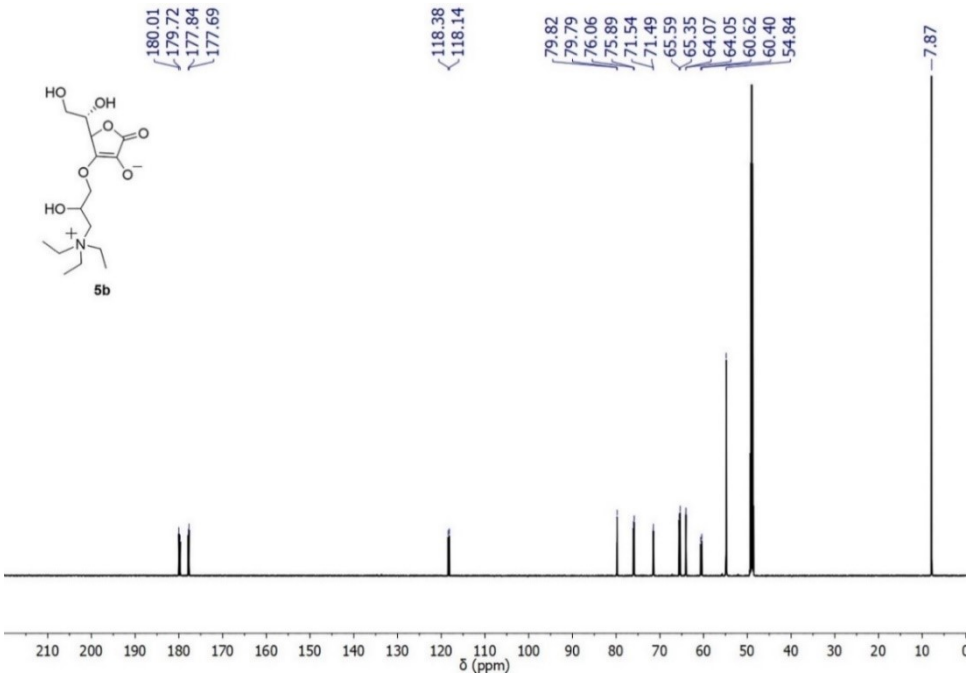


Figure S8. ^{13}C NMR (MeOD-d_4) spectrum of compound **5b**.

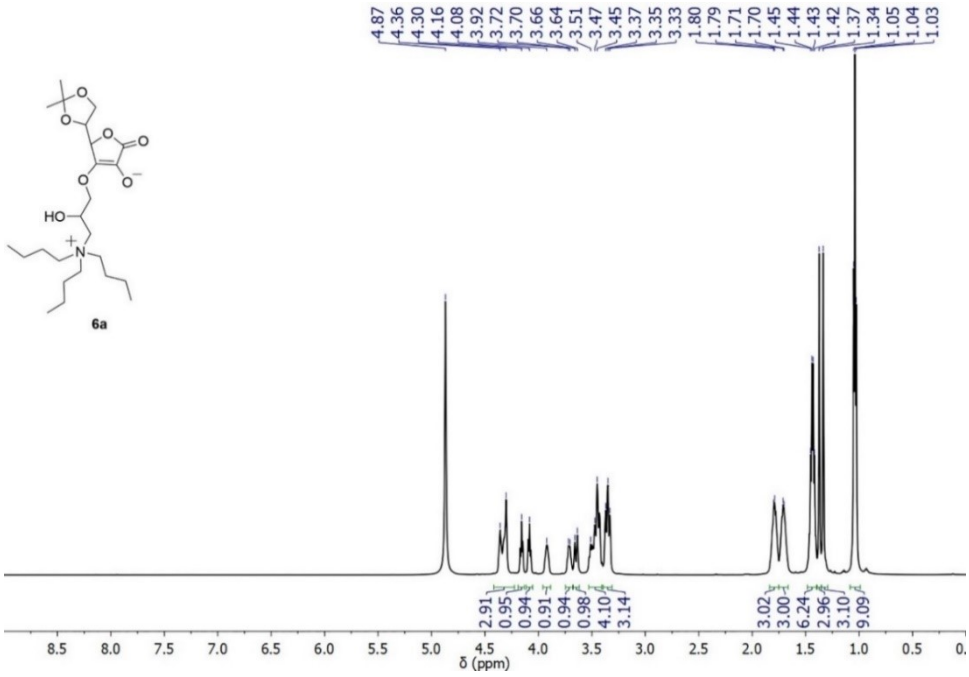


Figure S9. ^{1}H NMR (MeOD-d_4) spectrum of compound **6a**.

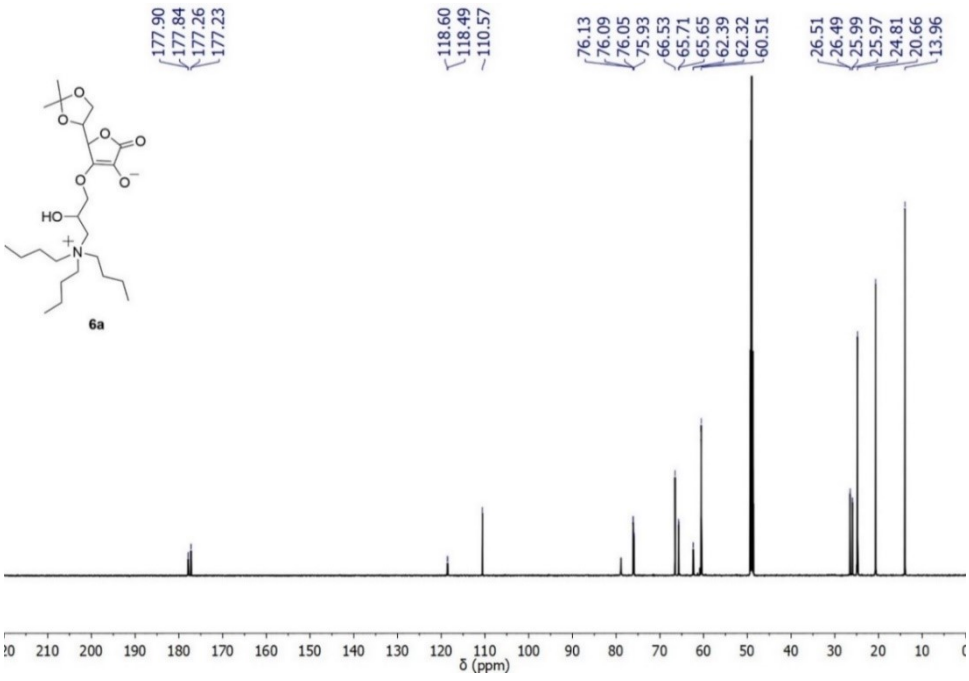


Figure S10. ^{13}C NMR (MeOD-d_4) spectrum of compound **6a**.

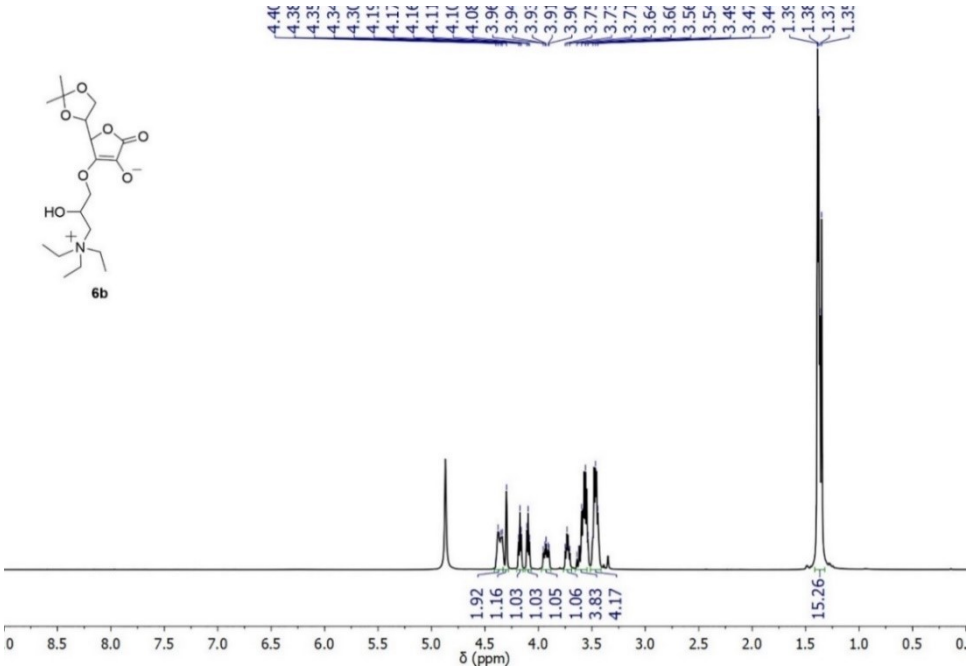


Figure S11. ^{1}H NMR (MeOD-d_4) spectrum of compound **6b**.

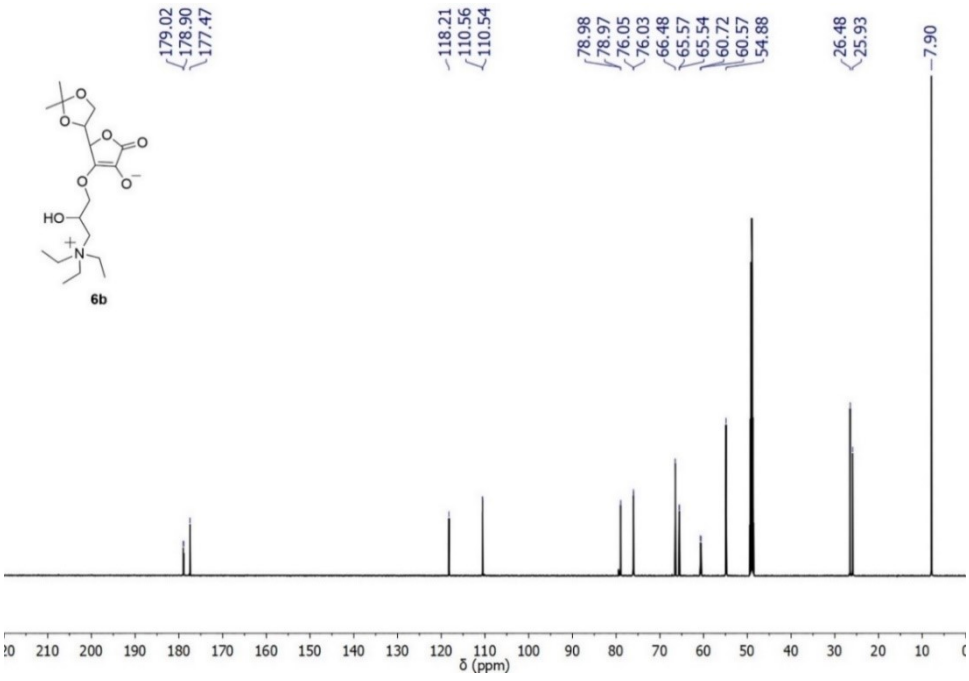


Figure S12. ^{13}C NMR (MeOD-d_4) spectrum of compound **6b**.

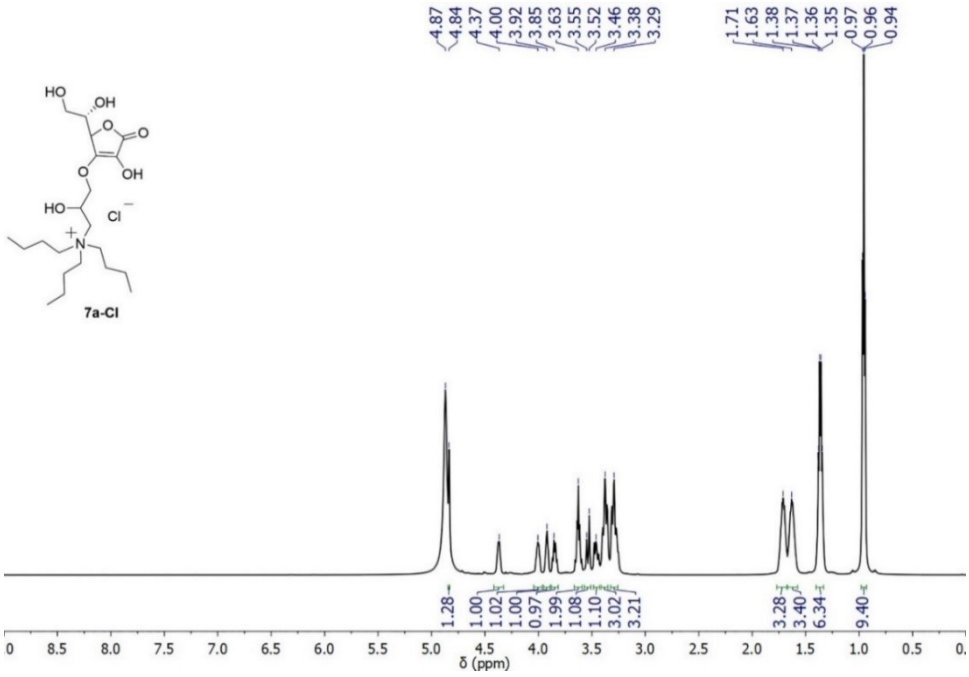


Figure S13. ^{1}H NMR (MeOD-d_4) spectrum of compound **7a-Cl**.

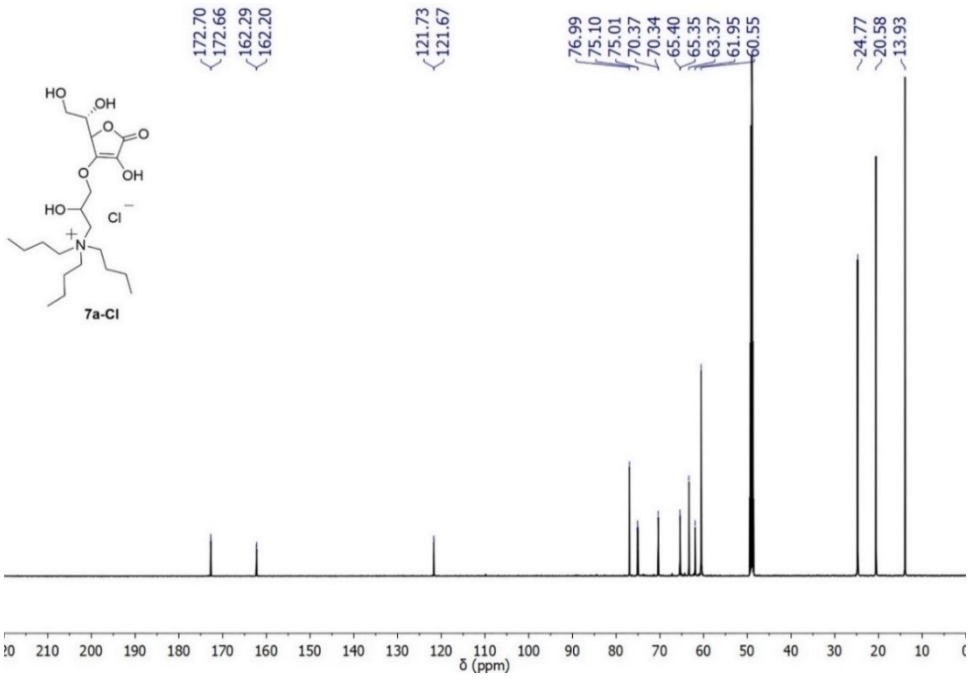


Figure S14. ^{13}C NMR (MeOD-d_4) spectrum of compound **7a-Cl**.

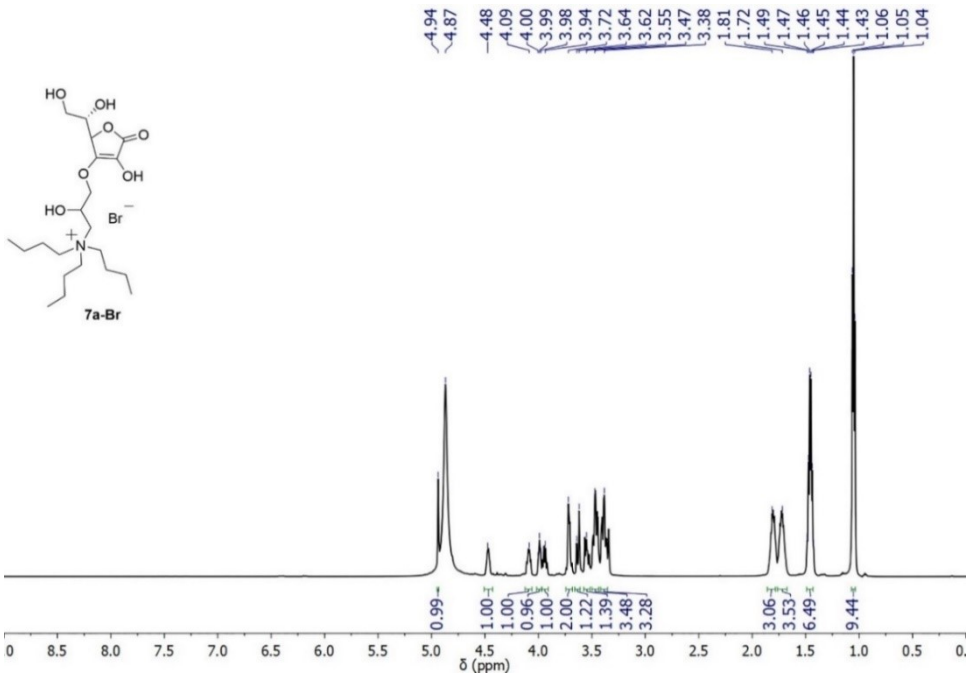


Figure S15. ^{1}H NMR (MeOD-d_4) spectrum of compound **7a-Br**.

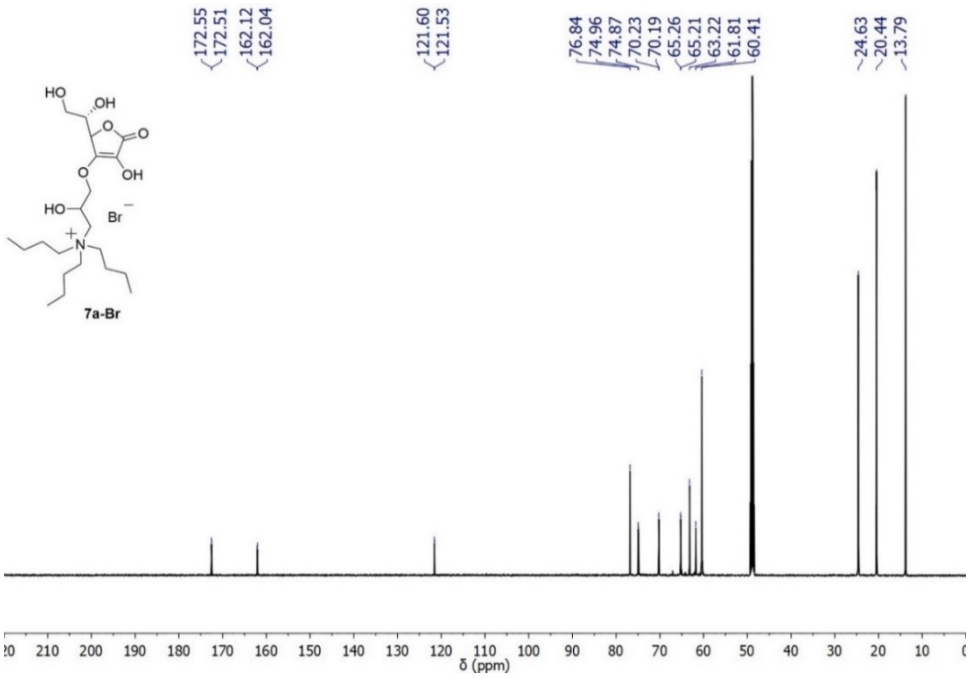


Figure S16. ^{13}C NMR (MeOD-d_4) spectrum of compound **7a-Br**.

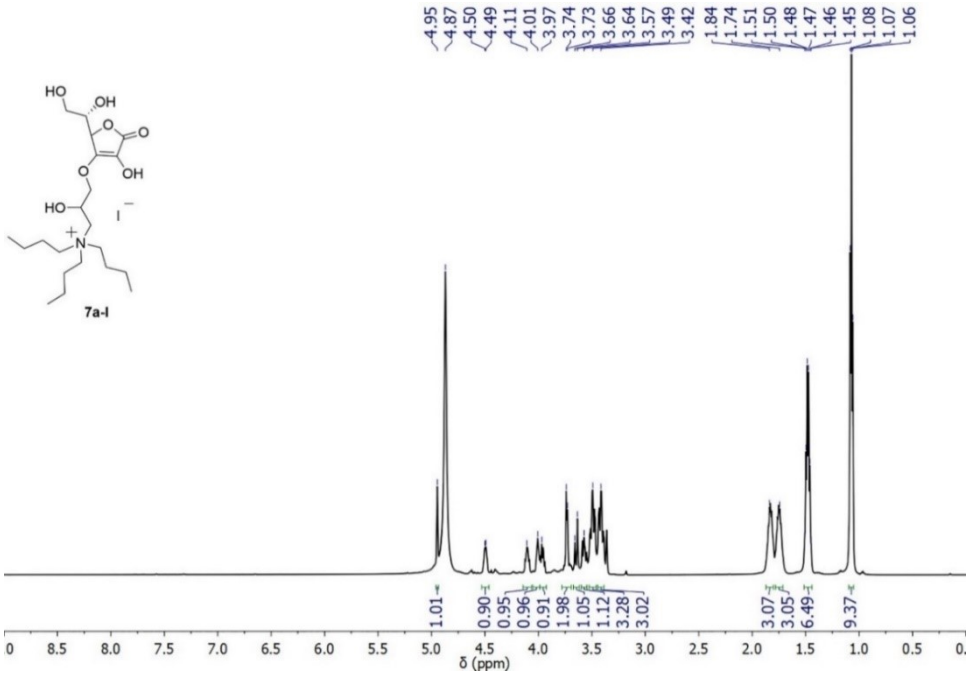


Figure S17. ^{1}H NMR (MeOD-d_4) spectrum of compound **7a-I**.

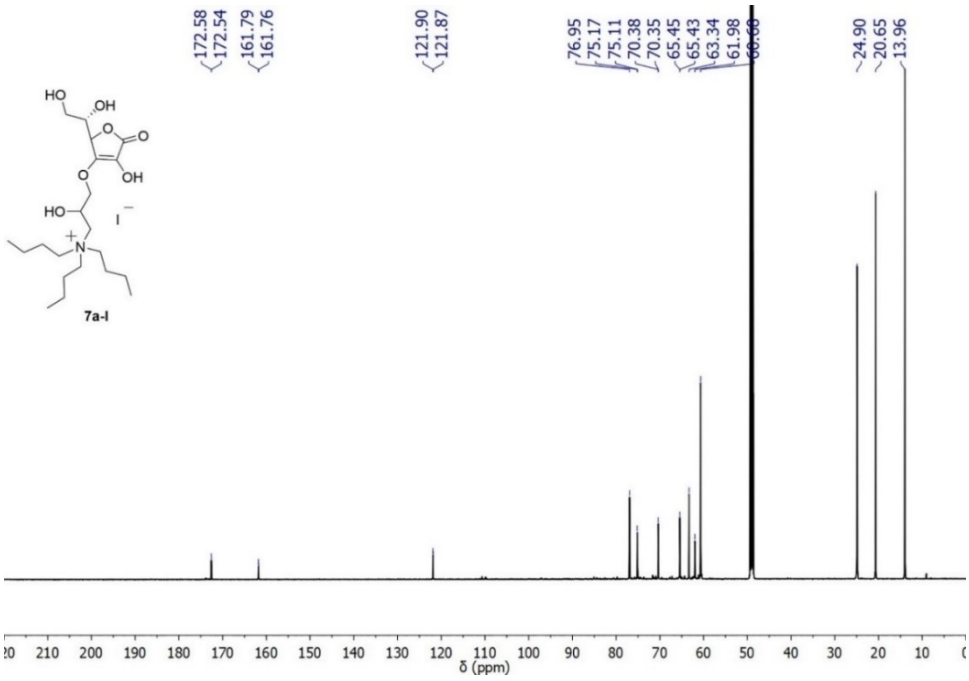


Figure S18. ^{13}C NMR (MeOD-d_4) spectrum of compound **7a-I**.

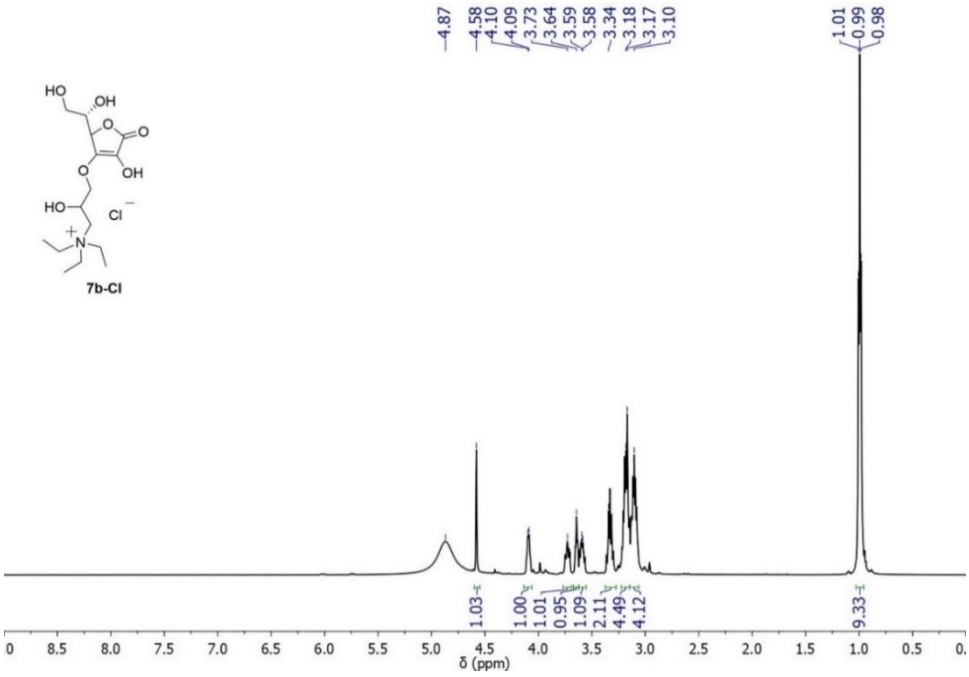


Figure S19. ^{1}H NMR (MeOD-d_4) spectrum of compound **7b-Cl**.

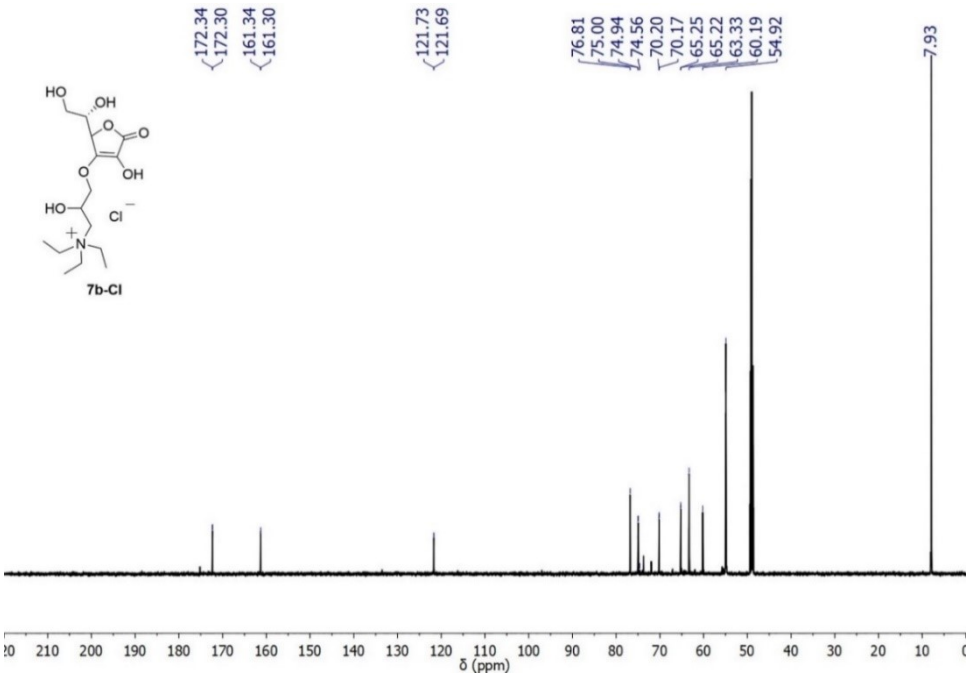


Figure S20. ^{13}C NMR (MeOD-d_4) spectrum of compound **7b-Cl**.

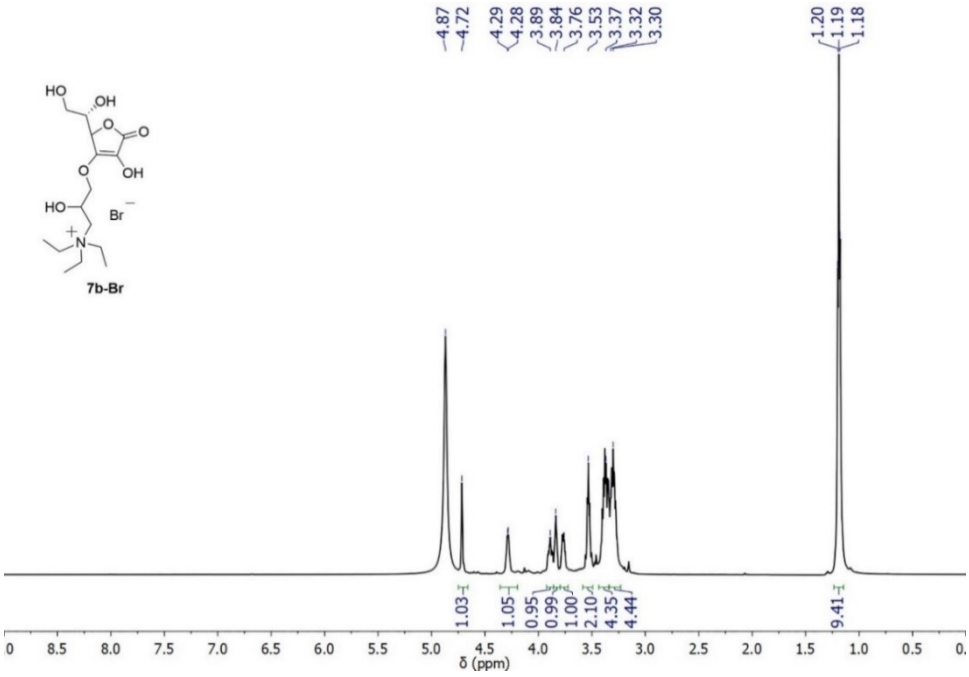


Figure S21. ^{1}H NMR (MeOD-d_4) spectrum of compound **7b-Br**.

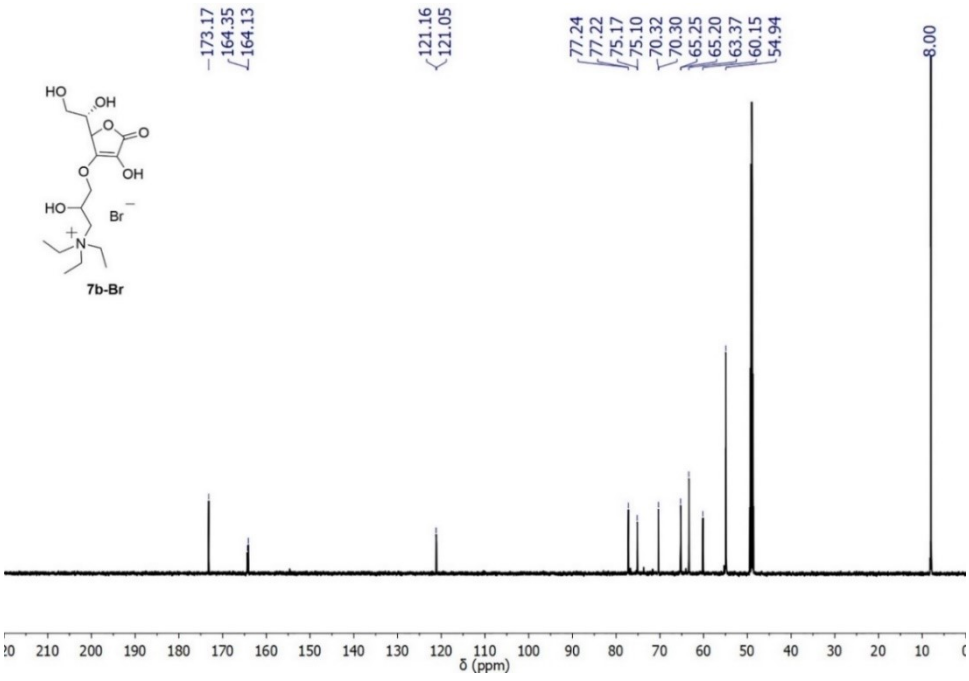


Figure S22. ^{13}C NMR (MeOD-d_4) spectrum of compound **7b-Br**.

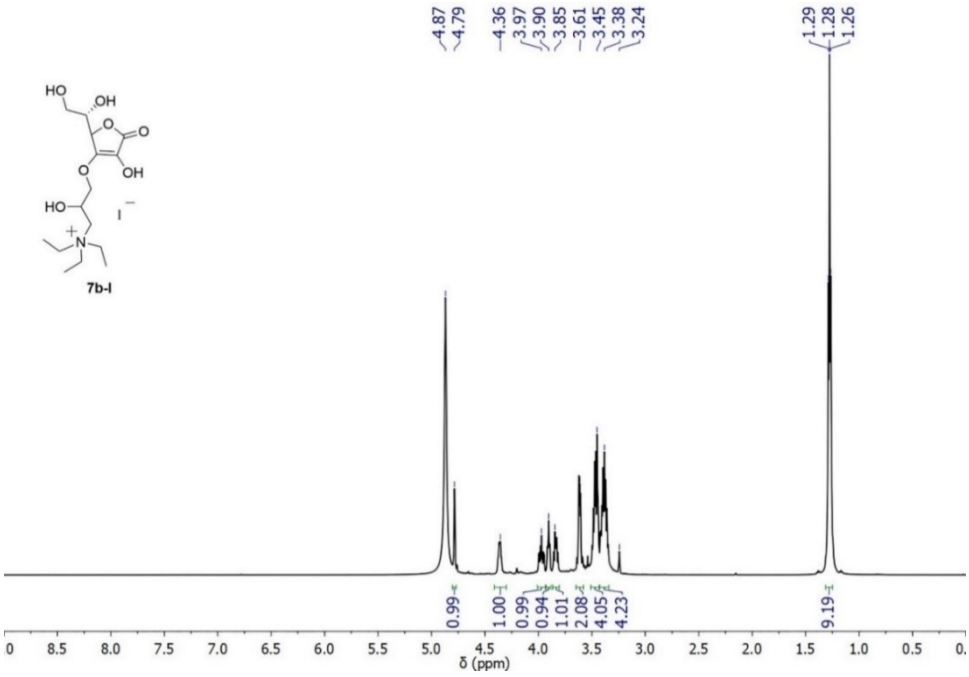


Figure S23. ^{1}H NMR (MeOD-d_4) spectrum of compound **7b-I**.

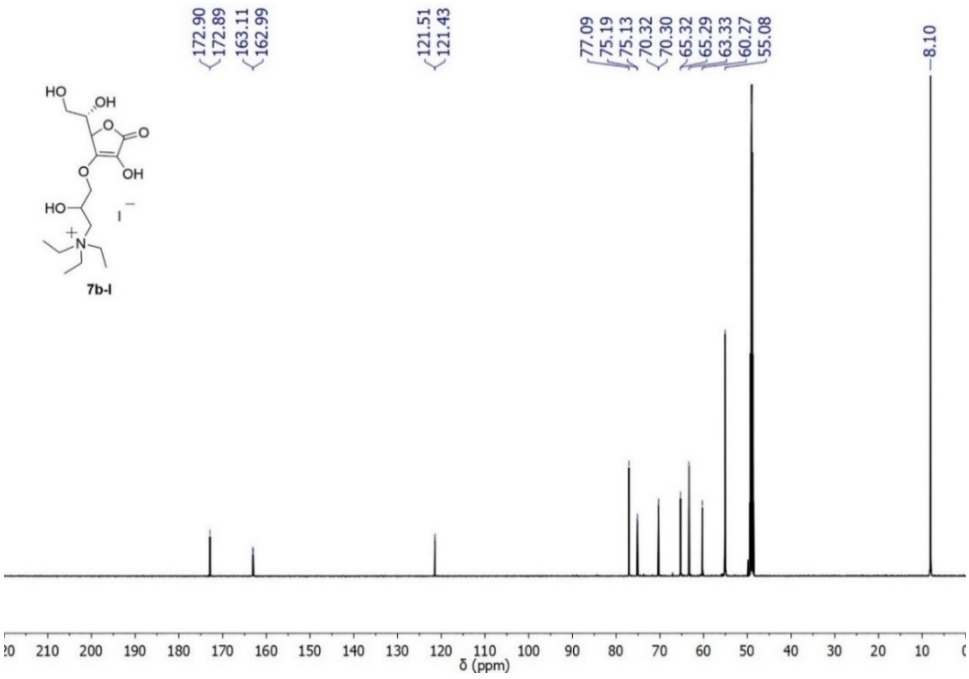


Figure S24. ^{13}C NMR (MeOD-d_4) spectrum of compound **7b-I.**

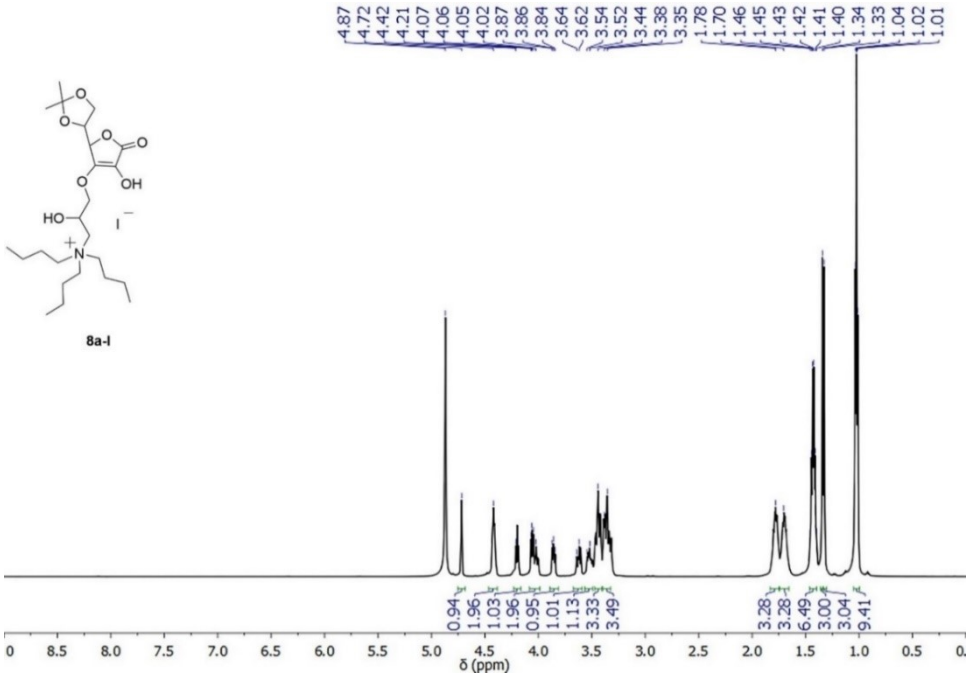


Figure S25. ^{1}H NMR (MeOD-d_4) spectrum of compound **8a-I**

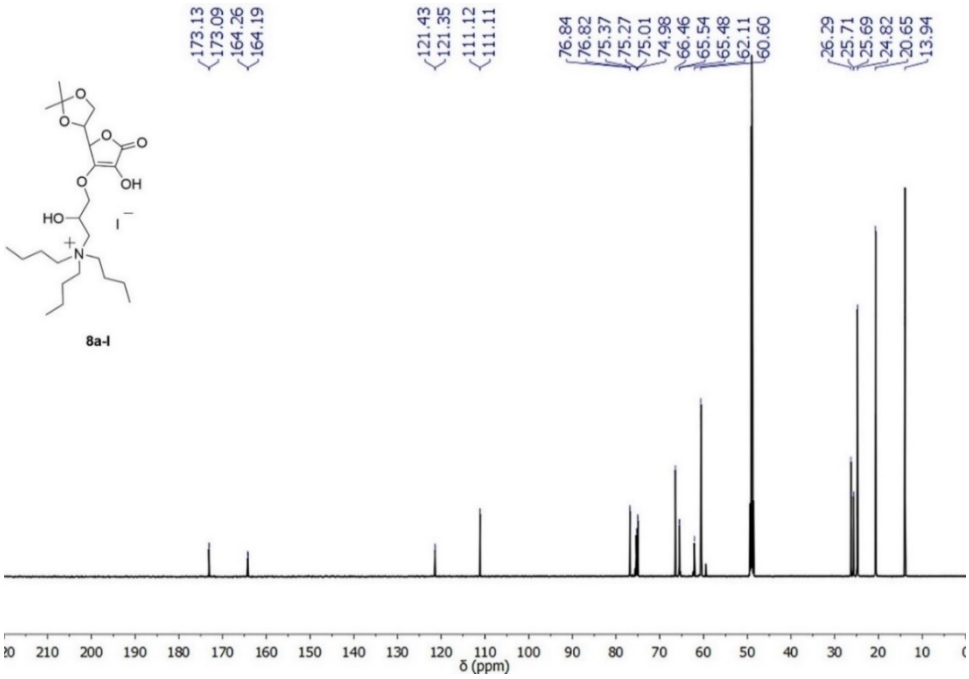


Figure S26. ^{13}C NMR (MeOD-d_4) spectrum of compound **8a-I**

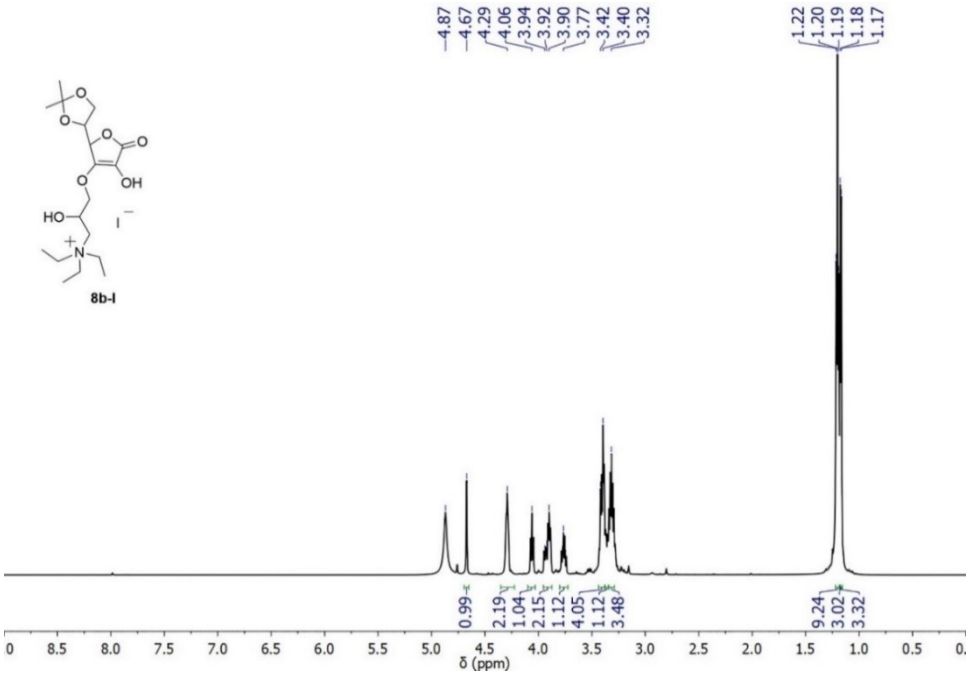


Figure S27. ^{1}H NMR (MeOD-d_4) spectrum of compound **8b-I**

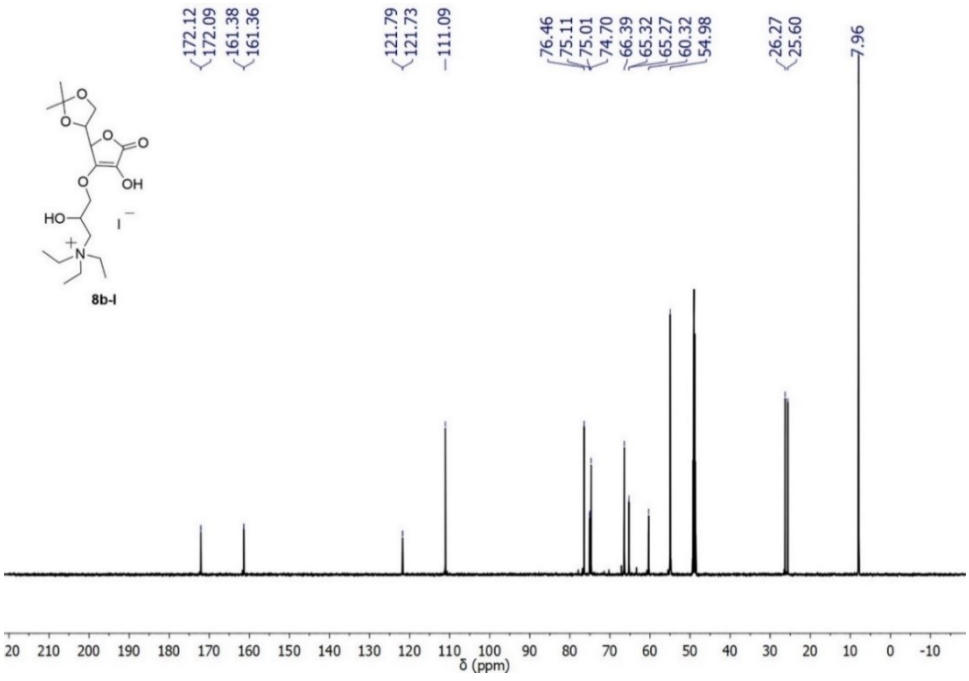


Figure S28. ^{13}C NMR (MeOD-d_4) spectrum of compound **8b-I**

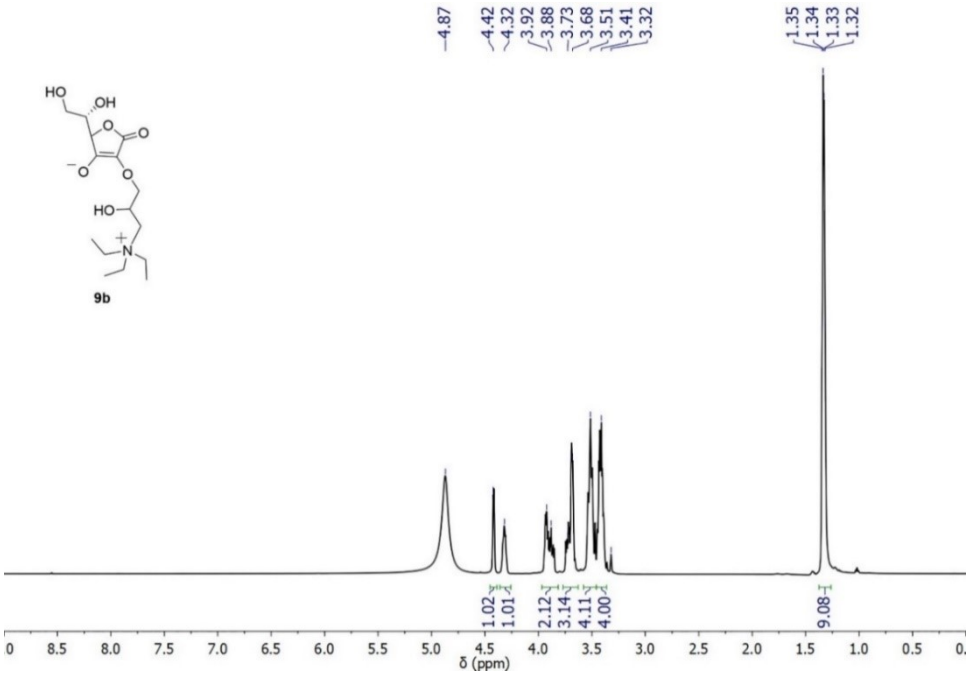


Figure S29. ^{1}H NMR (MeOD-d_4) spectrum of compound **9b**

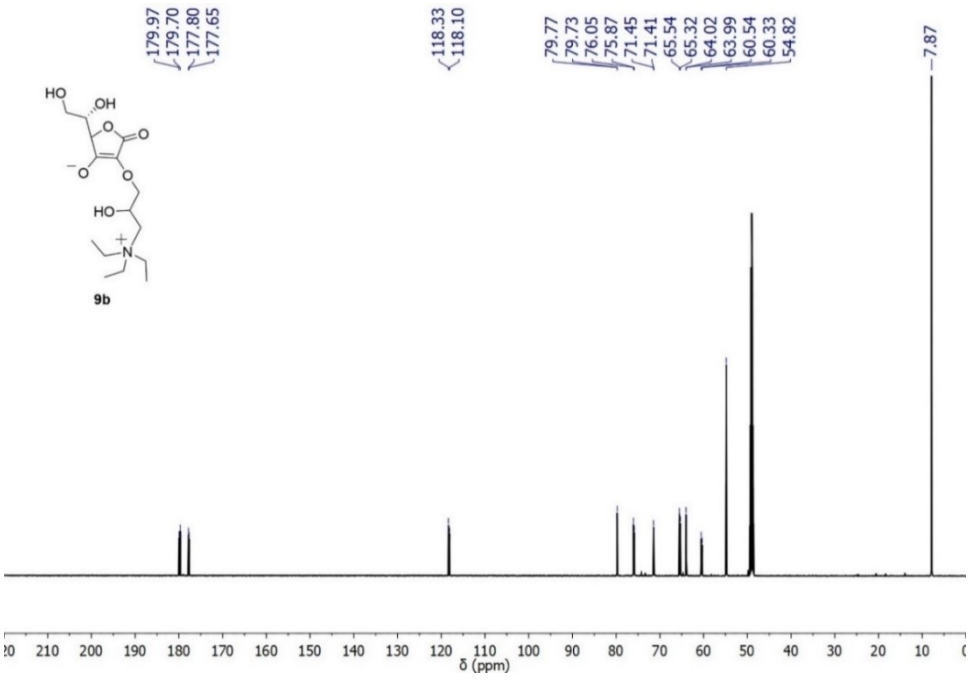


Figure S30. ^{13}C NMR (MeOD-d_4) spectrum of compound **9b**

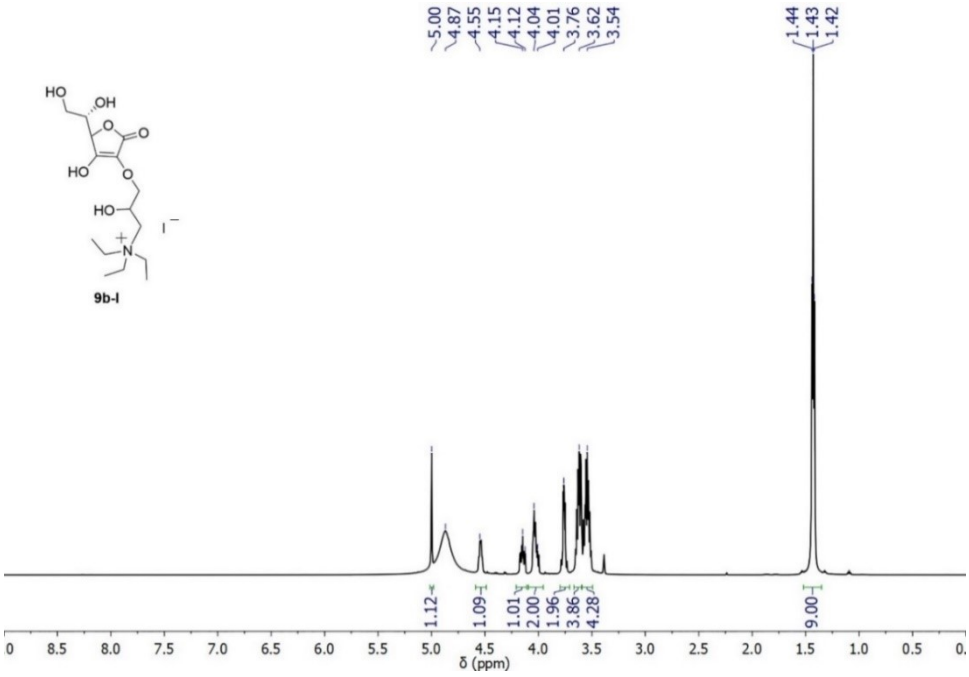


Figure S31. ^{1}H NMR (MeOD-d_4) spectrum of compound **9b-I**

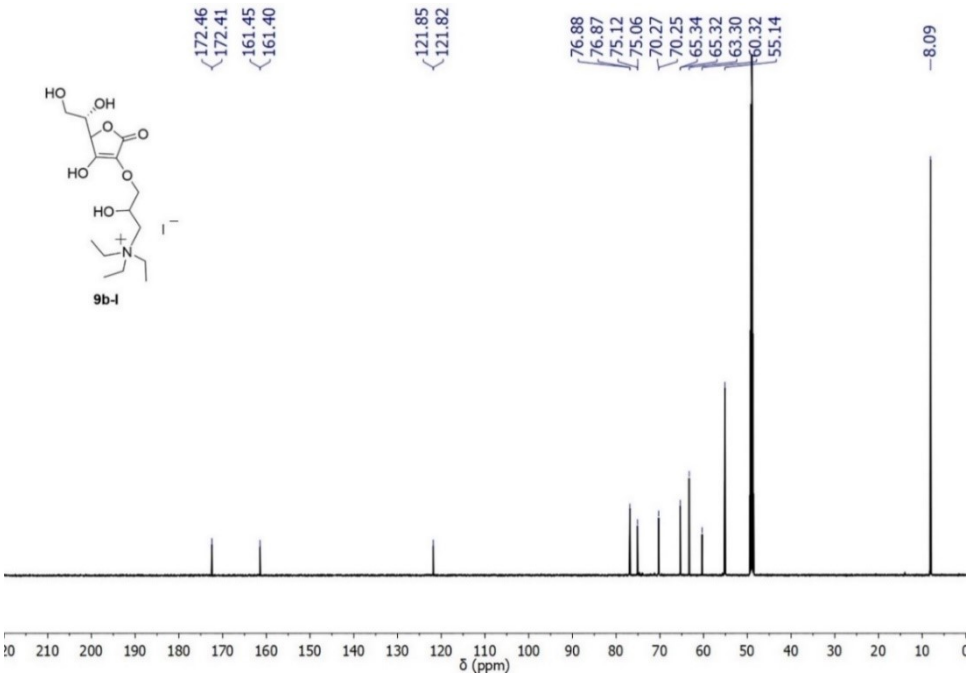


Figure S32. ^{13}C NMR (MeOD-d_4) spectrum of compound **9b-I**

S4. Solubility of the Catalysts in Epoxides and Cyclic Carbonates

All compounds could be dissolved in water with a solubility of at least 0.5 g/mL or higher. The solubility of the most promising catalysts **7a-I**, **7b-I,** and **8b-I** in several epoxides and carbonates was assessed by ^{1}H NMR using 1,3,5-trimethoxybenzene as the internal standard.

Sample preparation: In the absence of added water, an excess of catalyst (about 1 g) was dispersed into 100 μL epoxide or cyclic carbonate in a microtube. The mixture was shaken and equilibrated at 250 rpm under ambient temperature for 24 hours. For the case of water/cyclic carbonate biphasic systems, the catalyst (about 1g) was dissolved in 50 μL of water per mmol of carbonate in a microtube followed by adding 100 μL of carbonate. The mixture was equilibrated at 250 rpm under ambient temperature for 24 hours. For analysis, an aliquot of 25 μL of the supernatant from each sample was transferred into an NMR tube containing 500 μL DMSO-d_6. The quantification was carried out using 1,3,5-trimethoxybenzene as the internal standard. The concentration of soluble catalyst was calculated as in Equation (S1) based on the integration ratio of catalyst (a) and epoxide or cyclic carbonate (b) to the internal standard signal (δ 6.1 ppm, 3H).

Equation (S1):

$$\text{Solubility of catalyst} = \frac{I_a \times H_b \times MW_a}{I_b \times H_a \times MW_b}$$

Where I_a is the integral value of the protons signal of the catalyst, I_b is the integral value of the protons signal of an epoxide or cyclic carbonate, H_a is the number of protons of the catalyst, H_b is the number of protons of the epoxide or cyclic carbonate, MW_a is the molecular weight of the catalyst, and MW_b is the molecular weight of epoxide or cyclic carbonate.

For example: Calculation of catalyst **7a-I** in styrene oxide (**10a**)

$$\text{Solubility of } \mathbf{7a\text{-}I} = \frac{I_{\mathbf{7a\text{-}I}} \times H_{10a} \times MW_{\mathbf{7a\text{-}I}}}{I_{10a} \times H_{\mathbf{7a\text{-}I}} \times MW_{10a}}$$

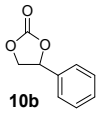
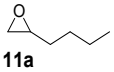
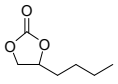
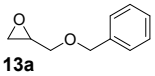
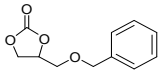
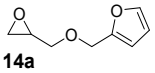
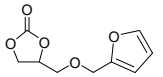
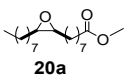
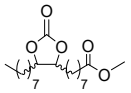
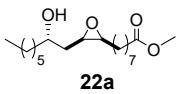
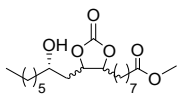
$$= \frac{0.40 \times 1 \times 545.45}{1.04 \times 9 \times 120.15}$$

$$= 0.1940 \text{ g/g styrene oxide}$$

$$\therefore \text{Solubility of } \mathbf{7a\text{-}I} = 194.01 \text{ mg/g } \mathbf{10a}$$

For terminal epoxides and carbonates, compound **7a-I** displayed some solubility in epoxide **10a** that was found to increase when the experiment was carried out at 60 °C, while no solubility in **11a** at room temperature was observed. **7a-I** displayed significant solubility in all terminal cyclic carbonates tested, indicating that this compound would be partially found in the product when used in biphasic reactions. On the other hand, **7b-I** was insoluble in any terminal epoxide at room temperature and 60 °C in 10a and 80 °C in **11a,** while some low solubility was observed in epoxides **13a** and **14a** at 100 °C. Interestingly, compound **7b-I** was very sparingly soluble (carbonates **10b**, **13b**, **14b**) or insoluble (**11b**, **12b**) in terminal carbonates. The solubility of **7b-I** in the carbonate phase decreased further in the presence of a water layer in the system (the carbonate/water volumetric ratio was similar to the case of the biphasic catalytic reactions) due to repartition between the phases; this was also the case of terminal carbonate **15b**. Catalyst **8b-I**, with an acetal-protected ethyldiol side chain, was not soluble in epoxides **10a** and **11a** but was slightly more soluble in cyclic carbonates than **7b-I** as observed for the cases of carbonates **10b** and **11b**. Finally, all catalysts were insoluble in non-polar epoxidized fatty acid esters (**20a**, **22a**) and their carbonated products (**20b**, **22b**) due to the presence of long aliphatic chains.

Table S1. Solubility of catalysts in epoxides and cyclic carbonates under various conditions.

Epoxide	Solubility of catalyst[a] (mg/g epoxide)[b]			Cyclic carbonate	Solubility of catalyst[a] (mg/g carbonate)[b]		
	7a-I	7b-I	8b-I		7a-I	7b-I	8b-I
 **10a**	184±28 (308)[c]	ND[d] (ND)[c]	ND	 **10b**	>1000	28±3 [25±2][e]	54±7
 **11a**	ND	ND (ND)[f]	ND	 **11b**	>1000	ND	16±3
 **12a**	-	ND	-	 **12b**	>1000	ND	-
 **13a**	-	ND (35)[g]	-	 **13b**	>1000	24±8 [4±2][e]	-
 **14a**	-	ND (37)[g]	-	 **14b**	>1000	22±3 [13±1][e]	-
 **20a**	ND	ND	ND	 **20b**	ND	ND	ND
 **22a**	ND	ND	ND	 **22b**	ND	ND	ND

[a] Epoxide or carbonate (100 µl), **7a-I**, **7b-I** or **8b-I** at room temperature, 250 rpm for 24 h. [b] Determined by ^{1}H NMR (see section S4 of the supporting information and Fig. S33-S34) using 1,3,5 trimethoxybenzene as the internal standard in DMSO-d_6. [c] Solubility in the epoxide at 60 °C. [d] ND: Not detected by ^{1}H-NMR measurement. [e] Solubility in the carbonate phase (100 µl) in the presence of 4 mol% **7b-I** and of 50 µL of water/mmol carbonate (30-40 µL of water depending on the epoxide). [f] Solubility in the epoxide at 80 °C. [g] Solubility in the epoxide at 100 °C.

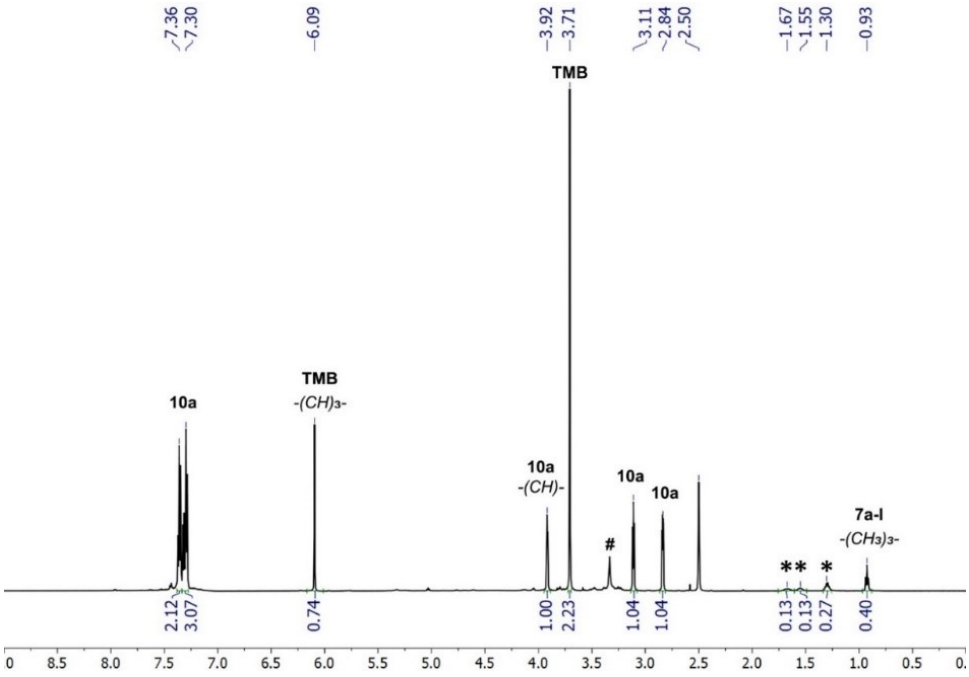


Figure S33. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7a-I** (*) in **10a** using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

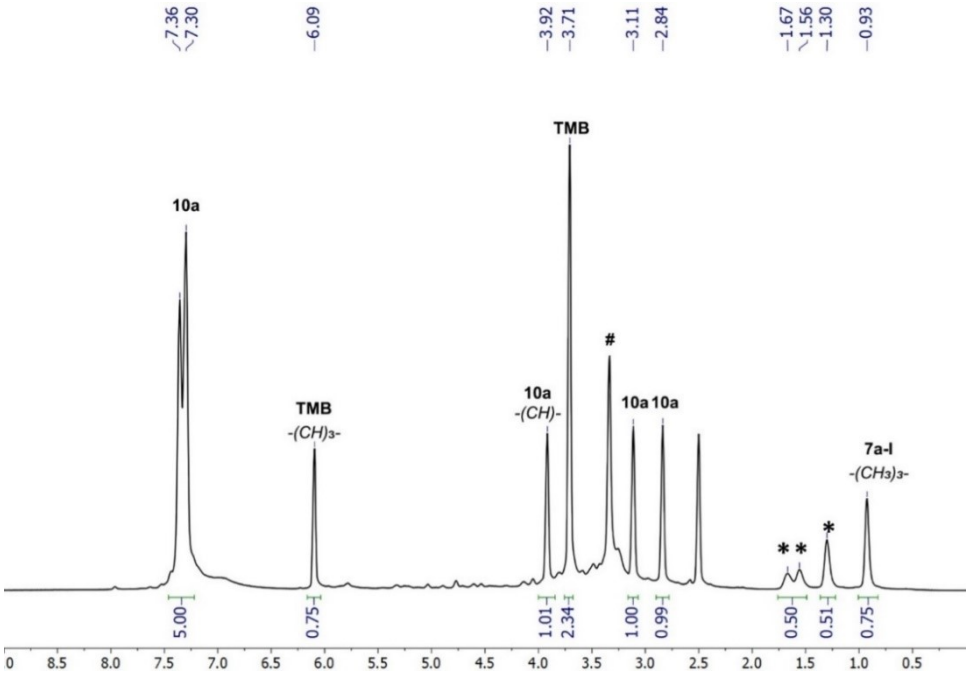


Figure S34. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7a-I** (*) in **10a** at 60 ºC using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

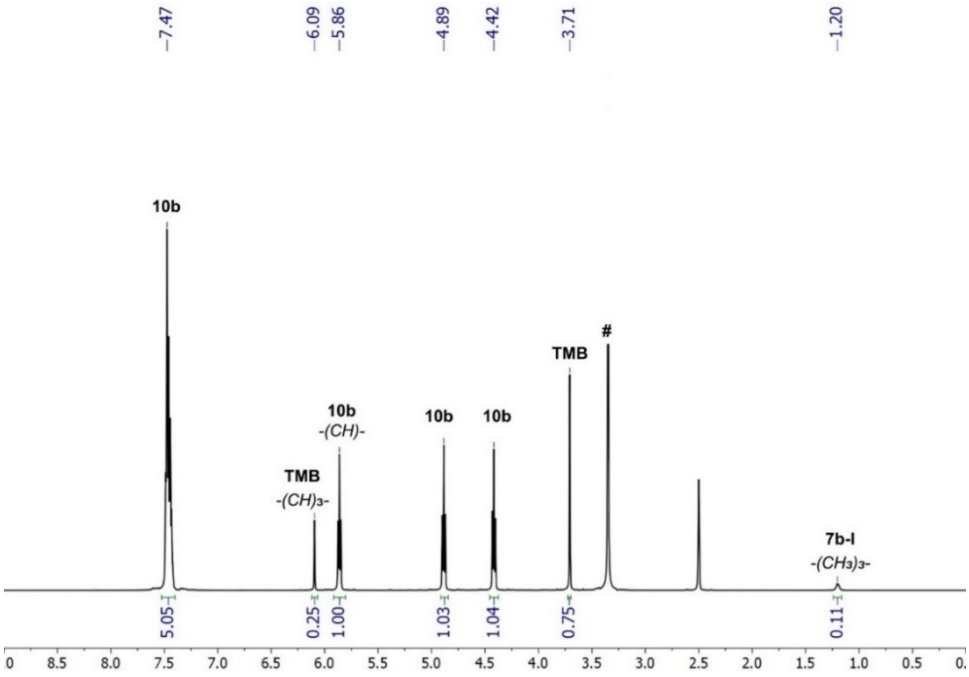


Figure S35. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **10b** using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

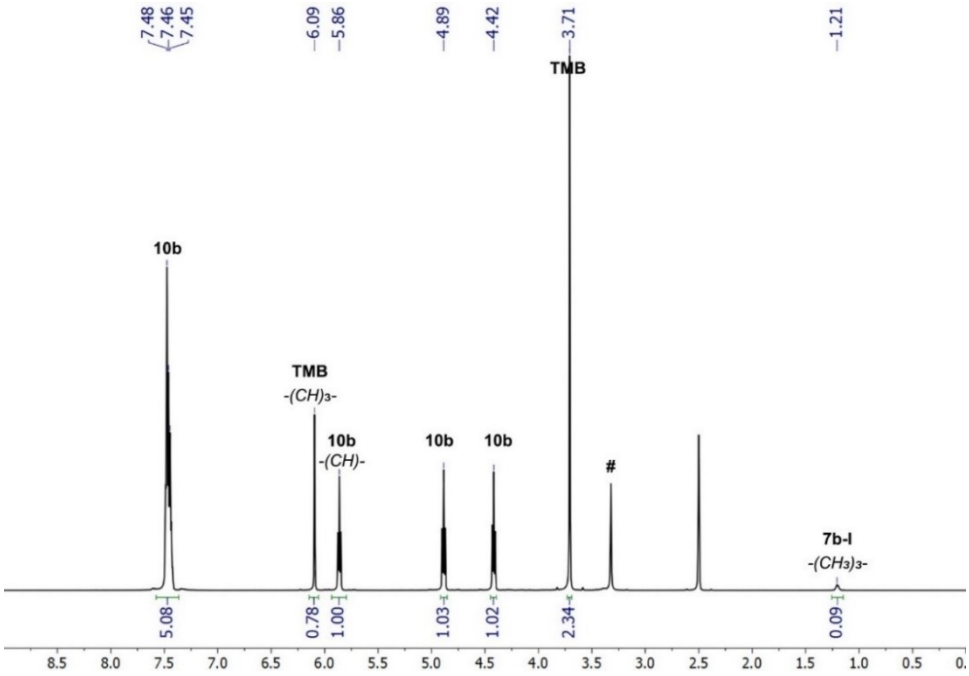


Figure S36. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **10b** and 50 µL of water/mmol carbonate using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

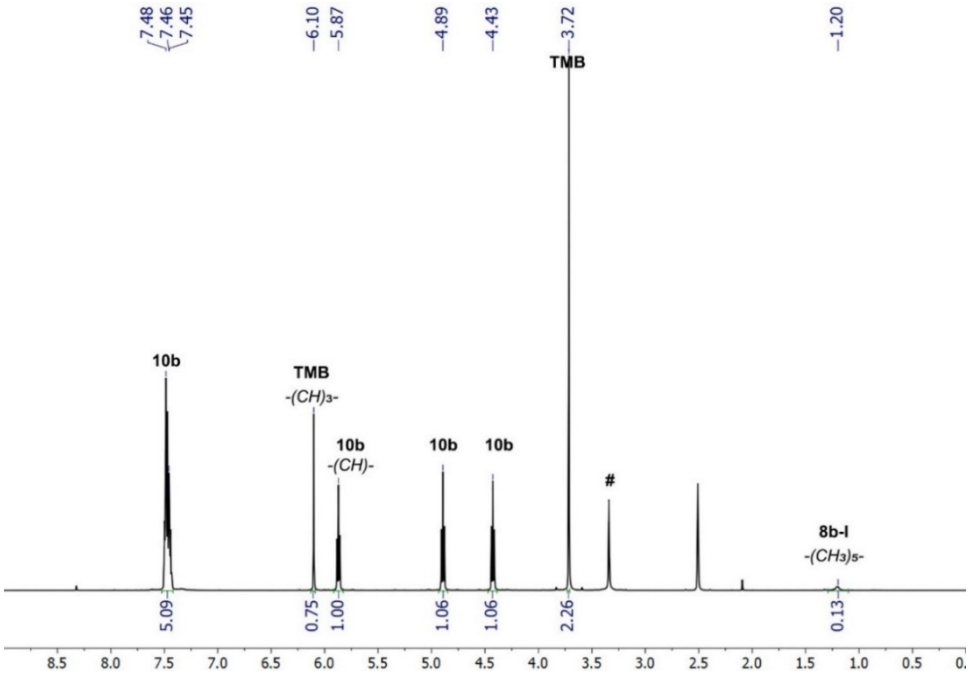


Figure S37. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **8b-I** in **10b** using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

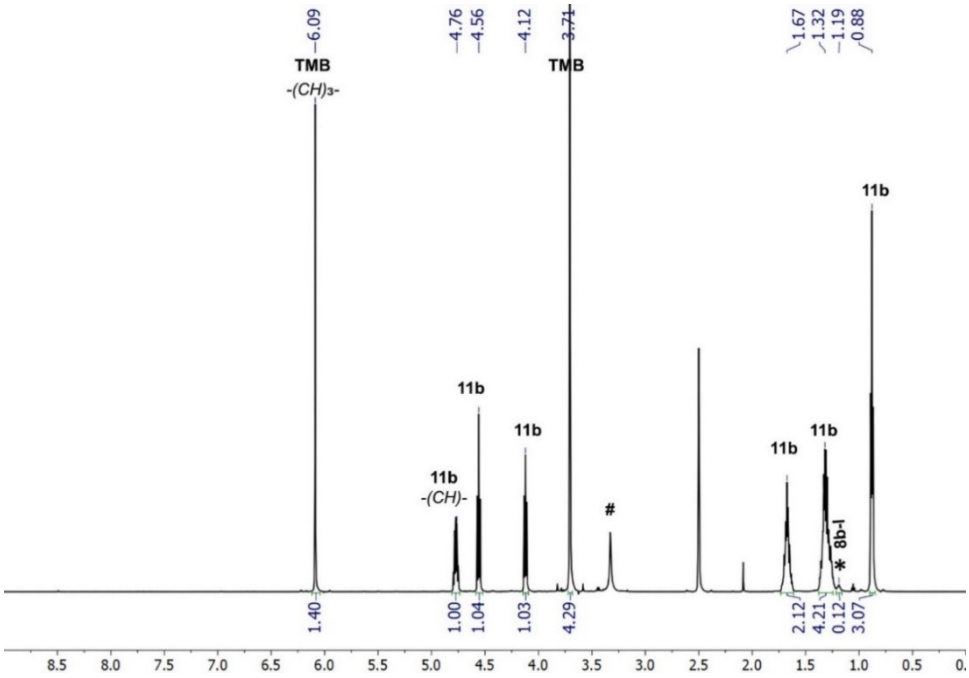


Figure S38. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **8b-I** in **11b** using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

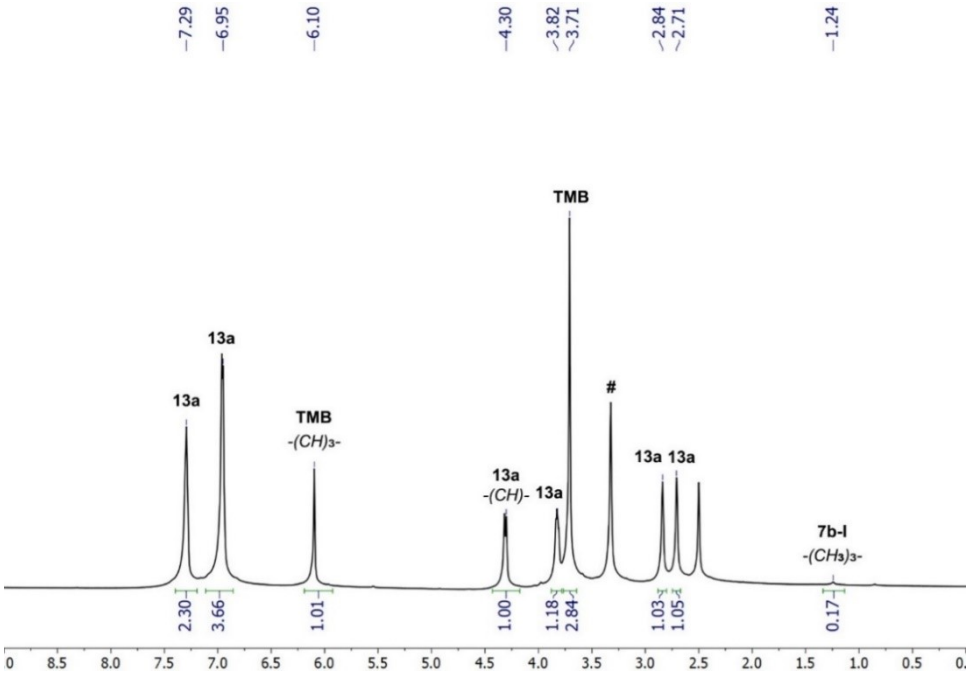


Figure S39. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **13a** at 100 ºC using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

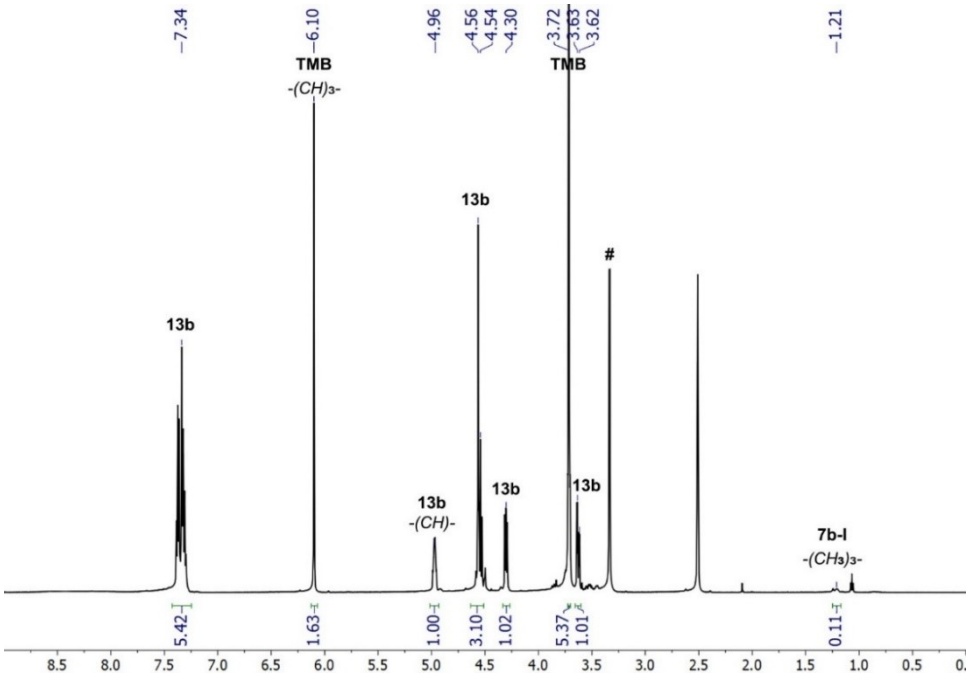


Figure S40. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **13b** using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

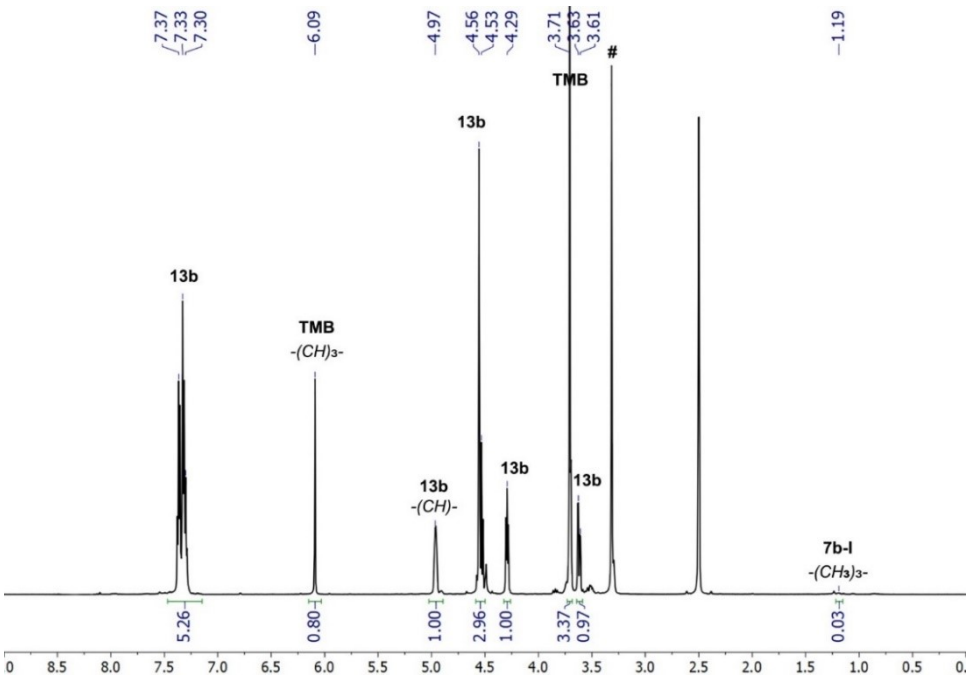


Figure S41. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **13b** and 50 µL of water/mmol carbonate using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

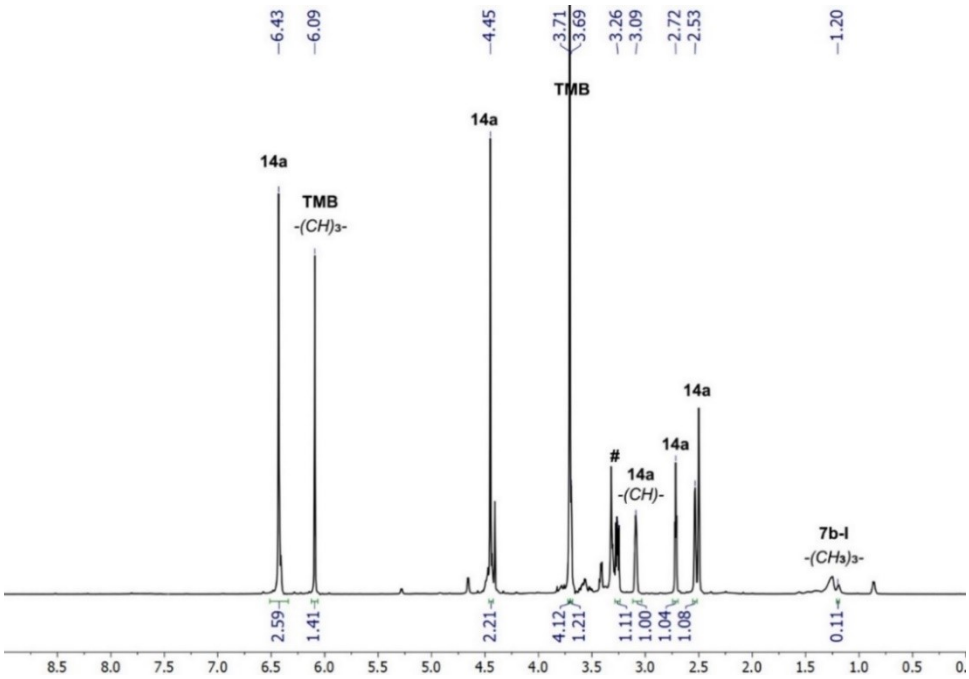


Figure S42. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **14a** at 100 ºC using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

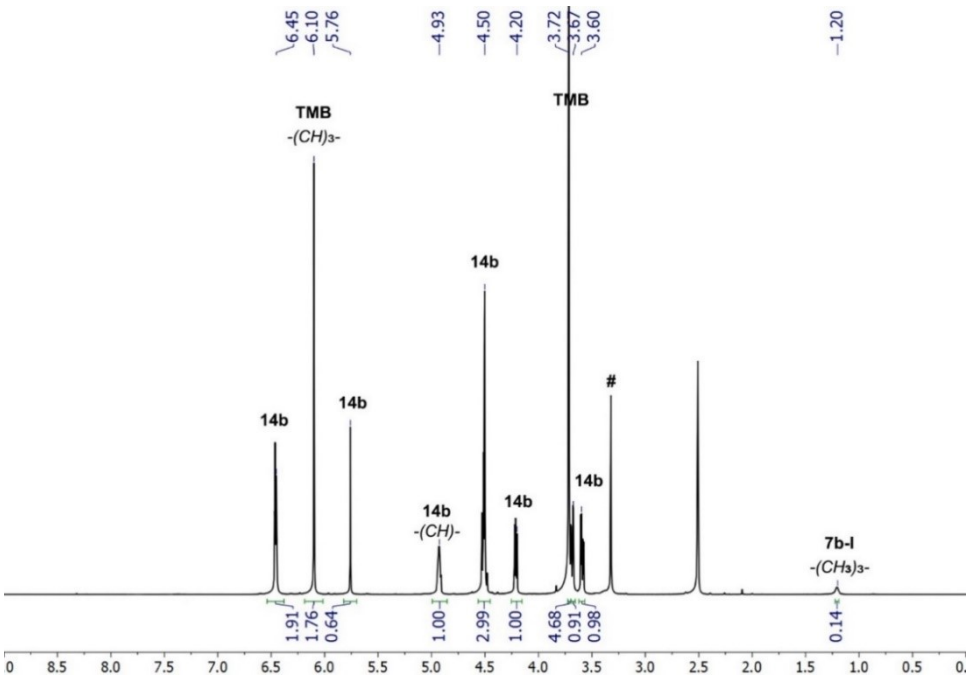


Figure S43. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **14b** using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

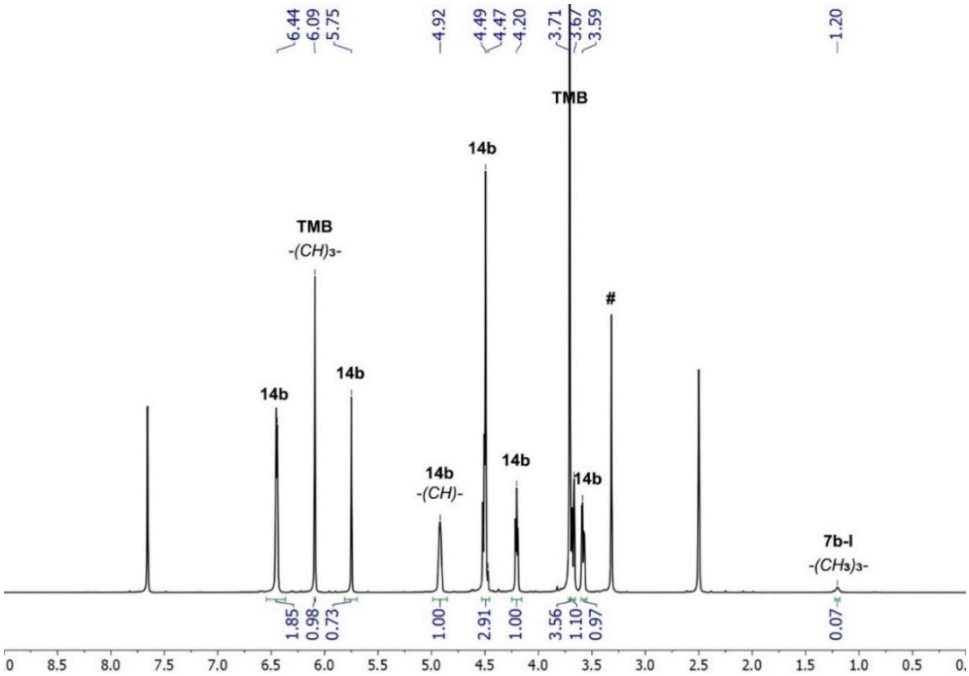


Figure S44. ^{1}H NMR (DMSO-d_6) solubility measurement of catalyst **7b-I** in **14b** and 50 µL of water/mmol carbonate using 1,3,5 trimethoxy benzene (TMB) as internal standard. (#) residual water signal in DMSO-d_6.

S5. General Procedure for the Synthesis of Cyclic Carbonates

5.1 CO_2 coupling reactions with epoxides at atmospheric pressure (1 bar)

Epoxide substrate (10 mmol), a stirring bar, 4 mol% (0.04 equiv.) of catalyst, and water (0-0.5 mL) were added into a 50 mL round bottom Schlenk flask. A rubber balloon containing CO_2 was connected to the Schlenk flask and part of the CO_2 was used for flushing the flask to replace air. The reaction vessel was well sealed to prevent losses of CO_2. The reaction mixture was stirred and heated at atmospheric pressure at the desired temperature. At the end of the reaction, an aliquot of the reaction mixture was analyzed by ^{1}H NMR to determine substrate conversion and selectivity. ^{1}H NMR spectra of crude products of the organic phases are shown in Figures S46-S61.

5.2 High-pressure reactions in biphasic systems (10-30 bar)

The epoxide substrate (10 mmol), catalyst (4 mol%; 0.04 equiv.), and deionized water (0-2 mL) were placed inside a 75 mL stainless steel autoclave containing a magnetic stirring bar. The autoclave was sealed and pressurized with CO_2 (10-30 bar), heated at the desired temperature (generally 60-100 °C for terminal epoxides, 100-120 °C for internal epoxides), and stirred for the desired reaction time. At the end of each run, the autoclave was cooled in an ice bath and carefully vented. Phase separation between the organic phase and the aqueous phase was generally observed. Then, the whole reaction mixture was carefully withdrawn using a glass Pasteur pipette and the aqueous phase was discarded. The obtained product was analyzed by ^{1}H NMR to calculate conversion and selectivity. ^{1}H NMR spectra of crude products in the separated organic phases are shown in Figures S62-S146. For the scale-up process (50 mmol of epoxide), a 200 mL stainless steel autoclave was used.

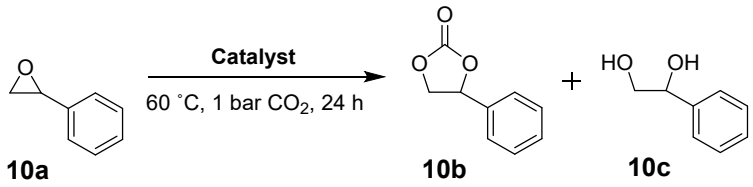
5.3 Recycling of the aqueous layer

The separation of the aqueous layer was carried out as in the procedure reported above. The used aqueous layer was readded into a reaction autoclave that was refilled with fresh substrate and the reactor pressurized again with CO_2.

S6. Kinetic profiles for Styrene Carbonate Synthesis Monitored by ^{1}H NMR

The kinetic comparison for the cycloaddition reaction of styrene oxide and CO_2 catalyzed by **7a-I** versus the previously reported binary system of ascorbic acid/TBAI[3] was performed under solvent-free conditions at 60 °C and 1 bar CO_2. ^{1}H NMR spectra were measured to observe epoxide conversion and selectivity after 2, 4, 6, 8, 12, and 24 hours as shown in Table S2 and Figure S45.

Table S2 Comparison of catalyst activity at various reaction times.[a]



Entry	Catalyst (mol%)	Additive (mol%)	Temp. (˚C)	P_{CO2} (bar)	Time (h)	Conversion [b] (%) ± S.D	Selectivity[c] (%) ± S.D
1	AsA (4)	TBAI (4)	60	1	2	19±1	85±1
2	AsA (4)	TBAI (4)	60	1	4	45±1	94±1
3	AsA (4)	TBAI (4)	60	1	6	64±1	95±1
4	AsA (4)	TBAI (4)	60	1	8	71±1	97±1
5	AsA (4)	TBAI (4)	60	1	12	82±1	98±1
6	AsA (4)	TBAI (4)	60	1	24	86±1	95±1
7	**7a-I** (4)	-	60	1	2	19±1	78±1
8	**7a-I** (4)	-	60	1	4	60±1	87±1
9	**7a-I** (4)	-	60	1	6	72±1	94±1
10	**7a-I** (4)	-	60	1	8	81±1	96±1
11	**7a-I** (4)	-	60	1	12	89±1	98±1
12	**7a-I** (4)	-	60	1	24	97±1	98±1

[a] Epoxide (10 mmol), Catalyst (4 mol%) at 60 °C, 1 bar CO_2, without solvent for 24 h. [b] Determined by ^{1}H NMR in $CDCl_3$. [c] Refers to the selectivity for cyclic carbonates (**10b**) versus 1,2-diol (**10c**).

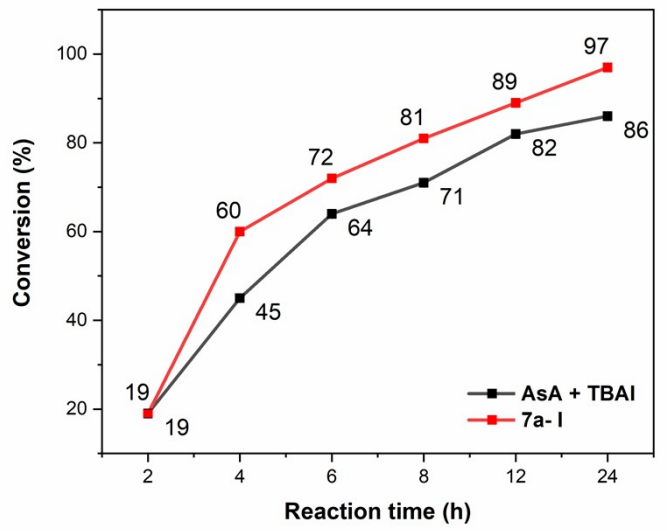


Figure S45. Kinetic profiles of styrene oxide conversion in the CO_2 cycloaddition reaction catalysed by the binary system of ascorbic acid/TBAI (black line) and **7a-I** (red line).

S7. ^{1}H NMR Spectra of Crude Reaction

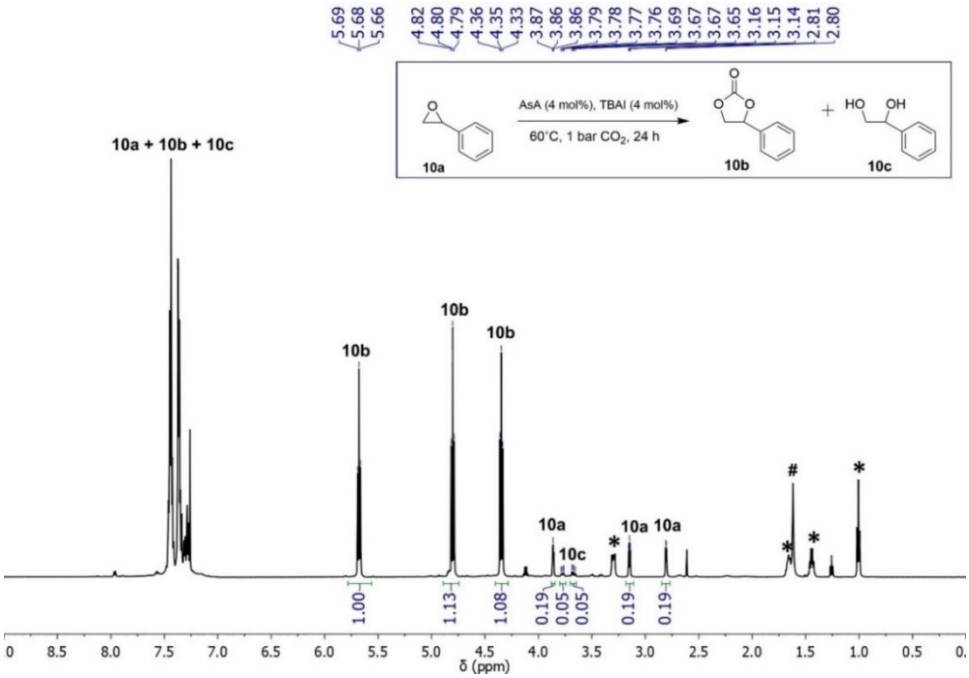


Figure S46. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% Ascorbic acid, 4 mol% TBAI **(*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 2. (#) residual water signal in $CDCl_3$.

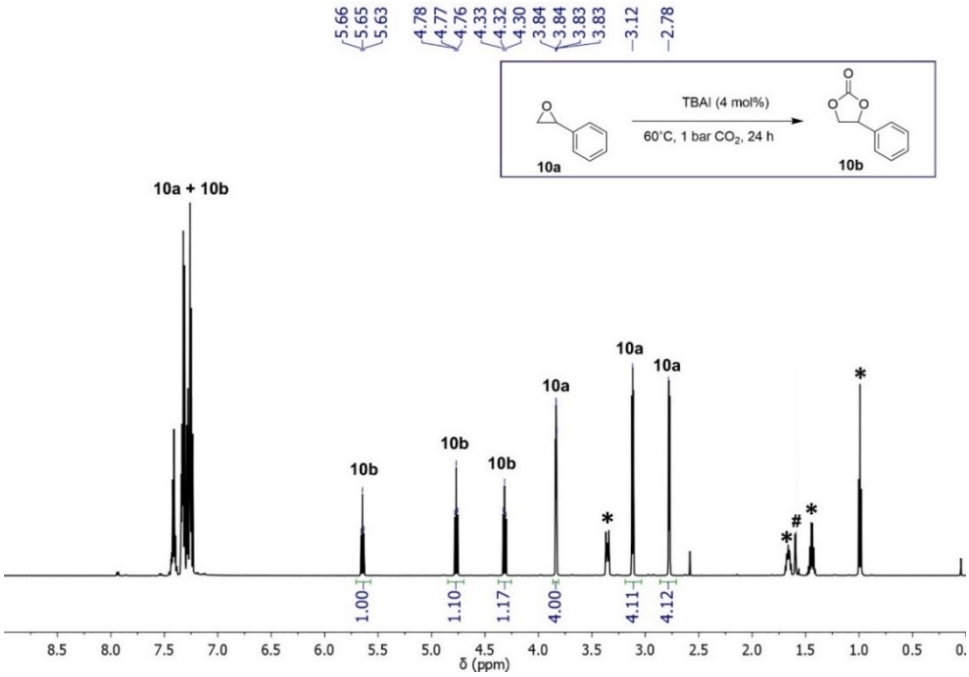


Figure S47. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% TBAI **(*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 3. (#) residual water signal in $CDCl_3$.

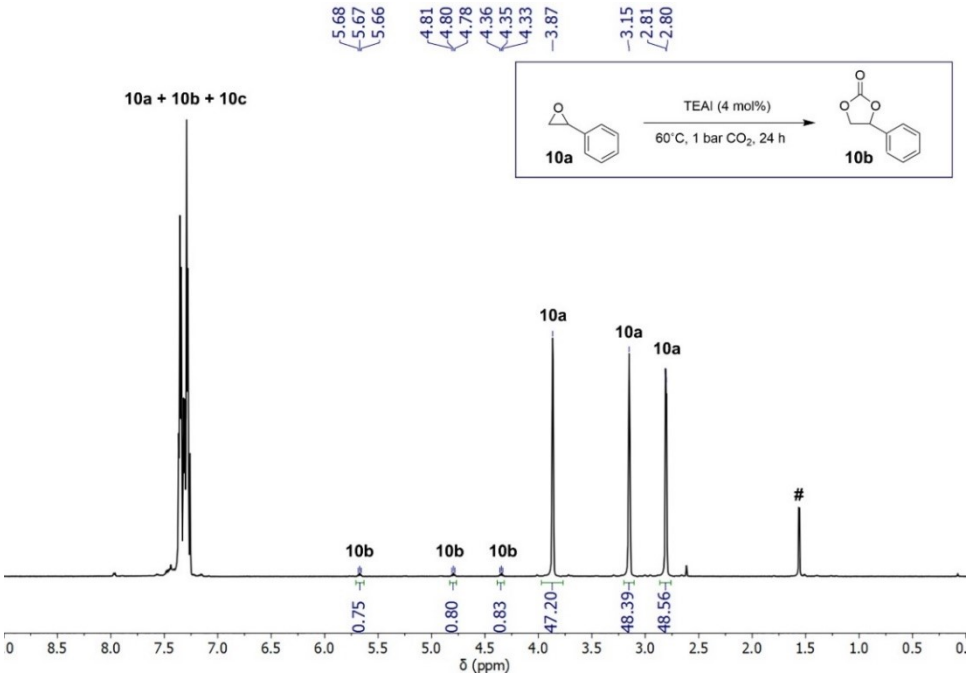


Figure S48. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% TEAI, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 4. (#) residual water signal in $CDCl_3$.

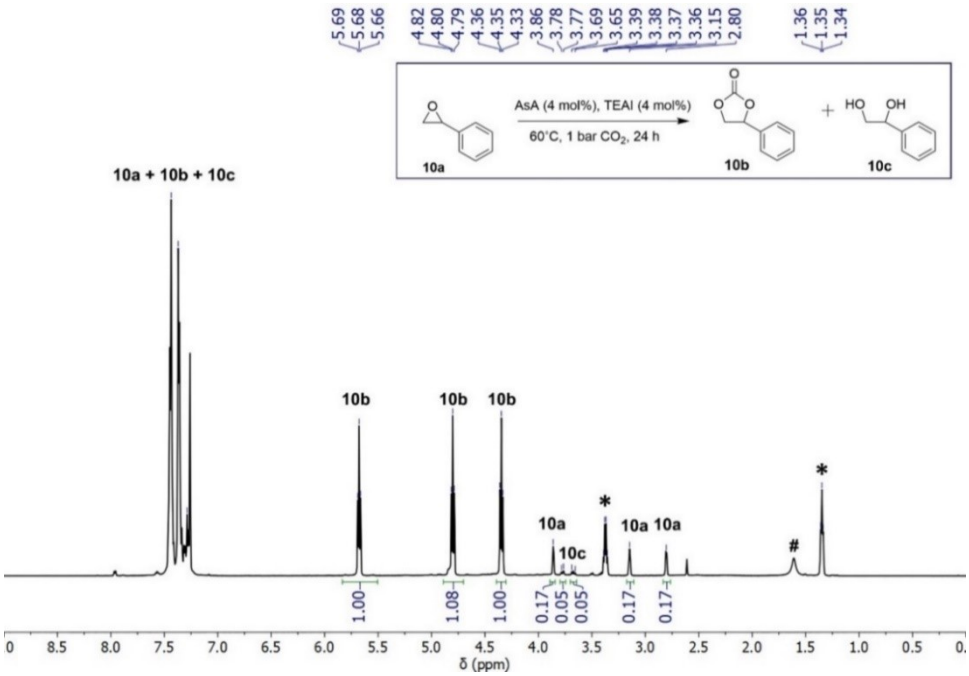


Figure S49. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% Ascorbic acid, 4 mol% TEAI **(*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 5. (#) residual water signal in $CDCl_3$.

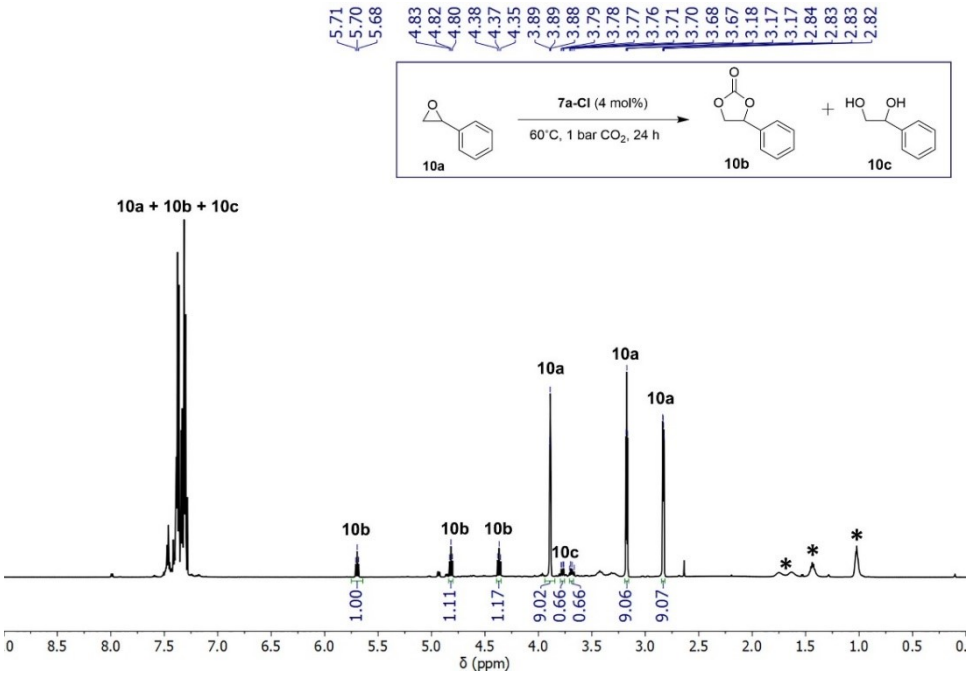


Figure S50. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7a-Cl (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 6.

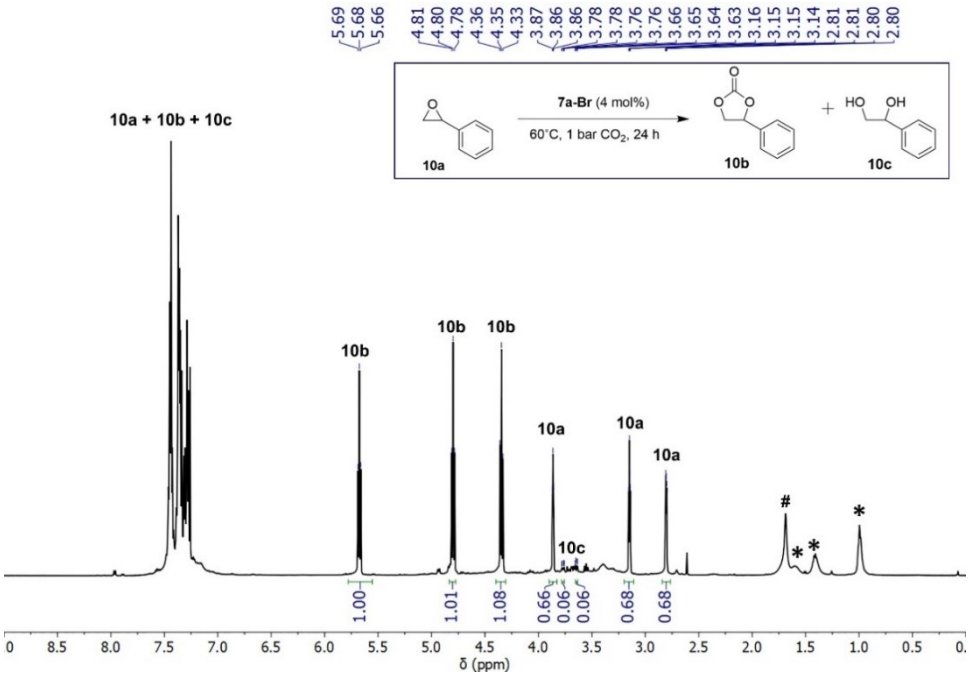


Figure S51. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7a-Br (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 7. (#) residual water signal in $CDCl_3$.

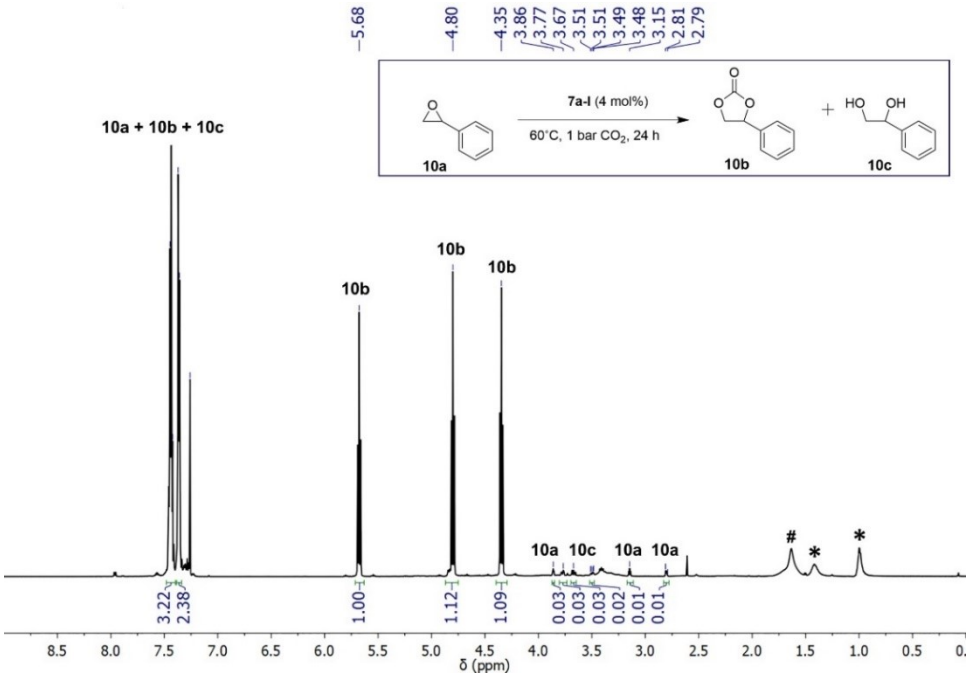


Figure S52. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7a-I (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 8. (#) residual water signal in $CDCl_3$.

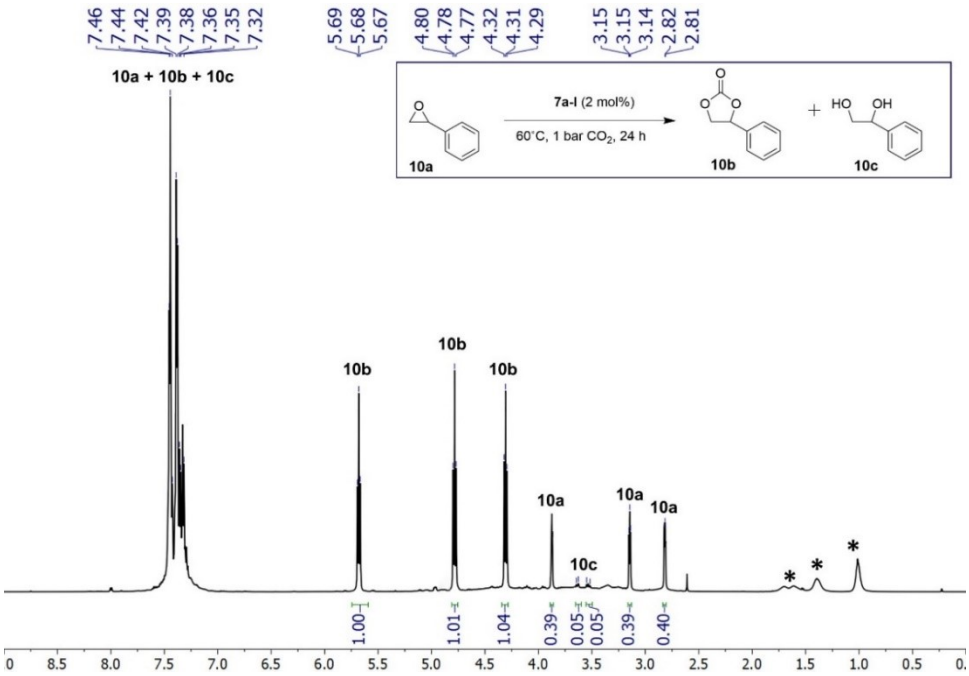


Figure S53. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 2 mol% **7a-I (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 9. (#) residual water signal in $CDCl_3$.

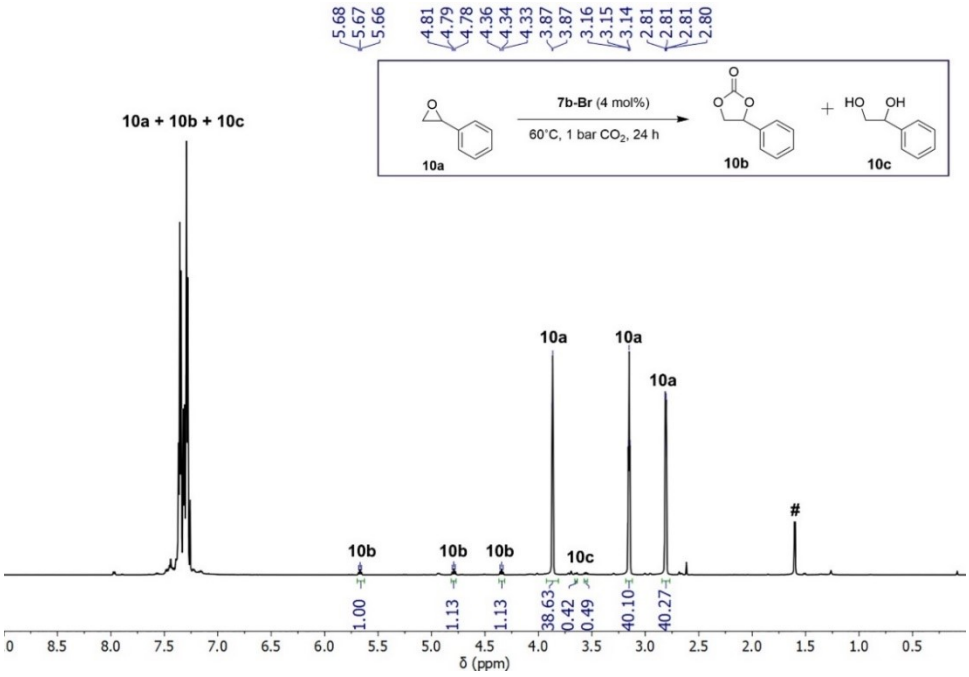


Figure S54. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7b-Br**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 11. (#) residual water signal in $CDCl_3$.

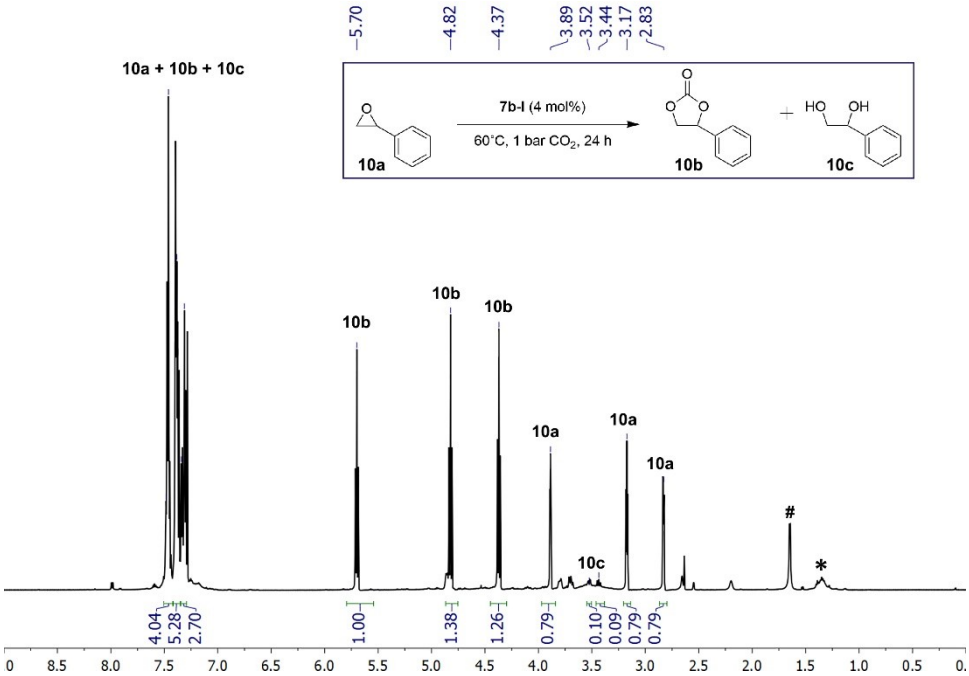


Figure S55. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7b-I (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 12. (#) residual water signal in $CDCl_3$.

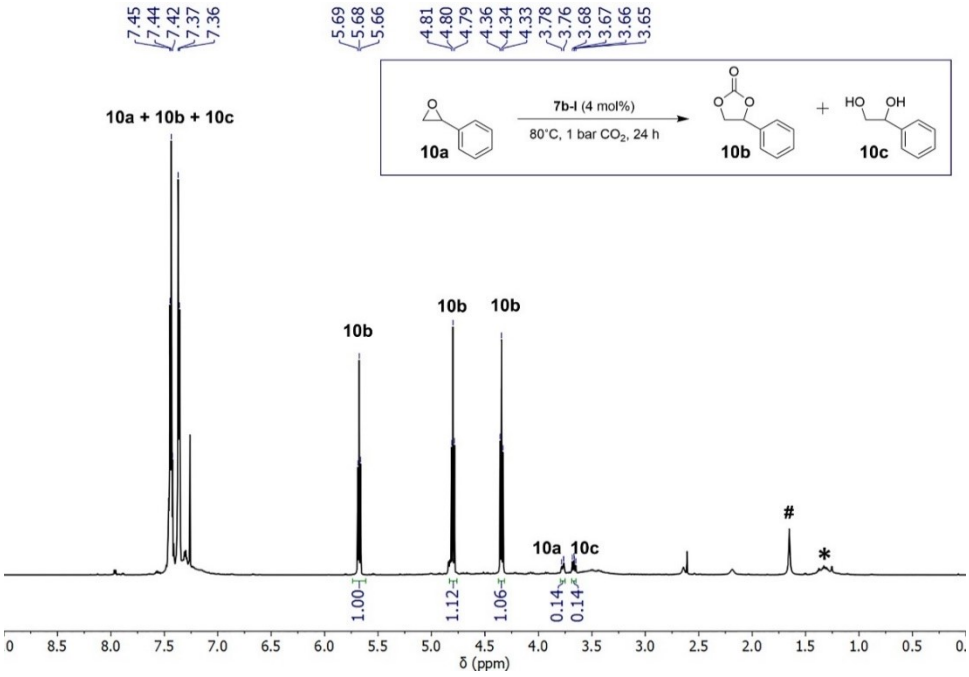


Figure S56. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7b-I (*)**, solvent-free, 80 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 13. (#) residual water signal in $CDCl_3$.

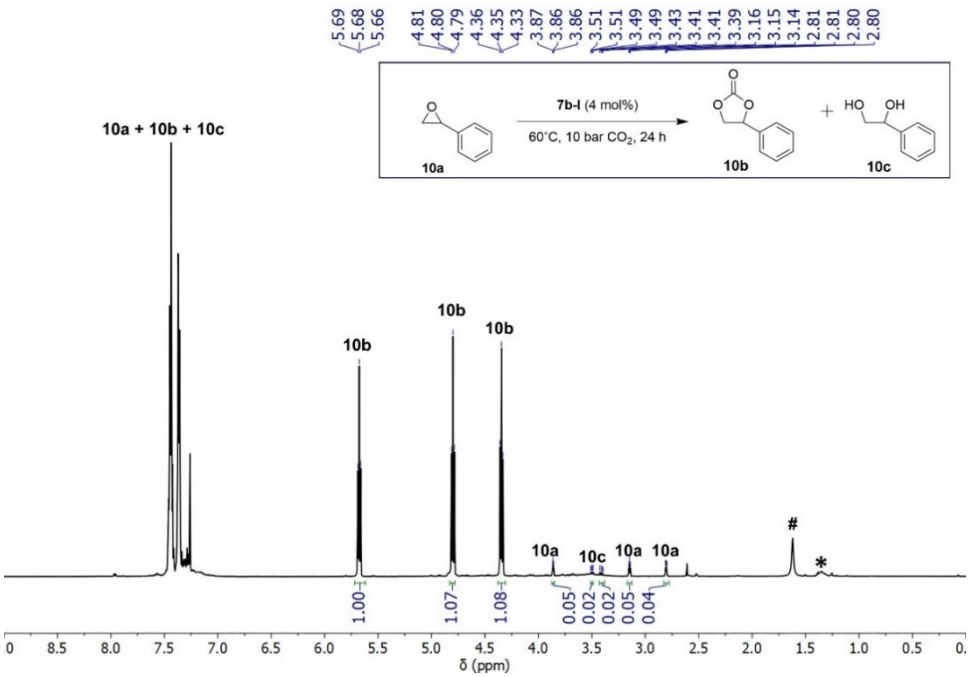


Figure S57. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7b-I (*)**, solvent-free, 60 °C, 10 bar CO_2, 24 h; Table 1, Entry 14. (#) residual water signal in $CDCl_3$.

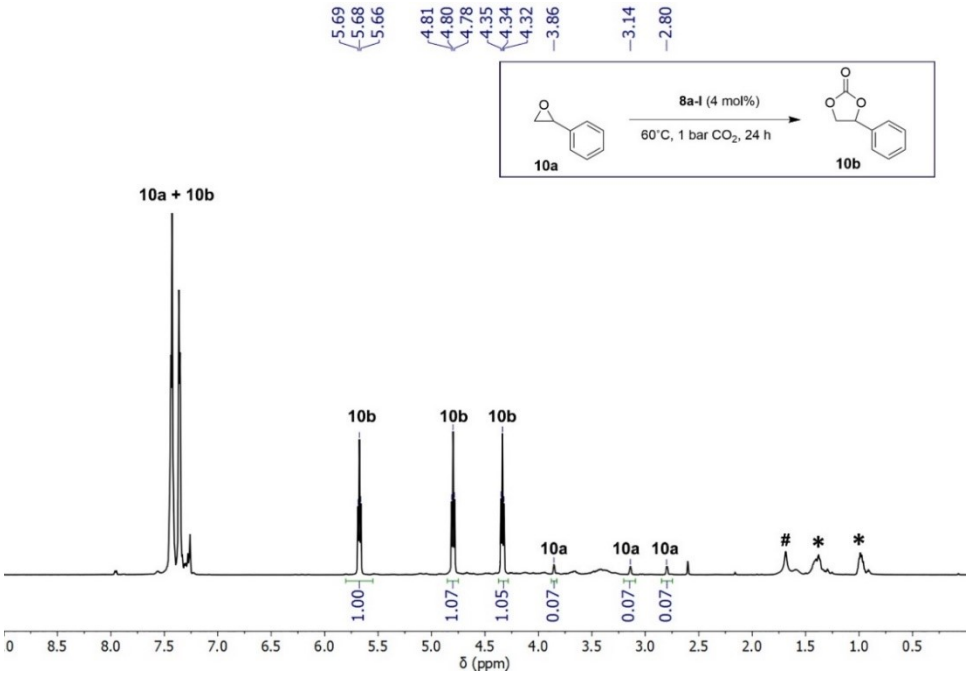


Figure S58. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **8a-I (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 15. (#) residual water signal in $CDCl_3$.

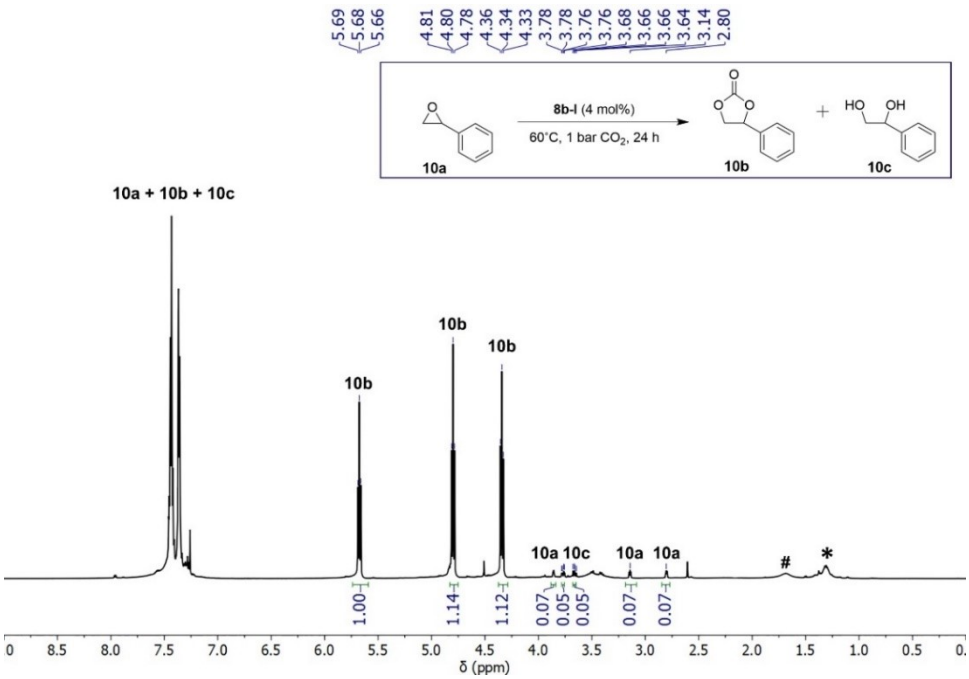


Figure S59. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **8b-I (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 16. (#) residual water signal in $CDCl_3$.

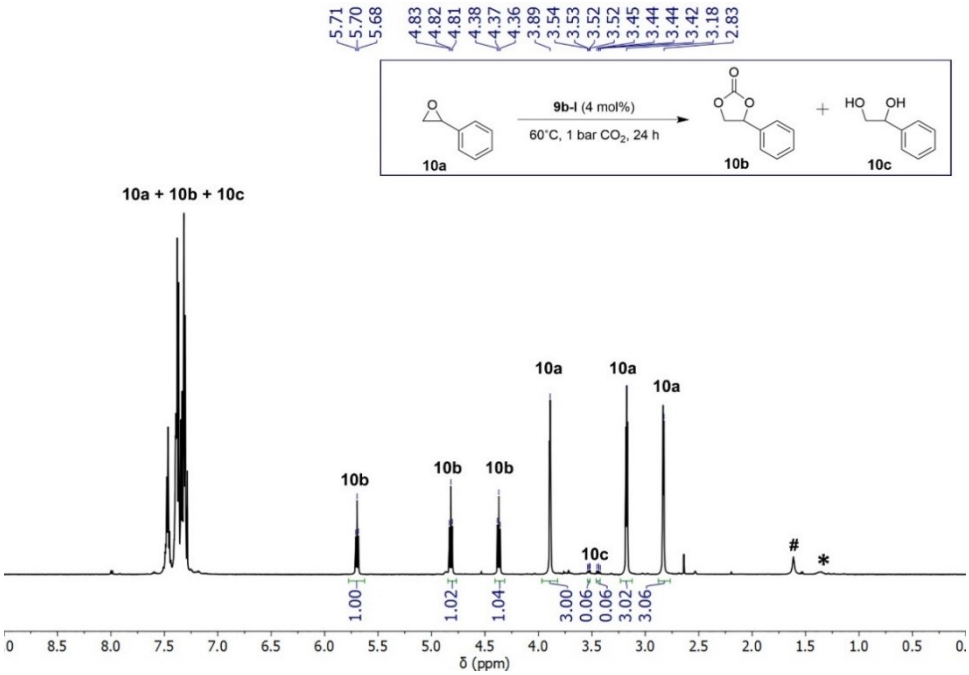


Figure S60. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **9b-I (*)**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 17. (#) residual water signal in $CDCl_3$.

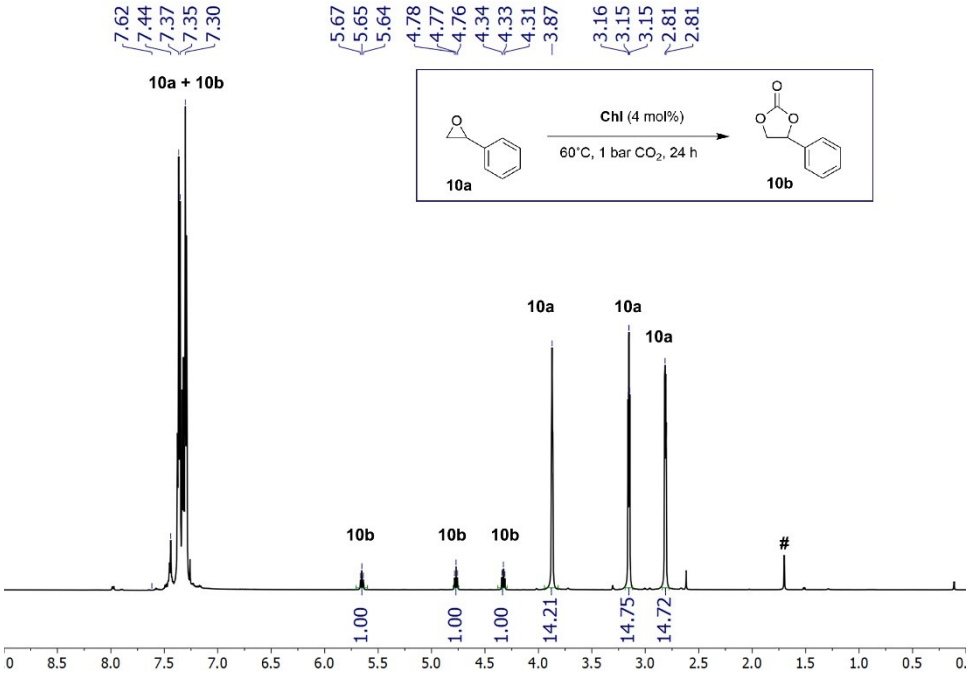


Figure S61. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **ChI**, solvent-free, 60 °C, 1 bar CO_2 (balloon), 24 h; Table 1, Entry 18. (#) residual water signal in $CDCl_3$.

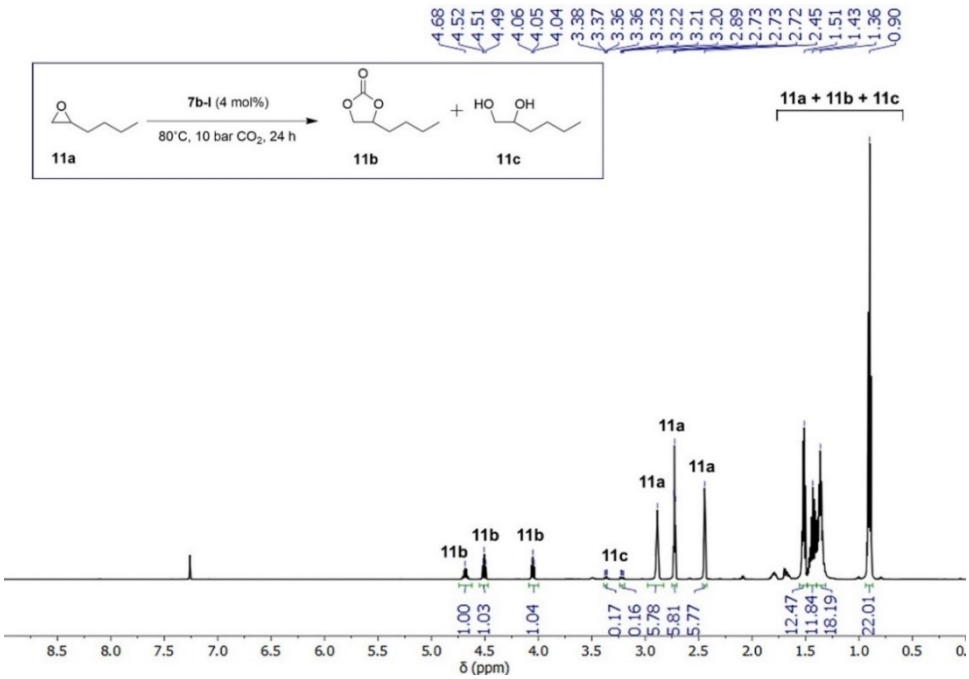


Figure S62. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, solvent-free, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 1.

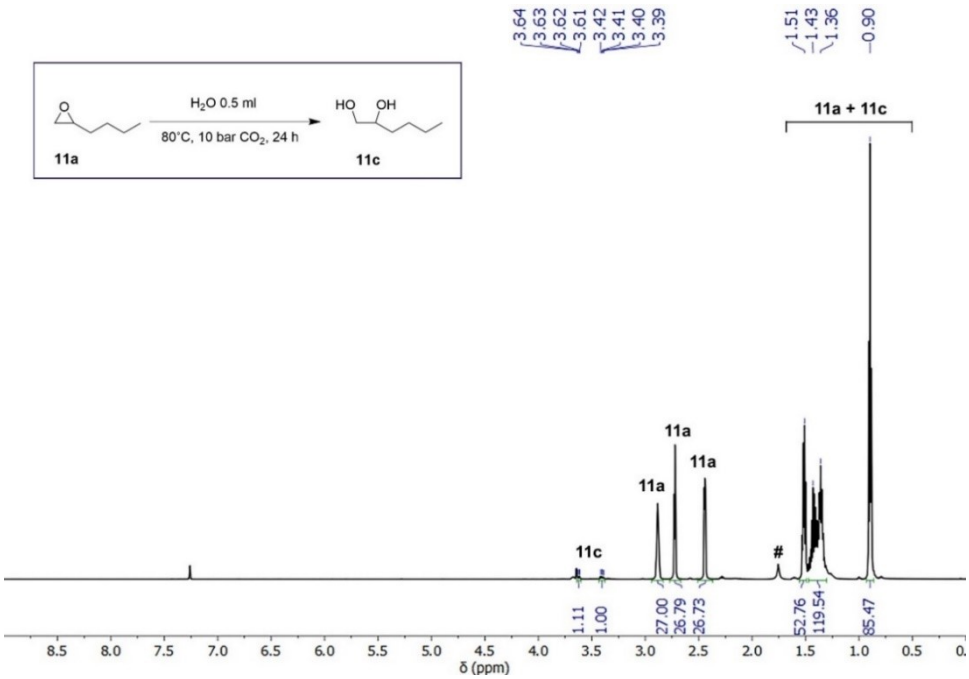


Figure S63. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 2. (#) residual water signal in $CDCl_3$.

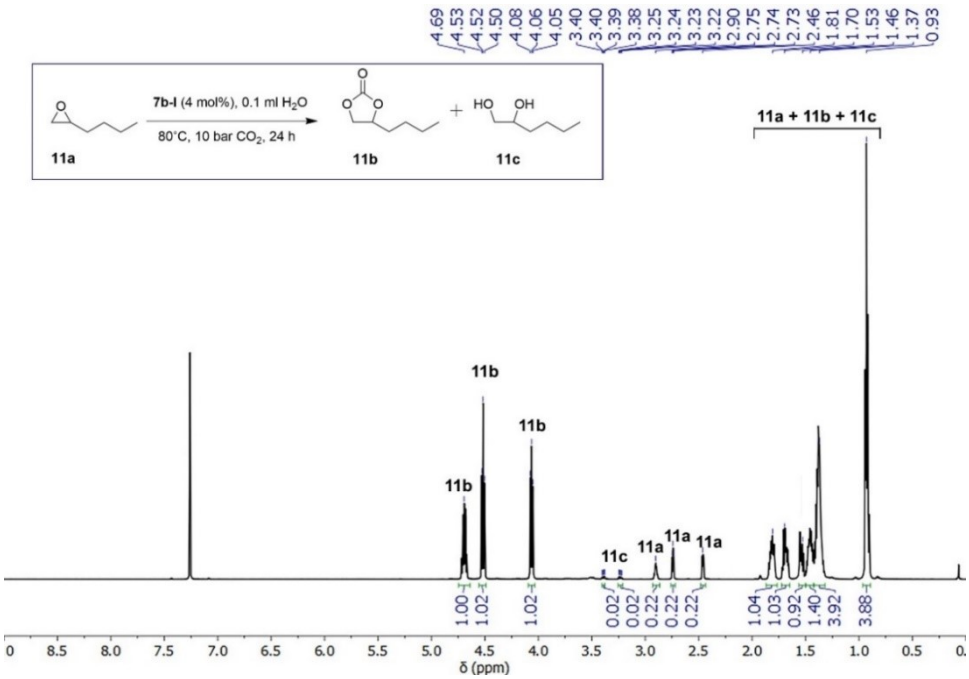


Figure S64. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.1 mL H_2O, 80 °C, 10 bar CO_2, 24 h (1st run); Table 2, Entry 3.

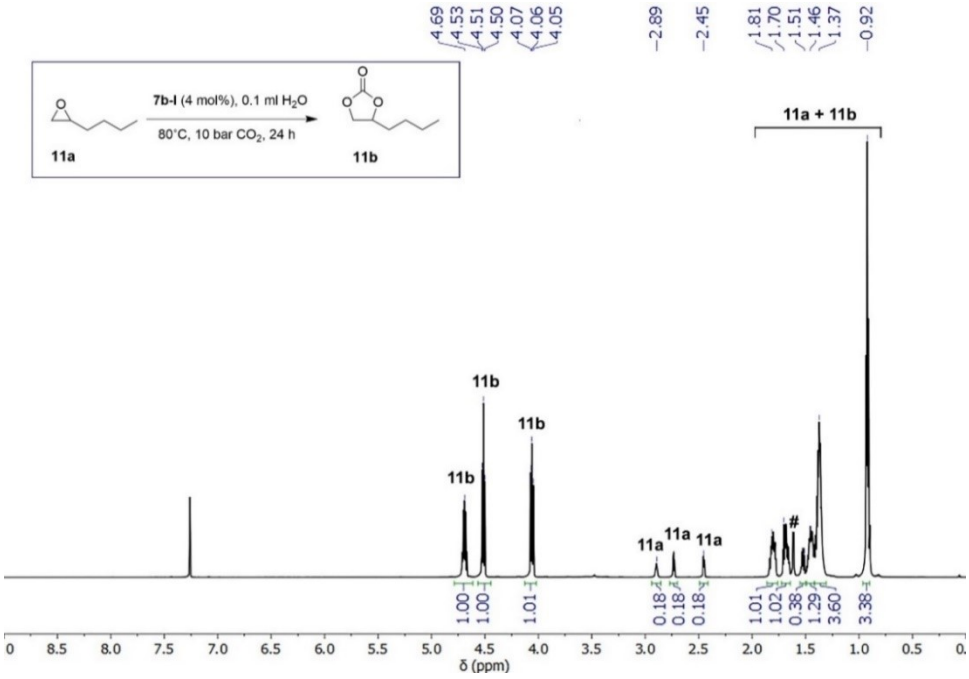


Figure S65. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.1 mL H_2O, 80 °C, 10 bar CO_2, 24 h (2nd run); Table 2, Entry 4. (#) residual water signal in $CDCl_3$.

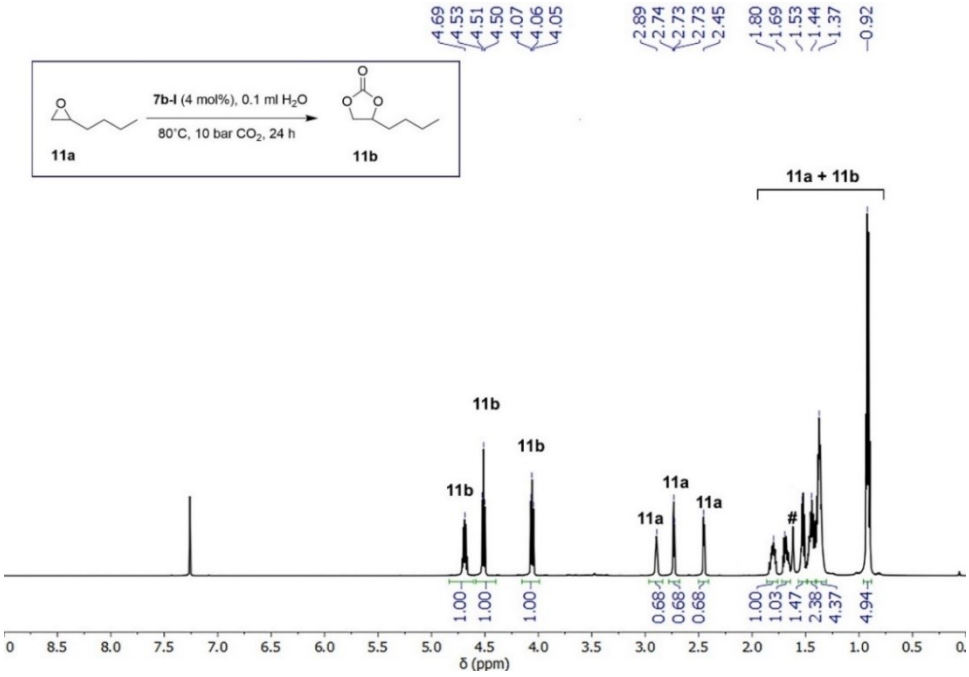


Figure S66. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.1 mL H_2O, 80 °C, 10 bar CO_2, 24 h (3rd run); Table 2, Entry 5. (#) residual water signal in $CDCl_3$.

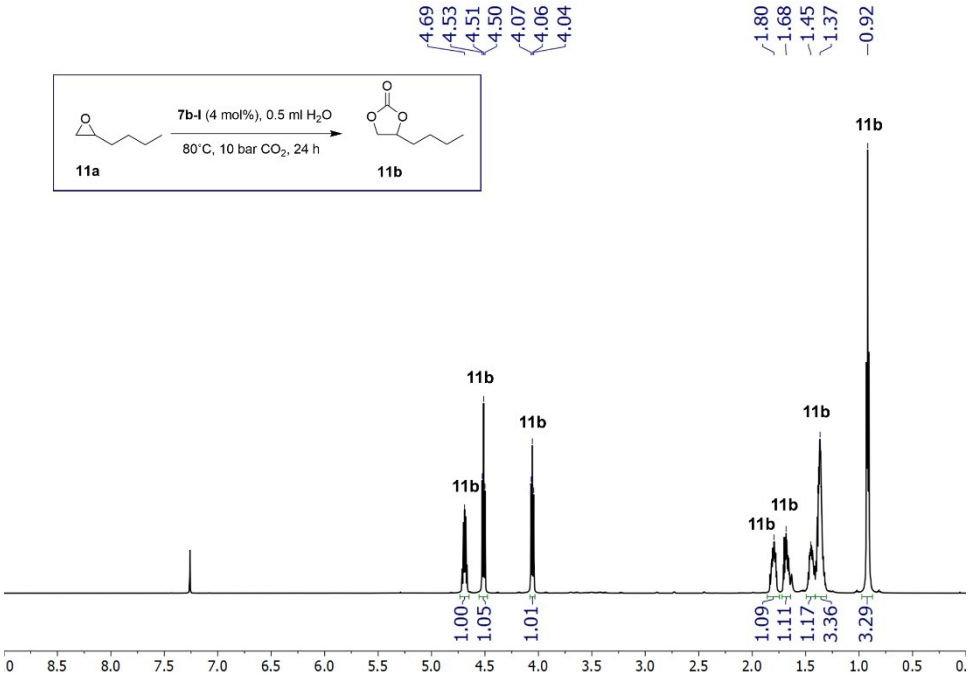


Figure S67. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (1st run); Table 2, Entry 6. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

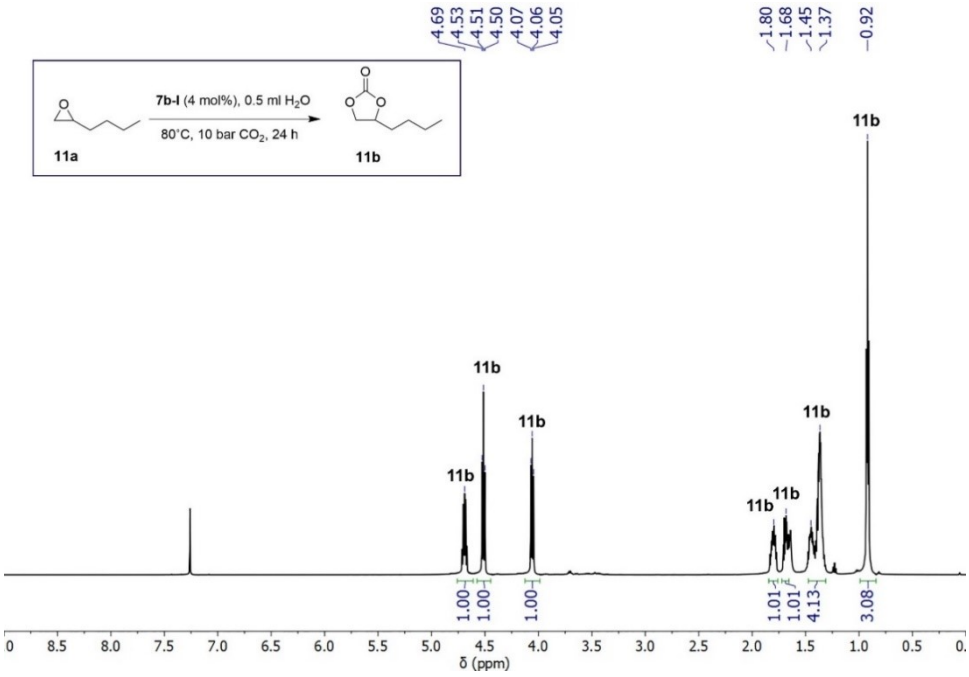


Figure S68. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (2nd run). The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

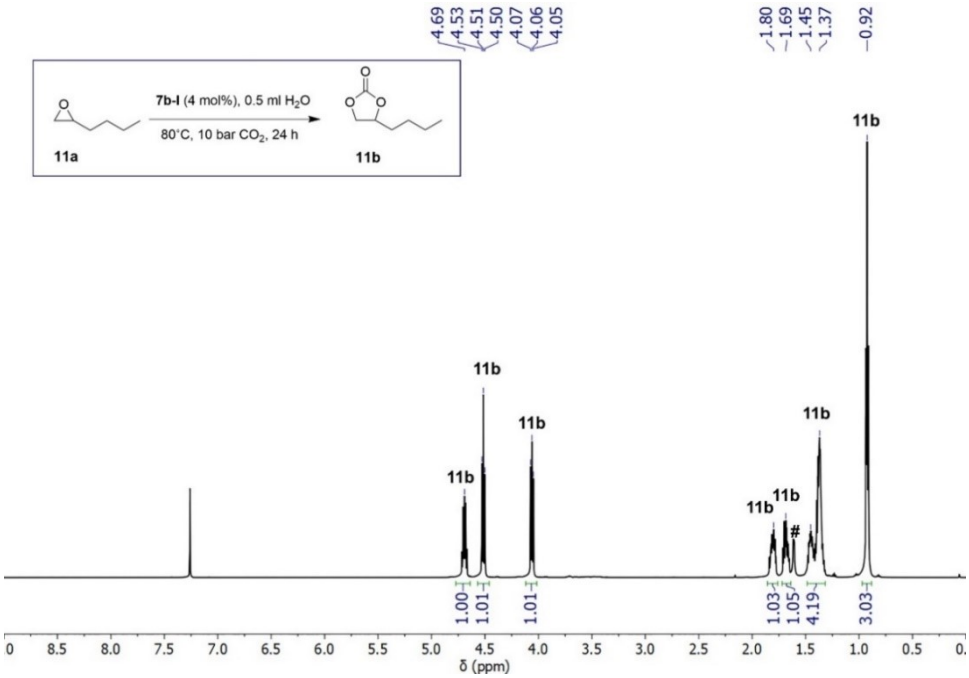


Figure S69. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (3rd run). (#) residual water signal in $CDCl_3$. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

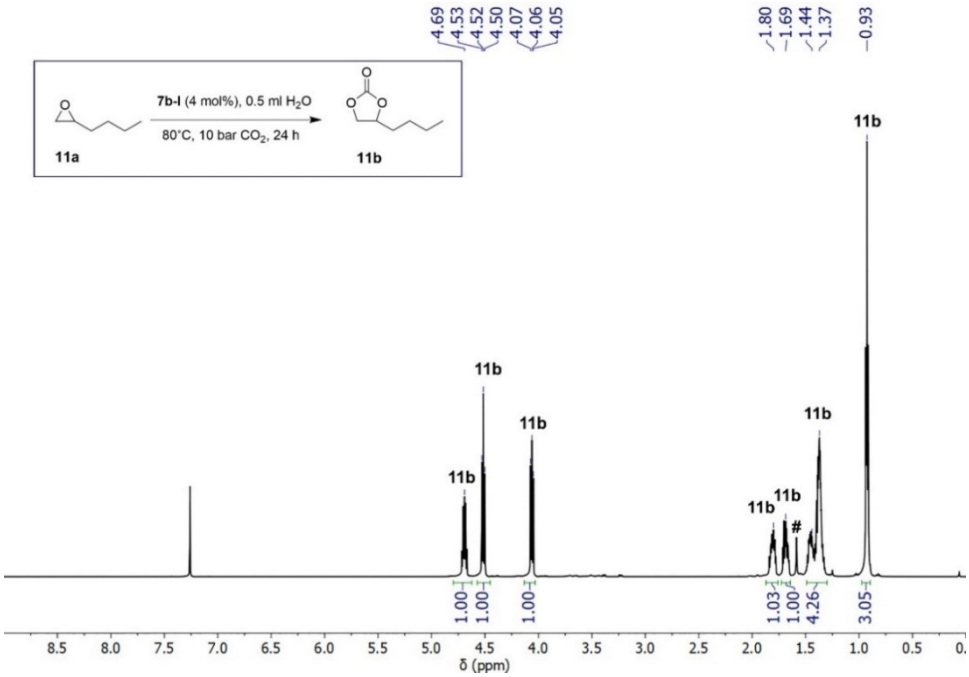


Figure S70. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (4^{th} run). (#) residual water signal in $CDCl_3$. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

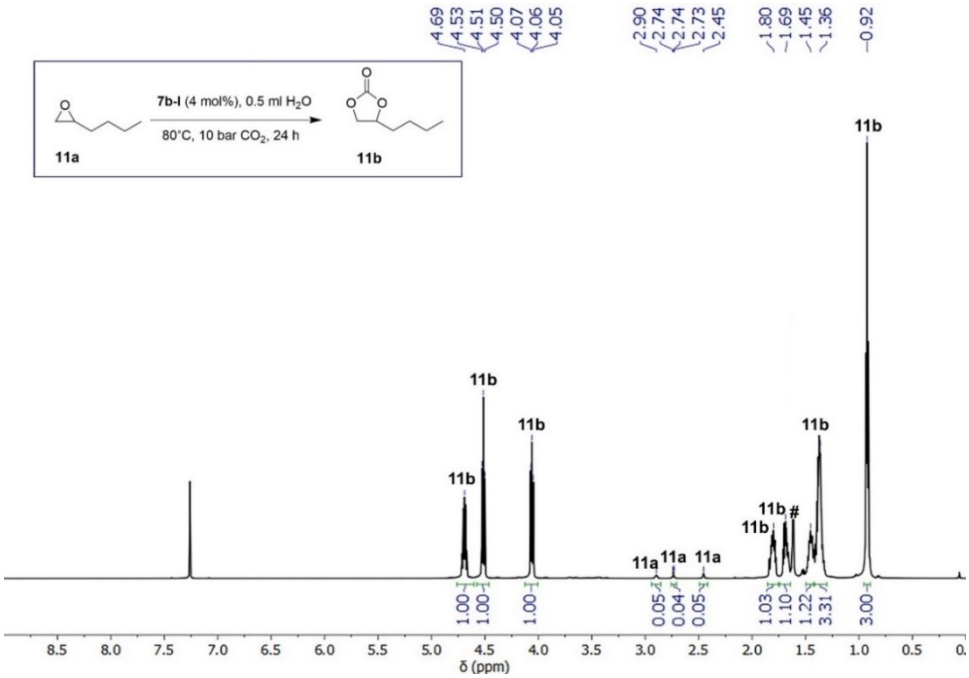


Figure S71. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (5^{th} run). (#) residual water signal in $CDCl_3$.

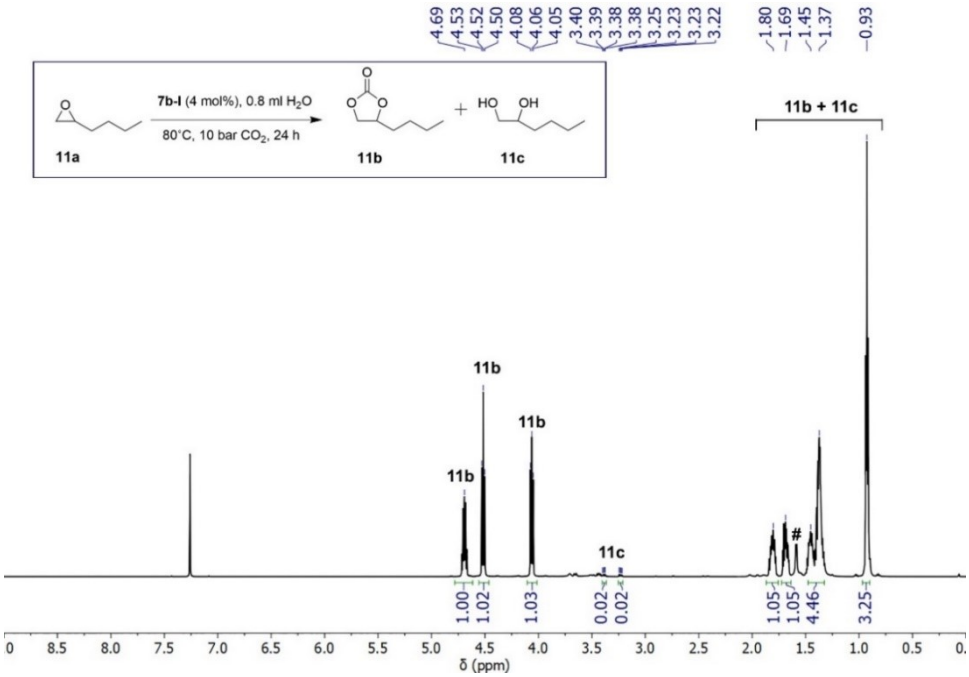


Figure S72. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.8 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 7. (#) residual water signal in $CDCl_3$.

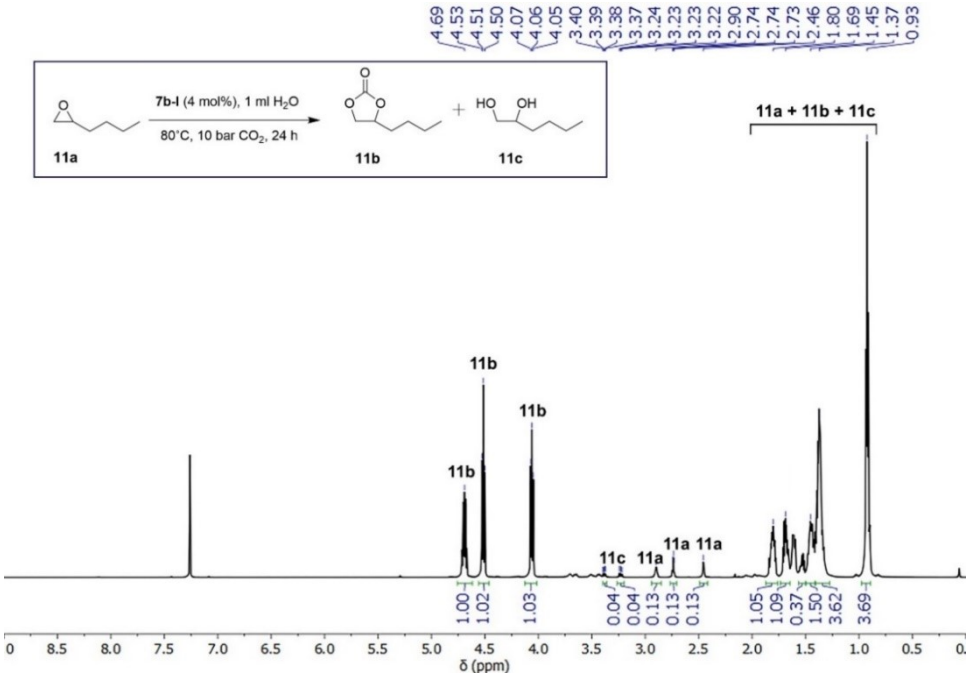


Figure S73. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 1 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 8.

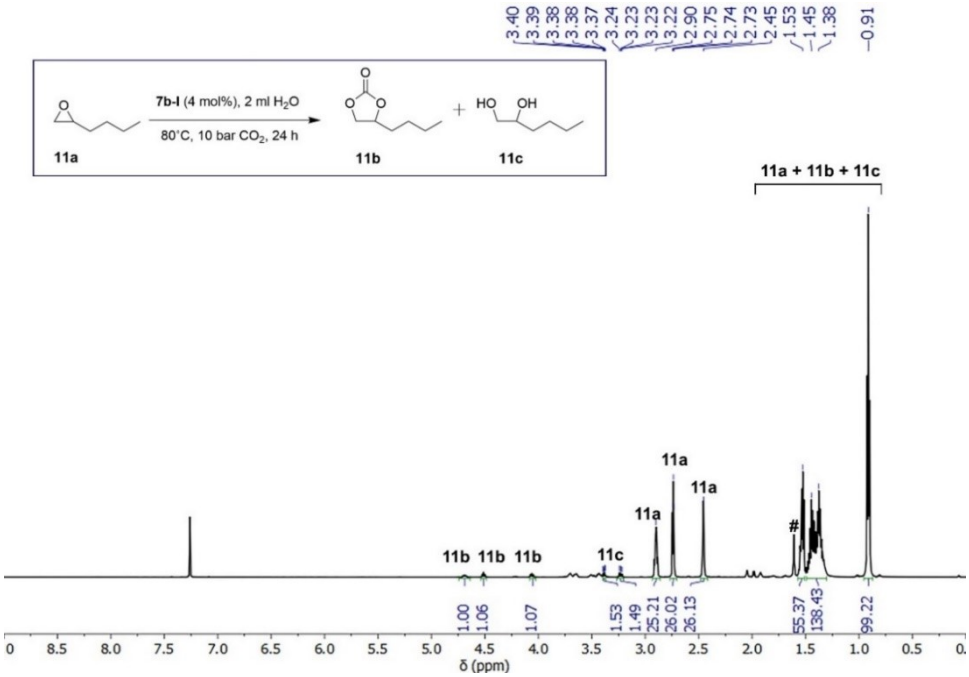


Figure S74. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 2 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 9. (#) residual water signal in $CDCl_3$.

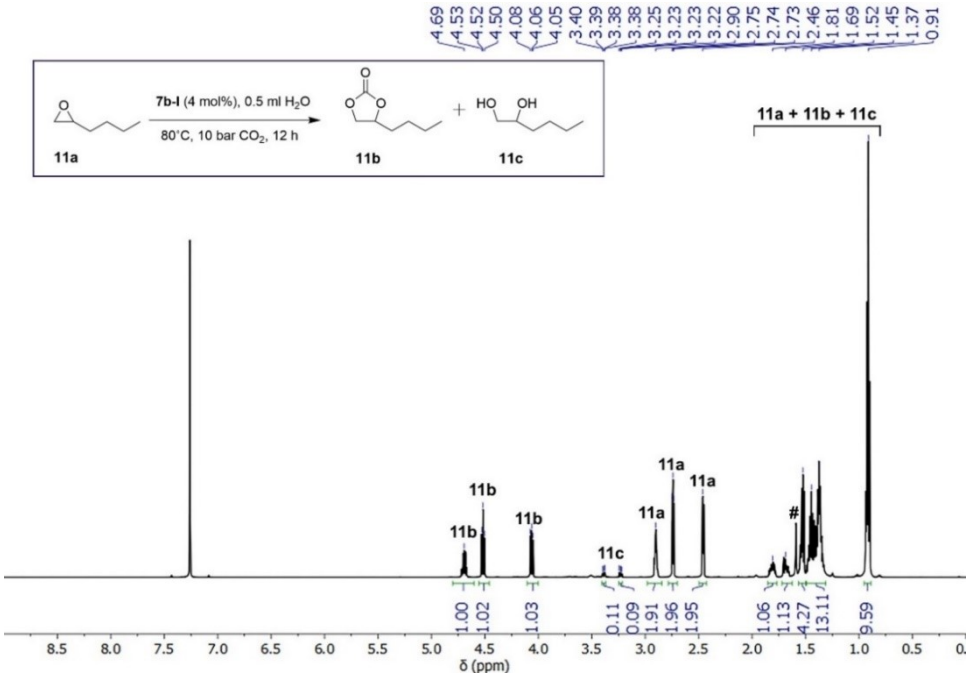


Figure S75. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 2, Entry 10. (#) residual water signal in $CDCl_3$.

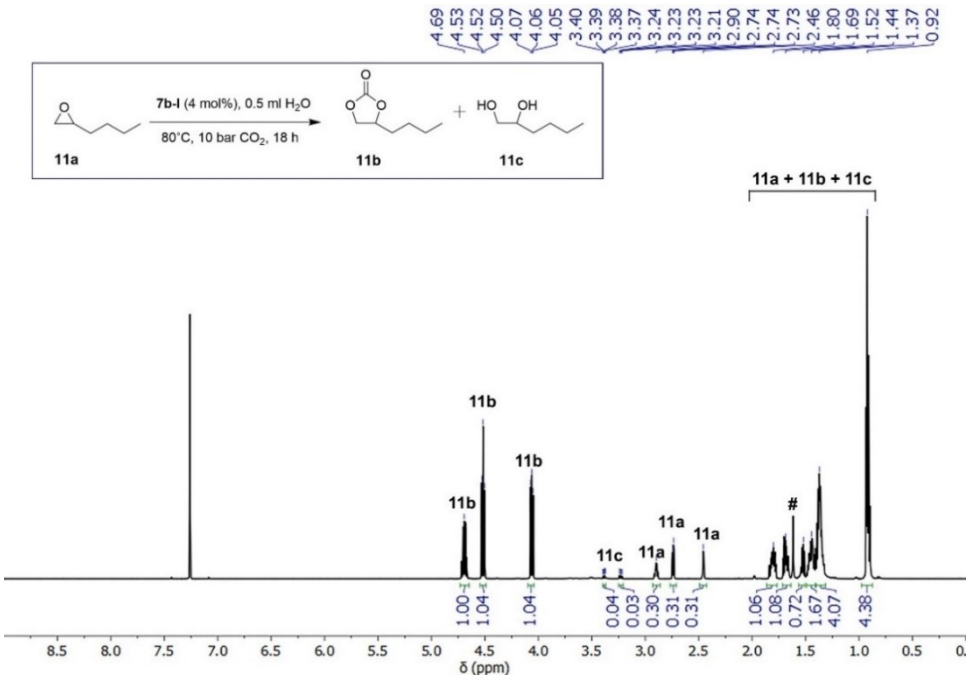


Figure S76. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 18 h; Table 2, Entry 11. (#) residual water signal in $CDCl_3$.

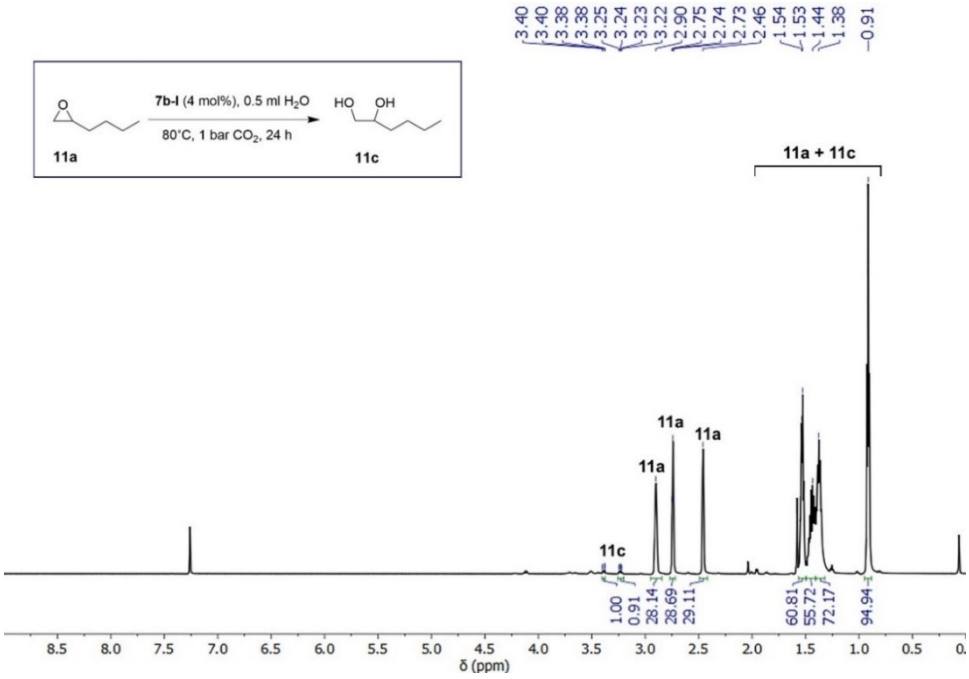


Figure S77. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 1 bar CO_2, 24 h; Table 2, Entry 12.

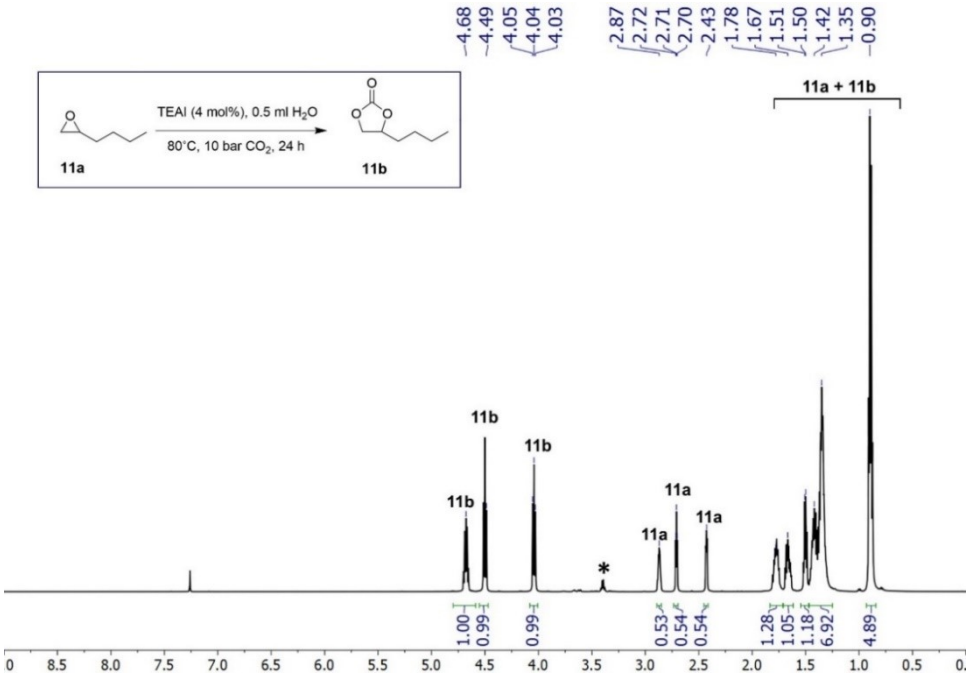


Figure S78. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **TEAI** (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (1st run); Table 2, Entry 13.

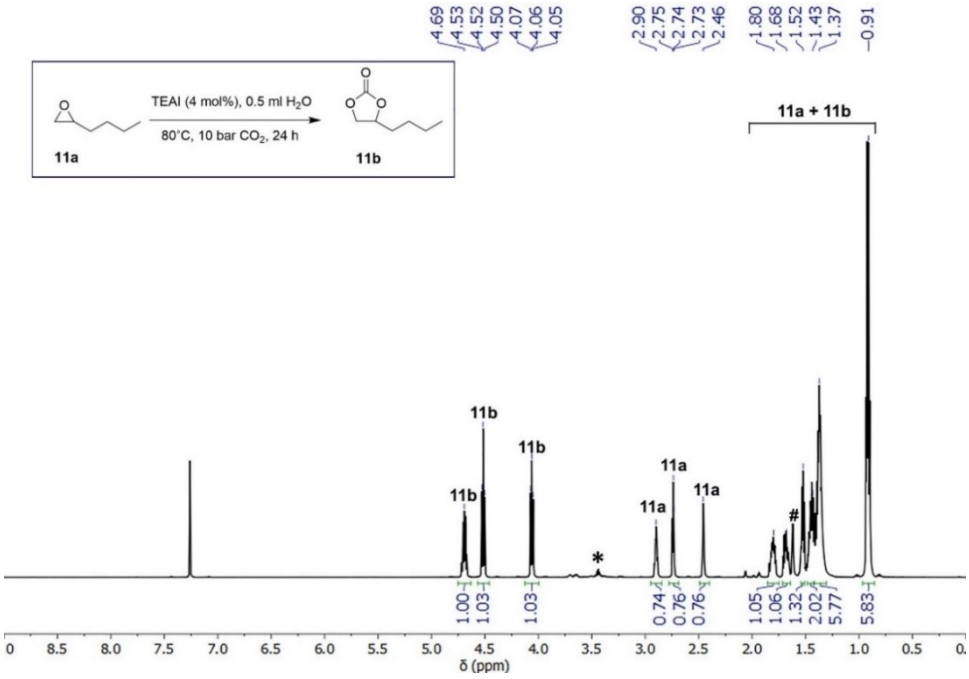


Figure S79. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **TEAI** (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (2nd run); Table 2, Entry 14. (#) residual water signal in $CDCl_3$.

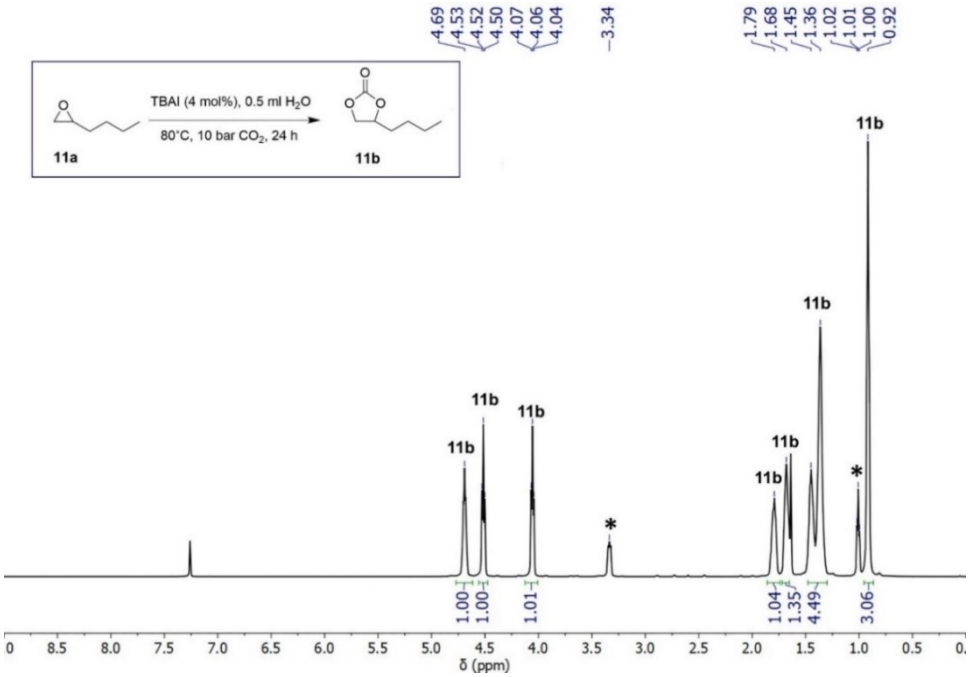


Figure S80. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **TBAI** (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (1st run); Table 2, Entry 15.

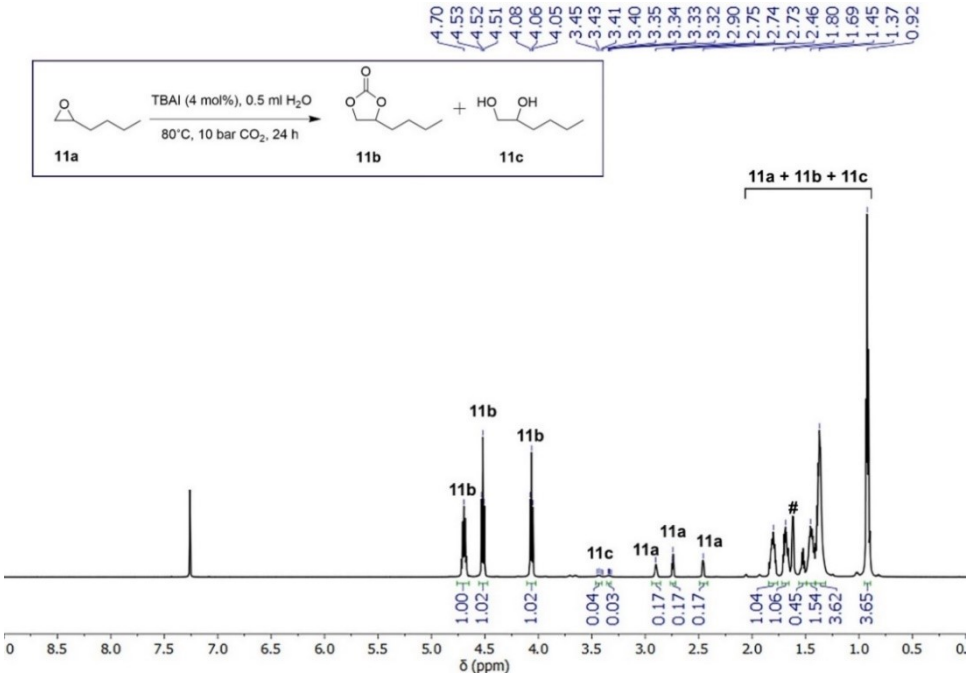


Figure S81. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **TBAI**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h (2nd run); Table 2, Entry 16. (#) residual water signal in $CDCl_3$.

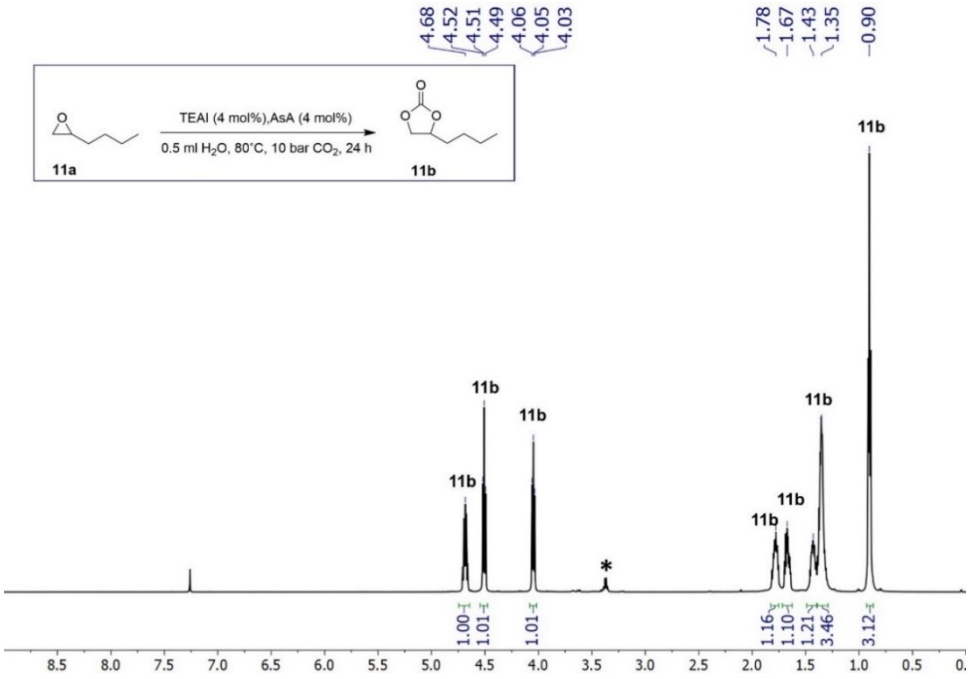


Figure S82. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% Ascorbic acid, 4 mol% **TEAI** (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 17.

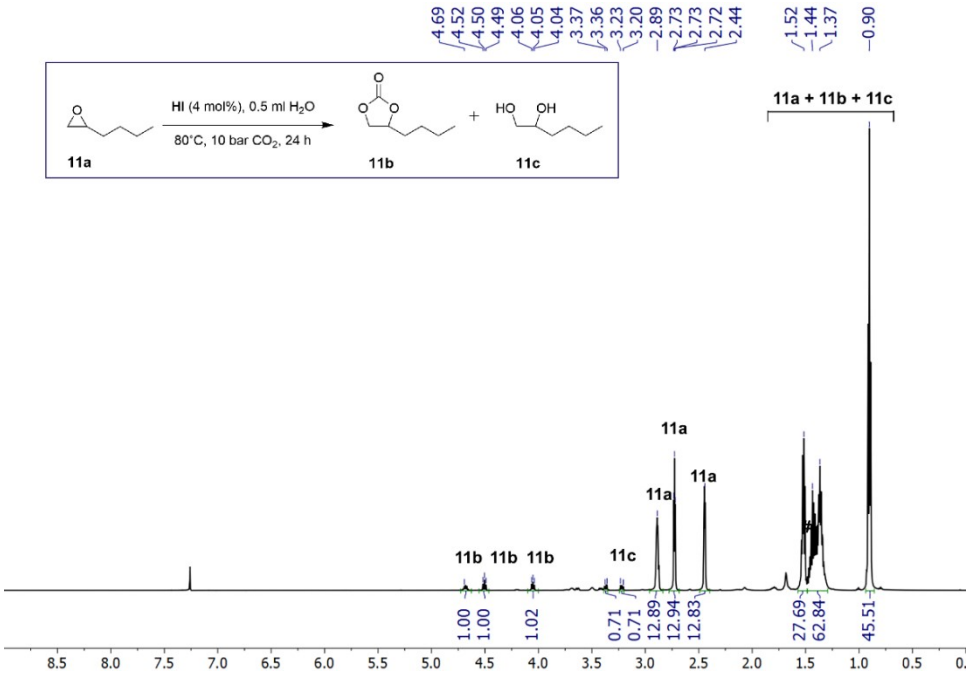


Figure S83. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% HI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 19.

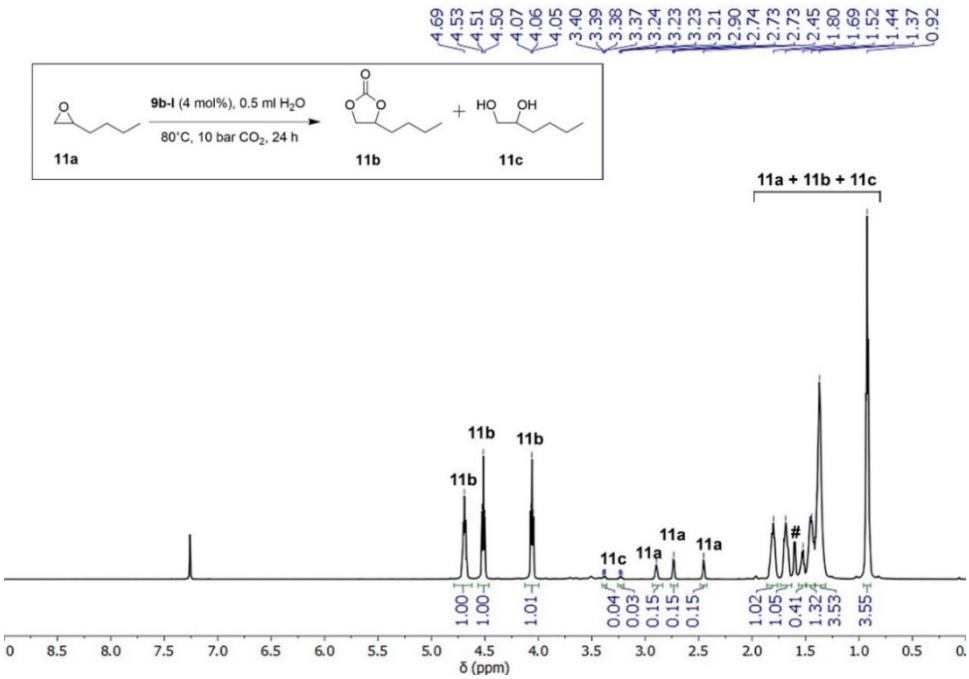


Figure S84. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **9b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 2, Entry 20. (#) residual water signal in $CDCl_3$.

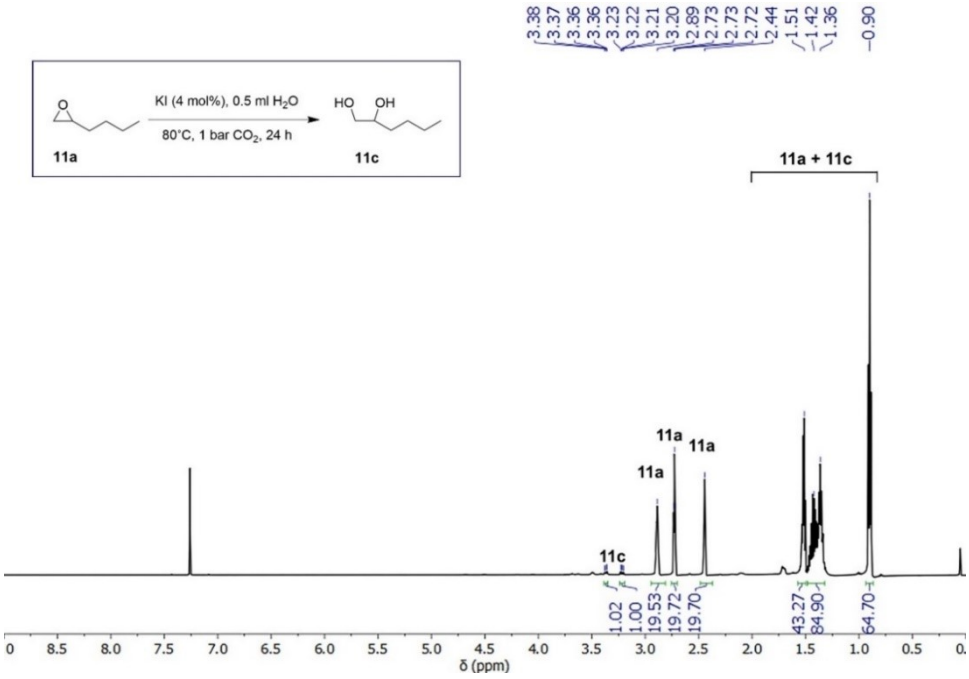


Figure S85. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% KI, 0.5 mL H_2O, 80 °C, 1 bar CO_2, 24 h; Table 3, Entry 1.

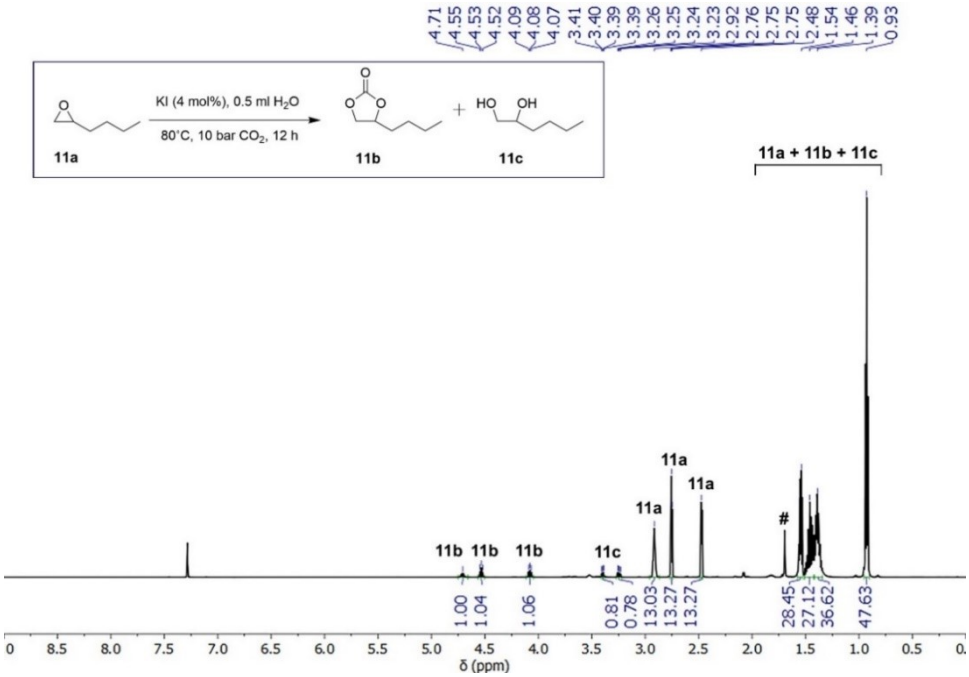


Figure S86. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% KI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 2. (#) residual water signal in $CDCl_3$.

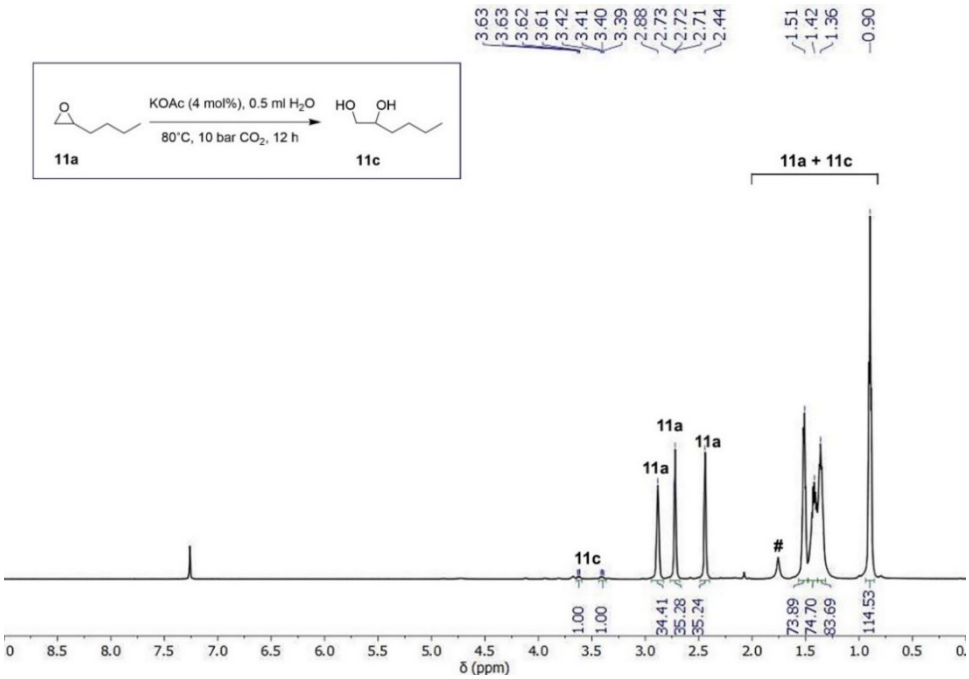


Figure S87. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% KOAc (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 3.

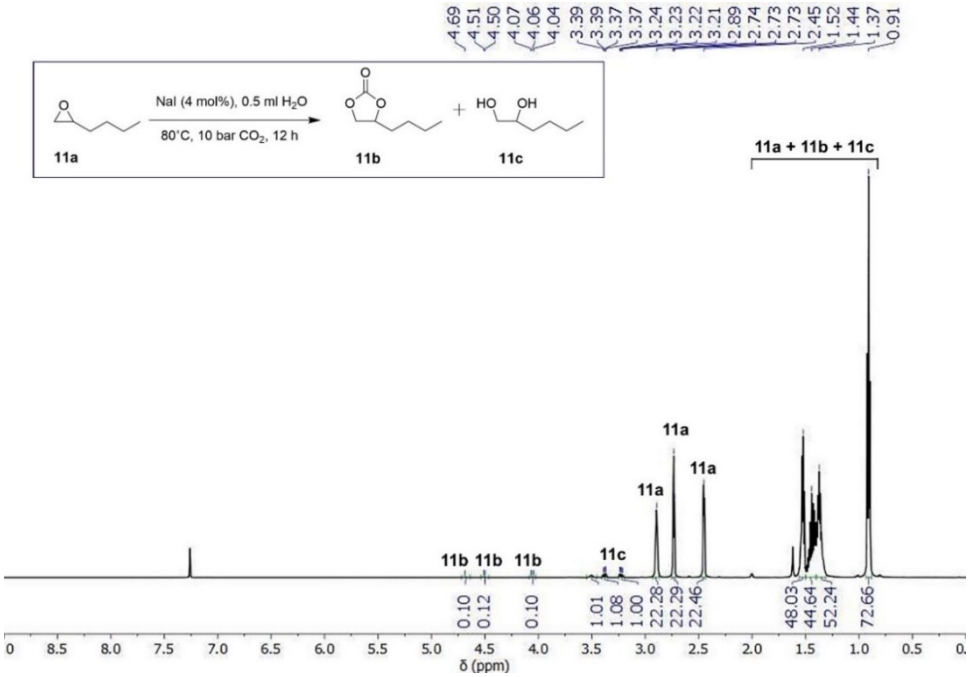


Figure S88. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% NaI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 5.

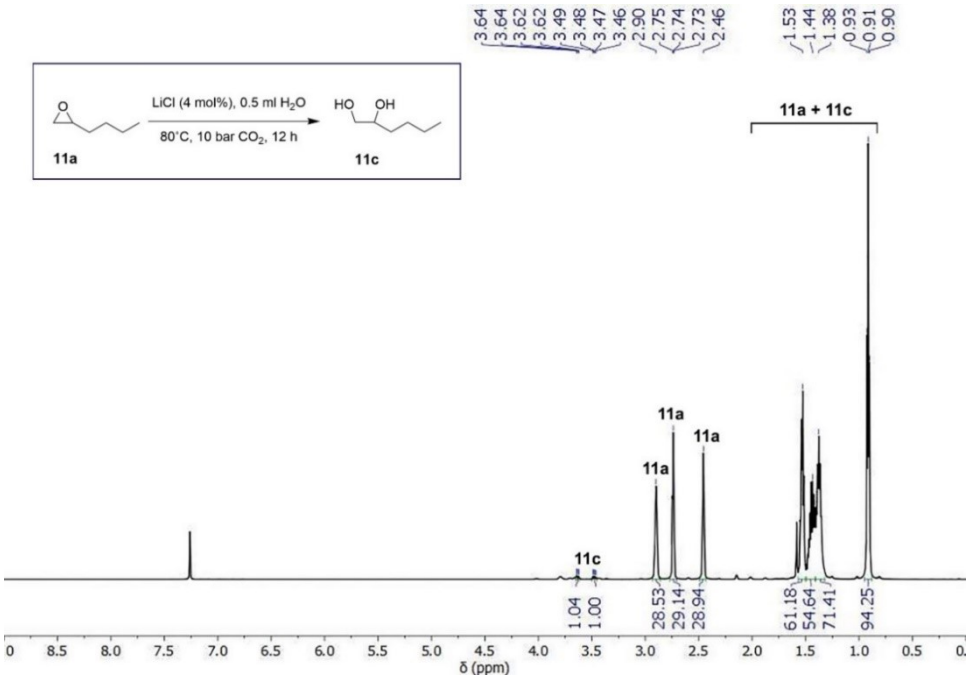


Figure S89. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% LiCl, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 6.

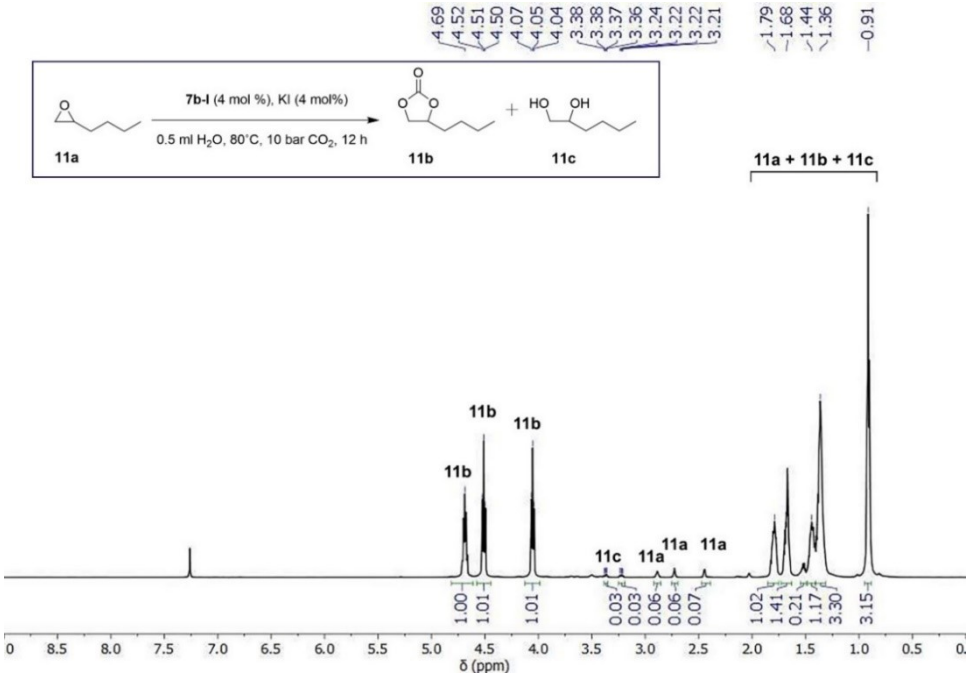


Figure S90. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (1st run); Table 3, Entry 9.

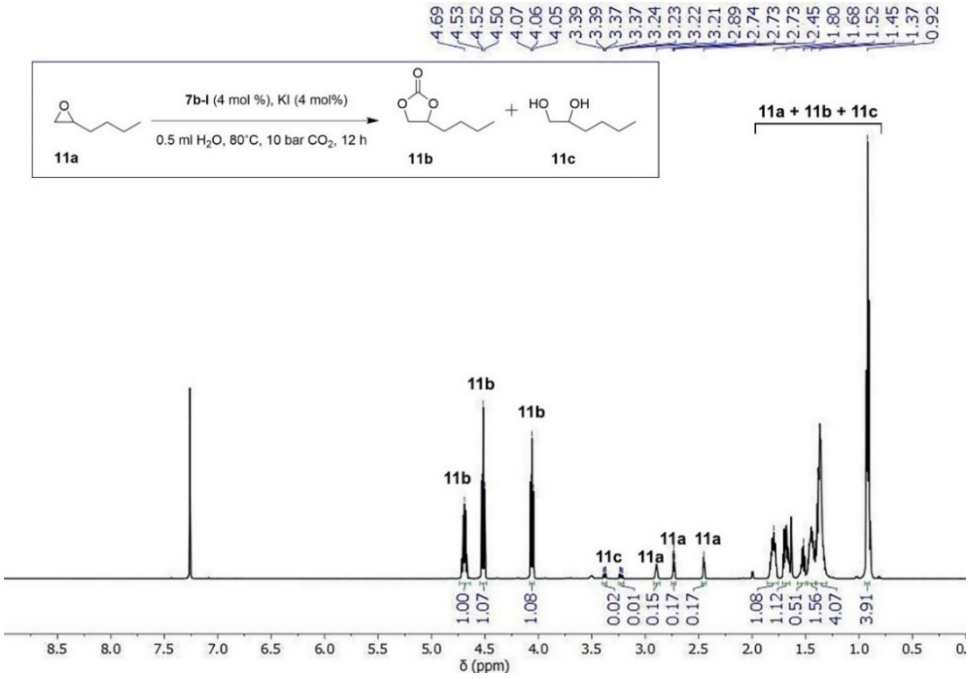


Figure S91. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (2nd run).

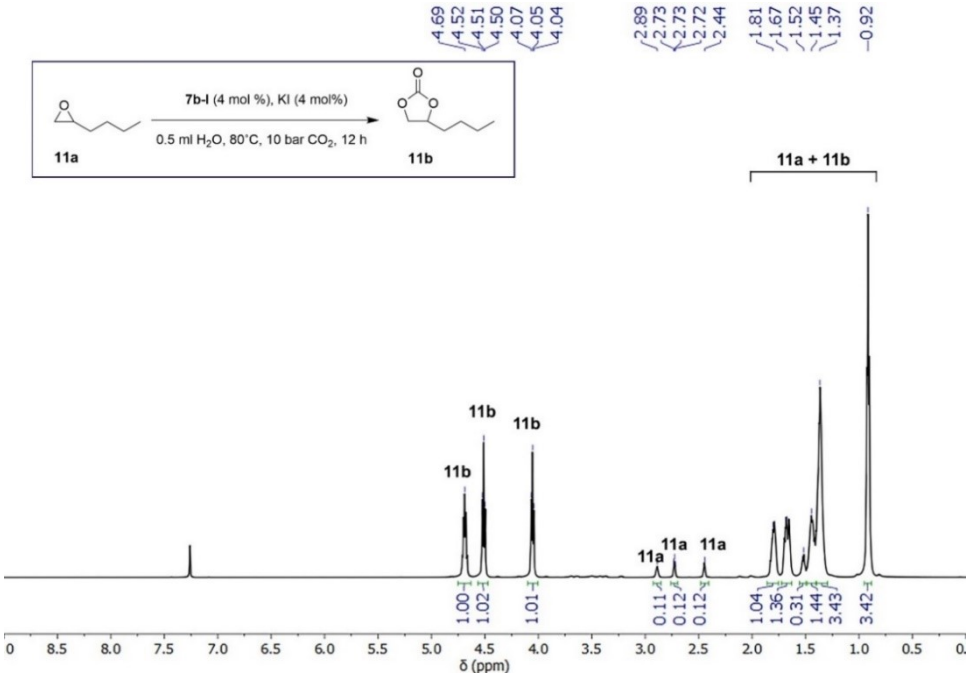


Figure S92. H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (3rd run).

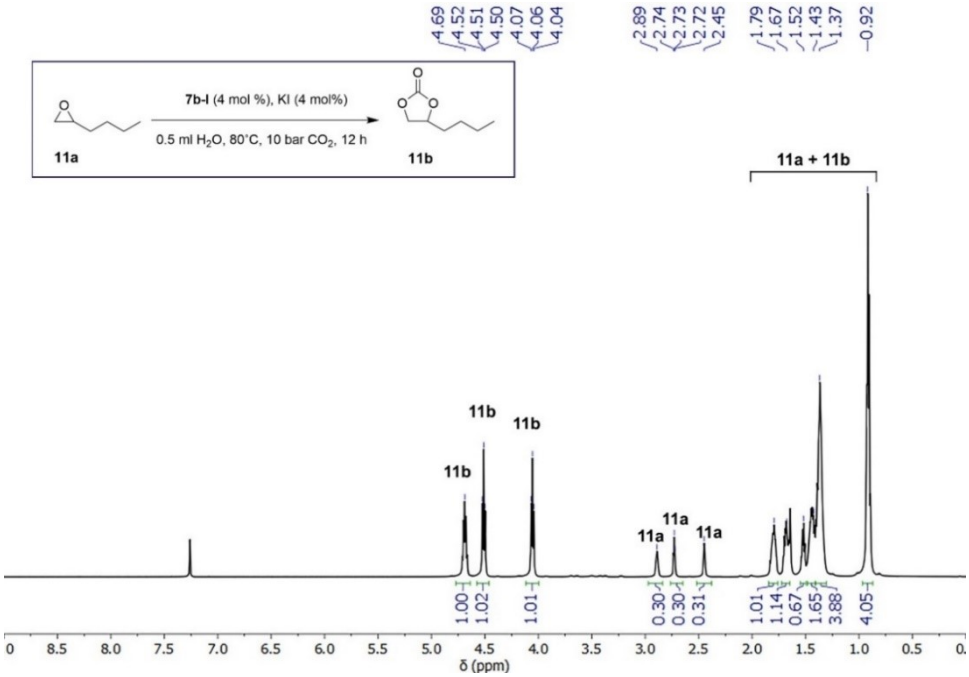


Figure S93. ^1H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (4th run).

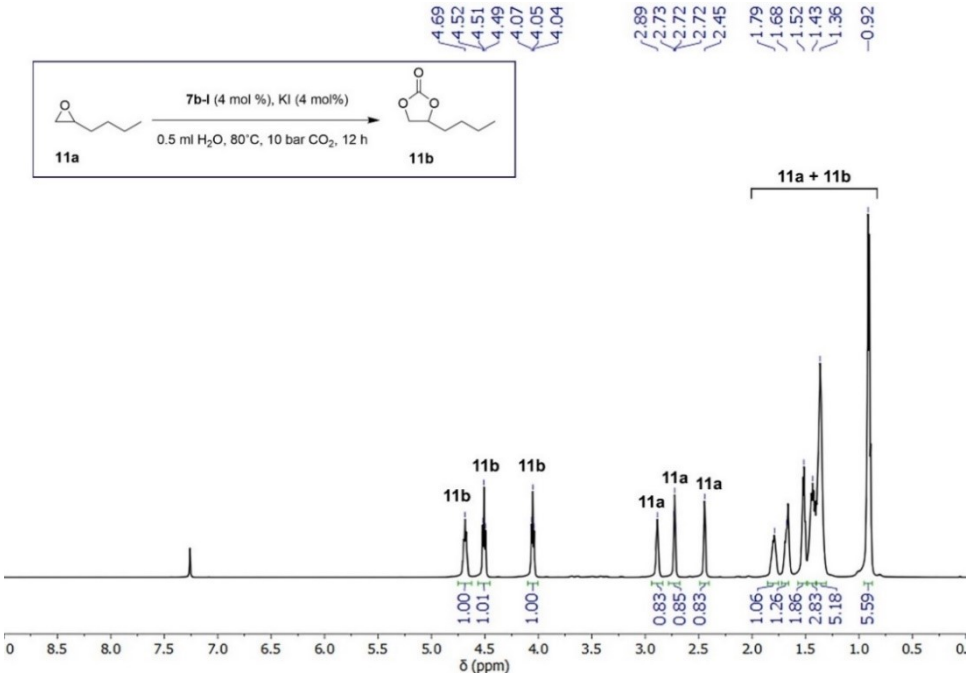


Figure S94. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (5th run).

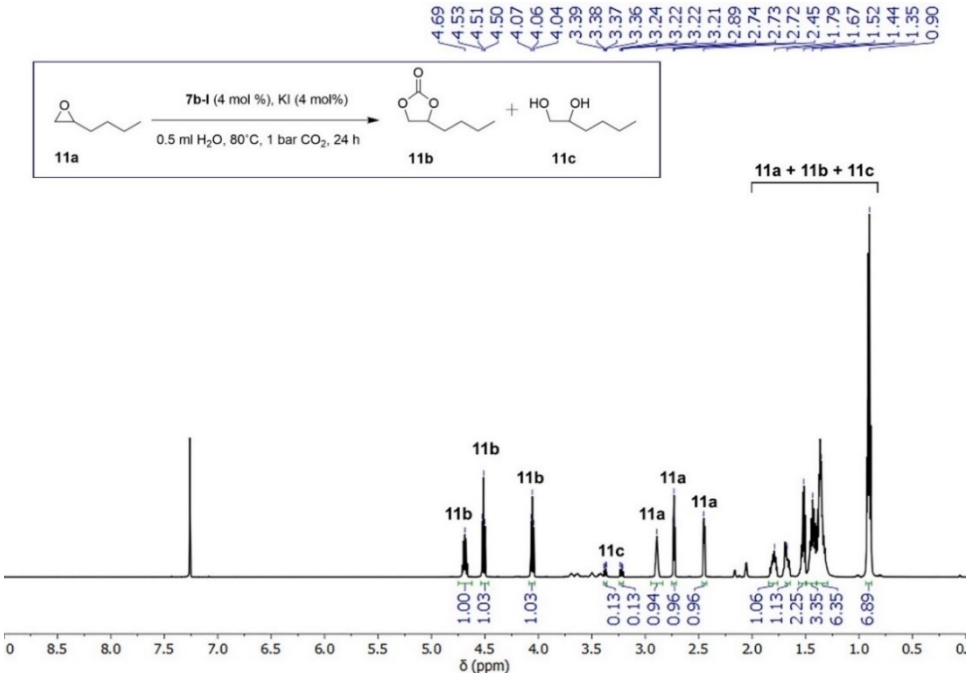


Figure S95. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KI, 0.5 mL H_2O, 80 °C, 1 bar CO_2 (ballon), 24 h; Table 3, Entry 10.

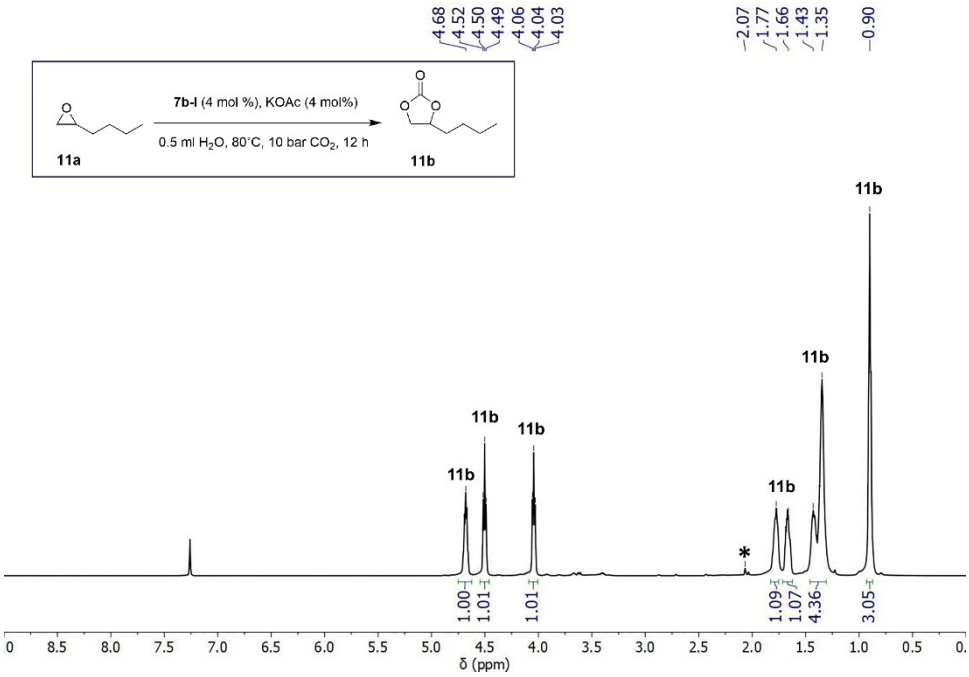


Figure S96. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KOAc (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (1st run); Table 3, Entry 11.

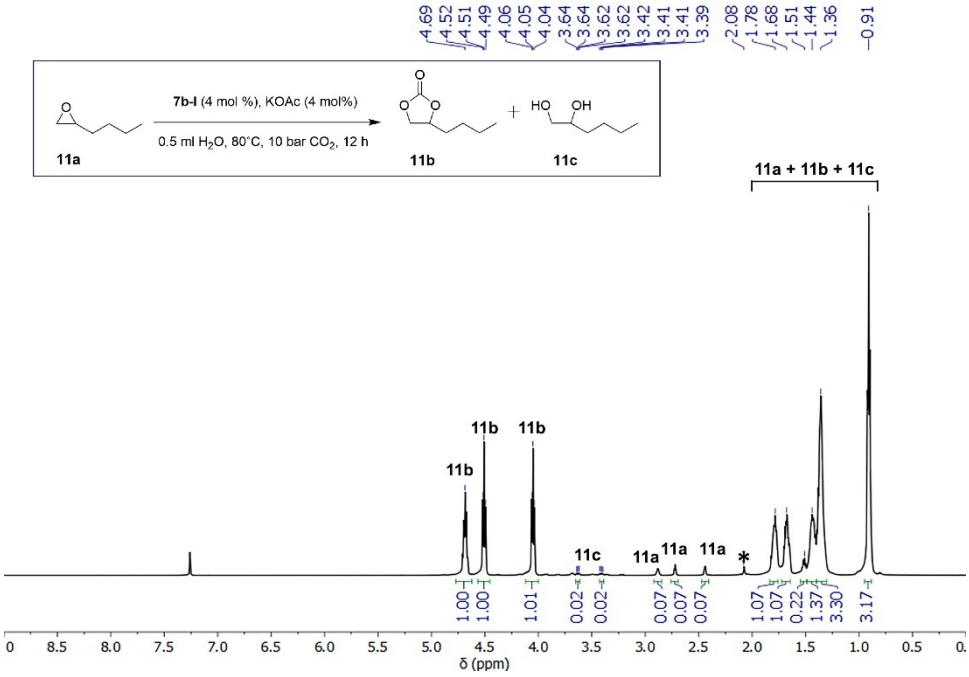


Figure S97. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KOAc (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (2nd run).

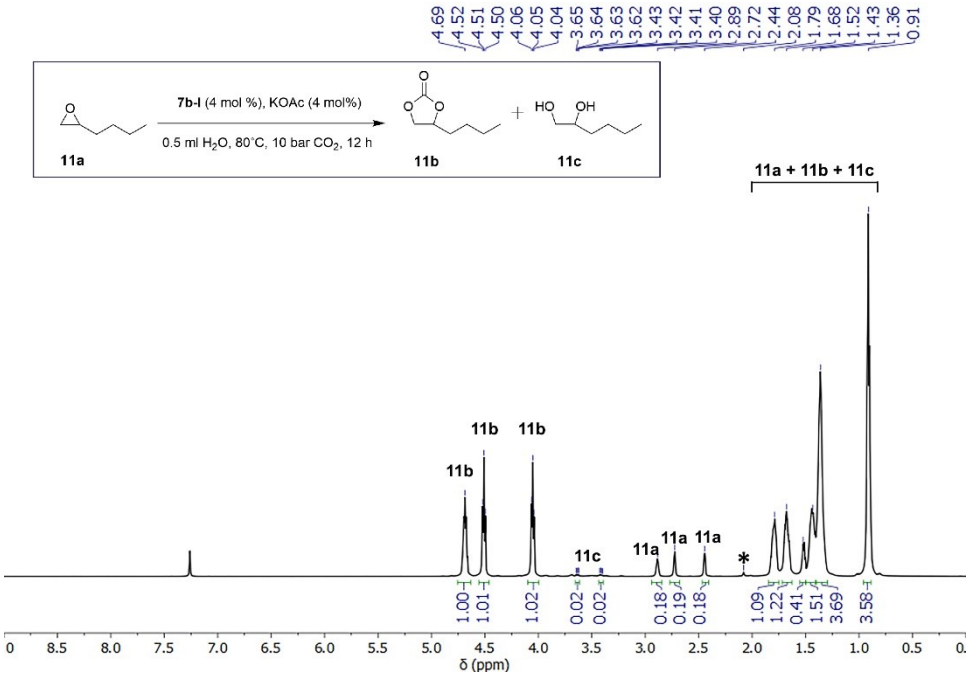


Figure S98. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KOAc (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (3rd run).

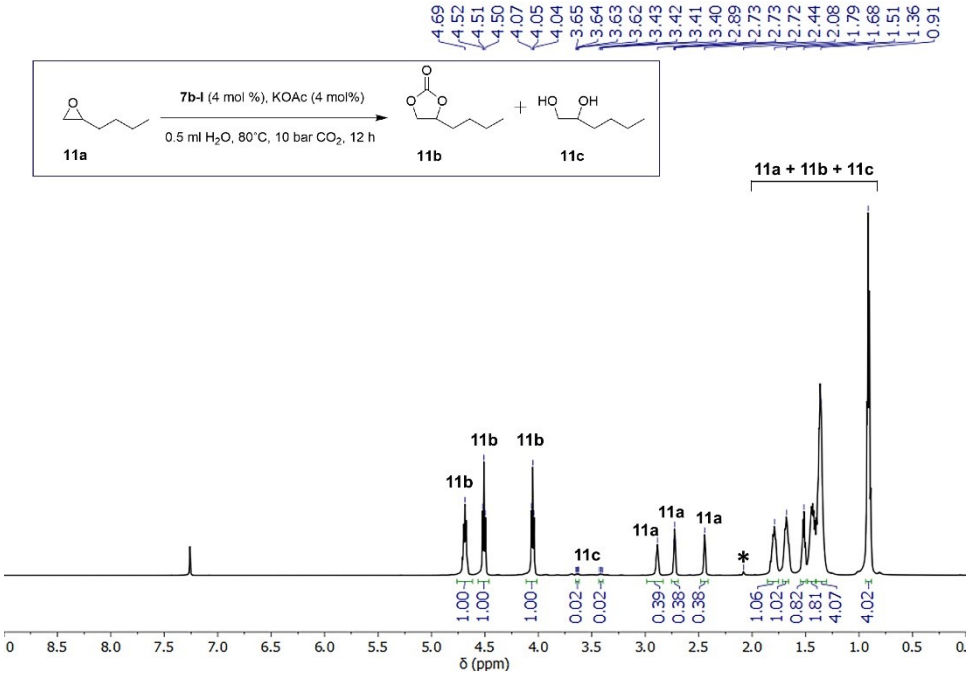


Figure S99. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KOAc (*), 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (4th run).

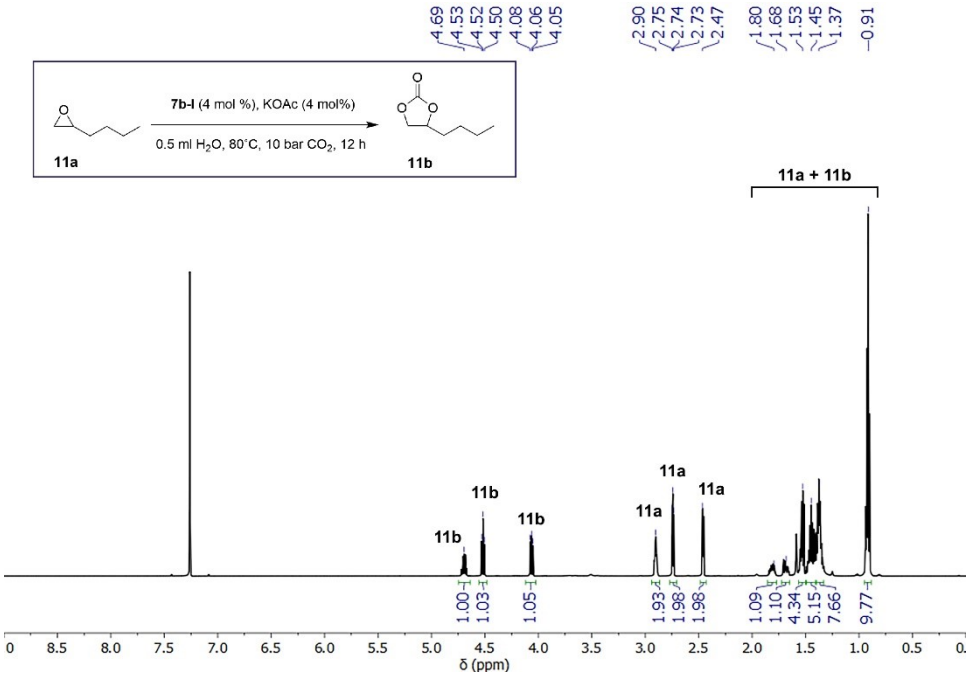


Figure S100. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KOAc, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h (5^{th} run).

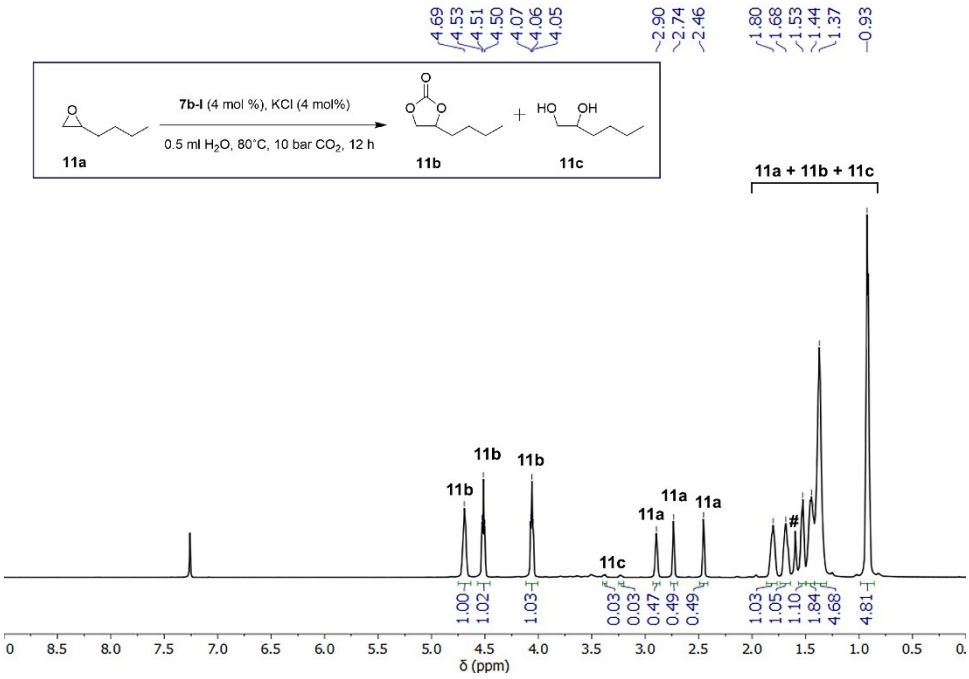


Figure S101. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KCl, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 12. (#) residual water signal in $CDCl_3$.

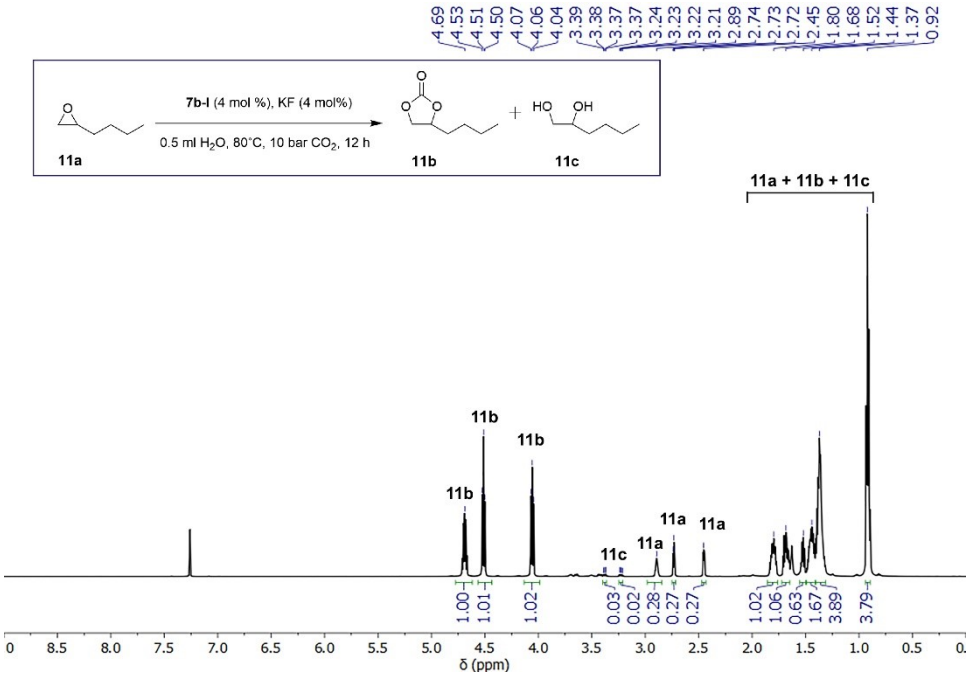


Figure S102. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% KF, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 13.

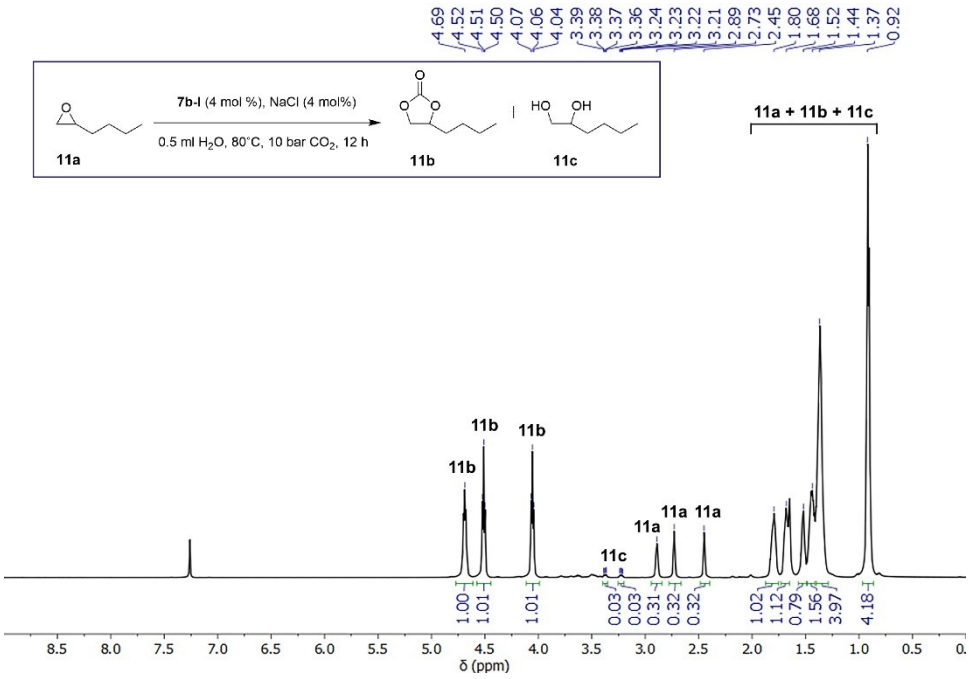


Figure S103. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% NaCl, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 14.

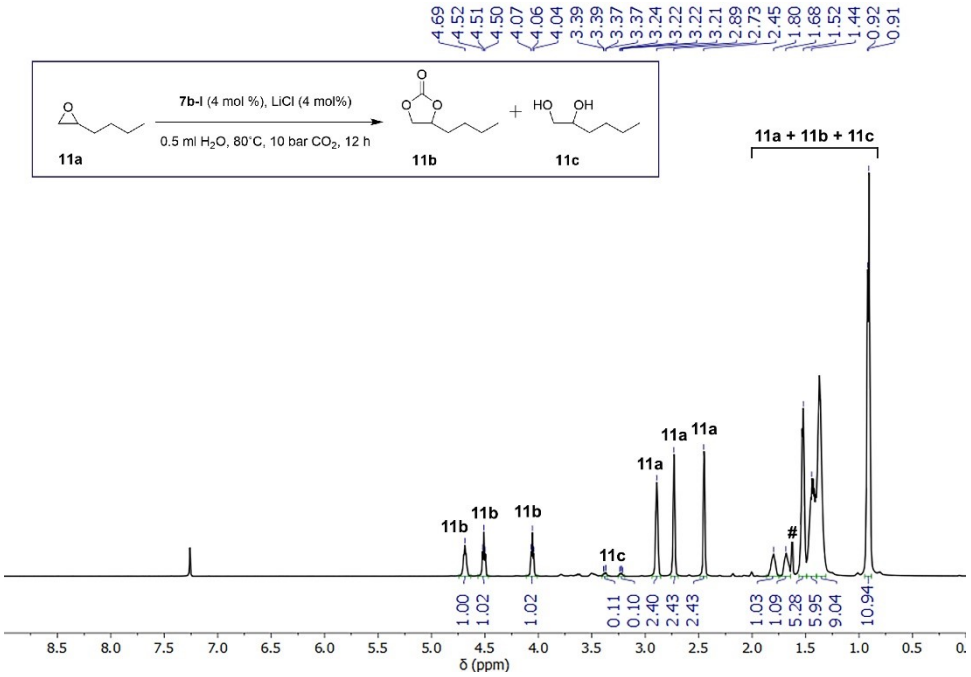


Figure S104. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% LiCl, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 15. (#) residual water signal in $CDCl_3$.

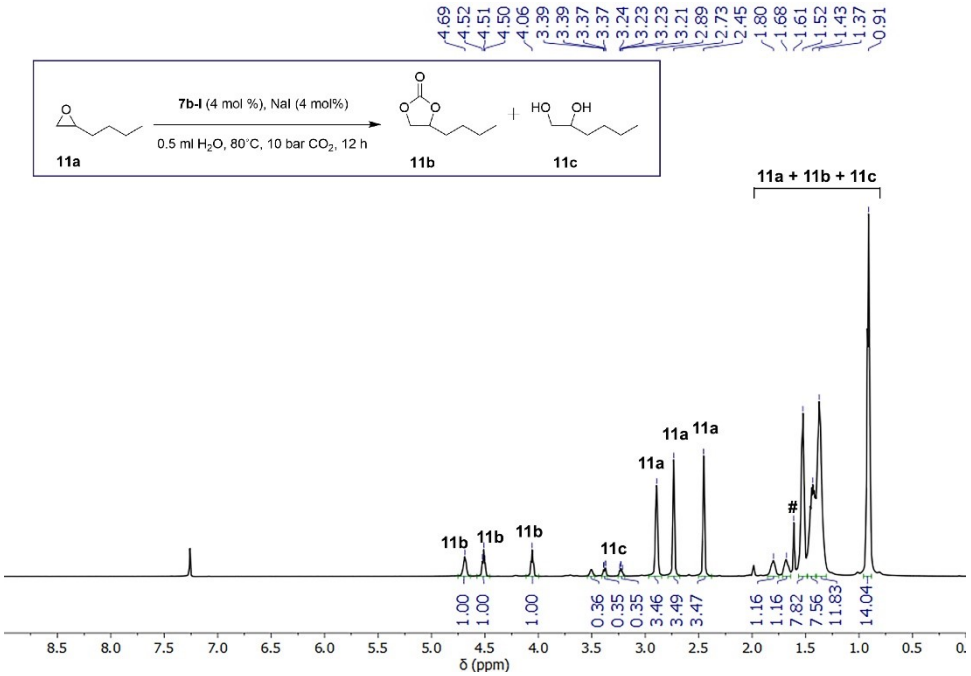


Figure S105. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% NaI, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 16. (#) residual water signal in $CDCl_3$.

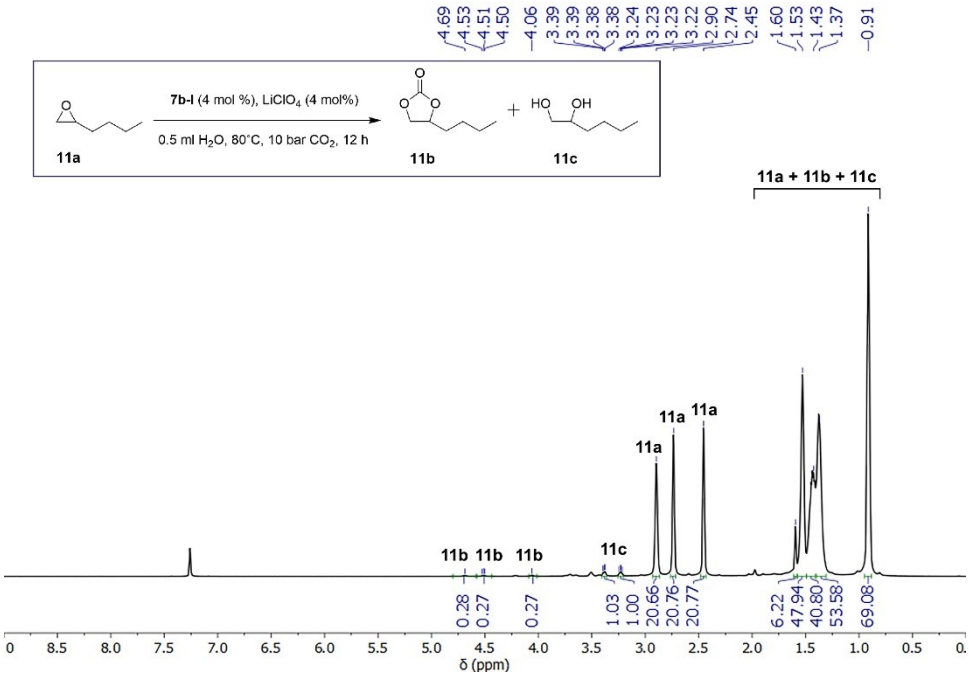


Figure S106. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 4 mol% $LiClO_4$, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 17.

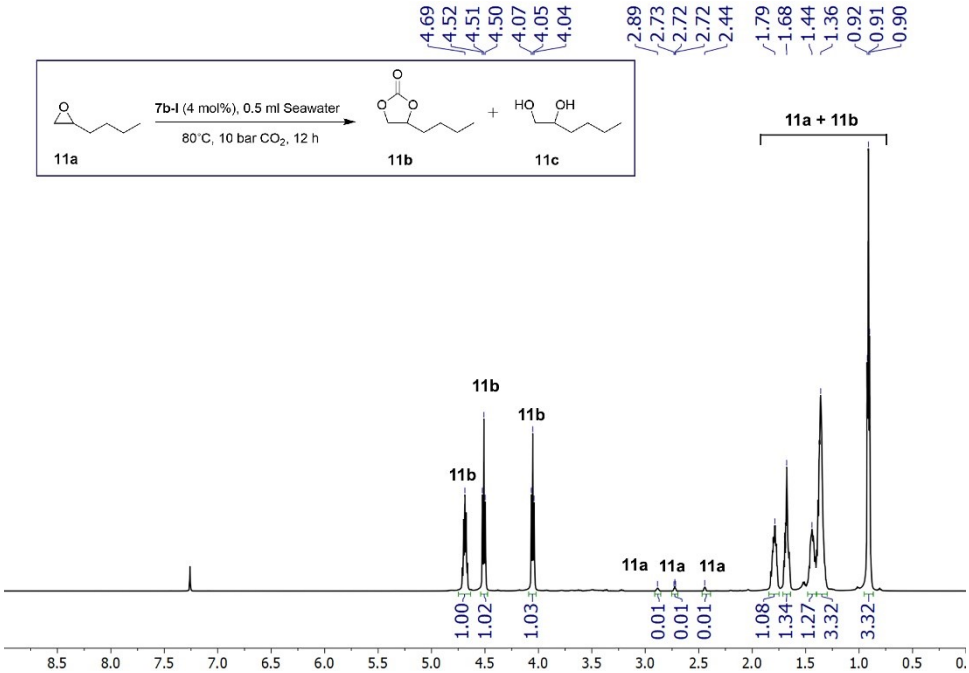


Figure S107. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 4 mol% **7b-I**, 0.5 mL seawater, 80 °C, 10 bar CO_2, 12 h; Table 3, Entry 19.

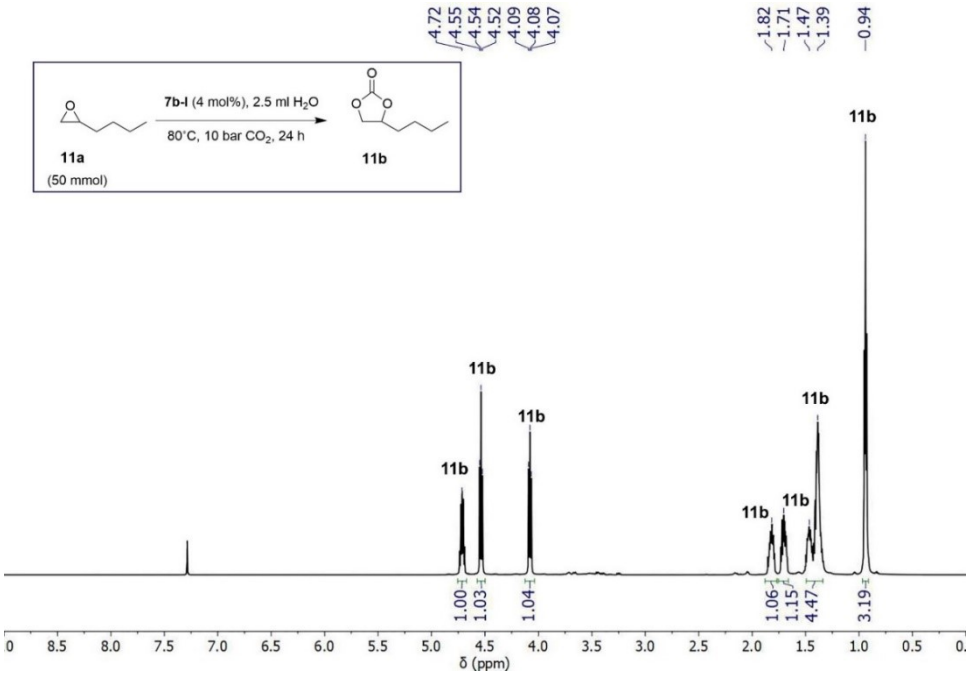


Figure S108. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **11a**; **11a** (50 mmol), 4 mol% **7b-I**, 2.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 1. The NMR spectrum matches the literature reference *J. Org. Chem*. 2005, 70, 1, 381–383.

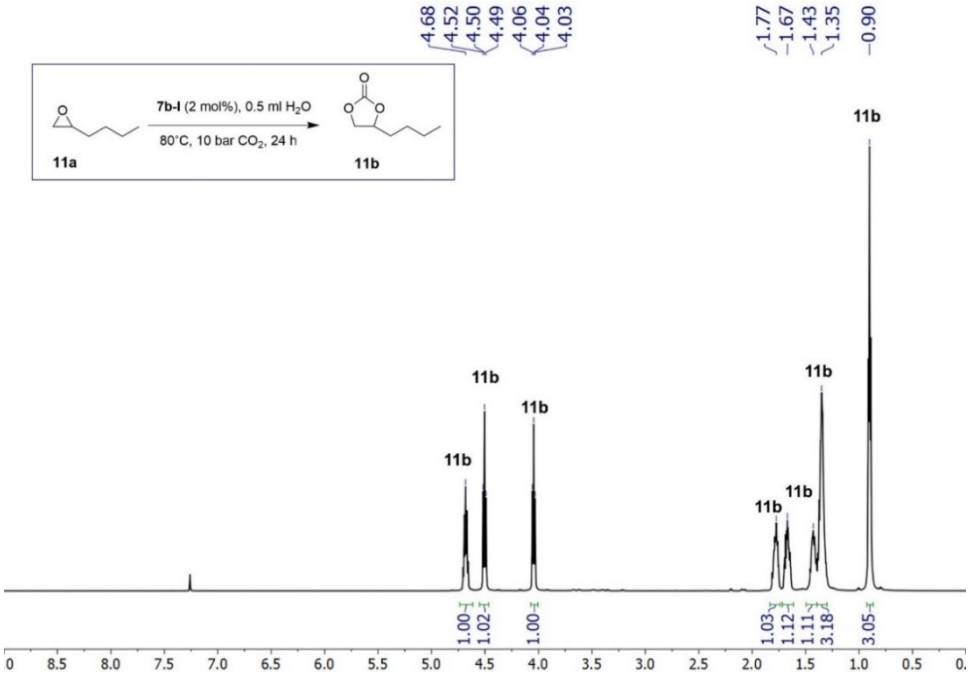


Figure S109. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 2 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 1a. The NMR spectrum matches the literature reference *J. Org. Chem*. 2005, 70, 1, 381–383.

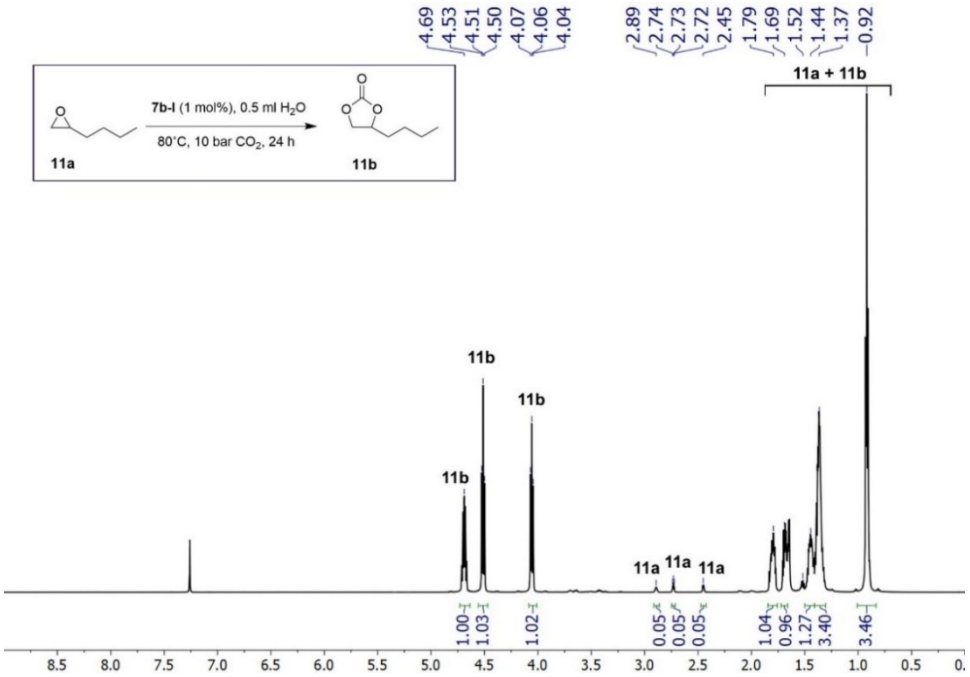


Figure S110. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **11a**; **11a** (10 mmol), 1 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 1b.

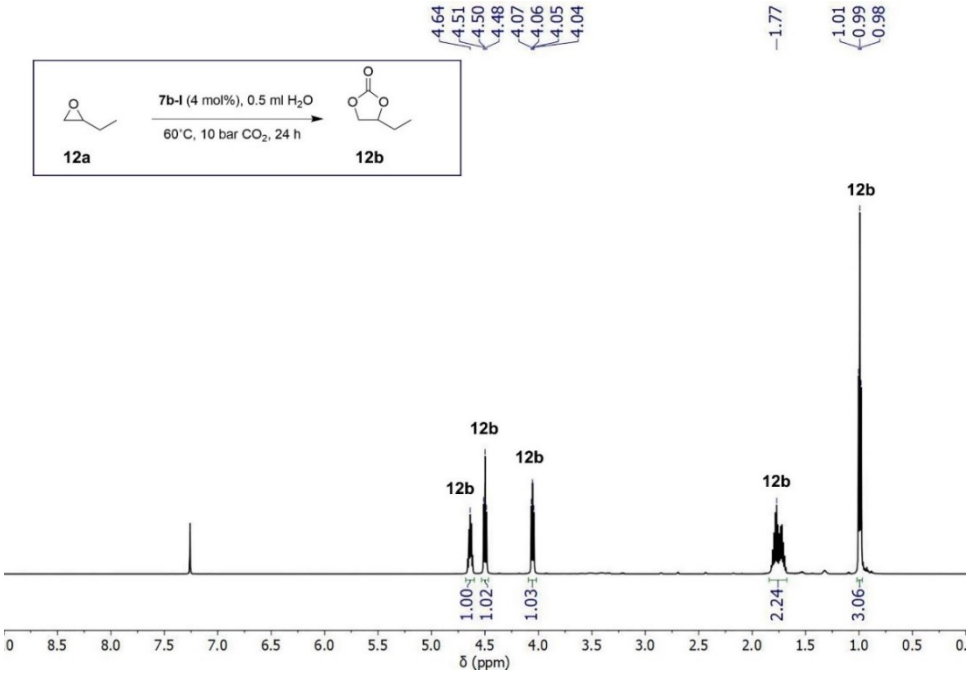


Figure S111. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **12a**; **12a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 60 °C, 10 bar CO_2, 24 h; Table 4, Entry 2. The NMR spectrum matches the literature reference *J. Org. Chem*. 2018, 83, 24, 14969–14977.

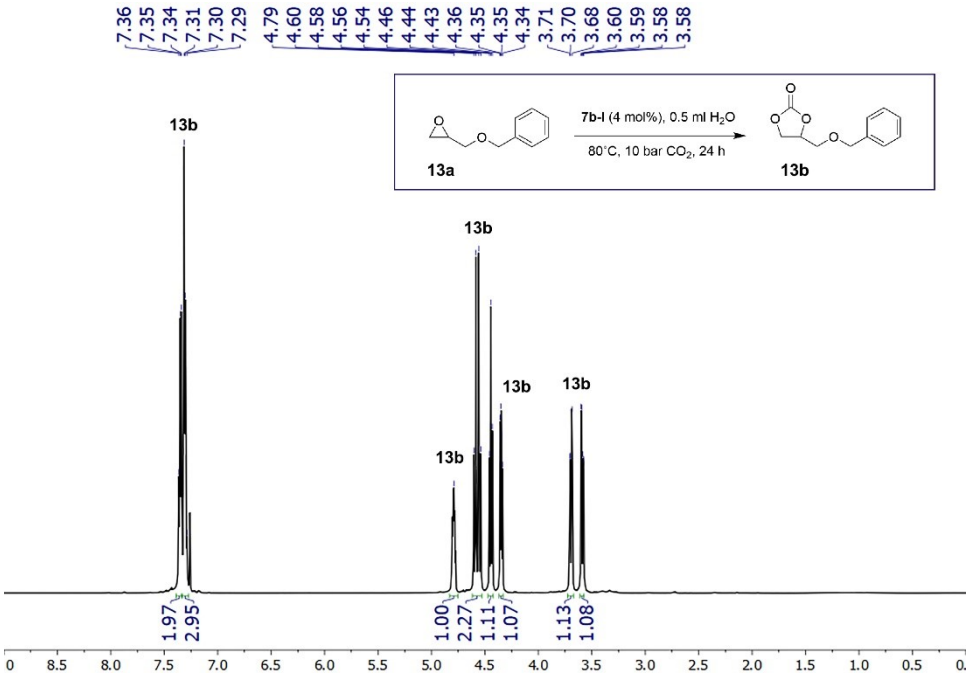


Figure S112. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic phase for the CO_2 cycloaddition reaction to **13a**; **13a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 3. The NMR spectrum matches the literature reference *J. Org. Chem. 2019*, 84, 23, 15578–15589.

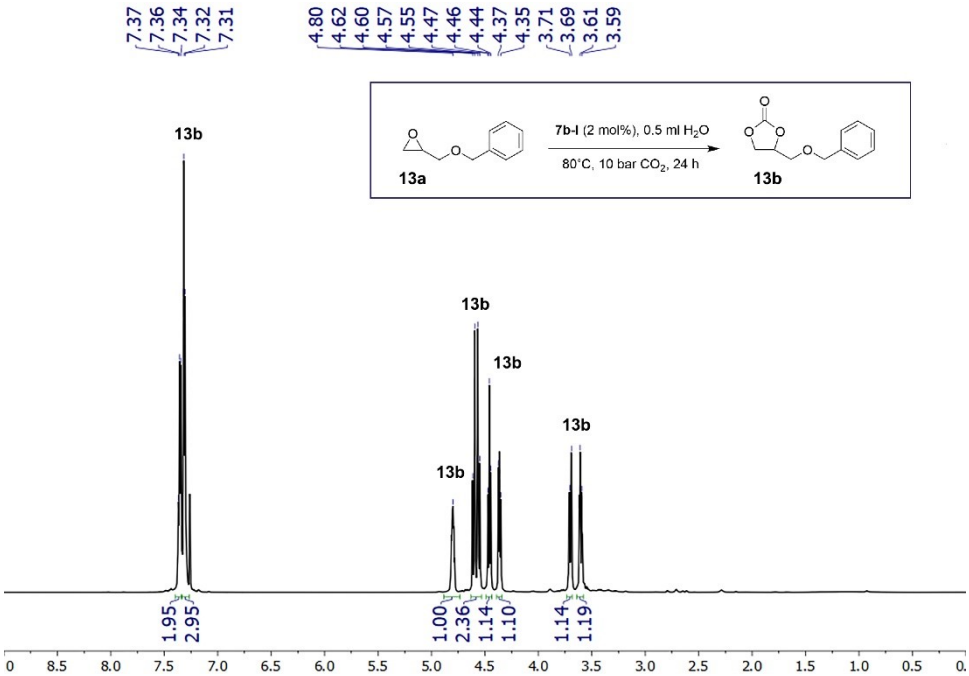


Figure S113. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic phase for the CO_2 cycloaddition reaction to **13a**; **13a** (10 mmol), 2 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 3a. The NMR spectrum matches the literature reference *J. Org. Chem. 2019*, 84, 23, 15578–15589.

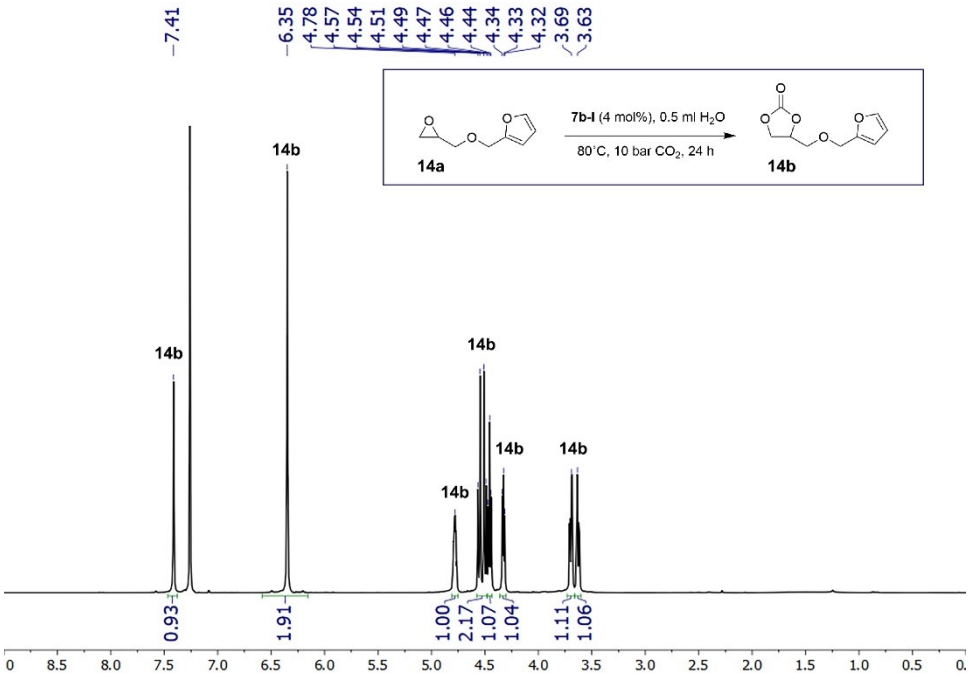


Figure S114. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **14a**; **14a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 4. The NMR spectrum matches the literature reference *Catal. Sci. Technol*. 2018, 8, 1981-1987.

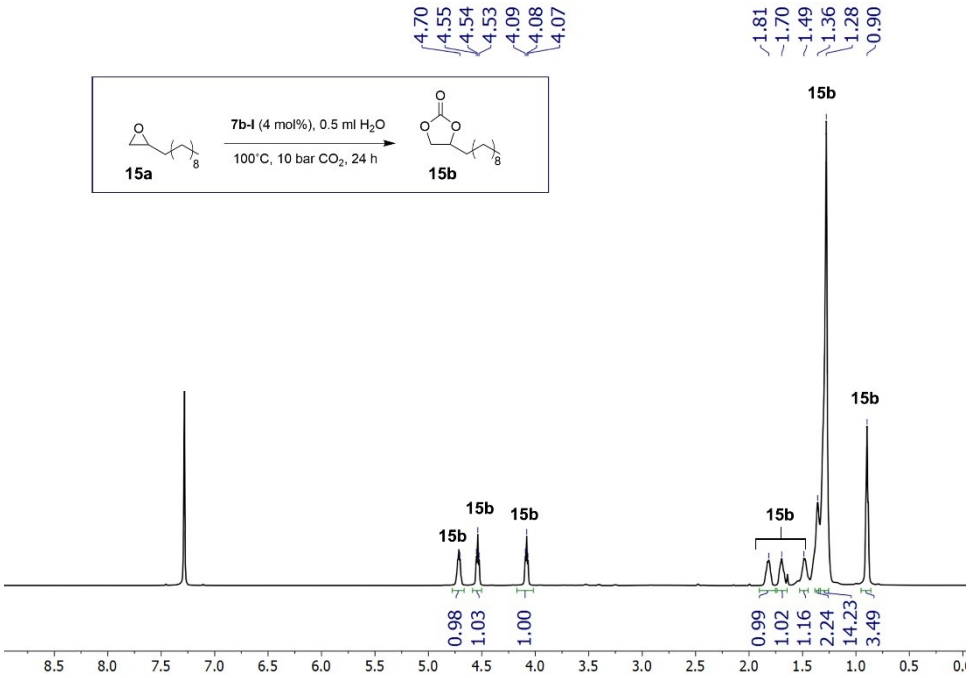


Figure S115. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **15a**; **15a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 100 °C, 10 bar CO_2, 24 h; Table 4, Entry 5. The NMR spectrum matches the literature reference *ChemSusChem.* 2016, 9, 749–755.

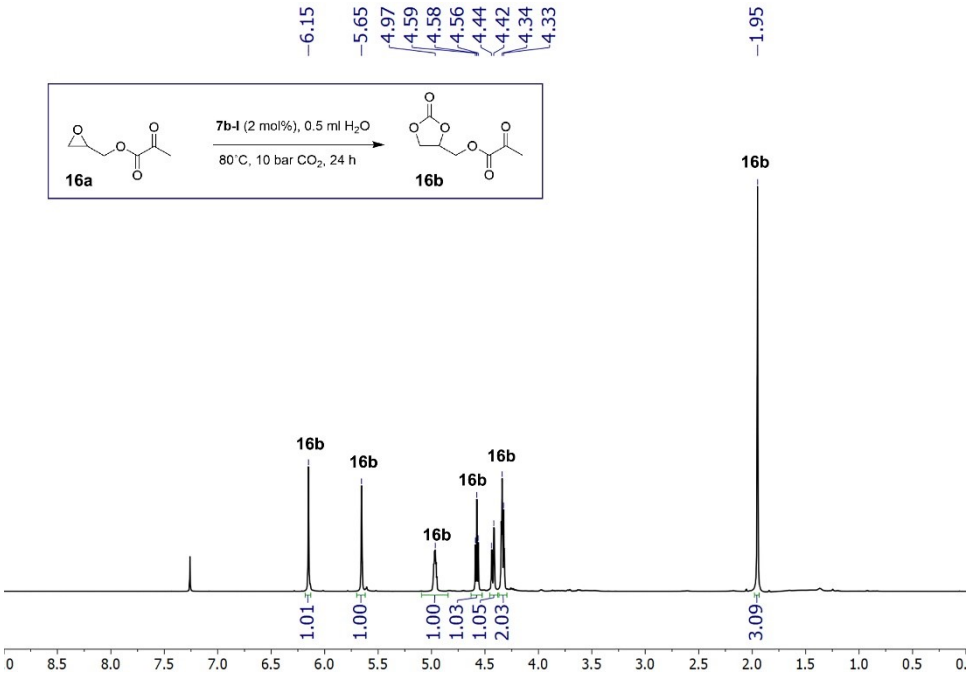


Figure S116. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **16a**; **16a** (10 mmol), 2 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 6. The NMR spectrum matches the literature reference *Eur. Polym. J.* 2014, 61, 133–144.

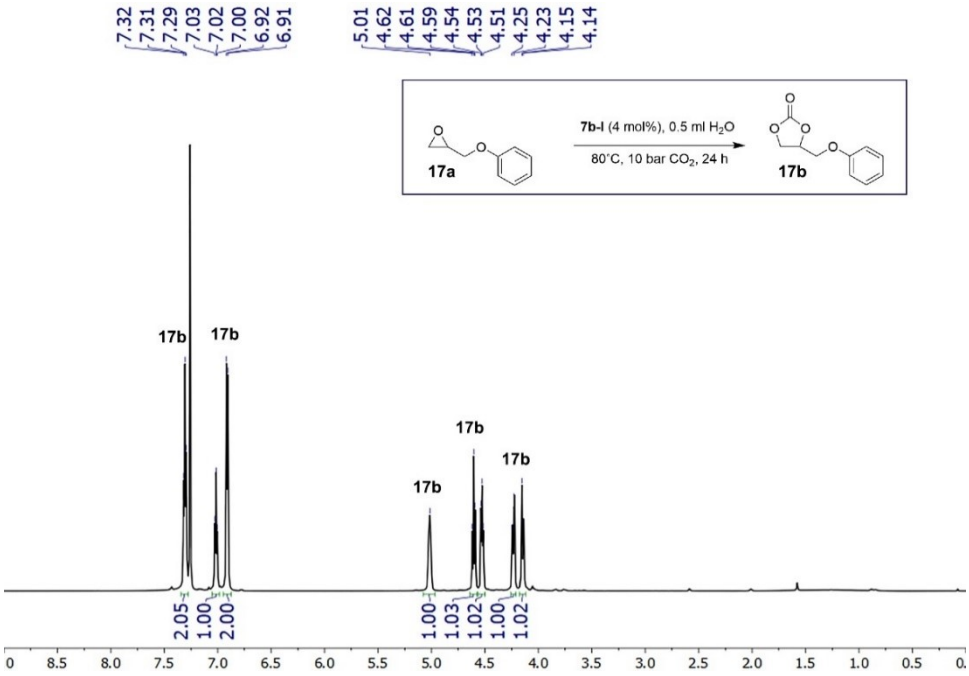


Figure S117. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **17a**; **17a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 80 °C, 10 bar CO_2, 24 h; Table 4, Entry 7. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

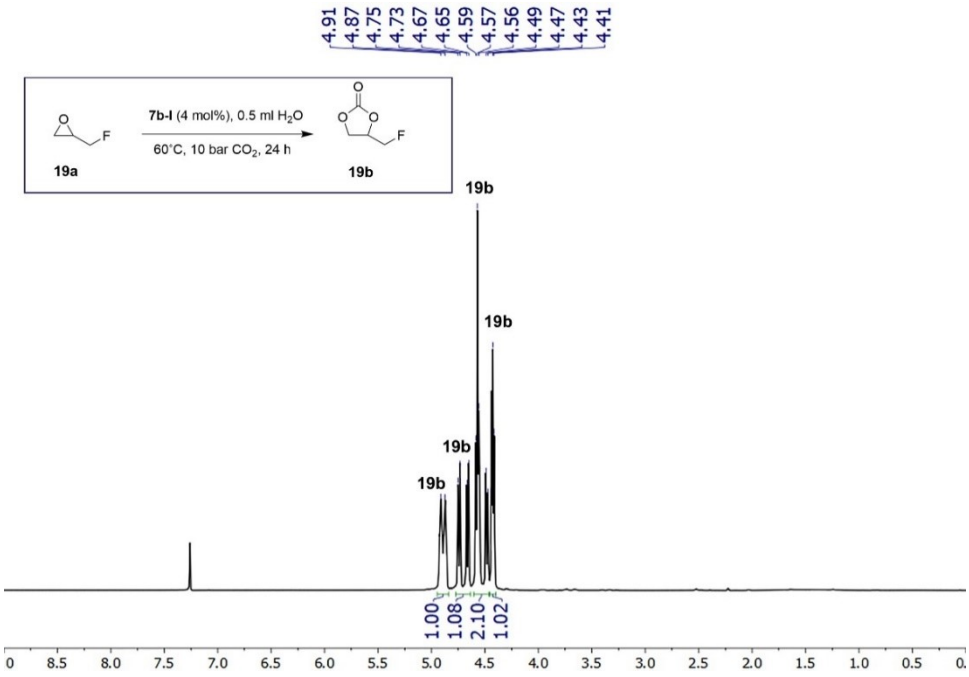


Figure S118. ^{1}H NMR ($CDCl_3$) spectrum of the isolated oraganic phase for the CO_2 cycloaddition reaction to **19a**; **19a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 60 °C, 10 bar CO_2, 24 h; Table 4, Entry 8. The NMR spectrum matches the literature reference *J. Am. Chem. Soc. 2015*, 137, 30, 9571–9574.

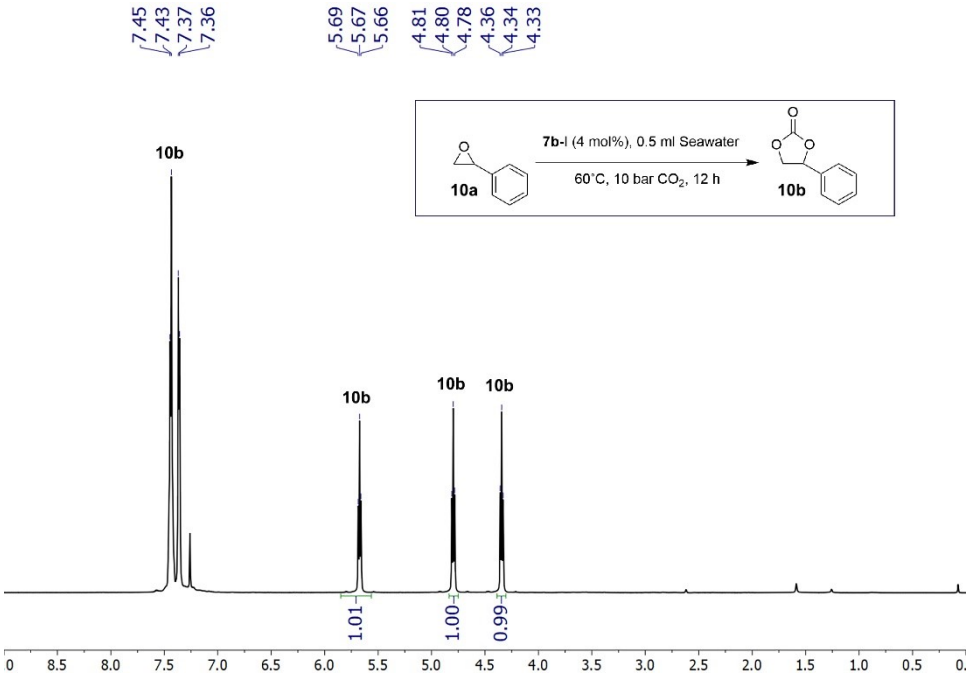


Figure S119. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **10a**; **10a** (10 mmol), 4 mol% **7b-I** (*), 0.5 mL seawater, 60 °C, 10 bar CO_2, 12 h; Table 4, Entry 9. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

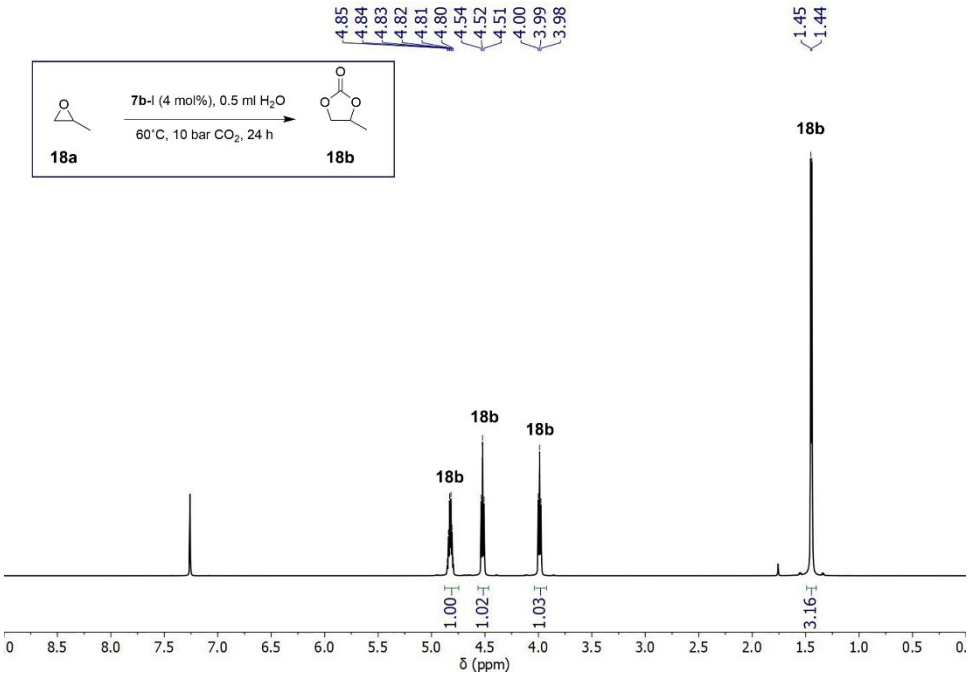


Figure S120. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **18a**; **18a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 60 °C, 10 bar CO_2, 24 h; Table 4, Entry 10. The NMR spectrum matches the literature reference *J. Org. Chem*. 2005, 70, 1, 381–383.

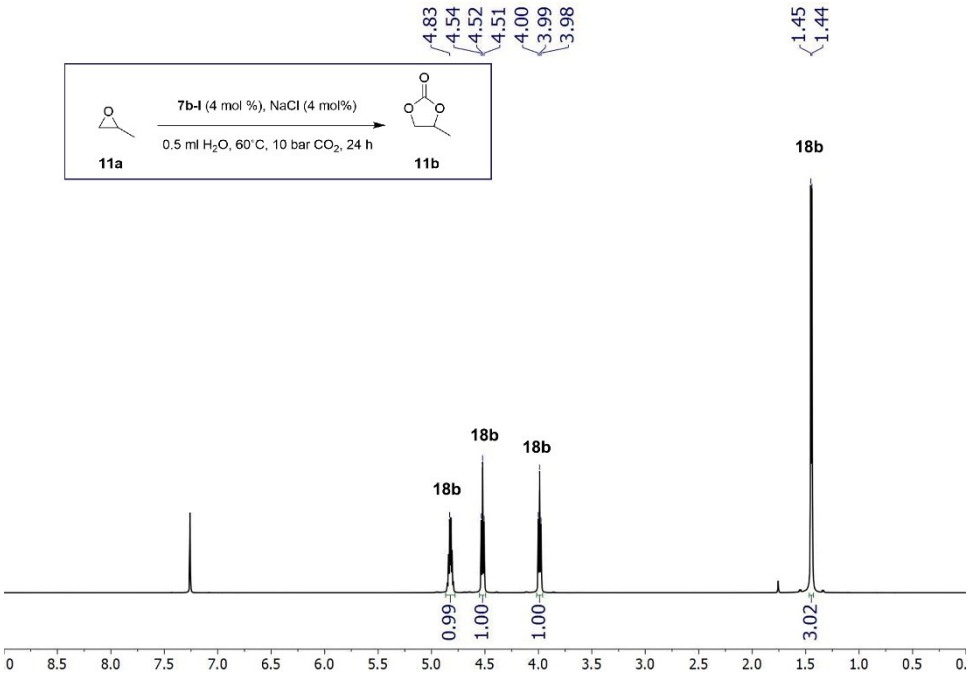


Figure S121. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **18a**; **18a** (10 mmol), 4 mol% **7b-I**, 4 mol% NaCl, 0.5 mL H_2O, 60 °C, 10 bar CO_2, 24 h; Table 4, Entry 10a. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

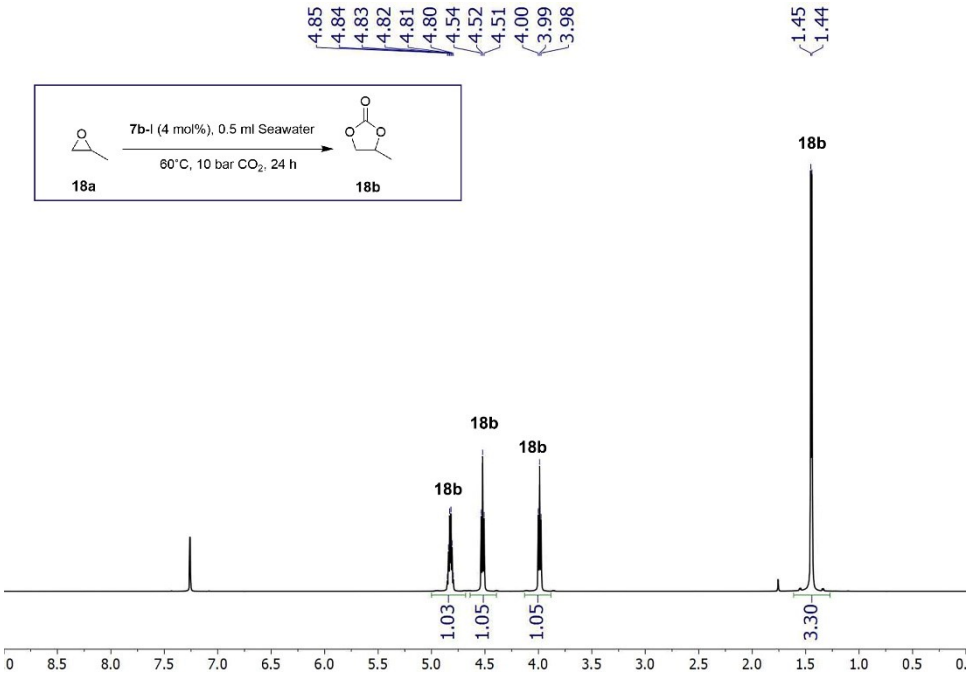


Figure S122. ^{1}H NMR ($CDCl_3$) spectrum of the isolated organic layer for the CO_2 cycloaddition reaction to **18a**; **18a** (10 mmol), 4 mol% **7b-I**, 0.5 mL seawater, 60 °C, 10 bar CO_2, 24 h; Table 4, Entry 10b. The NMR spectrum matches the literature reference *J. Org. Chem.* 2005, 70, 1, 381–383.

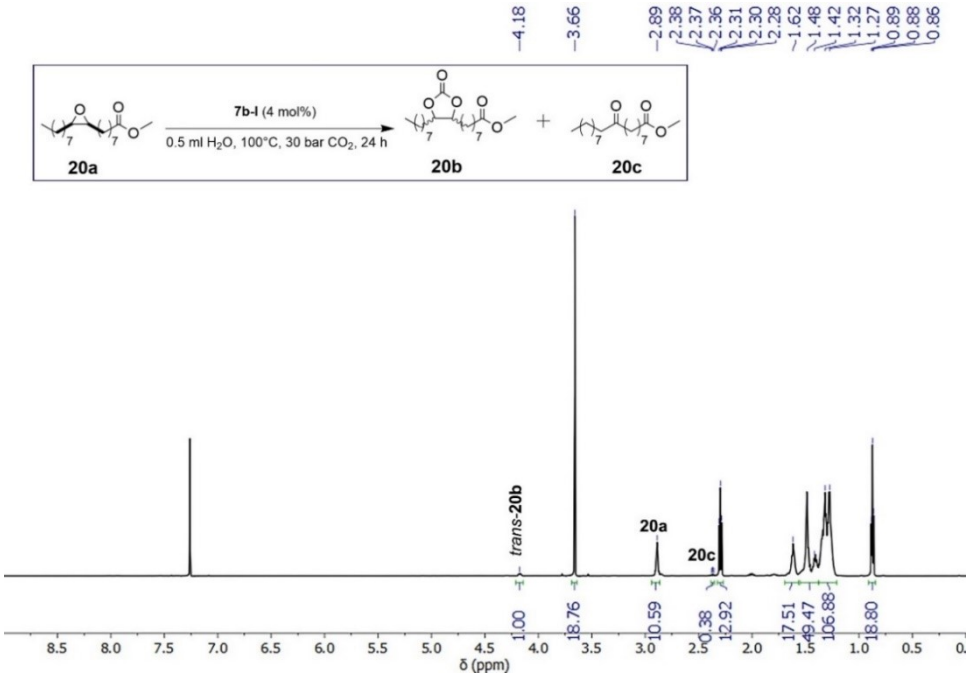


Figure S123. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 24 h; Table 5, Entry 1.

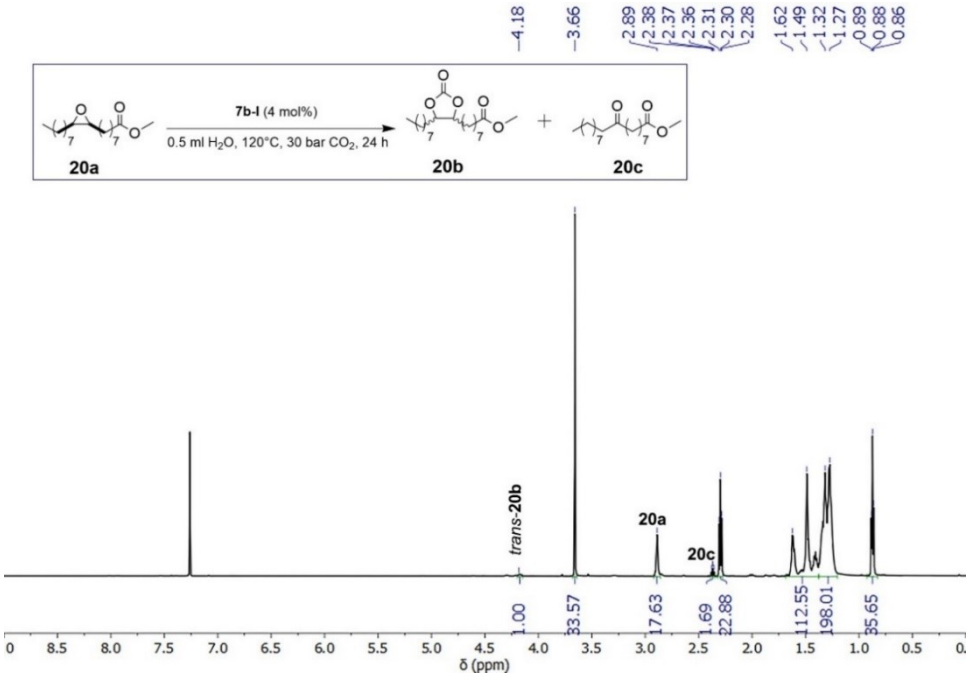


Figure S124. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 24 h; Table 5, Entry 2**.**

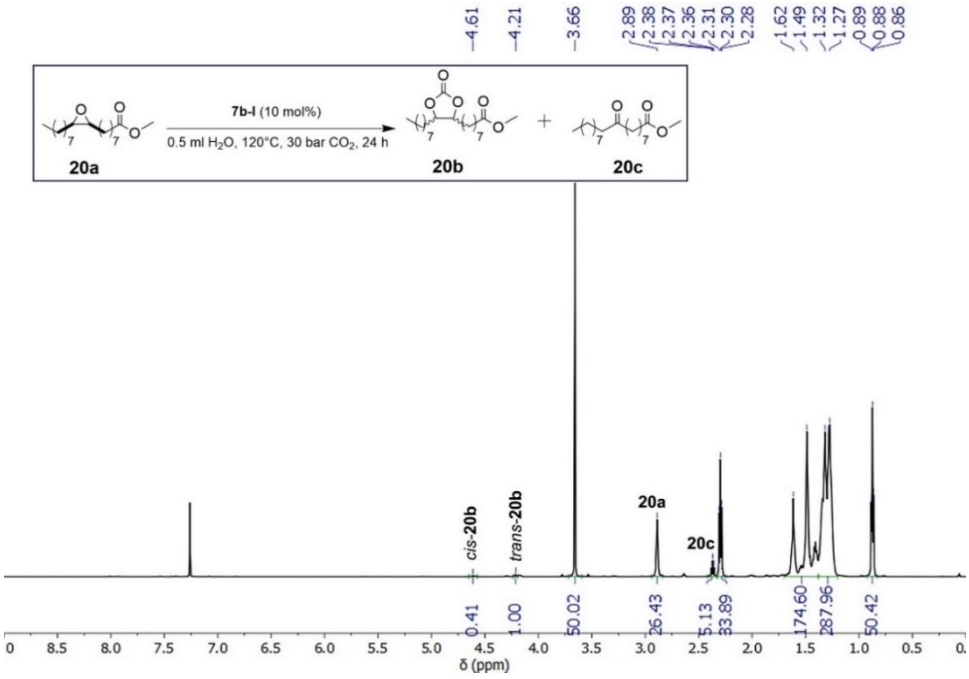


Figure S125. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7b-I**, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 24 h; Table 5, Entry 3.

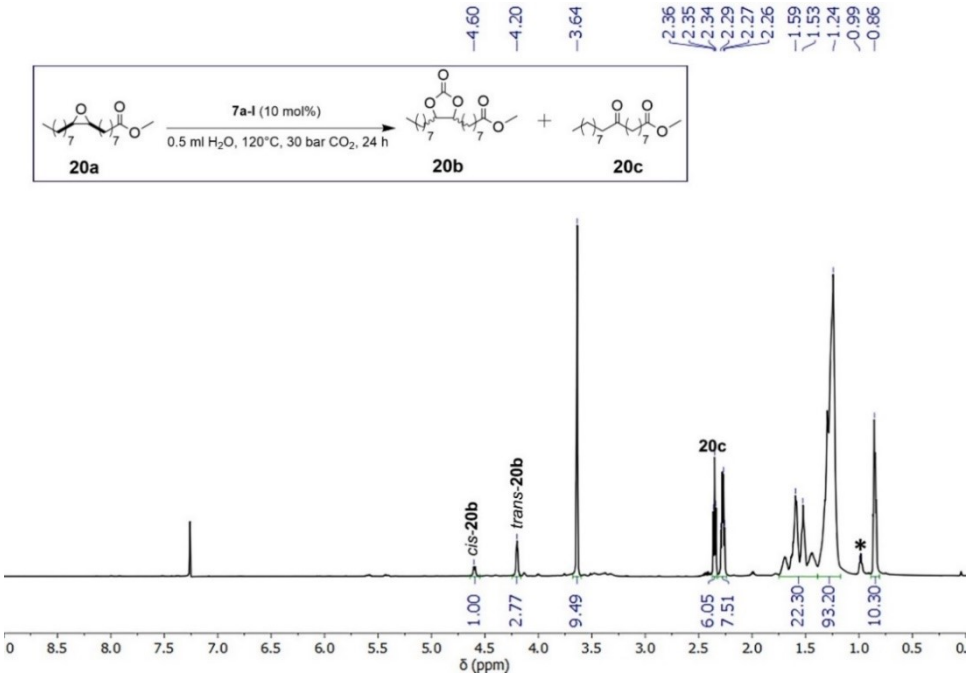


Figure S126. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-I (*)**, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 24 h; Table 5, Entry 6.

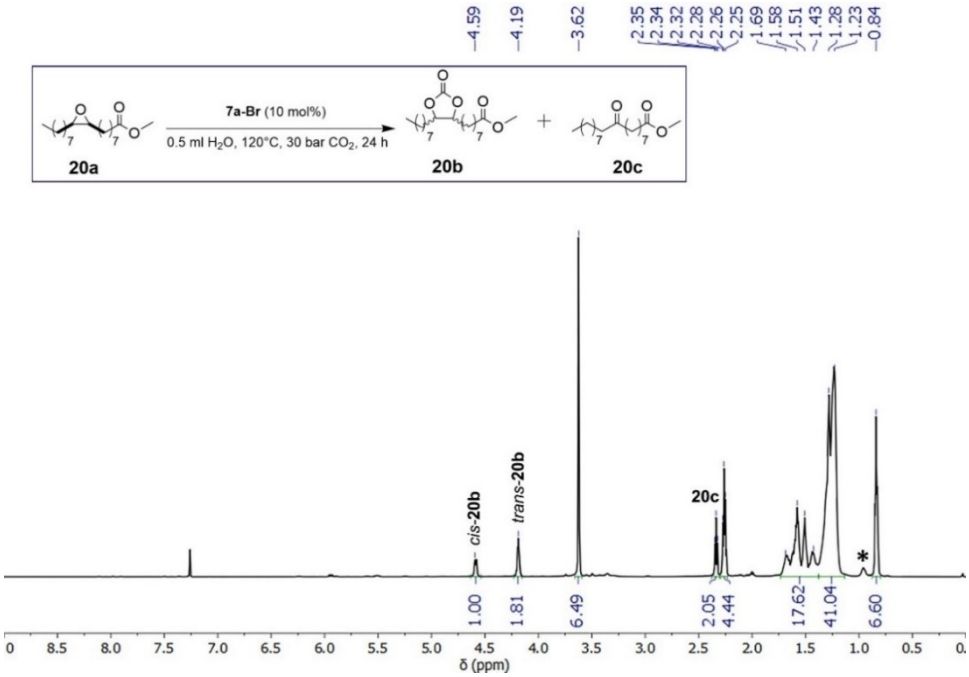


Figure S127. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Br (*)**, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 24 h; Table 5, Entry 7.

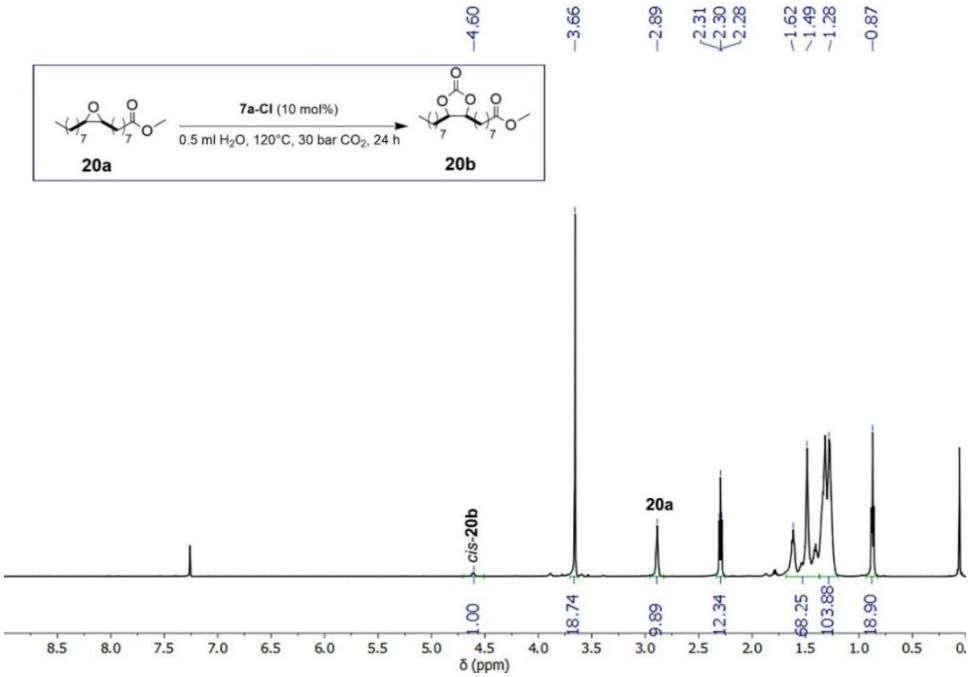


Figure S128. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 24 h; Table 5, Entry 8.

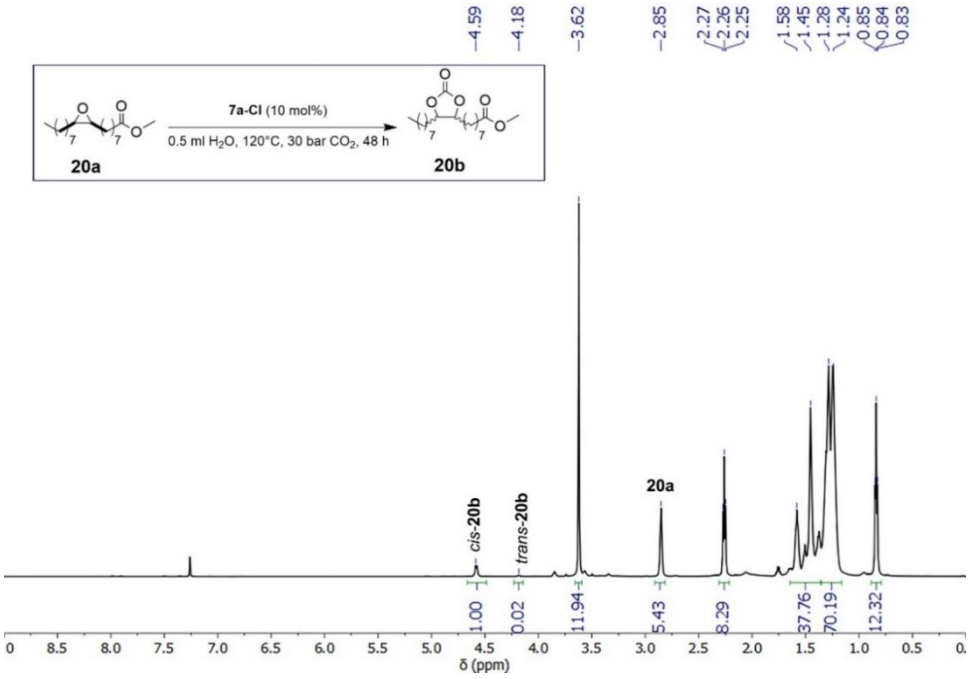


Figure S129. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **16a**; **16a** (1.5 mmol), 10 mol% **7a-Cl**, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 48 h; Table 5, Entry 9.

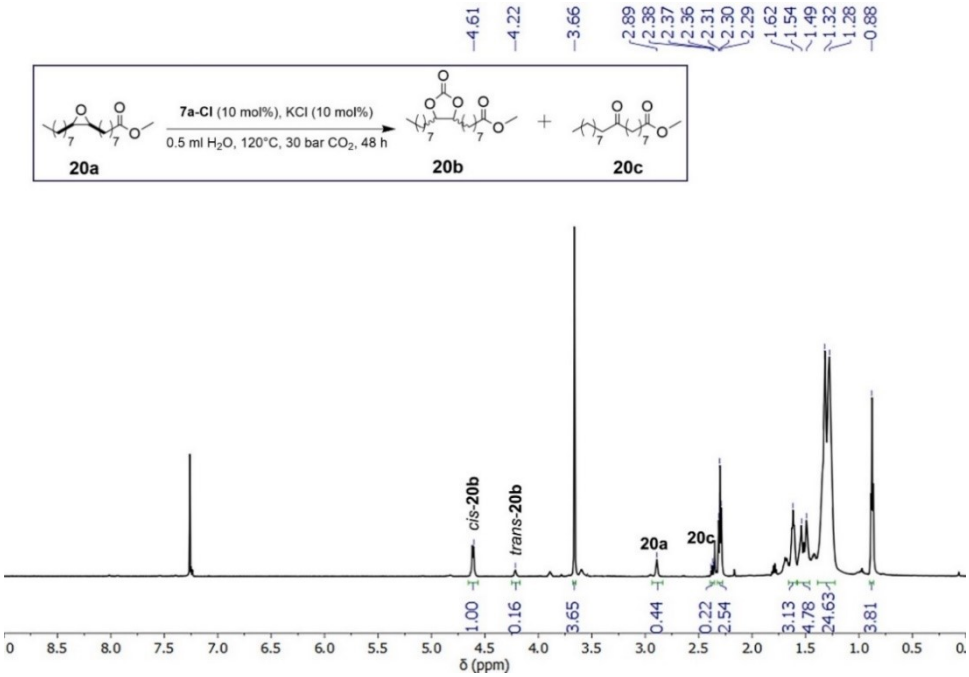


Figure S130. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 10 mol% KCl, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 48 h; Table 5, Entry 10.

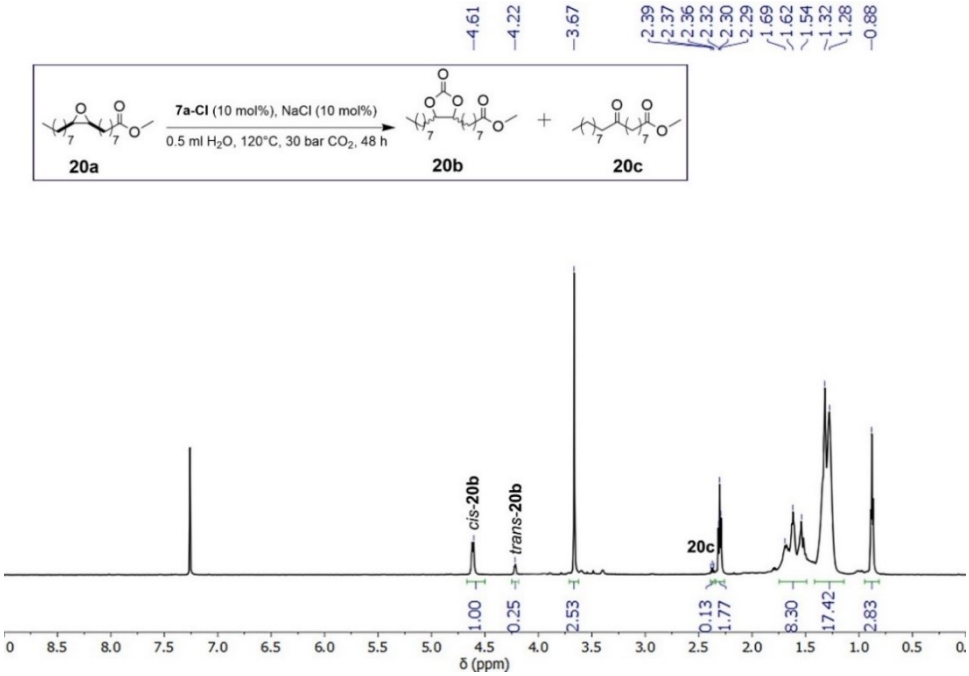


Figure S131. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 10 mol% NaCl, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 48 h; Table 5, Entry 11.

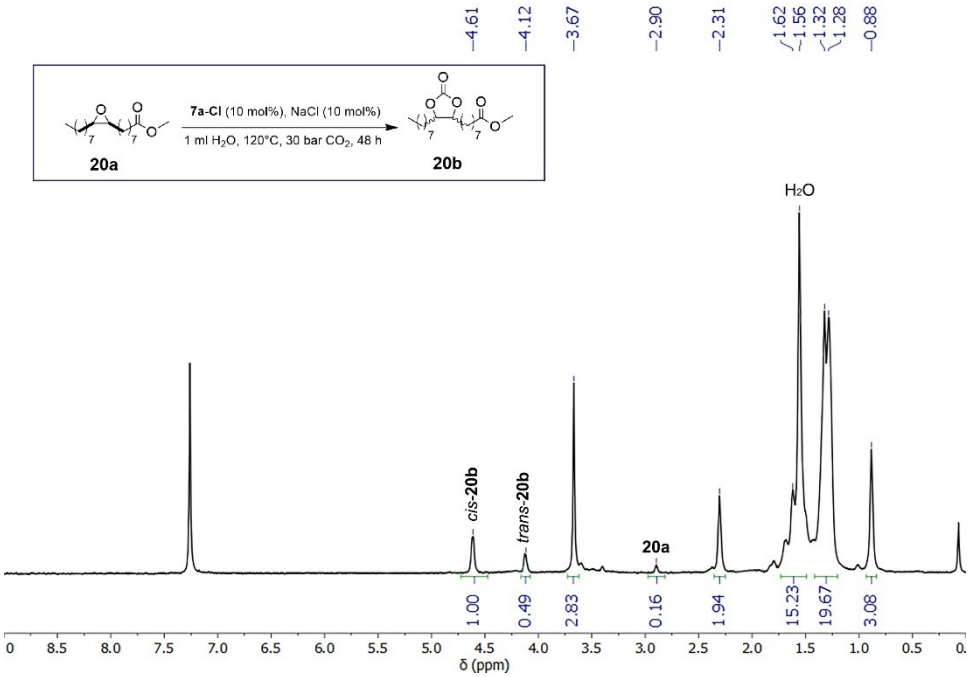


Figure S132. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 10 mol% NaCl, 1 mL H_2O, 120 °C, 30 bar CO_2, 48 h; Table 5, Entry 12.

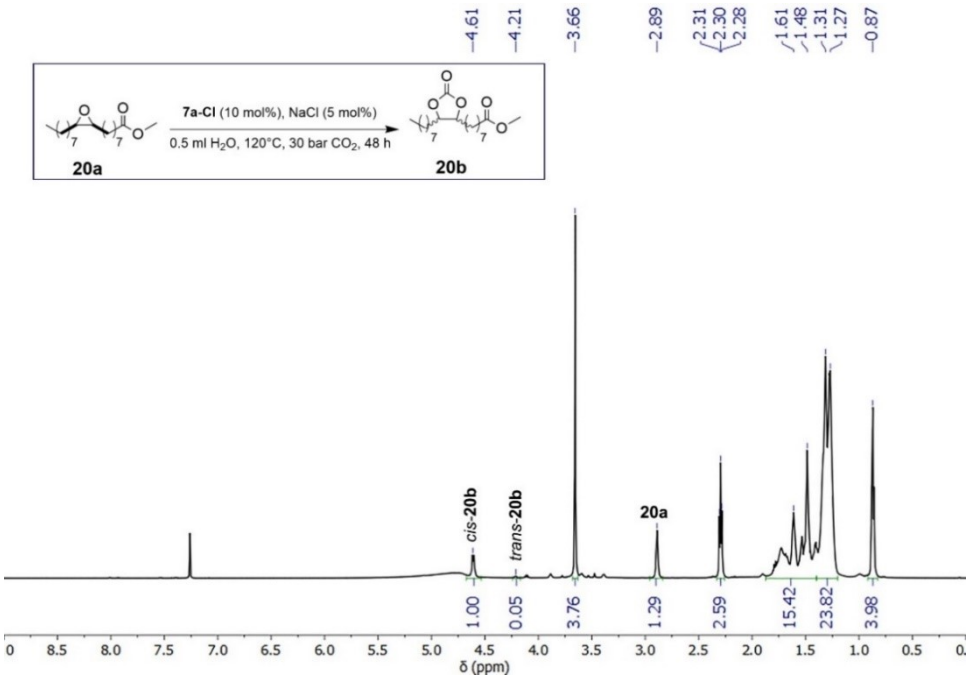


Figure S133. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 5 mol% NaCl, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 48 h; Table 5, Entry 14.

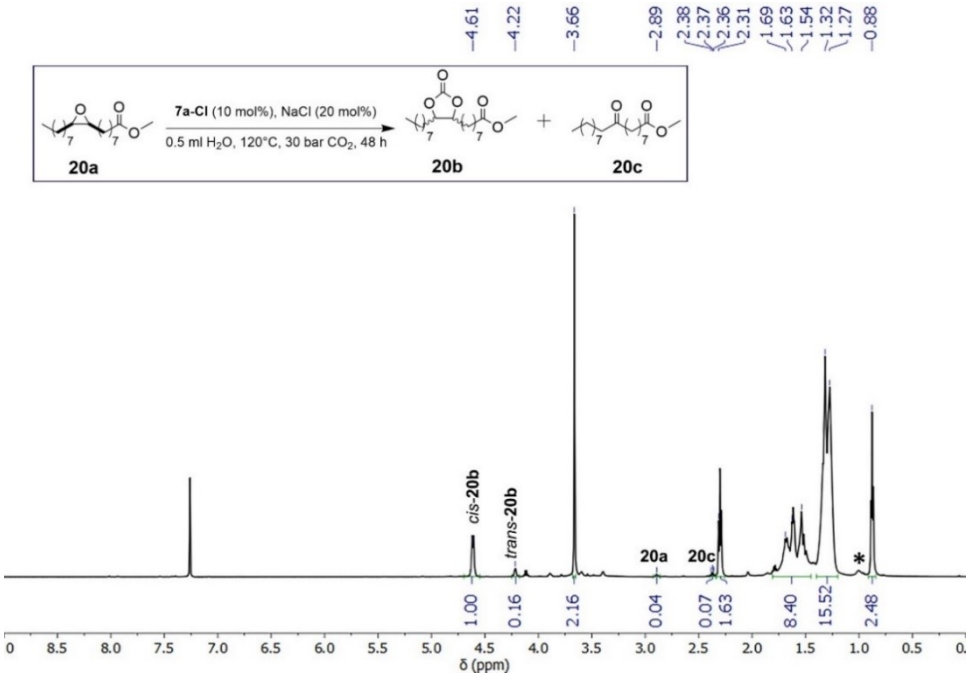


Figure S134. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl (*)**, 20 mol% NaCl, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 48 h; Table 5, Entry 15.

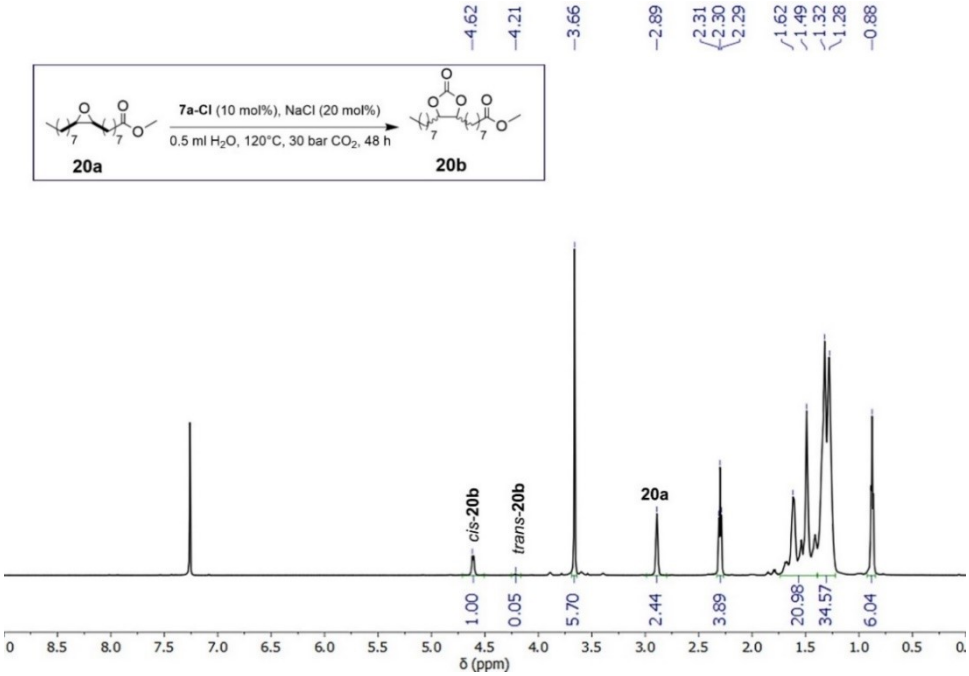


Figure S135. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 20 mol% NaCl, 0.5 mL H_2O, 120 °C, 30 bar CO_2, 48 h (2^{nd} run); Table 5, Entry 16.

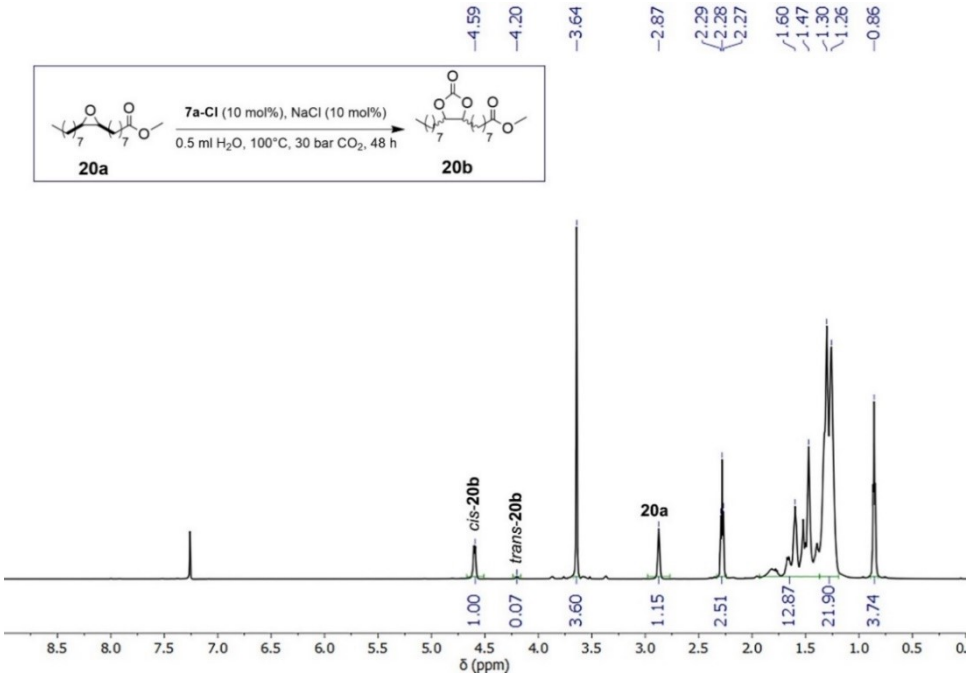


Figure S136. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 10 mol% NaCl, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 48 h; Table 5, Entry 17.

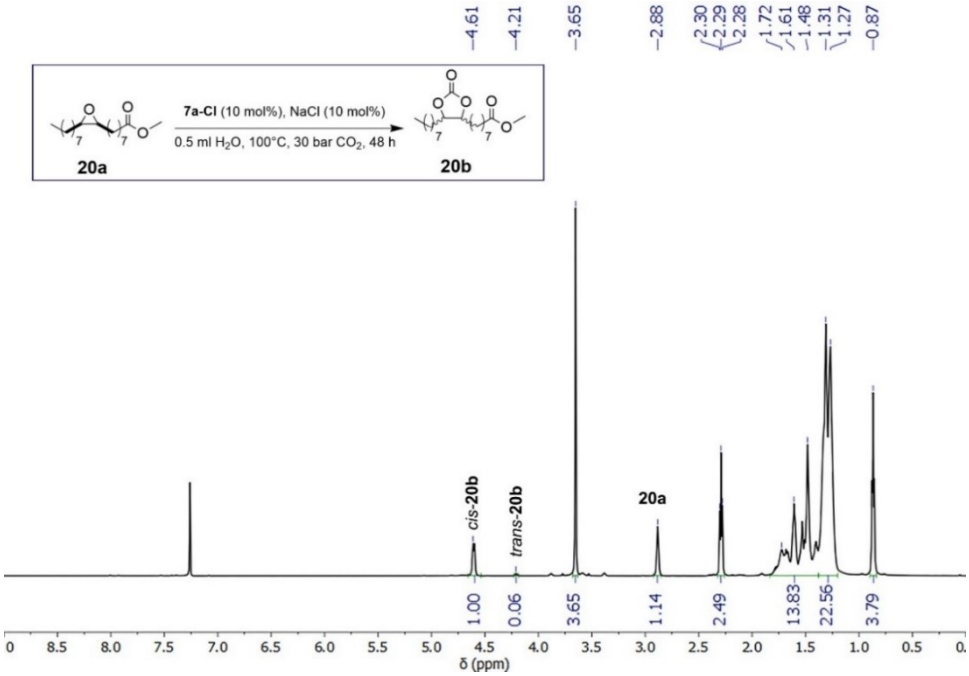


Figure S137. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 10 mol% NaCl, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 48 h (2^{nd} run); Table 5, Entry 18.

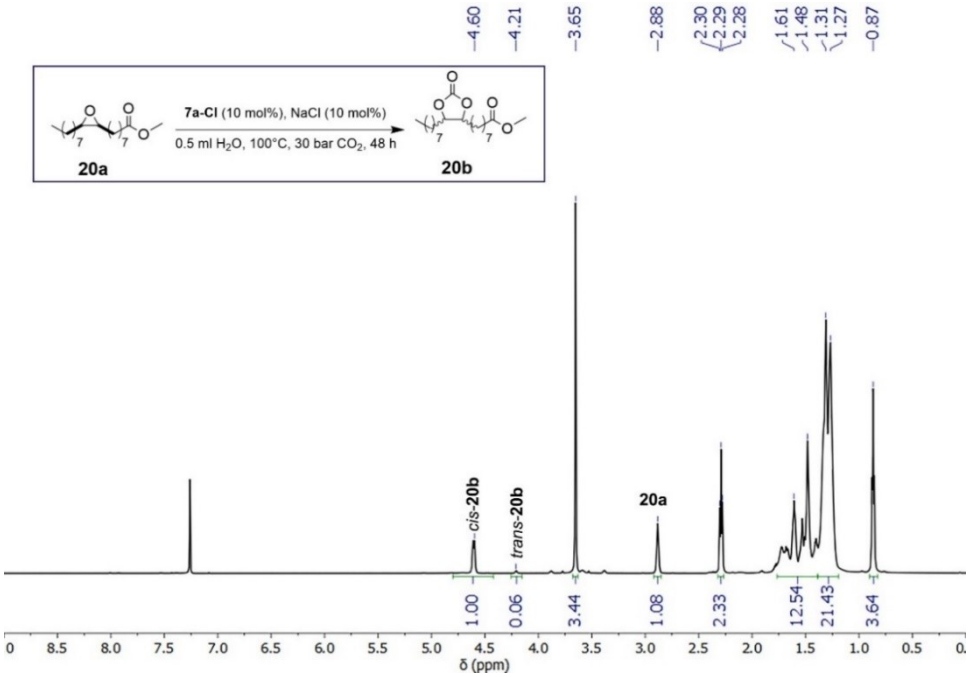


Figure S138. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl**, 10 mol% NaCl, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 48 h (3rd run); Table 5, Entry 19.

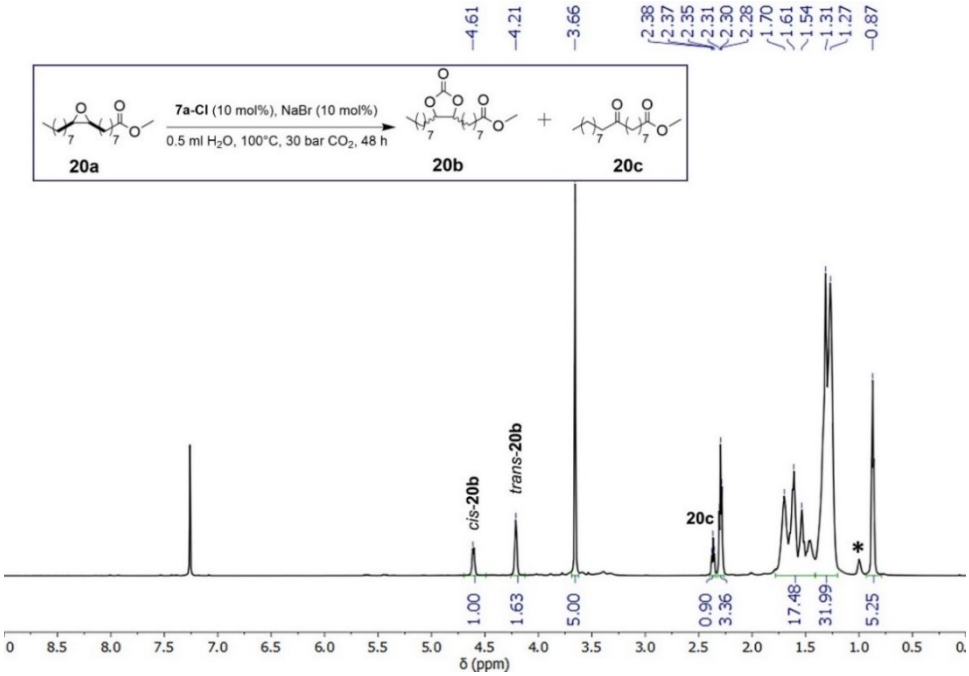


Figure S139. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl (*)**, 10 mol% NaBr, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 48 h; Table 5, Entry 20.

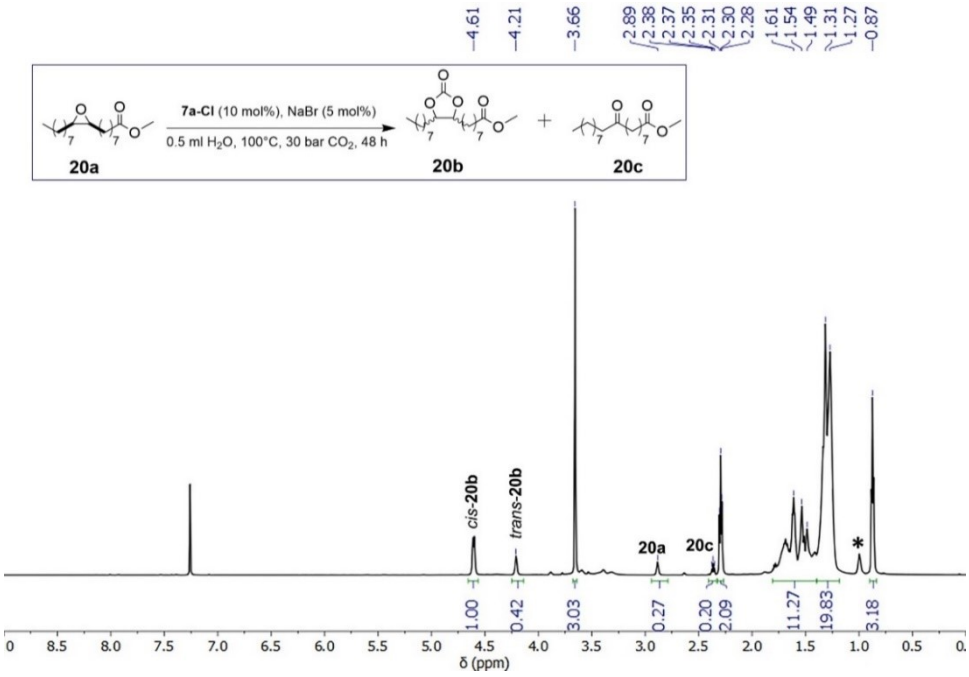


Figure S140. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl** (*), 5 mol% NaBr, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 48 h (1st run); Table 5, Entry 21.

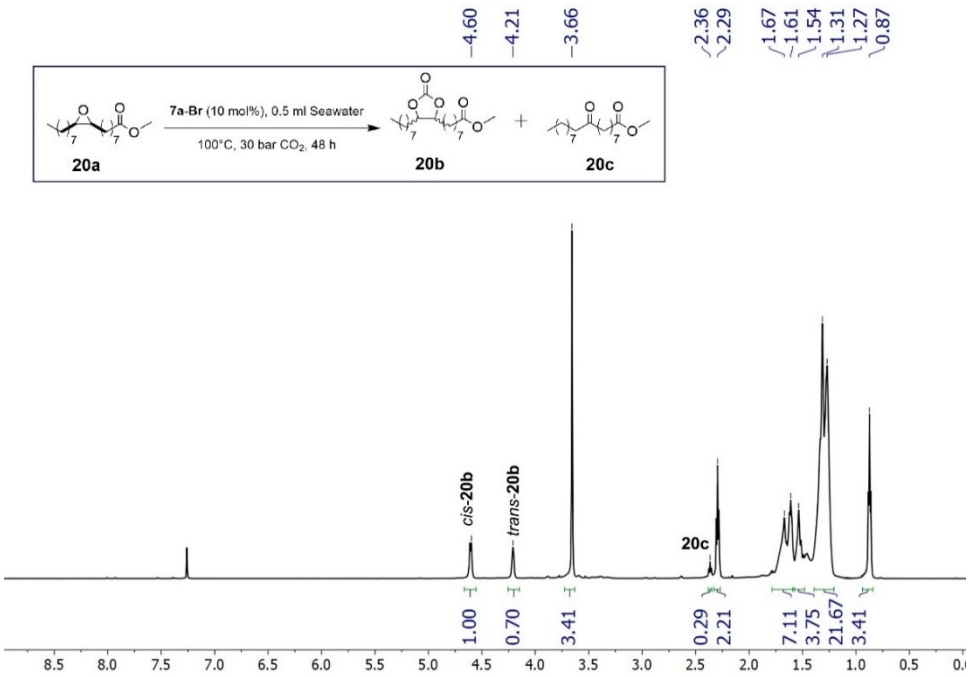


Figure S141. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Br**, 0.5 mL seawater, 100 °C, 30 bar CO_2, 48 h ; Table 5, Entry 22. The NMR spectrum of **20b** matches the literature reference *Asian J. Org. Chem.* 2020, 9, 801-810.

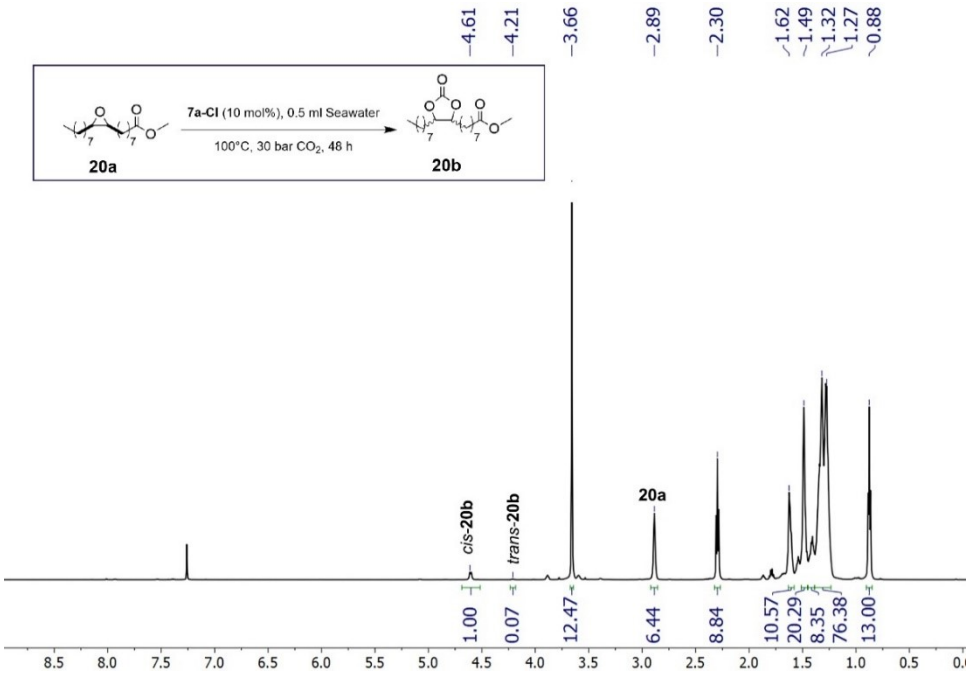


Figure S142. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **20a**; **20a** (1.5 mmol), 10 mol% **7a-Cl (*)**, 0.5 mL seawater, 100 °C, 30 bar CO_2, 48 h ; Table 5, Entry 23.

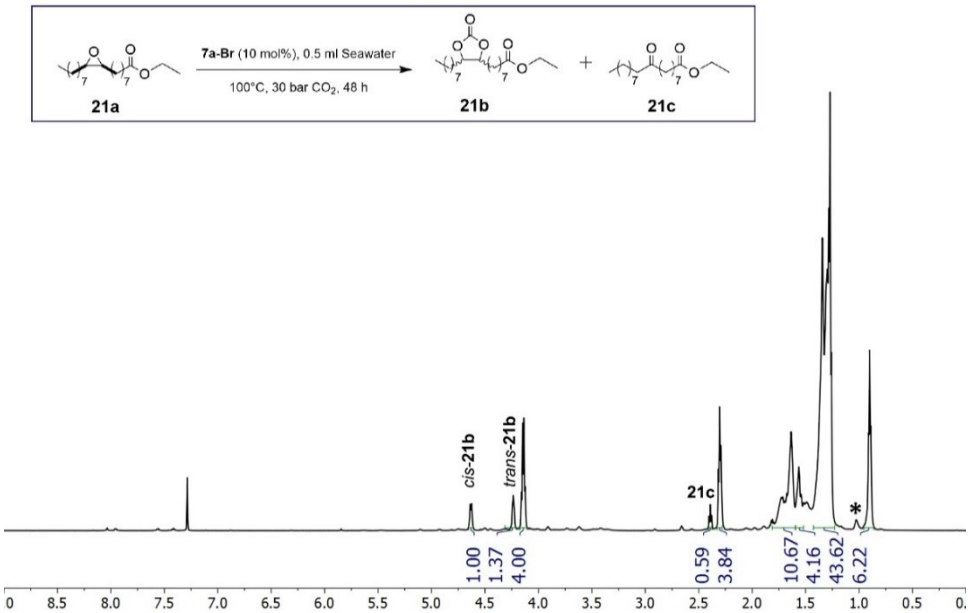


Figure S143. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **21a**; **21a** (1.5 mmol), 10 mol% **7a-Br**, 0.5 mL seawater, 100 °C, 30 bar CO_2, 48 h; Table S7 Entry 2.

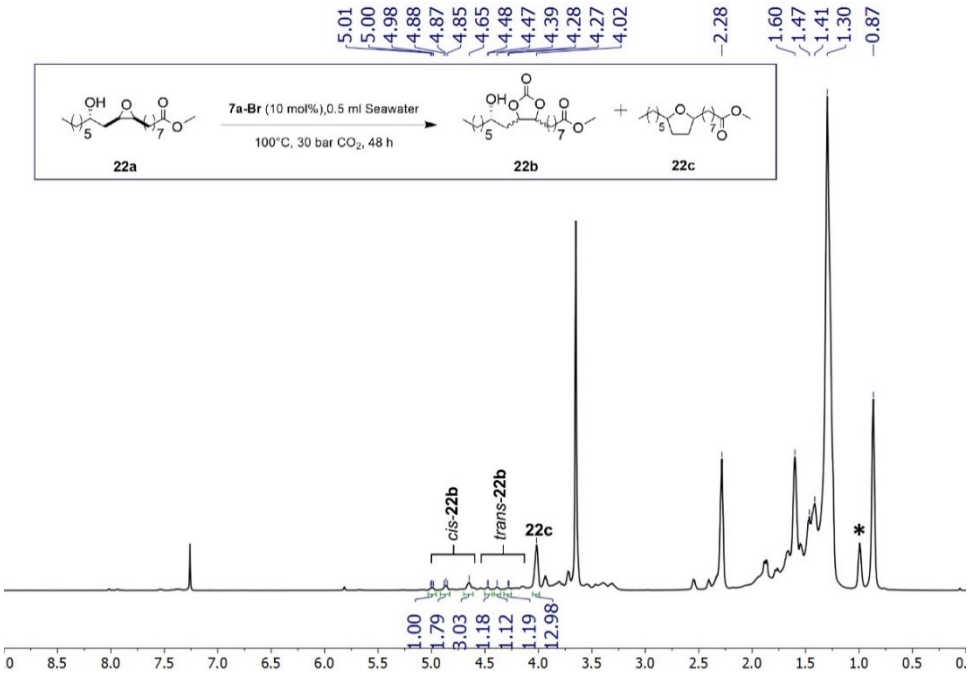


Figure S144. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **22a**; **22a** (1.5 mmol), 10 mol% **7a-Br (*)**, 0.5 mL seawater, 100 °C, 30 bar CO_2, 48 h; Table S7 Entry 3.

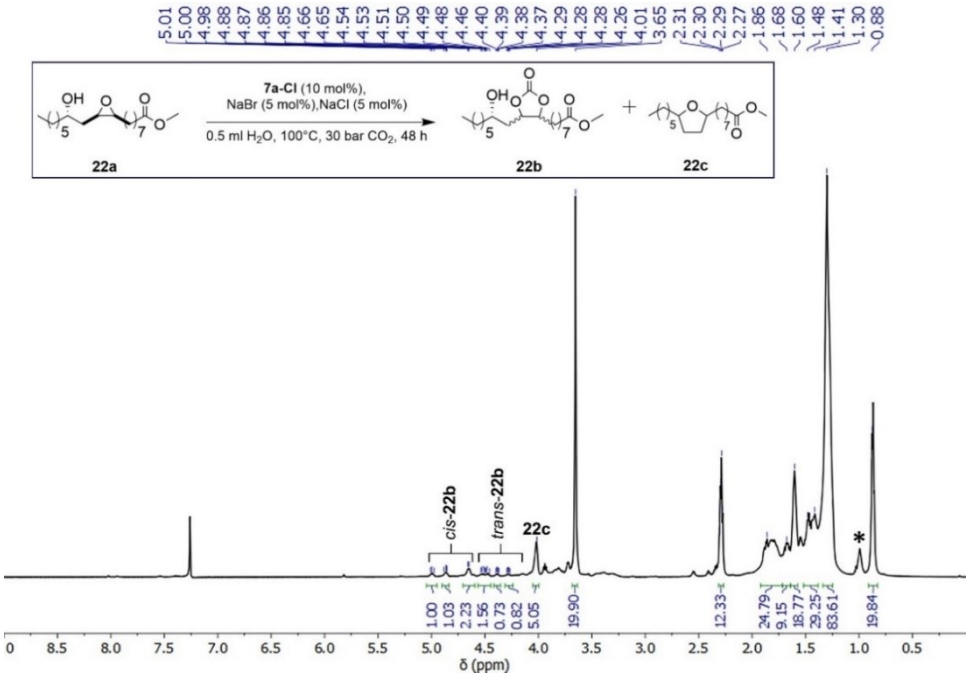


Figure S145. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **22a**; **22a** (1.5 mmol), 10 mol% **7a-Cl (*)**, 5 mol% NaBr, 5 mol% NaCl, 0.5 mL H_2O, 100 °C, 30 bar CO_2, 48 h; Table S7 Entry 3.

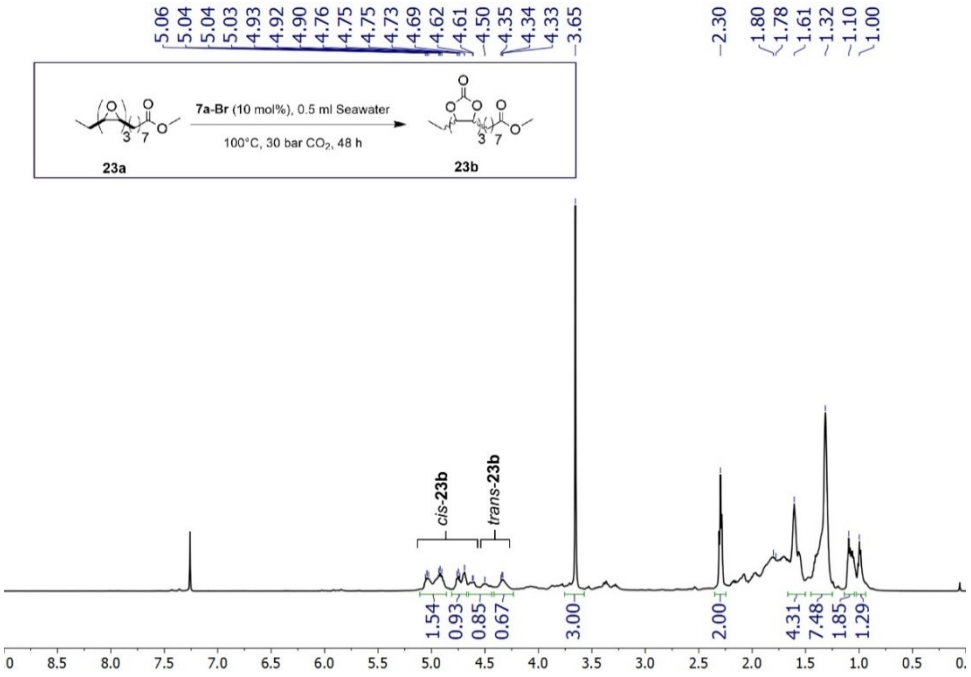
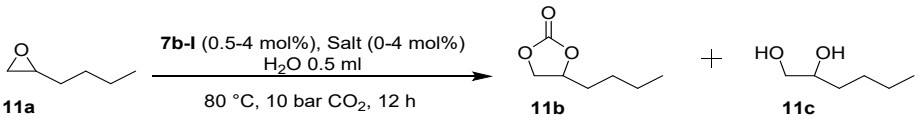


Figure S146. ^{1}H NMR ($CDCl_3$) spectrum of crude CO_2 cycloaddition reaction to **23a**; **23a** (1.5 mmol), 10 mol% **7a-Br**, 0.5 mL seawater, 100 °C, 30 bar CO_2, 48 h; Table S7 Entry 4.

S8. Supplementary Catalytic Results

Several experiments were conducted to investigate the salting in or salting out the behavior of salt additives at different concentrations (Table S3). When using just 1 mol% KI, the conversion of **11a** was basically identical as in the absence of KI but the selectivity for **11b** decreased (Table S3, entries 1, 2), indicating that, at this concentration, KI played a salting-in role similar to $LiClO_4$. Conversely, 2 mol% KI was sufficient to obtain the same enhancement of catalytic performance as when using 4 mol% KI achieving the carbonate product in high selectivity (Table S3, entries 3, 4). As **7b-I** was found to display moderate **11a** conversions to **11b** even when used in low catalytic loadings (0.5 mol%, Table S5), we also tested the effect of the addition of salts (KI, KOAc, 2 mol%) for this reduced **7b-I** loading (Table S3, entries 5-7); in the case of KI, the **11a** conversion even slightly decreased compared to the reaction carried out in the absence of salt indicating that, for this catalyst concentration, KI behaved as a salting-in additive such as NaI and $LiClO_4$ (Table 3). In the case of KOAc, instead, the conversion of **11a** increased significantly to about 80% with high **11b** selectivity confirming the positive effect of this salting-out additive even for low **7b-I** loadings.

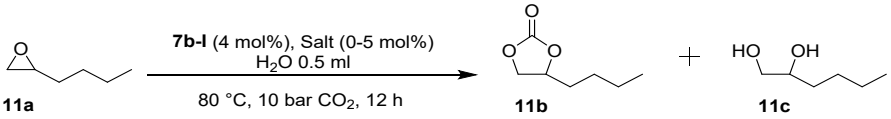
Table S3. Effect of salt addition on the cycloaddition of CO_2 to 1-hexene oxide (**11a**) catalyzed by **7b-I** in the aqueous biphasic environment.[a]



Entry	Catalyst (mol%)	Salt (mol%)	P_{CO2} (bar)	Time (h)	Conversion[b] (%)	Selectivity[c] (%)
1[d]	**7b-I** (4)	-	10	12	35±2	94±3
2	**7b-I** (4)	**KI** (1)	10	12	34±2	85±1
3	**7b-I** (4)	**KI** (2)	10	12	88±1	97±1
4[f]	**7b-I** (4)	**KI** (4)	10	12	87±1	98±1
5	**7b-I** (0.5)	-	10	24	54±1	99±1
6	**7b-I** (0.5)	**KI** (2)	10	24	27±1	90±1
7	**7b-I** (0.5)	**KOAc** (2)	10	24	79±1	97±1

[a] Reaction conditions: epoxide (10 mmol), **7b-I** (4 mol%), salt (0-4 mol%), H_2O 0.5 mL, at 80 °C, 10 bar CO_2 for 12-24 h. [b] Determined by ^{1}H NMR. [c]Refers to the selectivity for cyclic carbonate (**11b**) versus the corresponding 1,2-diol (**11c**). [d] Taken from Table 2. [f] Taken from Table 3.

Table S4 Effect of NaCl concentration on the cycloaddition of CO_2 with **11a** catalyzed by **7b-I.**[a]



Entry	Catalyst (mol%)	Salt (mol%)	Conversion[b] (%)	Selectivity[c] (%)
1[d]	**7b-I** (4)	-	35±2	94±3
2	**7b-I** (4)	**NaCl** (1)	47±1	94±1
3	**7b-I** (4)	**NaCl** (2)	65±1	96±1
4[e]	**7b-I** (4)	**NaCl** (2.45)	99±1	99±1
5	**7b-I** (4)	**NaCl** (2.5)	96±1	99±1
6[f]	**7b-I** (4)	**NaCl** (4)	77±1	97±1
7	**7b-I** (4)	**NaCl** (5)	66±1	97±1

[a] Reaction conditions: epoxide (10 mmol), **7b-I** (4 mol%), salt (0-4 mol%), H_2O 0.5 mL, at 80 °C, 10 bar CO_2 for 12 h. [b] Determined by ^{1}H NMR. [c]Refers to the selectivity for cyclic carbonate (**11b**) versus the corresponding 1,2-diol (**11c**). [d] Taken from Table 2. [e] Using 0.5 mL seawater (2.45 mol% NaCl) instead of DI water. [f] Taken from Table 3.

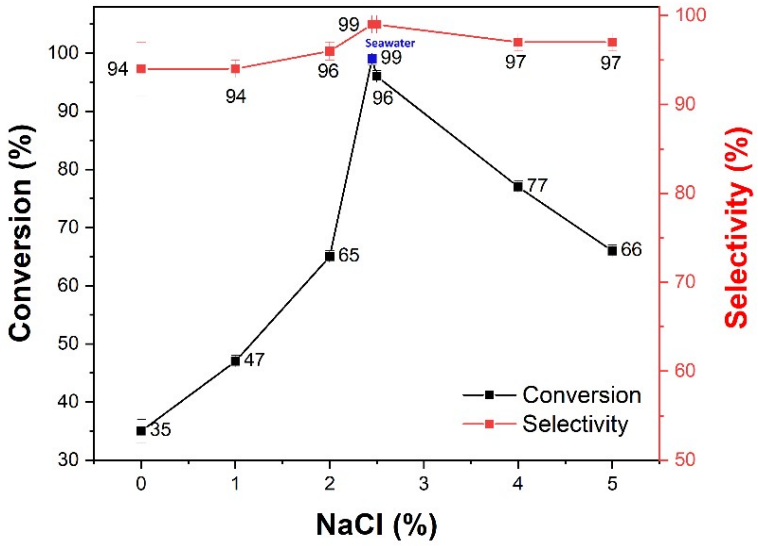
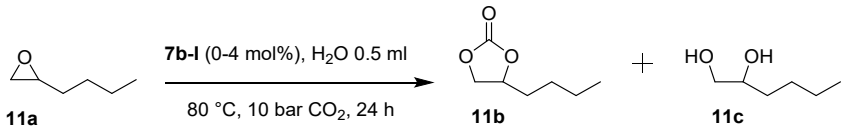


Figure S147. The effect of NaCl concentration to the biphasic catalytic system

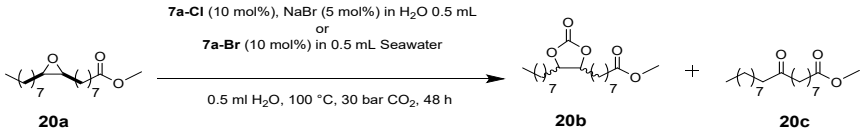
Table S5. Effect of catalyst amount on the cycloaddition of CO_2 to 1-hexene oxide (**11a**) catalyzed by **7b-I** in an aqueous biphasic environment.[a]



Entry	Catalyst (mol%)	Conversion[b] (%)	Selectivity[c] (%)	TON
1[d]	-	4±1	0	0
2	**7b-I** (0.25)	39±1	99±1	156
3	**7b-I** (0.5)	54±1	99±1	108
4	**7b-I** (1)	95±1	97±1	95
5	**7b-I** (2)	99±1	99±1	50
6[d]	**7b-I** (4)	99±1	99±1	25

[a] Reaction conditions: epoxide (10 mmol), **7b-I** (0-4 mol%), H_2O 0.5 mL, at 80 °C, 10 bar CO_2 for 24 h. [b] Determined by ^{1}H NMR. [c]Refers to the selectivity for cyclic carbonate (**11b**) versus the corresponding 1,2-diol (**11c**). [d] Taken from Table 2.

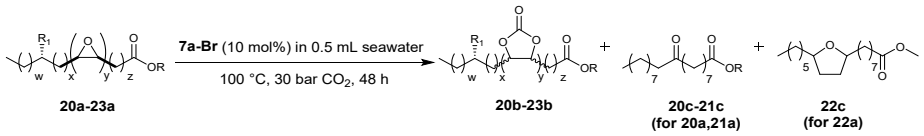
Table S6 Cycloaddition of CO_2 with internal epoxide catalyzed by **7a-Cl** [a] **and 7a-Br** [b].

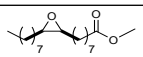
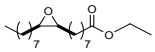
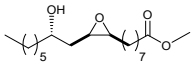
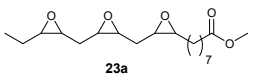


Entry	Catalyst (mol%)	Additive (mol %)	Conversion[c] (%)	Selectivity[c] (%)	*cis*/*trans*[c] (%)
1	-	NaCl(10)	0	0	-
2	-	NaBr(10)	0	0	-
3	**7a-Cl** (10) _(1st run)	NaBr(5)	86±1	88±1	70/30
4	**7a-Cl** (10)_(2nd run)	-	77±1	90±1	70/30
5	**7a-Cl** (10)_(3rd run)	-	69±1	92±1	80/20
6	**7a-Cl** (10)_(4th run)	-	62±1	93±1	85/15
7	**7a-Cl** (10)_(5th run)	-	55±1	94±1	89/11
8	**7a-Br** in seawater (10)_(1st run)	-	99±1	86±4	35/65
9	**7a-Br** in seawater (10)_(2nd run)	-	99±1	84±1	56/44
10	**7a-Br** in seawater (10)_(3rd run)	-	99±1	85±1	59/41
11	**7a-Br** in seawater (10)_(4th run)	-	90±1	88±1	59/41
12	**7a-Br** in seawater (10)_(5th run)	-	89±1	90±1	66/33

[a] Epoxide **20a** (1.5 mmol), **7a-Cl** (10 mol%), NaBr (5 mol%), T= 100 °C, 30 bar CO_2, 48 h, 0.5 mL water. [b]Epoxide **20a** (1.5 mmol), **7a-Br** (10 mol%), T= 100 °C, 30 bar CO_2, 48 h, 0.5 mL seawater. [c]Determined by ^{1}H NMR, see reference [4].

Table S7. Cycloaddition of CO_2 to epoxidized fatty acids **20a-23a** catalysed by **7a-Br** under optimized biphasic reaction conditions.[a]



Entry	Substrate	Conversion (%)[b]	Selectivity (%)[b]	*cis*/*trans* (%)[b]
1[c]	 **20a**	99±1	86±3 [c]	35/65
2	 **21a**	99±1	83±1	45/55
3	 **22a**	99±1	47±1 (60±1)[d]	62/38 (58/42)[d]
4	 **23a**	99±1	99±1	65/35

[a] Epoxide (1.5 mmol), catalyst **7a-Br** (10 mol%), seawater 0.5 mL, for at 100 °C, 30 bar CO_2 for 48 h.[b] Determined by ^{1}H NMR, see reference[4]. [c] Taken from Table 5. [d] Epoxide (1.5 mmol), catalyst **7a-Cl** (10 mol%), NaBr (5 mol%), NaCl (5 mol%), H_2O 0.5 mL, at 100 °C, 30 bar CO_2 for 48 h.

For epoxidized ethyl oleate (**21a**), a similar result as for **20a** was observed, although with a slightly lower **21b** selectivity (Table S7, entries 1, 2). For **22a** (Table S7, entry 3), complete substrate conversion was observed but with moderate **22b** selectivity due to the formation of a cyclic ether by-product via intramolecular cycloaddition of the alcohol group to the epoxide.[4, 5] The **22b** selectivity could be increased by using **7a-Cl** in the presence of NaBr and NaCl (5 mol% each) in the aqueous layer. For *cis*-epoxidized methyl linolenate (**23a**), a substrate with multiple epoxide functionalities, the triscarbonate **23b** was obtained with quantitative conversion and selectivity as the *cis*-isomer (Table S7, entry 4, Figure S146).

S9. Control Experiments for the Reaction Phase

The following spectra refer to control experiments to check for the phase in which the catalytic reaction takes place (epoxide phase or aqueous phase); the experimental details for each run are given in the captions of the spectra.

Experiment 1: **11a** (10 mmol), 4 mol% **7b-I** were stirred at 80 °C for 30 min, then the hot organic phase was filtrated and reacted with CO_2 (10 bar) for 24 h (Figure S148).

Experiment 2: **11a** (10 mmol), 4 mol% **7b-I** and H_2O (0.5 mL) stirred at 80 °C for 30 min, then the hot organic phase was filtrated and reacted with CO_2 (10 bar) for 24 h (Figure S149).

Experiment 3: **11a** (0.1 mmol) in D_2O (0.5 mL) stirred at 80 °C for 24 h (Figure S150).

Experiment 4: **11a** (0.1 mmol), 4 mol% **7b-I,** and D_2O (0.5 mL) stirred at 80 °C under 10 bar CO_2 for 24 h (Figure S151).

Experiment 5: **11a** (10 mmol), 4 mol% **7b-I,** 4 mol% KI, and D_2O (0.5 mL) stirred at 80 °C for 30 min, then the hot organic phase was filtrated and reacted with CO_2 (10 bar) for 24 h (Figure S152).

Experiment 6: **11a** (10 mmol), 4 mol% **7b-I,** 4 mol% KOAc, and D_2O (0.5 mL) stirred at 80 °C for 30 min, then the hot organic phase was filtrated and reacted with CO_2 (10 bar) for 24 h (Figure S153).

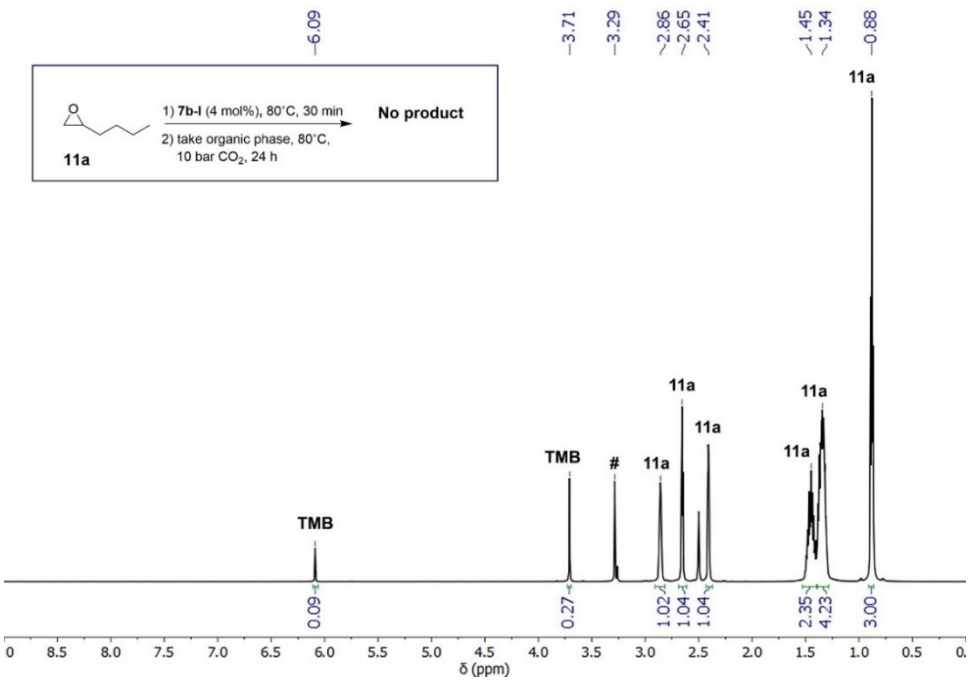


Figure S148. ^{1}H NMR (DMSO-d_6) spectrum of experiment 1; 1,3,5 trimethoxy benzene (TMB) was added as internal standard; Table 6 Entry 1. (#) residual water signal in DMSO-d_6.

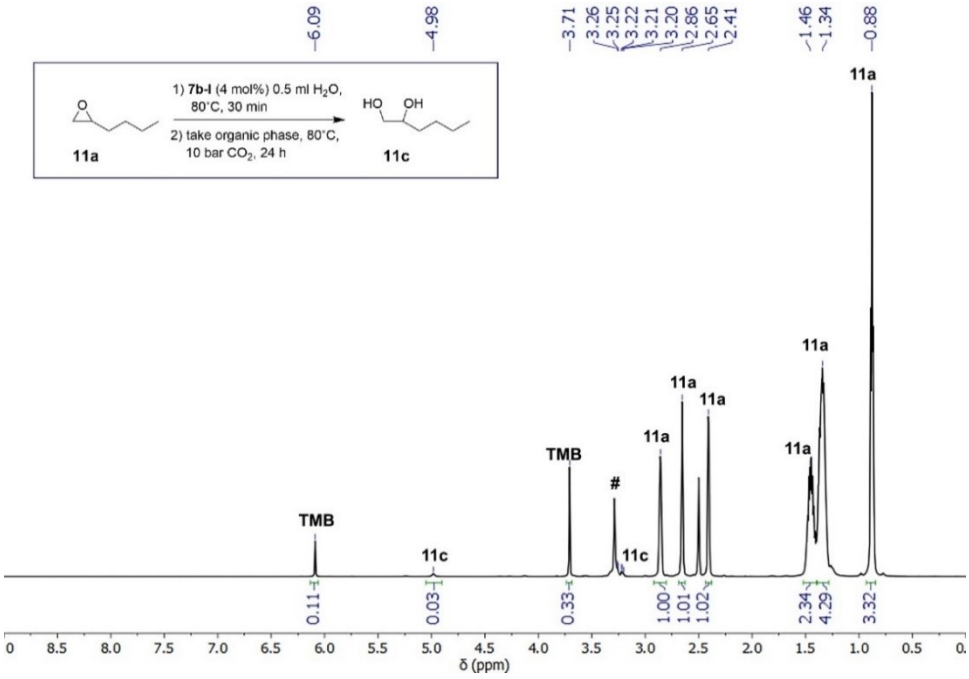


Figure S149. ^{1}H NMR (DMSO-d_6) spectrum of experiments 2. 1,3,5 trimethoxy benzene (TMB) was added as internal standard; Table 6 Entry 2. (#) residual water signal in DMSO-d_6.

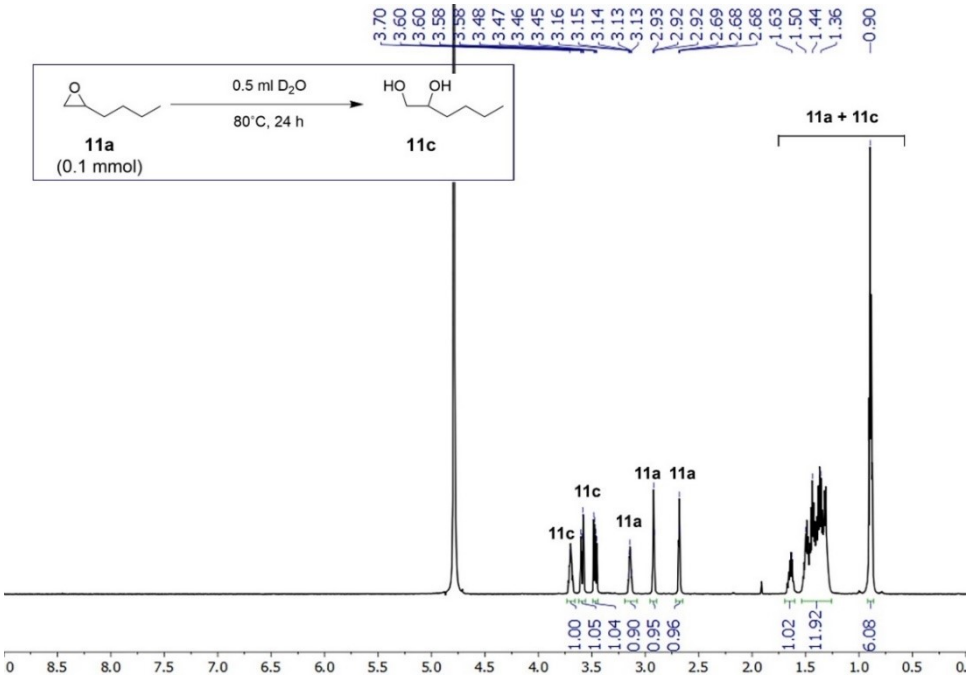


Figure S150. ^{1}H NMR (D_2O) spectrum of experiment 3; Table 6 Entry 3.

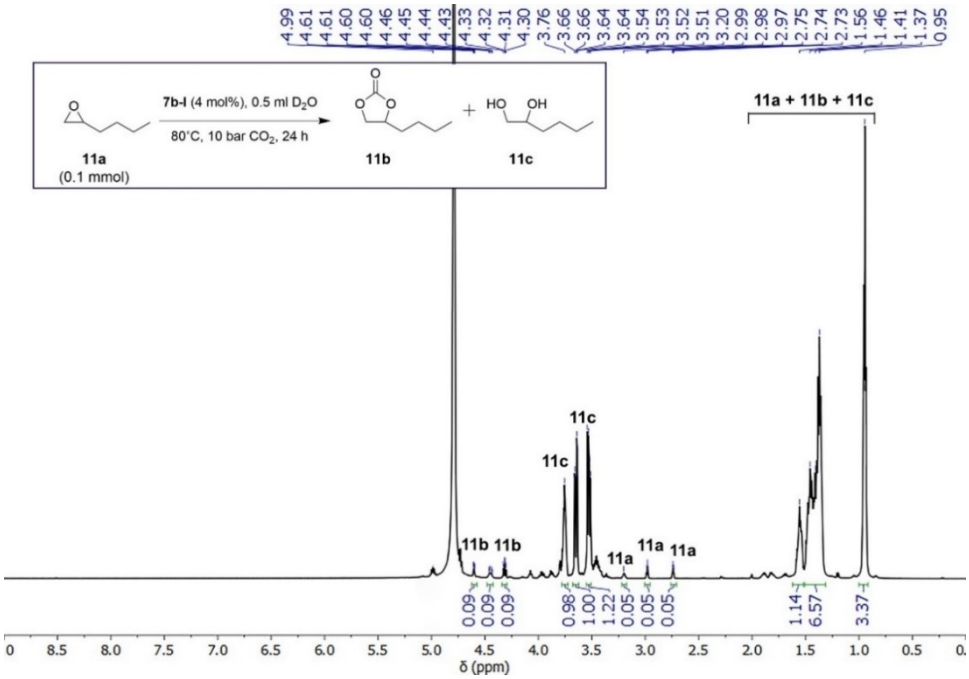


Figure S151. ^{1}H NMR (D_2O) spectrum of experiment 4.; Table 6 Entry 4.

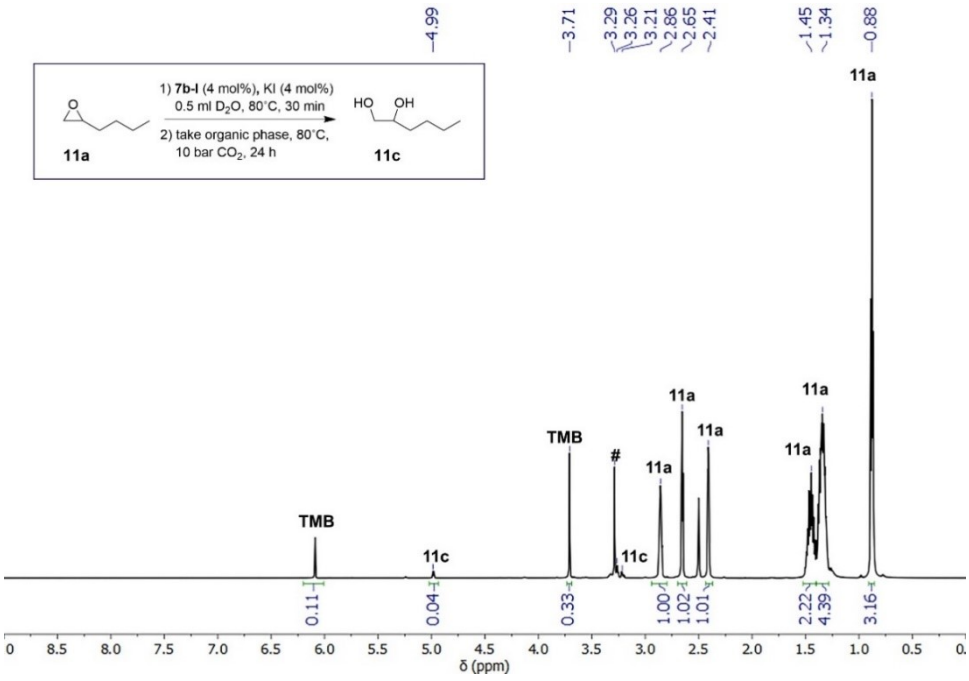


Figure S152. ^{1}H NMR (DMSO-d_6) spectrum of experiment 5; 1,3,5 trimethoxy benzene (TMB) was added as internal standard; Table 6 Entry 5. (#) residual water signal in DMSO-d_6.

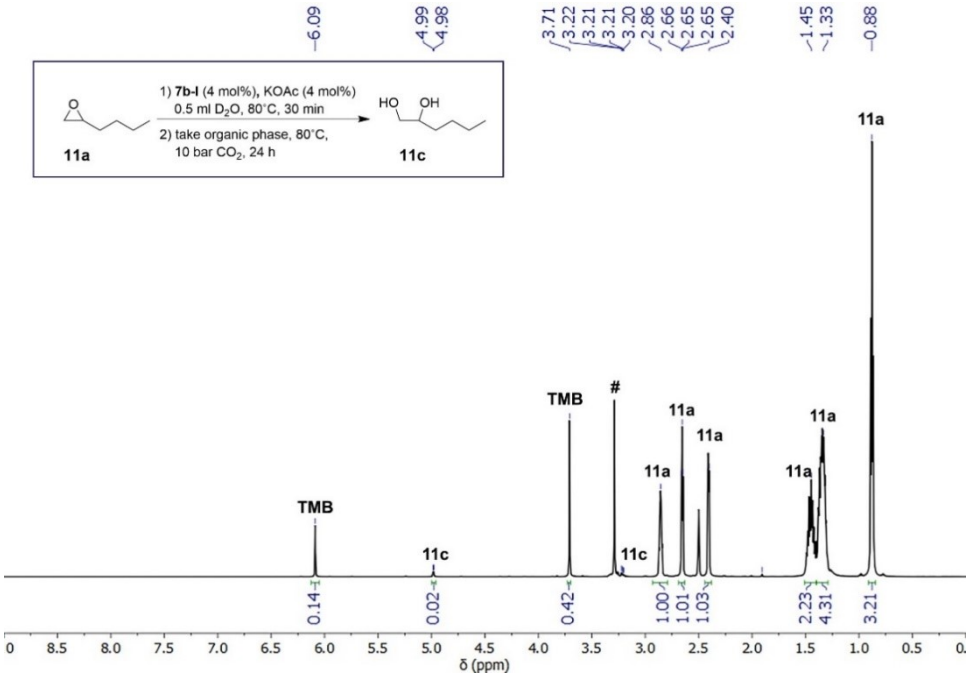


Figure S153. ^{1}H NMR (DMSO-d_6) spectrum of experiment 6; 1,3,5 trimethoxy benzene (TMB) was added as internal standard; Table 6 Entry 6. (#) residual water signal in DMSO-d_6.

S10. Quantification of Catalyst Concentration in the Aqueous Phase

The variation of catalyst concentration in the aqueous layer after stirring with the epoxide (80 °C, 30 min) or after catalytic reaction (80 °C, 10 bar, 24 h without added salts, and 12 h in the presence of salts; for detailed description of experiments see Table S8) was quantified by ^{1}H NMR spectroscopy using D_2O as the aqueous phase. In a general procedure, the aqueous phase after reaction (25 µL) and 1,3,5 trimethoxy benzene (~3 mg, internal standard) were added into an NMR tube. The catalyst concentration in the aqueous phase was calculated according to Equation (S2) from the ^{1}H NMR spectrum (Figure S154) compared to the initial loading. The results are given in Figure S155 and Table S8.

Equation (S2);

$$\text{Concentration of catalyst in the aqueous phase (mol/L)} = \frac{I_a \times H_{std} \times N_{std} \times 106}{I_{std} \times H_a \times 25}$$

Where I_a is the integral of protons signal $(CH_3)_3$ of **7b-I** at 1.35 ppm, I_{std} is the integral of protons signal $(CH)_3$ of 1,3,5 trimethoxy benzene (TMB) at 6.10 ppm, H_a is the number of protons in **7b-I** (H_a =9) at 1.35 ppm, H_{std} is the number of protons of TMB (H_{std} =3) at 6.10 ppm, N_{std} is the number of moles of TMB.

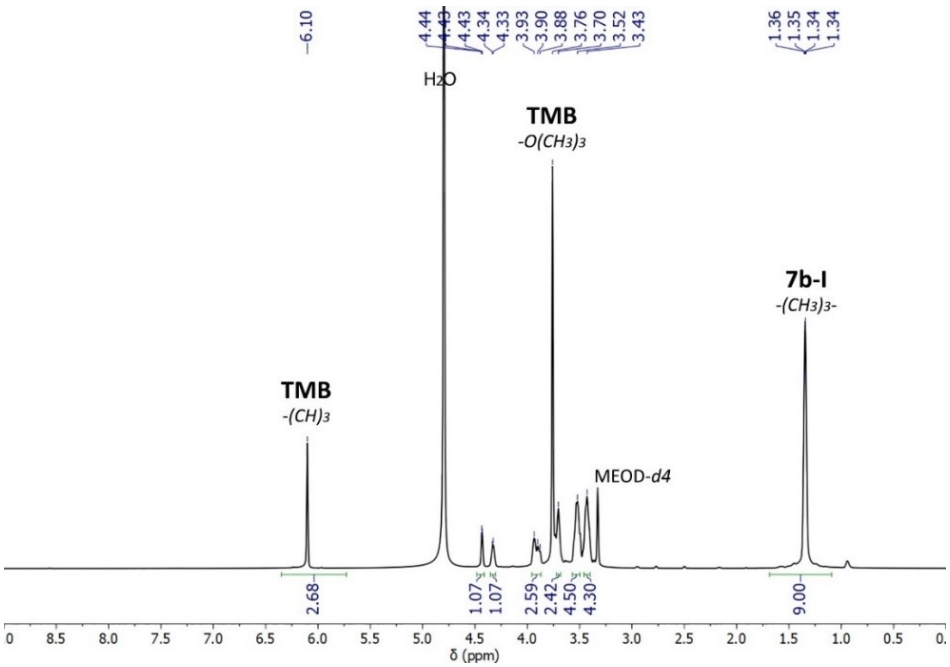


Figure S154. Representative ^{1}H NMR spectrum of **7b-I** obtained by sampling the aqueous layer to determine [**7b-I**] after the CO_2 cycloaddition reaction at 80 °C, 10 bar CO_2 for 24 h using 2.94 mg of 1,3,5 trimethoxy benzene (TMB) as an internal standard in MeOD-d_4.

Table S8 Concentration of **7b-I** in aqueous, epoxide **11a,** and carbonate **11b** in different control experiments.

Entry	Catalyst (mol%)	Cycle	7b-I transfer to epoxide phase (no reaction)[a]		7b-I transfer to carbonate phase (after reaction)[b]	
			[7b-I] (mol/L)[c]	(Δ[7b-I])-epoxide (%)[d]	[7b-I] (mol/L)[c]	(Δ[7b-I])-carbonate (%)[e]
1	**7b-I** (4)	1st run	0.80±0.01	0	0.77±0.01	4.34±0.70
2		2nd run	-	-	0.75±0.02	7.54±0.06
3		3rd run	-	-	0.70±0.02	13.08±2.04
4 [f]	**7b-I** (4) + KOAc (4)		0.69±0.01	14.20±0.38	0.69±0.01	15.02±0.33
5 [f]	**7b-I** (4) + KF (4)		0.78±0.01	2.16±0.52	0.73±0.01	9.03±0.64
6 [f]	**7b-I** (4) + KCl (4)		0.77±0.01	3.24±0.50	0.74±0.01	7.41±0.99
7 [f]	**7b-I** (4) + KI (4)		0.79±0.01	1.61±0.78	0.76±0.01	5.24±0.70
8 [g]	**7b-I** in seawater		0.80±0.01	0	0.78±0.01	2.34±1.00

[a]Reaction mixture of **11a** (10 mmol), **7b-I** (0.4 mmol, [**7b-I**]$_0$= 0.8 M) in 0.5 mL D_2O heated at 80 °C for 30 minutes followed by a sampling of the aqueous layer to determine [**7b-I**]; the same reaction mixture was used for the CO_2 cycloaddition reaction under the conditions in footnote b, recovered and reused two times. [b]Reaction conditions at 80 °C, 10 bar CO_2 for 24 h in the absence of salts, 12 h in the presence of salt followed by a sampling of the aqueous layer to determine [**7b-I**]. [c] Residual **7b-I** concentration in the aqueous phase as determined by ^{1}H NMR (see section S10) using 1,3,5 trimethoxy benzene as an internal standard in MeOD-d_4. [d] Percent loss of **7b-I** to the epoxide phase calculated as 100·([**7b-I**]$_0$-[**7b-I**])/[**7b-I**]$_0$. [e] Percent loss of **7b-I** to the final reaction product calculated as 100·([**7b-I**]$_0$-[**7b-I**])/[**7b-I**]$_0$. [f] Reaction mixture of **11a** (10 mmol), **7b-I** (0.4 mmol, [7b-I]$_0$= 0.8 M) in 0.5 mL D_2O containing 0.4 mmol salt heated at 80 °C for 30 minutes [g] Reaction mixture of **11a** (10 mmol), **7b-I** (0.4 mmol, [7b-I]$_0$= 0.8 M) in 0.5 mL Seawater heated at 80 °C for 30 minutes followed by a sampling of the aqueous layer to determine [**7b-I**]; the same reaction mixture was used for the CO_2 cycloaddition reaction under the conditions in footnote b.

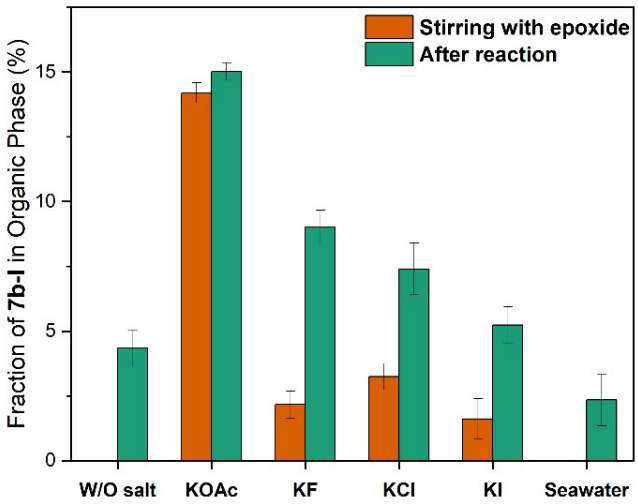


Figure S155. Fraction of **7b-I** in the organic phase after stirring with epoxide (80 °C, 30 min) or after catalytic reaction (80 °C, 10 bar, 12-24 h) as calculated from the variation of concentration in the aqueous layer.

S11. Substrate and Product Concentration Profile in the Aqueous Phase

The concentration of cyclic carbonate and diol in the aqueous layer after the biphasic cycloaddition reaction was quantified by ^{1}H NMR spectroscopy. In a general procedure, the aqueous phase after reaction (50 µL), 1,3,5 trimethyl benzene (1 uL, internal standard), and 450 uL DMSO-d_6 were added into an NMR tube. The concentration of epoxide, carbonate, and diol in the aqueous phase was calculated according to Equation (S3) from the ^{1}H NMR spectrum (Figure S156) compared to the initial loading. The results are given in Table S9.

Equation (S3);

$$\text{Concentration of } \textbf{epoxide/carbonate/diol} \text{ in the aqueous phase (mol/L)} = \frac{I_X \times H_{std} \times N_{std} \times 106}{I_{std} \times H_X \times 50}$$

Where I_X is the integral value of the protons signal of the epoxide, carbonate, or diol, I_{std} is the integral value of protons signal $(CH)_3$ of 1,3,5 trimethyl benzene at 6.75 ppm, H_a is the number of protons of epoxide, carbonate, or diol, H_{std} is number of protons of 1,3,5 trimethyl benzene (H_{std} =3) at 6.75 ppm, N_{std} is the number of moles of 1,3,5 trimethyl benzene.

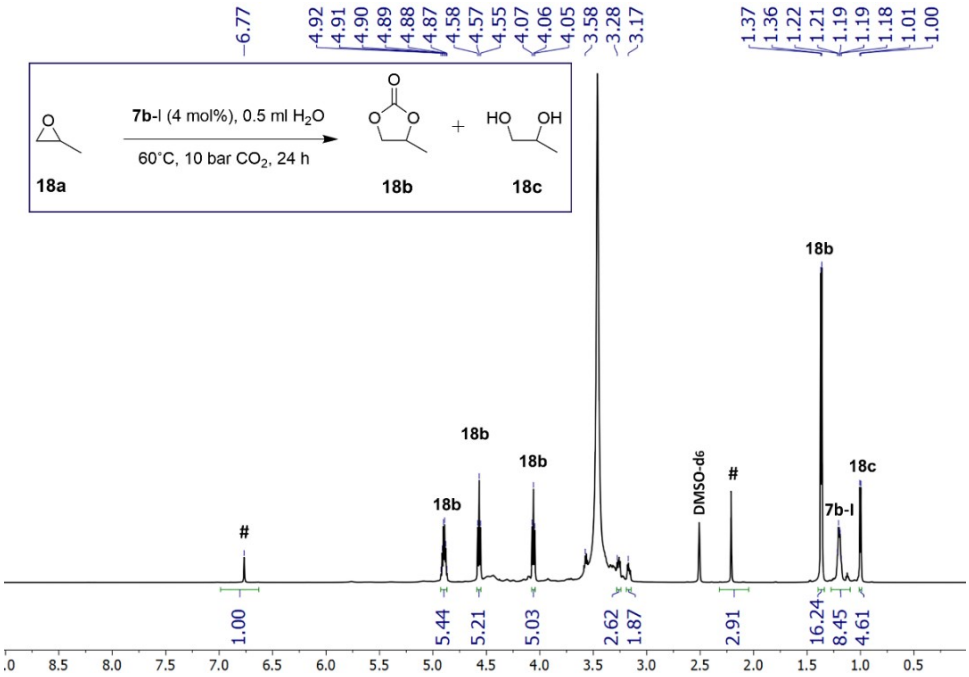


Figure S156. Representative ^{1}H NMR spectrum of the aqueous layer of crude CO_2 cycloaddition reaction to **18a**; **18a** (10 mmol), 4 mol% **7b-I**, 0.5 mL H_2O, 60 °C, 10 bar CO_2, 24 h by using 1 uL of 1,3,5 trimethyl benzene (#) as an internal standard in DMSO-d_6; Table 4, Entry 10.

Table S9 Concentration of cyclic carbonate and diol in aqueous layer after the biphasic reaction.[a]

Entry	Epoxide	Conv.	[Carbonate]$_{aq}$		[Diol]$_{aq}$		Selectivity[e]
	(10 mmol)	(%)	(mmol) [b]	(mol%) [c]	(mmol) [b]	(mol %) [d]	(%)
1	**11a**	99±1	0.17±0.05	1.69±0.50	ND [f]	-	99±1
2	**14a**	99±1	0.20±0.01	1.95±0.05	ND [f]	-	99±1
3[g]	**16a**	99±1	0.32±0.02	3.17±0.03	0.22±0.01	2.20±0.12	98±1
4	**18a**	99±1	1.28±0.15	12.76±1.53	0.42±0.12	4.15±1.18	96±1
5[h]	**18a**	99±1	0.77±0.03	7.71±0.27	0.36±0.02	3.57±0.20	96±1

[a] Reaction conditions: Epoxide (10 mmol), catalyst **7b-I** (4 mol%), H_2O 0.5 mL, at 60-80 °C, 10 bar CO_2 for 24 h followed by a sampling of the aqueous layer to determine [Carbonate] and [Diol]. [b] Residual [Carbonate] and [Diol] concentration in the aqueous phase as determined by ^{1}H NMR using 1,3,5 trimethyl benzene as an internal standard in DMSO-d_6.[c] Percent loss of carbonate to the aqueous phase calculated as $100\cdot([Carbonate]_{aq})/[Epoxide]_0$. [d]Percent loss of Diol to the aqueous phase calculated as $100\cdot([Diol]_{aq})/[Epoxide]_0$. [e]The selectivity for cyclic carbonates versus 1,2-diols was calculated as $100\cdot([Epoxide]_0-[Diol]_{aq})/[Epoxide]_0$. [f] ND: Not detected by ^{1}H-NMR measurement. [g] Using catalyst **7b-I** (2 mol%) [h] Using 4 mol% NaCl as an additive.

S12. Calculation of the isolated yield of cyclic carbonate product

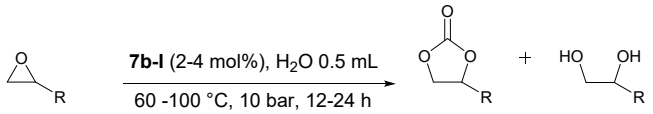
The organic phase was isolated and weighed on an analytical balance after completing the biphasic reaction, as shown in Table S10. Equation (S4) was used to calculate the percentage of isolation yield based on the initial concentration of epoxide substrate and weight of isolated cyclic carbonate.

Equation (S4);

$$\textbf{Isolated yield of cyclic carbonate}\ (\%) = \frac{g_p}{\mathrm{MW_p} \times\ \mathrm{mol_s}} \times 100$$

Where g_p is the weight of the isolated cyclic carbonate product, MW_p is the molecular weight of the cyclic carbonate product, and $\mathrm{mol_s}$ is the initial mole of the epoxide substrate.

Table S10 Isolated yield of cyclic carbonate product from the cycloaddition of CO_2 to terminal epoxides catalysed by 7**b-I** under biphasic reaction conditions.[a]



11a-19a **11b-19b** **11c-19c**

Entry	Substrate	Catalyst (mol%)	Temp. (˚C)	Isolated Yield (g)	(%)[b]
1	11a	**7b-I** (4)	80	1.312±0.020[c]	90±1
2	11a	**7b-I** (4)	80	7.010±0.025[c,d]	97±1
3	11a	**7b-I** (2)	80	1.376±0.010[c]	95±1
4	12a	**7b-I** (4)	60	1.051±0.008[c]	90±1
5	13a	**7b-I** (4)	80	1.811±0.059[c]	88±3
6	13a	**7b-I** (2)	80	1.822±0.074[c]	87±3
7	14a	**7b-I** (4)	80	1.793±0.042[c]	91±2
8	15a	**7b-I** (4)	100	2.043±0.016[c]	90±1
9	16a	**7b-I** (2)	80	1.684±0.013[c]	90±1
10	17a	**7b-I** (4)	80	1.842±0.004[e]	95±1
11	19a	**7b-I** (4)	60	1.129±0.013[c]	94±1
12	10a	**7b-I** in seawater (4)	60	1.485±0.012[c,f]	91±1
13	18a	**7b-I** (4)	60	0.817±0.029[c]	80±3
14	18a	**7b-I**+**NaCl** (4)	60	0.873±0.007[c]	86±1
15	18a	**7b-I** in seawater (4)	60	0.884±0.006[c]	87±1

[a] Reaction conditions: Epoxide (10 mmol), Catalyst **7b-I** (4 mol%), 0.5 mL H_2O, 10 bar CO_2 for 24 h. [b] Calculated according to Equation (S4). [c] Isolated from phase separation. [d] Results for an experiment carried out in a larger scale: Epoxide (50 mmol), **7b-I** (4 mol%), H_2O (2.5 mL) at 80 °C, 10 bar for 24 h. [e] Due to the solid nature of the product it formed as a precipitate that was filtrated and dried under vacuum.[f] Reaction conditions: Epoxide (10 mmol), Catalyst **7b-I** (4 mol%), Seawater 0.5 mL H_2O, 10 bar CO_2 for 12 h.

S13. Determination of Chloride Ion Concentration in Seawater by Titration (Mohr's Method)

The seawater sample was prepared according to the reported procedure. In this study, 20 mL seawater sample was diluted to 100 mL in a volumetric flask. Then 10 mL aliquot of diluted seawater was pipetted into a conical flask and added about 50 mL of distilled water, and 1 mL of K_2CrO_4 (C= 0.25 mol/L) was used as an indicator. The solution was titrated with $AgNO_3$ solution (C= 0.1 mol/L).

Table S11. Titration of seawater Mohr's method.

Entry	Volume of seawater (mL)	Volume of $AgNO_3$ (mL)
1	10	9.8
2	10	9.8
3	10	9.8
Average		**9.8**

Calculation:

Calculate the moles of reacted $\mathbf{AgNO_3}$ $= 9.8\,\text{mL} \times \frac{0.1\,\text{mol}}{1\,\text{L}} \times \frac{1\,\text{L}}{1000\,\text{mL}}$

$= 0.00098$ mol

Equation (S5); $\mathbf{Ag^+}\,(aq) + \mathbf{Cl^-}\,(aq) \rightarrow \mathbf{AgCl}\,(s)$

According to Equation (S5), one mole $\mathbf{Ag^+}$ions consumes one mol of $\mathbf{Cl^-}$ ions.

$[\mathbf{Cl^-}]$ in diluted seawater $= \frac{0.00098\,mol}{10\,mL} \times \frac{1000\,mL}{1\,L} = 0.098$ mol/L

$[\mathbf{Cl^-}]$ in original seawater $= \frac{C_{diluted}\ V_{diluted}}{V_{original}} = \frac{0.098\,\text{mol}}{1\,\text{L}} \times \frac{100\,mL}{20\,mL}$

$= 0.49$ mol/L

$[\ \mathbf{NaCl}\ ]$ in original seawater $= \frac{0.49\,\text{mol}}{1\,\text{L}} \times \frac{58.44\,g}{1\,mol} = 28.64$ g/L

$= 2.86$ %

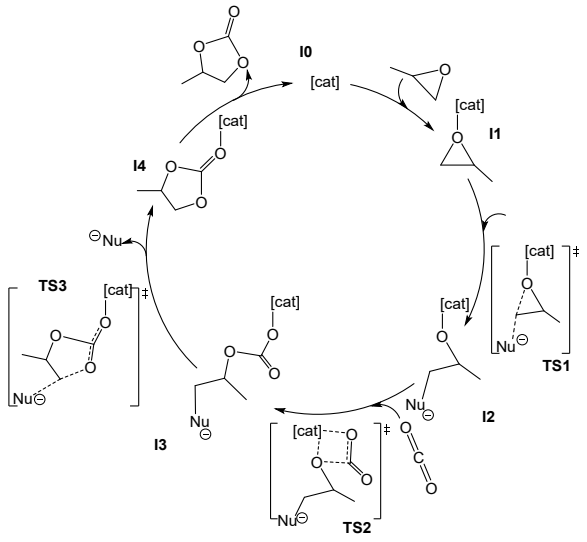
S14. Supplementary Computational Results and Data

The reaction barriers for the monomeric **7-Me-X** model catalysts are discussed in this section. All catalysts in this study are supposed to operate through the typical CO_2-epoxide reaction mechanism and thus, via a succession of three reaction energy barriers relative to three transition states (see Scheme of Table S12); the first corresponding to the opening of the epoxide (**TS1**), the second to the insertion of CO_2 (**TS2**), and finally the closing of the cyclic carbonate ring (**TS3**).[6, 7] First, the analysis of the reaction barriers (Table S12) for the typical neutral ascorbic acid was performed as a reference system to better understand the mechanistic differences with the single-component **7-Me-X** catalysts. Initially, there is the formation of a coordination intermediate **I1** where the epoxide forms a relatively stable adduct with ascorbic acid releasing 0.5 kcal/mol, following which, the opening of the epoxide by the iodide anion provided by tetramethylammonium iodide, as a simplified form of the TBAI reagent, implies to overcome a substantial energy barrier of 27.8 kcal/mol followed by two milder barriers of 10.6 and 7.1 kcal/mol for **TS2** and **TS3**, respectively. Overall, the rate determining step (rds) is the first, *i.e.,* the opening of the epoxide ring. Moving to **7-Me-I**, even though the formation of **I1** was disadvantaged by 1.8 kcal/mol, a strongly reduced kinetic cost of 18.4 kcal/mol was calculated for the epoxide ring-opening, indicating that the latter step is kinetically much more favorable compared to ascorbic acid. The CO_2 insertion step is feasible with an energy barrier of 13.5 kcal/mol while the ring-closure of the cyclic carbonate apparently requires an energy barrier of just 12.7 kcal/mol, that however, increases to 21.4 kcal/mol when calculated from the most stable previous intermediate or computed species, in particular for this system **I0**, thus representing the rds of the reaction. For the catalysts bearing different halides, i.e., **7-Me-Cl** and **7-Me-Br**, the barrier for **TS1** was less energetically favorable when compared to the case of **7-Me-I**, being, respectively, 3.7 and 2.2 kcal/mol higher in energy when calculated from **I0**. For **TS2**, moderate reaction barriers were observed in both cases with no defined trend based on the halogen anion, with the CO_2 insertion barrier being slightly higher for bromine than for chlorine and iodine which displayed identical values. Also for these halides, **TS3** remains the crucial rds with the barriers for chlorine and bromine anions being, respectively, 0.8 and 1.4 kcal/mol higher than for iodine. In addition, for chlorine, the results in Table S12 suggest that the opening of the epoxide is also energetically important, as it is only 0.1 kcal/mol less demanding than the ring closure step, so it is necessary to consider both energy barriers as postulated by Kozuch and Shaik.[8]

In order to understand the different roles of the two parts of the **7-Me-I** catalyst (*i.e.* the ascorbate-based scaffold and the quaternary ammonium salt), the mechanism of the reaction catalyzed only by tetramethylammonium iodide (Me_4NI) was also calculated. However, the kinetics worsened, with

energy barriers increasing up to energy limits of 28.3, 28.8 and 22.4 kcal/mol for **TS1**, **TS2** and **TS3**, respectively. Thus, the CO_2 insertion step, where the ascorbic acid scaffold participates the most, became the rds. Beside the results for the **7-Me-I** dimer, that is discussed in greater detail in the main text, Table S12 also includes the energy barrier values calculated for the dimeric version of catalyst **7b-I**. For dimeric **7b-I**, a slightly higher rate-limiting barrier for **TS3** compared to the **7-Me-I** dimer was calculated despite a lower energy barrier for **TS1** (ring-opening). Nevertheless, it should be noted that for dimeric **7b-I**, the complex arrangement of the ethyl side chains makes the identification of the most stable conformation much more complex than for the case of dimeric **7-Me-I**.

Table S12. Computed free energy surface for the cycloaddition of CO_2 to propylene oxide by several hydrogen bond donor catalysts [cat] in the presence of a nucleophile [Nu]. Free energies in solution are given in kcal/mol relative to the starting point. The cationic tetramethylammonium moiety is omitted for the sake of clarity.



I or TS	AsA/ Me_4NI	7-Me-Cl	7-Me-Br	7-Me-I	Me_4NI	7-Me-I dimer[a]	7-Et-I dimer[a]
I0	0.0	0.0	0.0	0.0	0.0	0.0 (4.2)	0.0
I1	-0.5	5.6	3.8	1.8	3.4	4.7 (12.1)	0.1
TS1	27.3	22.1	20.6	18.4	28.3	18.6 (24.5)	14.6
I2	0.1	3.0	4.2	2.3	28.1	1.5 (6.6)	-1.0
TS2	10.7	15.8	17.5	15.8	28.8	13.6 (15.5)	14.5
I3	12.1	8.7	10.4	8.7	16.1	2.5 (8.9)	7.0
TS3	19.2	22.2	22.8	21.4	22.4	22.1 (21.3)	27.0
I4	1.4	4.2	2.9	1.5	2.5	-0.2 (3.5)	2.2

[a] The plain values refer to a "stacked" form of the **7-Me-I** dimer; the values in brackets to a "planar" dimer, see Figure 5 of the manuscript.

Computational details:

All theoretical calculations were performed by means of the Gaussian16 software package.[9] For the geometry optimizations, the B3LYP functional,[10-13] and the 6-31G(d) basis set were used,[14] together with the Grimme D3 correction term for the electronic energy.[15, 16] In addition, for the halides we used the small-core quasi-relativistic Stuttgart/Dresden effective core potential, with an associated valence basis set (standard SDD keywords in Gaussian16).[17, 18]

The stationary points were characterized using analytical frequency calculations. The nature of the transition states was confirmed by the corresponding negative vibrational frequency along with the intrinsic reaction coordinates (IRC). Energies were obtained by single-point calculations on the optimized geometries with the B3LYP-D3 functional and the 6-311+G(d,p) basis set and by estimating solvent effects with the polarizable continuous solvation model (PCM) as implemented in Gaussian16,[19, 20] using water as a solvent.[19, 20] The reported free Gibbs free energies in this work include electronic energies obtained at the B3LYP-d3/6-311+G(d,p)~sdd(pcm-H_2O)//B3LYP-d3/6-31G(d)~sdd level of theory corrected with zero-point energies, thermal corrections and entropy effects computed with the B3LYP-d3/6-31G(d)~sdd level.

Table S13. Coordinate data sets and absolute energies **(**a.u.**)** for DFT optimized complexes for the cycloaddition of CO_2 to epoxides “around water”.

ASCORBIC ACID

I0				**I1**			
38				48			
AsAc-I0 SCF Done: -910.629713244 A.U.				AsAc-I1 SCF Done: -1103.75017279 A.U.			
O	-4.566795000	3.581894000	-2.959312000	O	-2.101150000	0.618224000	-1.205936000
O	-2.066163000	2.461232000	-4.380848000	O	-3.461787000	-2.253308000	-0.777738000
H	-1.521015000	1.742051000	-4.756382000	H	-2.505099000	-2.176032000	-0.564922000
C	-4.139589000	2.316062000	-3.052230000	C	-3.346835000	0.143896000	-1.416366000
O	-2.006308000	-0.313020000	-3.692529000	O	-6.182518000	-1.827891000	-1.688963000
C	-3.054017000	1.828105000	-3.678641000	C	-3.916967000	-1.070252000	-1.241163000
O	-3.967290000	0.025630000	-2.563313000	O	-5.559766000	0.308879000	-2.125720000
C	-2.921885000	0.411471000	-3.356717000	C	-5.322238000	-0.987767000	-1.678615000
O	-5.633957000	2.664517000	-0.698250000	O	-3.641597000	3.201117000	-1.039448000
H	-5.918919000	2.679649000	0.239592000	H	-4.054075000	4.035287000	-0.739337000
O	-5.728357000	0.987784000	1.353468000	O	-6.096197000	4.259900000	-0.828046000
H	-4.875289000	1.150063000	1.814332000	H	-6.494340000	4.059887000	0.034229000
C	-4.793468000	1.174681000	-2.300750000	C	-4.374493000	1.095870000	-1.967940000
H	-5.806373000	0.967939000	-2.666498000	H	-4.071246000	1.486829000	-2.949965000
C	-4.831132000	1.482937000	-0.804906000	C	-4.730681000	2.280394000	-1.062441000
H	-3.808950000	1.688113000	-0.459647000	H	-4.919154000	1.890215000	-0.048604000
C	-5.432183000	0.398606000	0.094161000	C	-5.974715000	3.030034000	-1.555788000
H	-6.385213000	0.049100000	-0.319032000	H	-5.839175000	3.317195000	-2.603524000
H	-4.745148000	-0.452388000	0.174657000	H	-6.870338000	2.406647000	-1.476522000
C	-1.714871000	4.074020000	-1.110470000	O	-0.836794000	-1.637795000	-0.416823000
N	-0.326358000	3.481053000	-1.182439000	C	0.311386000	-2.408287000	-0.879138000
C	0.371553000	4.006980000	-2.403285000	H	1.009501000	-1.836499000	-1.486177000
H	-0.218683000	3.731756000	-3.279571000	H	0.050446000	-3.408938000	-1.220037000
H	0.449406000	5.093215000	-2.324953000	C	0.181129000	-2.071916000	0.543218000

H	1.368636000	3.565042000	-2.457507000
C	-0.411119000	1.973710000	-1.265751000
H	0.603962000	1.573304000	-1.231669000
H	-0.987058000	1.615404000	-0.407932000
H	-0.883013000	1.701950000	-2.207485000
C	0.434116000	3.860207000	0.063712000
H	0.486204000	4.949191000	0.120709000
H	-0.101536000	3.454753000	0.927330000
H	1.438673000	3.437522000	-0.000028000
H	-5.163040000	3.622198000	-2.172374000
H	-2.249333000	3.835754000	-2.027737000
H	-2.218210000	3.655354000	-0.234399000
I	-2.331327000	2.005787000	2.163730000
H	-1.615840000	5.156590000	-1.008236000

Zero-point correction=	0.814184 (Hartree/Particle)
Thermal correction to Energy=	0.340588
Thermal correction to Enthalpy=	0.341532
Thermal correction to Gibbs Free Energy=	0.267066
Sum of electronic and zero-point Energies=	-910.310328
Sum of electronic and thermal Energies=	-910.289125
Sum of electronic and thermal Enthalpies=	-910.288181
Sum of electronic and thermal Free Energies=	-910.362648

H	0.790160000	-1.236784000	0.886724000
I	2.526748000	0.767481000	-0.727187000
C	-0.286734000	-3.064895000	1.570702000
H	0.579846000	-3.532035000	2.052375000
H	-0.878954000	-2.569077000	2.347679000
H	-0.898553000	-3.849664000	1.113293000
C	-0.413656000	3.303379000	-0.487952000
N	-0.110734000	3.746299000	-1.904002000
C	-1.108856000	4.782922000	-2.328037000
H	-2.104567000	4.338806000	-2.282396000
H	-1.042116000	5.634250000	-1.646861000
H	-0.873241000	5.104401000	-3.344891000
C	-0.201376000	2.559496000	-2.834250000
H	-0.012696000	2.909762000	-3.851460000
H	0.555669000	1.832672000	-2.526741000
H	-1.194437000	2.124270000	-2.738102000
C	1.285014000	4.309982000	-1.959544000
H	1.338443000	5.172481000	-1.292000000
H	1.981502000	3.529704000	-1.638043000
H	1.497275000	4.615138000	-2.986446000
H	-1.488831000	-0.100300000	-0.908107000
H	-1.427802000	2.906661000	-0.461886000
H	0.319211000	2.539804000	-0.214558000
H	-0.316714000	4.177006000	0.161016000

Zero-point correction=	0.812939 (Hartree/Particle)
Thermal correction to Energy=	0.434272
Thermal correction to Enthalpy=	0.435216
Thermal correction to Gibbs Free Energy=	0.344292
Sum of electronic and zero-point Energies=	-1103.343285
Sum of electronic and thermal Energies=	-1103.315901
Sum of electronic and thermal Enthalpies=	-1103.314957
Sum of electronic and thermal Free Energies=	-1103.405881

TS1

48

AsAc-TS1 SCF Done: -1103.69690000 A.U.

O	-2.622053000	1.561457000	0.021450000
O	-2.744870000	-1.613423000	-0.157208000
H	-1.912287000	-1.258541000	0.314877000
C	-3.442035000	0.705951000	-0.668888000
O	-4.955352000	-2.128437000	-1.944117000
C	-3.451296000	-0.645698000	-0.721048000
O	-5.205112000	0.120566000	-2.079296000
C	-4.573481000	-1.037390000	-1.622551000
O	-4.763041000	3.216654000	-0.234811000
H	-5.419098000	3.890061000	0.025389000
O	-7.364961000	3.686889000	-0.893857000
H	-7.978993000	3.223207000	-0.302362000
C	-4.532028000	1.257414000	-1.548977000
H	-4.123506000	1.853136000	-2.381664000
C	-5.525969000	2.131941000	-0.782405000
H	-5.959529000	1.524729000	0.028564000
C	-6.645586000	2.704871000	-1.647284000
H	-6.214690000	3.240355000	-2.499581000
H	-7.291640000	1.904282000	-2.025857000
O	-0.605036000	-0.613978000	0.842405000
C	0.312415000	-1.105064000	-0.832958000
H	-0.130001000	-0.277309000	-1.348804000
H	-0.065037000	-2.082047000	-1.117863000
C	0.726014000	-0.910792000	0.570933000
H	1.401209000	-0.051114000	0.723503000
I	2.400838000	-0.867295000	-2.563370000
C	1.288985000	-2.140100000	1.271252000
H	2.293453000	-2.374025000	0.901271000
H	1.338042000	-1.958721000	2.350225000
H	0.634541000	-3.002144000	1.099799000

I2

48

AsAc-I2 SCF Done: -1103.74752185 A.U.

O	-1.909030000	0.734585000	-0.938554000
O	-3.258156000	-1.157779000	1.130468000
H	-2.396302000	-0.743090000	1.346246000
C	-3.088818000	0.167656000	-0.962852000
O	-5.852499000	-1.786880000	-0.104199000
C	-3.696428000	-0.667672000	-0.069287000
O	-5.188007000	-0.457131000	-1.821166000
C	-5.000495000	-1.069146000	-0.571499000
O	-3.545720000	2.632380000	-2.856837000
H	-4.050248000	3.310067000	-3.348713000
O	-6.040779000	3.180341000	-3.667509000
H	-6.518539000	3.588347000	-2.927547000
C	-4.050914000	0.360993000	-2.122043000
H	-3.599684000	0.022247000	-3.065936000
C	-4.572443000	1.790461000	-2.324469000
H	-4.905550000	2.172675000	-1.343728000
C	-5.755461000	1.819347000	-3.301729000
H	-5.473766000	1.319439000	-4.233765000
H	-6.627129000	1.310963000	-2.880739000
O	-0.640843000	-0.036086000	1.161303000
C	-0.424616000	-2.029366000	-0.145490000
H	-0.849869000	-1.503515000	-0.997929000
H	-1.198225000	-2.607808000	0.359110000
C	0.289321000	-1.058974000	0.800407000
H	1.142033000	-0.610686000	0.262534000
I	0.961294000	-3.511483000	-1.060476000
C	0.783019000	-1.700170000	2.089773000
H	1.547161000	-2.457079000	1.892561000
H	1.205012000	-0.930145000	2.743224000
H	-0.055749000	-2.172103000	2.613646000

C	-0.642499000	1.696316000	-2.851231000
N	0.030328000	2.763451000	-2.020764000
C	-0.954937000	3.863044000	-1.745275000
H	-1.284861000	4.289033000	-2.695136000
H	-1.799199000	3.432187000	-1.206738000
H	-0.467533000	4.631144000	-1.141777000
C	1.214555000	3.291339000	-2.785655000
H	1.708868000	4.055831000	-2.183341000
H	1.895250000	2.457268000	-2.975747000
H	0.865709000	3.721064000	-3.726867000
C	0.521325000	2.182386000	-0.709101000
H	-0.302815000	1.687853000	-0.188396000
H	1.311779000	1.467462000	-0.941555000
H	0.922604000	3.004019000	-0.112153000
H	-3.187947000	2.311960000	0.301136000
H	-1.003000000	2.157415000	-3.773291000
H	0.094433000	0.922568000	-3.081866000
H	-1.474681000	1.284638000	-2.280386000

Zero-point correction=	0.404739 (Hartree/Particle)
Thermal correction to Energy=	0.431268
Thermal correction to Enthalpy=	0.432212
Thermal correction to Gibbs Free Energy=	0.344673
Sum of electronic and zero-point Energies=	-1103.292161
Sum of electronic and thermal Energies=	-1103.265632
Sum of electronic and thermal Enthalpies=	-1103.264688
Sum of electronic and thermal Free Energies=	-1103.352227

C	0.744889000	2.664517000	-0.556917000
N	-0.159563000	3.397873000	-1.513937000
C	0.494458000	4.675296000	-1.943888000
H	0.667960000	5.303556000	-1.067798000
H	1.444161000	4.444579000	-2.430971000
H	-0.166428000	5.188734000	-2.644197000
C	-1.465032000	3.700169000	-0.811211000
H	-2.125139000	4.210267000	-1.510788000
H	-1.907536000	2.738109000	-0.540290000
H	-1.242980000	4.322618000	0.058446000
C	-0.420032000	2.528000000	-2.727412000
H	0.540088000	2.331602000	-3.209788000
H	-0.915841000	1.618473000	-2.373708000
H	-1.094810000	3.063148000	-3.394099000
H	-1.100294000	0.297384000	0.317434000
H	0.989171000	3.332467000	0.271714000
H	0.225701000	1.785426000	-0.177634000
H	1.655677000	2.377265000	-1.085833000

Zero-point correction=	0.407072 (Hartree/Particle)
Thermal correction to Energy=	0.433681
Thermal correction to Enthalpy=	0.434625
Thermal correction to Gibbs Free Energy=	0.346104
Sum of electronic and zero-point Energies=	-1103.340450
Sum of electronic and thermal Energies=	-1103.313841
Sum of electronic and thermal Enthalpies=	-1103.312896
Sum of electronic and thermal Free Energies=	-1103.401418

TS2

51

AsAc-TS2 SCF Done: -1292.33288884 A.U.

O	-0.001628000	2.758253000	-1.123582000
O	-3.092490000	3.516160000	-0.679889000
H	-2.479629000	4.053759000	-0.150528000
C	-1.132272000	2.403434000	-1.748419000
O	-4.441444000	1.902156000	-2.659392000
C	-2.435365000	2.716065000	-1.554778000
O	-2.389149000	1.140936000	-3.256978000
C	-3.249941000	1.931869000	-2.499680000
O	0.952192000	2.419861000	-3.948138000
H	1.406990000	2.260747000	-4.798533000
O	0.455631000	1.361628000	-6.375979000
H	-0.066049000	1.988653000	-6.902044000
C	-1.032864000	1.442338000	-2.904413000
H	-0.520823000	0.522592000	-2.593391000
C	-0.384529000	1.984019000	-4.188864000
H	-1.006344000	2.831741000	-4.526344000
C	-0.359285000	0.912552000	-5.286121000
H	0.133386000	0.012041000	-4.905368000
H	-1.375451000	0.652430000	-5.599311000
O	-0.632659000	3.994981000	1.120408000
C	-0.799267000	3.847548000	3.470738000
H	-0.802589000	4.933786000	3.533516000
H	0.206583000	3.447539000	3.600714000
C	-1.432277000	3.388324000	2.160592000
H	-2.453384000	3.775405000	2.100927000
I	-1.937578000	3.196824000	5.262253000
C	-1.400361000	1.884797000	1.925321000
H	-1.953782000	1.360067000	2.708226000
H	-1.862529000	1.645972000	0.963479000
H	-0.366776000	1.520132000	1.920754000
C	0.043839000	5.498221000	-2.852099000
N	1.518387000	5.798610000	-2.715131000
C	1.682392000	7.175496000	-2.125434000
H	1.242354000	7.902154000	-2.812132000
H	1.165671000	7.184906000	-1.163160000
H	2.748896000	7.376219000	-2.003026000

I3

51

AsAc-I3 SCF Done: -1292.32942907 A.U.

O	-2.020159000	1.749913000	-0.825713000
O	-2.022590000	1.302246000	2.220661000
H	-1.054179000	1.095256000	2.020726000
C	-2.739964000	0.869304000	-0.078616000
O	-4.083251000	-0.818223000	2.620867000
C	-2.745156000	0.694632000	1.254141000
O	-4.252181000	-0.842089000	0.356548000
C	-3.719050000	-0.375971000	1.564280000
O	-3.889490000	1.112941000	-2.681727000
H	-4.443037000	1.131597000	-3.484240000
O	-6.161399000	-0.149437000	-3.499235000
H	-6.929708000	0.311082000	-3.125424000
C	-3.595129000	-0.184444000	-0.723525000
H	-2.949835000	-0.904929000	-1.247708000
C	-4.626197000	0.364331000	-1.706623000
H	-5.313624000	1.030679000	-1.159859000
C	-5.422647000	-0.727397000	-2.416904000
H	-4.734022000	-1.442199000	-2.878089000
H	-6.062767000	-1.263313000	-1.706114000
O	0.398888000	1.021577000	1.269718000
C	0.406736000	0.109178000	0.383423000
O	1.284973000	0.454288000	-0.671417000
O	-0.237427000	-0.936948000	0.319247000
C	-0.038790000	-0.667687000	-2.388663000
H	-0.672846000	0.208321000	-2.276762000
H	-0.529541000	-1.546156000	-1.984650000
C	1.361489000	-0.427787000	-1.807184000
H	1.942963000	0.161016000	-2.523724000
I	0.029419000	-1.019759000	-4.600146000
C	2.108028000	-1.718735000	-1.484262000
H	2.226756000	-2.324170000	-2.389439000
H	3.101087000	-1.483874000	-1.088256000
H	1.552307000	-2.288672000	-0.736831000
C	0.593405000	3.520923000	-1.087500000
N	0.671994000	4.235220000	0.239264000
C	0.885533000	5.700136000	0.012461000

C	2.159016000	5.720539000	-4.066792000
H	3.225962000	5.931365000	-3.969778000
H	2.002936000	4.711754000	-4.451887000
H	1.693288000	6.455855000	-4.726549000
C	2.166217000	4.780959000	-1.797544000
H	1.692896000	4.884799000	-0.820123000
H	1.983410000	3.788940000	-2.208137000
H	3.234091000	5.008515000	-1.754789000
H	-0.198774000	3.219585000	-0.256707000
H	-0.393949000	6.244807000	-3.518559000
H	-0.052729000	4.498823000	-3.266029000
C	-0.814086000	5.455745000	0.863583000
O	0.127465000	5.875347000	0.162544000
O	-1.838123000	5.946517000	1.319732000
H	-0.391101000	5.557638000	-1.855489000

Zero-point correction= 0.421726 (Hartree/Particle)
Thermal correction to Energy= 0.450409
Thermal correction to Enthalpy= 0.451353
Thermal correction to Gibbs Free Energy= 0.359761
Sum of electronic and zero-point Energies= -1291.911163
Sum of electronic and thermal Energies= -1291.882480
Sum of electronic and thermal Enthalpies= -1291.881536
Sum of electronic and thermal Free Energies= -1291.973128

H	1.825461000	5.845402000	-0.523592000
H	0.055562000	6.093377000	-0.578089000
H	0.926829000	6.207404000	0.978216000
C	1.822016000	3.659820000	1.035291000
H	1.883830000	4.199721000	1.982685000
H	1.606087000	2.595945000	1.195923000
H	2.739445000	3.802145000	0.460266000
C	-0.615079000	4.022912000	1.001434000
H	-1.437457000	4.432827000	0.413712000
H	-0.761143000	2.957140000	1.151481000
H	-0.533992000	4.539300000	1.959811000
H	-2.446627000	1.768494000	-1.709431000
H	1.502570000	3.746380000	-1.649075000
H	0.520565000	2.449881000	-0.902374000
H	-0.285210000	3.883921000	-1.622421000

Zero-point correction= 0.421381 (Hartree/Particle)
Thermal correction to Energy= 0.450920
Thermal correction to Enthalpy= 0.451864
Thermal correction to Gibbs Free Energy= 0.356628
Sum of electronic and zero-point Energies= -1291.908048
Sum of electronic and thermal Energies= -1291.878509
Sum of electronic and thermal Enthalpies= -1291.877565
Sum of electronic and thermal Free Energies= -1291.972801

TS3

51
AsAc-TS3 SCF Done: -1292.32272320 A.U.

O	-2.352725000	0.798832000	0.029694000
O	-3.474525000	-2.152650000	0.425692000
H	-2.612291000	-1.955061000	0.859633000
C	-3.323457000	0.099738000	-0.591067000
O	-5.662269000	-2.282227000	-1.505544000
C	-3.803368000	-1.152316000	-0.413417000
O	-5.073394000	-0.172141000	-2.097510000
C	-4.930346000	-1.342535000	-1.346023000
O	-3.646742000	3.091012000	-1.353943000
H	-4.117871000	3.936204000	-1.494154000
O	-6.028409000	3.928896000	-2.266288000
H	-6.678765000	3.981089000	-1.547691000
C	-4.054619000	0.757788000	-1.727139000
H	-3.395372000	0.910804000	-2.597500000
C	-4.689386000	2.112254000	-1.403270000
H	-5.191082000	2.048193000	-0.424595000
C	-5.701285000	2.547437000	-2.469044000
H	-5.239354000	2.493784000	-3.460115000
H	-6.584546000	1.901375000	-2.462312000
O	-1.187874000	-1.043292000	1.458406000
C	0.031613000	-1.038493000	1.186007000
O	0.631219000	0.210060000	1.172969000
O	0.790908000	-2.002223000	0.894786000
C	2.312204000	-1.018881000	-0.006146000
H	1.749827000	-1.085663000	-0.922821000
H	3.003684000	-1.818613000	0.207606000
C	2.063542000	0.097297000	0.993042000
H	2.353279000	1.063173000	0.583665000
I	4.219490000	0.216170000	-1.529848000
C	2.772442000	-0.137710000	2.320286000
H	3.855872000	-0.127019000	2.164561000
H	2.507952000	0.652054000	3.029183000
H	2.480157000	-1.104976000	2.738432000
C	-0.052668000	1.393930000	-2.035729000
N	0.107475000	2.857743000	-1.709395000
C	-0.374802000	3.120053000	-0.298912000
H	-1.443078000	2.909400000	-0.254238000
H	0.155107000	2.451756000	0.380339000
H	-0.166380000	4.165590000	-0.063251000

I4

51
AsAc-I4 SCF Done: -1292.36909062 A.U.

O	-3.279715000	2.644233000	-0.589146000
O	-2.553684000	0.937060000	1.827375000
H	-1.857701000	0.310530000	2.120950000
C	-3.297413000	1.300947000	-0.466222000
O	-3.090627000	-1.851475000	0.936948000
C	-2.966593000	0.542064000	0.594970000
O	-3.615090000	-0.929269000	-1.077124000
C	-3.205753000	-0.869643000	0.247090000
O	-5.084844000	2.061328000	-2.529594000
H	-5.718131000	2.147357000	-3.265857000
O	-6.520454000	0.350230000	-4.086923000
H	-7.292582000	0.077692000	-3.565334000
C	-3.669395000	0.399129000	-1.612696000
H	-2.917317000	0.498701000	-2.407157000
C	-5.057828000	0.672762000	-2.189165000
H	-5.813634000	0.460718000	-1.414465000
C	-5.347816000	-0.156154000	-3.439882000
H	-4.534101000	-0.027658000	-4.160106000
H	-5.431549000	-1.220373000	-3.187865000
O	0.039558000	-0.107278000	1.925781000
C	0.414942000	-0.574857000	0.871735000
O	1.470396000	-0.099073000	0.181552000
O	-0.166952000	-1.602800000	0.244588000
C	0.405180000	-1.745188000	-1.076144000
H	-0.290537000	-1.316649000	-1.801678000
H	0.556695000	-2.809759000	-1.263637000
C	1.714149000	-0.941451000	-0.986450000
H	1.814494000	-0.267191000	-1.839085000
I	-0.260280000	1.416996000	-3.333608000
C	2.961341000	-1.775563000	-0.750563000
H	3.176149000	-2.378115000	-1.640152000
H	3.823617000	-1.131868000	-0.552201000
H	2.823300000	-2.449857000	0.102522000
C	-0.666334000	4.534695000	-0.986440000
N	0.277938000	3.911885000	0.012478000
C	0.503685000	4.855215000	1.154051000
H	0.942535000	5.780039000	0.773827000
H	-0.455082000	5.063411000	1.632286000
H	1.180042000	4.386020000	1.870984000

C	-0.718764000	3.671919000	-2.669248000
H	-0.563867000	4.730010000	-2.447717000
H	-0.387243000	3.454788000	-3.686559000
H	-1.770045000	3.408547000	-2.531545000
C	1.559031000	3.235425000	-1.838350000
H	2.163257000	2.591754000	-1.197750000
H	1.873864000	3.084634000	-2.872090000
H	1.675219000	4.283357000	-1.555992000
H	-1.916634000	0.222390000	0.724383000
H	-1.107140000	1.140446000	-1.967909000
H	0.346557000	1.214776000	-3.035071000
H	0.499341000	0.818131000	-1.296430000

Zero-point correction= 0.421565 (Hartree/Particle)
Thermal correction to Energy= 0.450552
Thermal correction to Enthalpy= 0.451496
Thermal correction to Gibbs Free Energy= 0.357930
Sum of electronic and zero-point Energies= -1291.901158
Sum of electronic and thermal Energies= -1291.872171
Sum of electronic and thermal Enthalpies= -1291.871227
Sum of electronic and thermal Free Energies= -1291.964793

C	1.588772000	3.599007000	-0.663226000
H	2.242159000	3.110530000	0.061871000
H	1.385378000	2.930047000	-1.504537000
H	2.032752000	4.533018000	-1.014333000
C	-0.323973000	2.631435000	0.539733000
H	-1.272731000	2.851290000	1.023985000
H	-0.485532000	1.966893000	-0.309908000
H	0.368475000	2.179552000	1.247955000
H	-3.794082000	2.856437000	-1.397738000
H	-0.232326000	5.475909000	-1.330920000
H	-0.788645000	3.836281000	-1.818487000
H	-1.625017000	4.698915000	-0.494453000

Zero-point correction= 0.423635 (Hartree/Particle)
Thermal correction to Energy= 0.453362
Thermal correction to Enthalpy= 0.454306
Thermal correction to Gibbs Free Energy= 0.358541
Sum of electronic and zero-point Energies= -1291.945455
Sum of electronic and thermal Energies= -1291.915728
Sum of electronic and thermal Enthalpies= -1291.914784
Sum of electronic and thermal Free Energies= -1292.010549

7-Me-Cl

I0

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7-Me-Cl I0 SCF Done: -1511.99908216 A.U.

O	-2.876651000	1.874170000	-1.713946000
O	-1.999601000	-1.028435000	-1.225855000
H	-1.263158000	-0.366801000	-1.308143000
C	-3.657744000	0.764033000	-1.585609000
O	-4.412705000	-2.613982000	-1.395434000
C	-3.202711000	-0.497056000	-1.422256000
O	-5.489055000	-0.660723000	-1.781446000
C	-4.363568000	-1.418794000	-1.514674000
O	-5.933568000	2.862794000	-1.069502000
H	-6.771845000	3.238737000	-0.740255000
O	-8.372524000	1.981852000	-0.330474000
H	-8.331250000	1.717447000	0.602615000
C	-5.147191000	0.734060000	-1.852864000
H	-5.371609000	1.104675000	-2.863058000
C	-6.069918000	1.464543000	-0.867852000
H	-5.769734000	1.183209000	0.157928000
C	-7.542045000	1.082656000	-1.077346000
H	-7.813966000	1.233862000	-2.126763000
H	-7.722447000	0.035591000	-0.815165000
C	-3.041258000	2.962776000	-0.792303000
C	-1.646244000	3.454803000	-0.383140000
C	-0.820505000	3.650125000	-1.662489000
N	0.542478000	4.341883000	-1.508192000
O	-1.034863000	2.586763000	0.539061000
H	-0.652508000	1.816592000	0.048584000
C	0.348250000	5.822163000	-1.385299000
H	-0.159918000	6.193667000	-2.277291000
H	-0.256001000	6.026083000	-0.500408000
H	1.322620000	6.304383000	-1.285288000
C	1.327220000	4.023747000	-2.757353000
H	2.281567000	4.553499000	-2.718745000
H	1.478711000	2.941051000	-2.780247000
H	0.751194000	4.348971000	-3.625974000
C	1.350323000	3.852332000	-0.321630000
H	0.810469000	4.074766000	0.594969000
H	1.475277000	2.772157000	-0.421205000
H	2.310838000	4.372408000	-0.353659000
H	-3.563365000	2.638736000	0.111162000
H	-3.630875000	3.752961000	-1.268907000
H	-1.368793000	4.250786000	-2.393977000

I1

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7-Me-Cl I1 SCF Done: -1705.12827488 A.U.

O	-2.380611000	1.067403000	0.125256000
O	-2.959979000	-1.643469000	1.054840000
H	-2.108818000	-1.178532000	1.224368000
C	-3.429499000	0.324084000	-0.300316000
O	-5.194773000	-2.639943000	-0.643540000
C	-3.622497000	-0.941107000	0.112631000
O	-5.048988000	-0.617245000	-1.662841000
C	-4.685245000	-1.550842000	-0.712375000
O	-4.498956000	2.979179000	-1.462497000
H	-5.089219000	3.635457000	-1.880332000
O	-6.754534000	3.020734000	-2.940027000
H	-7.517552000	2.961837000	-2.342866000
C	-4.245283000	0.579848000	-1.543025000
H	-3.559054000	0.652118000	-2.401465000
C	-5.223456000	1.754954000	-1.556936000
H	-5.909875000	1.649469000	-0.698210000
C	-6.036004000	1.781296000	-2.856602000
H	-5.351021000	1.776962000	-3.709707000
H	-6.696875000	0.911144000	-2.927120000
O	-0.339909000	-0.587403000	0.703934000
C	-0.296147000	-1.085397000	-0.669080000
H	0.003592000	-0.358286000	-1.419602000
H	-1.165010000	-1.676552000	-0.949494000
C	0.621937000	-1.616452000	0.345217000
H	1.648549000	-1.246520000	0.344534000
Cl	-1.162622000	0.883756000	-3.498406000
C	0.401438000	-2.961538000	0.987401000
H	0.969121000	-3.732848000	0.453987000
H	0.733580000	-2.954524000	2.031832000
H	-0.660399000	-3.226323000	0.959444000
C	-2.518709000	2.347776000	0.747368000
C	-1.205448000	3.058591000	0.409536000
C	-1.192598000	3.263737000	-1.113469000
N	0.100563000	3.812674000	-1.715392000
O	-0.088602000	2.338610000	0.904337000
H	-0.236301000	1.375811000	0.765125000
C	0.610118000	4.981134000	-0.933481000
H	-0.186117000	5.723514000	-0.842939000
H	0.920655000	4.635012000	0.052642000
H	1.461945000	5.414491000	-1.461862000

H	-0.611265000	2.663724000	-2.077784000
H	-1.794699000	4.411123000	0.141515000
Cl	0.601428000	0.691244000	-1.403206000

Zero-point correction=	0.360191 (Hartree/Particle)
Thermal correction to Energy=	0.382845
Thermal correction to Enthalpy=	0.383789
Thermal correction to Gibbs Free Energy=	0.307588
Sum of electronic and zero-point Energies=	-1511.638891
Sum of electronic and thermal Energies=	-1511.616237
Sum of electronic and thermal Enthalpies=	-1511.615293
Sum of electronic and thermal Free Energies=	-1511.691494

C	-0.218949000	4.227844000	-3.132224000
H	0.705028000	4.560868000	-3.610447000
H	-0.631736000	3.348930000	-3.643149000
H	-0.941702000	5.045939000	-3.101988000
C	1.169391000	2.739529000	-1.781471000
H	1.369286000	2.408797000	-0.765472000
H	0.769246000	1.927702000	-2.399827000
H	2.057865000	3.183537000	-2.237314000
H	-2.598500000	2.214611000	1.833517000
H	-3.384393000	2.890337000	0.362075000
H	-1.982542000	3.969704000	-1.383432000
H	-1.380888000	2.328431000	-1.653667000
H	-1.196908000	4.025717000	0.928270000

Zero-point correction=	0.449121 (Hartree/Particle)
Thermal correction to Energy=	0.477635
Thermal correction to Enthalpy=	0.478579
Thermal correction to Gibbs Free Energy=	0.388939
Sum of electronic and zero-point Energies=	-1704.679154
Sum of electronic and thermal Energies=	-1704.650640
Sum of electronic and thermal Enthalpies=	-1704.649696
Sum of electronic and thermal Free Energies=	-1704.739336

TS1

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7-Me-Cl TS1 SCF Done: -1705.09829096 A.U.

O	-2.720746000	1.026088000	-0.869106000
O	-3.202082000	-1.635118000	0.679211000
H	-2.275090000	-1.269483000	0.753037000
C	-3.840481000	0.246283000	-0.794098000
O	-5.864088000	-2.466637000	-0.057228000
C	-3.976949000	-0.924169000	-0.132925000
O	-5.929786000	-0.613298000	-1.355364000
C	-5.324320000	-1.470300000	-0.457091000
O	-5.107760000	2.880435000	-1.888335000
H	-5.777497000	3.569959000	-2.059314000
O	-7.791465000	3.073893000	-2.051309000
H	-8.157689000	3.208005000	-1.162498000
C	-5.061599000	0.494294000	-1.648689000
H	-4.802795000	0.469711000	-2.716579000
C	-5.857376000	1.779560000	-1.389882000
H	-6.019394000	1.876105000	-0.301281000
C	-7.218830000	1.760461000	-2.097704000
H	-7.076005000	1.537924000	-3.159747000
H	-7.879603000	1.002153000	-1.666054000
O	-0.742499000	-0.671971000	0.925504000
C	-0.294727000	-0.834394000	-0.857136000
H	-0.738629000	0.081208000	-1.173727000
H	-0.741696000	-1.749536000	-1.228617000
C	0.534422000	-0.899387000	0.338721000
H	1.215959000	-0.054489000	0.485453000
Cl	1.153180000	-0.315033000	-2.843551000
C	1.188701000	-2.219963000	0.684023000
H	2.054809000	-2.385817000	0.033894000
H	1.518722000	-2.218835000	1.728249000
H	0.479040000	-3.043017000	0.547892000
C	-2.697626000	2.244884000	-0.109539000
C	-1.241039000	2.709421000	-0.007641000
C	-0.624164000	2.726380000	-1.426197000
N	0.784676000	3.313623000	-1.550561000
O	-0.492399000	1.986341000	0.932832000
H	-0.731051000	1.007119000	0.936170000
C	0.826083000	4.716908000	-1.029543000
H	0.041039000	5.302818000	-1.512691000
H	0.676214000	4.702695000	0.049879000
H	1.803287000	5.146338000	-1.257529000
C	1.139009000	3.299355000	-3.019756000
H	2.145564000	3.707098000	-3.134232000

I2

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7-Me-Cl I2 SCF Done: -1705.12229892 A.U.

O	-2.474199000	1.084292000	-0.810303000
O	-2.750525000	-1.555149000	0.732236000
H	-1.577412000	-0.786820000	1.153060000
C	-3.510056000	0.165023000	-0.813049000
O	-5.284229000	-2.750678000	-0.250138000
C	-3.539688000	-1.014273000	-0.124272000
O	-5.426162000	-0.906201000	-1.547808000
C	-4.807795000	-1.697721000	-0.585020000
O	-4.911470000	2.689317000	-1.808595000
H	-5.620985000	3.334391000	-1.988490000
O	-7.587039000	2.652665000	-2.294685000
H	-8.040599000	2.653585000	-1.436438000
C	-4.665739000	0.297318000	-1.754204000
H	-4.347982000	0.335493000	-2.809108000
C	-5.612183000	1.480405000	-1.515311000
H	-5.917064000	1.457269000	-0.454150000
C	-6.861211000	1.417164000	-2.397169000
H	-6.565327000	1.338851000	-3.448292000
H	-7.478804000	0.549993000	-2.140229000
O	-0.647378000	-0.338941000	1.361768000
C	-0.096465000	-0.995612000	-0.874120000
H	-0.510671000	-0.025847000	-1.132632000
H	-0.805099000	-1.781164000	-1.132171000
C	0.326928000	-1.041506000	0.598574000
H	1.269074000	-0.487116000	0.704517000
Cl	1.391290000	-1.229580000	-2.019015000
C	0.498477000	-2.469329000	1.107653000
H	1.233773000	-3.013458000	0.504282000
H	0.829880000	-2.457429000	2.150409000
H	-0.466045000	-2.985426000	1.053789000
C	-2.558276000	2.127823000	0.159328000
C	-1.208586000	2.853128000	0.161543000
C	-0.881228000	3.211892000	-1.308679000
N	0.585446000	3.546252000	-1.594089000
O	-0.170208000	2.123016000	0.760430000
H	-0.462741000	1.181632000	1.020512000
C	1.152871000	4.446791000	-0.529740000
H	0.517855000	5.331110000	-0.446656000
H	1.166697000	3.893433000	0.408356000
H	2.162938000	4.738727000	-0.824337000
C	0.652079000	4.240347000	-2.924085000
H	1.698831000	4.406530000	-3.186646000

H	1.110817000	2.258902000	-3.361479000
H	0.419957000	3.916789000	-3.562138000
C	1.816735000	2.473906000	-0.820637000
H	1.524356000	2.411815000	0.224495000
H	1.825501000	1.482752000	-1.286879000
H	2.784397000	2.965221000	-0.946904000
H	-3.066186000	2.064967000	0.907919000
H	-3.328176000	2.992594000	-0.600121000
H	-1.254949000	3.332054000	-2.084865000
H	-0.543819000	1.729941000	-1.856954000
H	-1.292778000	3.743969000	0.362315000

Zero-point correction= 0.447540 (Hartree/Particle)
Thermal correction to Energy= 0.475303
Thermal correction to Enthalpy= 0.476248
Thermal correction to Gibbs Free Energy= 0.389163
Sum of electronic and zero-point Energies= -1704.650751
Sum of electronic and thermal Energies= -1704.622988
Sum of electronic and thermal Enthalpies= -1704.622043
Sum of electronic and thermal Free Energies= -1704.709128

H	0.177043000	3.606038000	-3.674228000
H	0.126803000	5.194902000	-2.858468000
C	1.408521000	2.275128000	-1.673816000
H	1.312740000	1.764060000	-0.720239000
H	1.015703000	1.646287000	-2.472894000
H	2.443985000	2.550154000	-1.885029000
H	-2.737137000	1.714414000	1.159730000
H	-3.371564000	2.815326000	-0.101678000
H	-1.467162000	4.084489000	-1.611692000
H	-1.133666000	2.377747000	-1.962812000
H	-1.341540000	3.792167000	0.723245000

Zero-point correction= 0.447796 (Hartree/Particle)
Thermal correction to Energy= 0.475501
Thermal correction to Enthalpy= 0.476445
Thermal correction to Gibbs Free Energy= 0.388578
Sum of electronic and zero-point Energies= -1704.674502
Sum of electronic and thermal Energies= -1704.646798
Sum of electronic and thermal Enthalpies= -1704.645854
Sum of electronic and thermal Free Energies= -1704.733721

TS2

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7-Me-Cl TS2 SCF Done: -1893.70354080 A.U.

O	-2.226349000	1.256730000	-0.814084000
O	-4.390894000	3.009306000	0.593138000
H	-3.450938000	3.353071000	0.694222000
C	-3.454551000	0.944452000	-0.340880000
O	-6.631609000	1.132404000	1.004545000
C	-4.383105000	1.717390000	0.257013000
O	-5.272252000	-0.429073000	0.073957000
C	-5.569788000	0.861581000	0.515097000
O	-2.681517000	-1.129895000	-2.420453000
H	-2.785631000	-1.816000000	-3.109820000
O	-4.489377000	-2.916616000	-3.286104000
H	-5.112427000	-2.497244000	-3.901077000
C	-3.945219000	-0.465767000	-0.464843000
H	-3.342206000	-1.170149000	0.127521000
C	-4.011736000	-0.987751000	-1.905393000
H	-4.574002000	-0.257311000	-2.510133000
C	-4.702725000	-2.353712000	-1.984616000
H	-4.228292000	-3.046894000	-1.282574000
H	-5.764387000	-2.271042000	-1.731090000
O	-1.856994000	3.820898000	1.017771000
C	-1.197799000	2.103827000	2.416067000
H	-0.397892000	1.900822000	1.705455000
H	-2.060145000	1.469297000	2.205365000
C	-1.563476000	3.584467000	2.399323000
H	-0.686654000	4.179531000	2.678585000
Cl	-0.548858000	1.548031000	4.082466000
C	-2.731433000	3.951766000	3.307299000
H	-2.483029000	3.754693000	4.354932000
H	-2.942384000	5.016005000	3.181779000
H	-3.626825000	3.378501000	3.042756000
C	-2.166983000	2.362278000	-1.727514000
C	-0.695746000	2.535379000	-2.071194000
C	-0.174146000	1.268006000	-2.821638000
N	0.819363000	0.349970000	-2.106418000
O	0.073161000	2.793855000	-0.916873000
H	-0.455363000	3.424121000	-0.374786000
C	2.133967000	1.057964000	-1.886315000
H	2.533637000	1.353723000	-2.858691000
H	1.943614000	1.933189000	-1.268836000
H	2.820641000	0.364847000	-1.396353000
C	1.046637000	-0.836515000	-3.003853000
H	1.787582000	-1.490516000	-2.540239000
H	0.101157000	-1.367737000	-3.121736000

I3

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7-Me-Cl I3 SCF Done: -1893.72498732 A.U.

O	-2.163060000	1.344231000	-0.554084000
O	-2.704479000	0.133364000	2.254206000
H	-1.765443000	0.458749000	2.145482000
C	-3.061251000	0.385047000	-0.167574000
O	-4.795315000	-1.854408000	1.819883000
C	-3.244655000	-0.126786000	1.066369000
O	-4.651851000	-1.296563000	-0.370186000
C	-4.291177000	-1.180956000	0.961587000
O	-4.225324000	1.372411000	-2.798502000
H	-4.858021000	1.578626000	-3.511806000
O	-6.626719000	0.444912000	-3.671618000
H	-7.323039000	0.868519000	-3.144469000
C	-3.912682000	-0.354407000	-1.164536000
H	-3.291652000	-0.904712000	-1.885542000
C	-4.931167000	0.484726000	-1.943518000
H	-5.539043000	1.046136000	-1.210368000
C	-5.860322000	-0.389262000	-2.793087000
H	-5.261015000	-1.031189000	-3.446523000
H	-6.492734000	-1.022024000	-2.161194000
O	-0.215817000	1.057654000	1.750038000
C	0.160997000	0.189338000	0.897969000
O	1.177143000	0.717363000	0.049445000
O	-0.231460000	-0.955822000	0.712231000
C	0.422419000	-0.537041000	-1.921631000
H	-0.358153000	0.222846000	-1.950594000
H	0.004235000	-1.493451000	-1.625574000
C	1.613013000	-0.101621000	-1.056950000
H	2.209507000	0.596391000	-1.655980000
Cl	1.003379000	-0.751968000	-3.698853000
C	2.494506000	-1.261505000	-0.608498000
H	2.867367000	-1.802093000	-1.484968000
H	3.349720000	-0.885125000	-0.037713000
H	1.917858000	-1.942483000	0.020256000
C	-2.643383000	2.698137000	-0.608236000
C	-1.617440000	3.609675000	0.078666000
C	-0.259712000	3.399681000	-0.608086000
N	0.928085000	4.189455000	-0.044587000
O	-1.569530000	3.395237000	1.465114000
H	-1.183220000	2.493139000	1.609702000
C	0.679915000	5.663092000	-0.145280000
H	0.469346000	5.920915000	-1.185460000
H	-0.169835000	5.920746000	0.486408000
H	1.568608000	6.196021000	0.198733000

H	1.411794000	-0.491923000	-3.973107000
C	0.280056000	-0.166500000	-0.789681000
H	0.110165000	0.686294000	-0.141234000
H	-0.661766000	-0.674941000	-0.990687000
H	1.024103000	-0.850233000	-0.375108000
H	-2.537781000	3.285350000	-1.281377000
H	-2.754147000	2.127313000	-2.627067000
H	0.337191000	1.554614000	-3.744242000
H	-1.020463000	0.623104000	-3.068374000
H	-0.630279000	3.379425000	-2.773285000
C	-1.594584000	5.319223000	0.479272000
O	-1.547910000	5.239890000	-0.747892000
O	-1.480520000	6.135934000	1.366655000

Zero-point correction= 0.463291 (Hartree/Particle)
Thermal correction to Energy= 0.493735
Thermal correction to Enthalpy= 0.494679
Thermal correction to Gibbs Free Energy= 0.400531
Sum of electronic and zero-point Energies= -1893.240250
Sum of electronic and thermal Energies= -1893.209805
Sum of electronic and thermal Enthalpies= -1893.208861
Sum of electronic and thermal Free Energies= -1893.303010

C	2.126939000	3.812155000	-0.875084000
H	2.988918000	4.389353000	-0.534436000
H	2.300845000	2.745612000	-0.731984000
H	1.921749000	4.029978000	-1.924805000
C	1.243192000	3.830797000	1.398012000
H	0.441441000	4.204768000	2.027739000
H	1.279773000	2.744341000	1.484329000
H	2.201551000	4.293537000	1.644299000
H	-3.585414000	2.785556000	-0.058033000
H	-2.816414000	2.972712000	-1.653912000
H	-0.326045000	3.682128000	-1.663698000
H	0.035993000	2.354921000	-0.531869000
H	-1.966277000	4.641111000	-0.069708000

Zero-point correction= 0.465074 (Hartree/Particle)
Thermal correction to Energy= 0.495442
Thermal correction to Enthalpy= 0.496386
Thermal correction to Gibbs Free Energy= 0.402536
Sum of electronic and zero-point Energies= -1893.259913
Sum of electronic and thermal Energies= -1893.229545
Sum of electronic and thermal Enthalpies= -1893.228601
Sum of electronic and thermal Free Energies= -1893.322451

TS3

56
7-Me-Cl TS3 SCF Done: -1893.71218575 A.U.

O	-2.178810000	0.954745000	-0.124824000
O	-3.294247000	-1.004901000	1.995121000
H	-2.394686000	-0.609408000	2.176561000
C	-3.152464000	0.002381000	-0.233347000
O	-5.325214000	-2.567915000	0.554583000
C	-3.604122000	-0.844410000	0.709979000
O	-4.739187000	-1.339186000	-1.258948000
C	-4.644191000	-1.700247000	0.078128000
O	-3.836823000	2.034663000	-2.305470000
H	-4.323206000	2.562046000	-2.967177000
O	-6.008854000	1.742536000	-3.916014000
H	-6.806516000	1.944804000	-3.401167000
C	-3.842660000	-0.251998000	-1.540230000
H	-3.135907000	-0.563363000	-2.322001000
C	-4.686414000	0.917208000	-2.064107000
H	-5.431122000	1.158949000	-1.285032000
C	-5.417044000	0.560719000	-3.361806000
H	-4.692072000	0.218476000	-4.107232000
H	-6.150887000	-0.234986000	-3.191829000
O	-0.827728000	0.074361000	2.325093000
C	-0.136139000	-0.418603000	1.404760000
O	1.081732000	0.182194000	1.184125000
O	-0.436565000	-1.352253000	0.603037000
C	0.599830000	-0.640650000	-0.982053000
H	-0.231882000	0.031107000	-1.082061000
H	0.573950000	-1.553279000	-1.559480000
C	1.711983000	-0.384498000	0.015604000
H	2.380952000	0.391537000	-0.346645000
Cl	1.468328000	0.620183000	-2.825502000
C	2.517153000	-1.635228000	0.352208000
H	3.051012000	-1.979267000	-0.540294000
H	3.250225000	-1.402134000	1.130168000
H	1.859253000	-2.431772000	0.707377000
C	-2.585448000	2.148870000	0.554792000
C	-1.376580000	3.079289000	0.656502000
C	-0.685892000	3.112486000	-0.722343000
N	0.587224000	3.956214000	-0.794176000
O	-0.494509000	2.784499000	1.714962000
H	-0.575781000	1.837386000	1.992206000
C	0.438256000	5.242810000	-0.039023000

I4

56
7-Me-Cl I4 SCF Done: -1893.75525078 A.U.

O	-2.264081000	0.994953000	0.408008000
O	-3.400896000	-1.379600000	1.897802000
H	-2.594143000	-0.932315000	2.230105000
C	-3.149400000	0.071628000	-0.048650000
O	-4.940024000	-2.886739000	-0.145440000
C	-3.596755000	-1.002264000	0.621190000
O	-4.258488000	-1.264444000	-1.579174000
C	-4.351175000	-1.853582000	-0.331870000
O	-3.899917000	2.355865000	-1.686539000
H	-4.183038000	2.952935000	-2.404554000
O	-4.996411000	2.170170000	-4.172848000
H	-5.950572000	2.037420000	-4.051741000
C	-3.497704000	-0.038326000	-1.502751000
H	-2.576376000	-0.134615000	-2.092791000
C	-4.367128000	1.075792000	-2.103246000
H	-5.399529000	0.919214000	-1.745822000
C	-4.323359000	1.024723000	-3.632104000
H	-3.279977000	1.110691000	-3.952439000
H	-4.741322000	0.081624000	-4.006484000
O	-0.652965000	-0.135379000	2.387495000
C	-0.133782000	-0.565410000	1.371647000
O	0.919053000	0.003659000	0.773096000
O	-0.555601000	-1.654252000	0.724941000
C	0.125446000	-1.732237000	-0.554101000
H	-0.534623000	-1.335495000	-1.328676000
H	0.373886000	-2.778706000	-0.737178000
C	1.347596000	-0.824407000	-0.357624000
H	1.453538000	-0.157055000	-1.214708000
Cl	-0.272622000	1.001863000	-2.797742000
C	2.633546000	-1.540114000	0.014564000
H	2.986887000	-2.129304000	-0.838924000
H	3.411994000	-0.819474000	0.283021000
H	2.474945000	-2.215886000	0.862971000
C	-2.749916000	2.155696000	1.092064000
C	-1.583179000	3.143094000	1.090650000
C	-1.161081000	3.331072000	-0.381559000
N	0.176783000	4.025729000	-0.616353000
O	-0.527310000	2.741638000	1.948089000
H	-0.551647000	1.771814000	2.090109000
C	0.343861000	5.216174000	0.275839000

H	-0.457903000	5.759967000	-0.388150000
H	0.360801000	5.014474000	1.023871000
H	1.318585000	5.859641000	-0.229278000
C	0.865176000	4.238045000	-2.249093000
H	1.824445000	4.754547000	-2.324536000
H	0.910953000	3.281709000	-2.777868000
H	0.066622000	4.868434000	-2.645434000
C	1.761019000	3.175895000	-0.236720000
H	1.477213000	2.791944000	0.741068000
H	1.967797000	2.365360000	-0.937245000
H	2.615571000	3.853475000	-0.174781000
H	-2.940514000	1.913034000	1.564888000
H	-3.383453000	2.630630000	-0.020258000
H	-1.384605000	3.520918000	-1.457928000
H	-0.390938000	2.122595000	-1.061728000
H	-1.787264000	4.078423000	0.861599000

Zero-point correction= 0.464947 (Hartree/Particle)
Thermal correction to Energy= 0.494505
Thermal correction to Enthalpy= 0.495449
Thermal correction to Gibbs Free Energy= 0.405092
Sum of electronic and zero-point Energies= -1893.247239
Sum of electronic and thermal Energies= -1893.217681
Sum of electronic and thermal Enthalpies= -1893.216737
Sum of electronic and thermal Free Energies= -1893.307093

H	-0.516767000	5.876739000	0.148529000
H	0.411304000	4.871117000	1.307336000
H	1.258110000	5.741812000	-0.007974000
C	0.204485000	4.448467000	-2.065012000
H	1.189084000	4.868233000	-2.283351000
H	0.017349000	3.556110000	-2.673563000
H	-0.567799000	5.204010000	-2.224179000
C	1.316697000	3.052045000	-0.399772000
H	1.248360000	2.673077000	0.615753000
H	1.186658000	2.247208000	-1.128156000
H	2.252535000	3.591453000	-0.566132000
H	-3.019593000	1.903735000	2.125692000
H	-3.613263000	2.568081000	0.564206000
H	-1.919853000	3.935721000	-0.883836000
H	-1.090645000	2.381991000	-0.917957000
H	-1.954715000	4.096791000	1.489922000

Zero-point correction= 0.466350 (Hartree/Particle)
Thermal correction to Energy= 0.496954
Thermal correction to Enthalpy= 0.497898
Thermal correction to Gibbs Free Energy= 0.403810
Sum of electronic and zero-point Energies= -1893.288901
Sum of electronic and thermal Energies= -1893.258297
Sum of electronic and thermal Enthalpies= -1893.257353
Sum of electronic and thermal Free Energies= -1893.351441

7-Me-Br

I0			
43			
7-Me-Br I0 SCF Done: -1065.19692242 A.U.			
O	-2.776409000	1.749541000	-1.578349000
O	-2.090616000	-1.190210000	-1.213883000
H	-1.333588000	-0.555079000	-1.236235000
C	-3.642526000	0.697859000	-1.533629000
O	-4.577127000	-2.641169000	-1.559510000
C	-3.263231000	-0.592872000	-1.422586000
O	-5.533951000	-0.613902000	-1.875463000
C	-4.461151000	-1.446024000	-1.609216000
O	-5.881691000	2.878168000	-0.989920000
H	-6.724586000	3.255362000	-0.672999000
O	-8.354426000	2.036948000	-0.366967000
H	-8.356370000	1.736168000	0.555956000
C	-5.122769000	0.763974000	-1.851156000
H	-5.292840000	1.203567000	-2.844076000
C	-6.051578000	1.475579000	-0.855630000
H	-5.784657000	1.142673000	0.163590000
C	-7.527469000	1.139500000	-1.119670000
H	-7.764837000	1.331282000	-2.170772000
H	-7.743441000	0.090399000	-0.897174000
C	-2.995549000	2.888708000	-0.735722000
C	-1.620741000	3.451911000	-0.356617000
C	-0.794968000	3.608069000	-1.641917000
N	0.528865000	4.374630000	-1.523956000
O	-0.974304000	2.662719000	0.613413000
H	-0.628765000	1.845953000	0.182652000
C	0.262409000	5.846288000	-1.428033000
H	-0.284563000	6.170760000	-2.315424000
H	-0.329110000	6.041743000	-0.533023000
H	1.213925000	6.377463000	-1.362998000
C	1.312485000	4.075076000	-2.779037000
H	2.238196000	4.654060000	-2.762593000
H	1.525033000	3.002765000	-2.790587000
H	0.709281000	4.353263000	-3.645375000
C	1.373585000	3.947102000	-0.339435000

I1			
53			
7-Me-Br I1 SCF Done: -1258.33245308 A.U.			
O	-2.354503000	1.072672000	-0.190695000
O	-2.950480000	-1.557469000	1.097043000
H	-2.081420000	-1.103587000	1.198556000
C	-3.428881000	0.281159000	-0.434255000
O	-5.330482000	-2.611285000	-0.327353000
C	-3.636077000	-0.921760000	0.127373000
O	-5.191224000	-0.711976000	-1.562835000
C	-4.789231000	-1.559591000	-0.549631000
O	-4.516520000	2.871124000	-1.571747000
H	-5.105420000	3.538669000	-1.972676000
O	-6.893026000	2.955845000	-2.866170000
H	-7.601920000	2.936780000	-2.203302000
C	-4.354226000	0.465659000	-1.605621000
H	-3.765171000	0.468735000	-2.534107000
C	-5.290958000	1.675422000	-1.581518000
H	-5.908668000	1.611856000	-0.667860000
C	-6.205911000	1.698257000	-2.810276000
H	-5.595554000	1.653579000	-3.717274000
H	-6.894498000	0.846223000	-2.803351000
O	-0.353912000	-0.548097000	0.708670000
C	-0.249849000	-1.056179000	-0.657156000
H	0.120678000	-0.342163000	-1.387783000
H	-1.120994000	-1.616933000	-0.987542000
C	0.599067000	-1.608579000	0.404706000
H	1.632530000	-1.263490000	0.456660000
Br	-1.076705000	0.842453000	-3.816518000
C	0.309862000	-2.942810000	1.040870000
H	0.879416000	-3.730744000	0.534758000
H	0.596032000	-2.940463000	2.098657000
H	-0.756408000	-3.178595000	0.967017000
C	-2.477759000	2.258415000	0.601510000
C	-1.173243000	3.013081000	0.343022000
C	-1.116271000	3.296288000	-1.169071000
N	0.190698000	3.884268000	-1.698238000

H	0.840814000	4.171076000	0.580770000
H	1.540227000	2.870833000	-0.411249000
H	2.314627000	4.498723000	-0.400189000
H	-3.513387000	2.605043000	0.184435000
H	-3.607702000	3.628032000	-1.262395000
H	-1.366769000	4.131595000	-2.413501000
H	-0.534205000	2.611204000	-1.999769000
H	-1.804278000	4.427092000	0.117165000
Br	0.786949000	0.492709000	-1.310832000

O	-0.048549000	2.307451000	0.838437000
H	-0.187341000	1.340035000	0.722792000
C	0.672079000	5.006761000	-0.833162000
H	-0.128686000	5.741959000	-0.726805000
H	0.950853000	4.603729000	0.140586000
H	1.539301000	5.469803000	-1.308431000
C	-0.084524000	4.384060000	-3.096346000
H	0.852467000	4.745026000	-3.525849000
H	-0.478568000	3.544902000	-3.679424000
H	-0.811378000	5.196945000	-3.041405000
C	1.264161000	2.818363000	-1.790874000
H	1.440404000	2.438175000	-0.788049000
H	0.889379000	2.033183000	-2.455121000
H	2.161744000	3.282798000	-2.205902000
H	-2.547225000	1.996834000	1.665290000
H	-3.348098000	2.843514000	0.293436000
H	-1.904706000	4.009377000	-1.425265000
H	-1.285398000	2.388771000	-1.755398000
H	-1.212286000	3.956104000	0.903362000

Zero-point correction=	0.359515 (Hartree/Particle)
Thermal correction to Energy=	0.382666
Thermal correction to Enthalpy=	0.383611
Thermal correction to Gibbs Free Energy=	0.304844
Sum of electronic and zero-point Energies=	-1064.837407
Sum of electronic and thermal Energies=	-1064.814256
Sum of electronic and thermal Enthalpies=	-1064.813312
Sum of electronic and thermal Free Energies=	-1064.892078

Zero-point correction=	0.448888 (Hartree/Particle)
Thermal correction to Energy=	0.477682
Thermal correction to Enthalpy=	0.478626
Thermal correction to Gibbs Free Energy=	0.387447
Sum of electronic and zero-point Energies=	-1257.883565
Sum of electronic and thermal Energies=	-1257.854771
Sum of electronic and thermal Enthalpies=	-1257.853827
Sum of electronic and thermal Free Energies=	-1257.945006

TS1

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7-Me-Br TS1 SCF Done: -1258.30215417 A.U.

O	-2.702541000	1.046230000	-0.846811000
O	-3.171108000	-1.592162000	0.747637000
H	-2.244201000	-1.219428000	0.808726000
C	-3.811943000	0.250744000	-0.770339000
O	-5.821526000	-2.461912000	0.001569000
C	-3.945036000	-0.907006000	-0.086988000
O	-5.888346000	-0.635578000	-1.334855000
C	-5.285531000	-1.469908000	-0.413416000
O	-5.072412000	2.857838000	-1.893685000
H	-5.740295000	3.544069000	-2.084204000
O	-7.754307000	3.041552000	-2.116864000
H	-8.141629000	3.177178000	-1.237279000
C	-5.025871000	0.473038000	-1.640375000
H	-4.757715000	0.431742000	-2.705442000
C	-5.830849000	1.757096000	-1.407543000
H	-6.017341000	1.858189000	-0.323308000
C	-7.175648000	1.730355000	-2.145630000
H	-7.008044000	1.504783000	-3.203436000
H	-7.842698000	0.970598000	-1.726085000
O	-0.722353000	-0.599314000	0.922245000
C	-0.303811000	-0.850286000	-0.889934000
H	-0.708217000	0.081850000	-1.217891000
H	-0.825103000	-1.744721000	-1.211965000
C	0.520202000	-0.920881000	0.315828000
H	1.256331000	-0.114866000	0.422036000
Br	1.193593000	-0.533738000	-3.024322000
C	1.100806000	-2.265368000	0.701195000
H	1.955023000	-2.505602000	0.059014000
H	1.431021000	-2.245890000	1.745099000
H	0.343658000	-3.049507000	0.594323000
C	-2.689556000	2.249544000	-0.063304000
C	-1.241181000	2.744673000	0.017430000
C	-0.651953000	2.777375000	-1.411954000
N	0.763771000	3.343447000	-1.550737000

I2

53

7-Me-Br I2 SCF Done: -1258.32041918 A.U.

O	-2.438500000	1.063729000	-0.781797000
O	-2.779704000	-1.517385000	0.847368000
H	-1.571727000	-0.779130000	1.213195000
C	-3.474545000	0.145339000	-0.786553000
O	-5.308179000	-2.717407000	-0.154137000
C	-3.539720000	-1.003652000	-0.051737000
O	-5.394236000	-0.917958000	-1.519131000
C	-4.807973000	-1.684672000	-0.515782000
O	-4.803996000	2.663834000	-1.838955000
H	-5.495065000	3.320356000	-2.047108000
O	-7.468185000	2.674791000	-2.397959000
H	-7.945529000	2.693478000	-1.552912000
C	-4.611972000	0.266755000	-1.749124000
H	-4.279676000	0.269402000	-2.800182000
C	-5.538683000	1.472987000	-1.552472000
H	-5.872767000	1.468867000	-0.499966000
C	-6.763759000	1.424795000	-2.467638000
H	-6.440736000	1.329677000	-3.509376000
H	-7.404605000	0.572030000	-2.218945000
O	-0.623795000	-0.352536000	1.392448000
C	-0.111108000	-1.036278000	-0.832961000
H	-0.465619000	-0.044906000	-1.095778000
H	-0.861935000	-1.781471000	-1.089820000
C	0.319690000	-1.105380000	0.636277000
H	1.286305000	-0.597544000	0.747975000
Br	1.457077000	-1.379922000	-2.108806000
C	0.413218000	-2.538328000	1.151155000
H	1.125208000	-3.123605000	0.558697000
H	0.735243000	-2.537140000	2.196847000
H	-0.576242000	-3.003952000	1.091567000
C	-2.516733000	2.084042000	0.211874000
C	-1.179720000	2.830395000	0.190729000
C	-0.924642000	3.255854000	-1.275646000
N	0.526037000	3.602440000	-1.619592000

O	-0.457031000	2.033341000	0.935780000
H	-0.678368000	1.046294000	0.936088000
C	0.841974000	4.726527000	-0.979249000
H	0.056483000	5.342519000	-1.422362000
H	0.715601000	4.672261000	0.101823000
H	1.821340000	5.147216000	-1.213962000
C	1.085679000	3.377867000	-3.025826000
H	2.098719000	3.765568000	-3.150157000
H	1.028264000	2.355636000	-3.411335000
H	0.368792000	4.028428000	-3.530640000
C	1.796393000	2.462139000	-0.873295000
H	1.529450000	2.375895000	0.176759000
H	1.775682000	1.484166000	-1.361566000
H	2.772407000	2.931674000	-1.014661000
H	-3.032205000	2.042683000	0.957949000
H	-3.345057000	2.992908000	-0.527557000
H	-1.286018000	3.399632000	-2.051500000
H	-0.601987000	1.784267000	-1.853769000
H	-1.306134000	3.777364000	0.390446000

Zero-point correction= 0.446914 (Hartree/Particle)
Thermal correction to Energy= 0.474996
Thermal correction to Enthalpy= 0.475941
Thermal correction to Gibbs Free Energy= 0.386807
Sum of electronic and zero-point Energies= -1257.855240
Sum of electronic and thermal Energies= -1257.827158
Sum of electronic and thermal Enthalpies= -1257.826214
Sum of electronic and thermal Free Energies= -1257.915347

O	-0.107206000	2.082485000	0.702813000
H	-0.402683000	1.156641000	1.009108000
C	1.147600000	4.457423000	-0.547611000
H	0.519505000	5.337761000	-0.397134000
H	1.205435000	3.865620000	0.365015000
H	2.142757000	4.760885000	-0.878965000
C	0.527572000	4.352560000	-2.920703000
H	1.560216000	4.529275000	-3.228348000
H	0.013215000	3.751439000	-3.672267000
H	0.008952000	5.303743000	-2.787859000
C	1.340875000	2.335354000	-1.793657000
H	1.289622000	1.783585000	-0.859288000
H	0.905011000	1.745156000	-2.600321000
H	2.365604000	2.617538000	-2.043940000
H	-2.663662000	1.645788000	1.206683000
H	-3.346701000	2.764253000	-0.014530000
H	-1.523302000	4.140849000	-1.509250000
H	-1.212430000	2.451248000	-1.952073000
H	-1.299109000	3.741801000	0.799714000

Zero-point correction= 0.447078 (Hartree/Particle)
Thermal correction to Energy= 0.475069
Thermal correction to Enthalpy= 0.476013
Thermal correction to Gibbs Free Energy= 0.386378
Sum of electronic and zero-point Energies= -1257.873341
Sum of electronic and thermal Energies= -1257.845350
Sum of electronic and thermal Enthalpies= -1257.844406
Sum of electronic and thermal Free Energies= -1257.934042

TS2

56
7-Me-Br TS2 SCF Done: -1446.90224969 A.U.

O	-2.228339000	1.262083000	-0.814949000
O	-4.397099000	3.015098000	0.587610000
H	-3.457587000	3.360513000	0.689606000
C	-3.457036000	0.949824000	-0.342630000
O	-6.635558000	1.136632000	0.999508000
C	-4.386985000	1.722739000	0.253311000
O	-5.273592000	-0.425054000	0.073088000
C	-5.573031000	0.865850000	0.511639000
O	-2.680167000	-1.126789000	-2.418211000
H	-2.782710000	-1.814770000	-3.105972000
O	-4.483585000	-2.919149000	-3.280490000
H	-5.107667000	-2.503016000	-3.896612000
C	-3.945948000	-0.461291000	-0.464256000
H	-3.342688000	-1.163639000	0.130262000
C	-4.010788000	-0.986342000	-1.903749000
H	-4.574395000	-0.258297000	-2.510136000
C	-4.698868000	-2.353956000	-1.980334000
H	-4.223323000	-3.044570000	-1.276524000
H	-5.760834000	-2.272995000	-1.727547000
O	-1.866577000	3.827173000	1.012811000
C	-1.215570000	2.097631000	2.379595000
H	-0.433538000	1.895149000	1.651426000
H	-2.085819000	1.468287000	2.192150000
C	-1.567648000	3.581164000	2.391559000
H	-0.686354000	4.170050000	2.669676000
Br	-0.458357000	1.437267000	4.150398000
C	-2.731239000	3.950609000	3.304104000
H	-2.480952000	3.760035000	4.352550000
H	-2.942091000	5.014381000	3.174495000
H	-3.627717000	3.376657000	3.044811000
C	-2.167492000	2.366213000	-1.729525000
C	-0.695778000	2.537676000	-2.072366000
C	-0.173774000	1.268342000	-2.819201000
N	0.818933000	0.351176000	-2.101774000

I3

56
7-Me-Br I3 SCF Done: -1446.92371062 A.U.

O	-2.162999000	1.354172000	-0.521005000
O	-2.719255000	0.154173000	2.283804000
H	-1.777987000	0.472668000	2.176542000
C	-3.060071000	0.391955000	-0.140115000
O	-4.809615000	-1.838497000	1.842727000
C	-3.252366000	-0.114481000	1.094260000
O	-4.644151000	-1.293554000	-0.349410000
C	-4.297158000	-1.169939000	0.985577000
O	-4.163010000	1.345303000	-2.802282000
H	-4.773035000	1.536949000	-3.539020000
O	-6.538870000	0.400946000	-3.729476000
H	-7.248546000	0.831539000	-3.226334000
C	-3.891036000	-0.361670000	-1.142784000
H	-3.254384000	-0.922515000	-1.842086000
C	-4.890668000	0.465763000	-1.956744000
H	-5.518525000	1.034839000	-1.246794000
C	-5.794920000	-0.420268000	-2.820292000
H	-5.176979000	-1.068979000	-3.449229000
H	-6.442778000	-1.046639000	-2.197558000
O	-0.216950000	1.058985000	1.777061000
C	0.147409000	0.193322000	0.918061000
O	1.163678000	0.716185000	0.065532000
O	-0.256191000	-0.947148000	0.724383000
C	0.347835000	-0.512586000	-1.890556000
H	-0.447261000	0.229582000	-1.855855000
H	-0.037094000	-1.495506000	-1.642114000
C	1.568223000	-0.098335000	-1.056951000
H	2.165738000	0.598555000	-1.654902000
Br	0.864509000	-0.631623000	-3.866548000
C	2.442601000	-1.273402000	-0.633881000
H	2.801192000	-1.808662000	-1.519783000
H	3.308113000	-0.911874000	-0.069219000
H	1.866828000	-1.955579000	-0.005801000
C	-2.646206000	2.707111000	-0.573493000

O	0.071926000	2.799493000	-0.917850000
H	-0.455740000	3.433871000	-0.380129000
C	2.133465000	1.059078000	-1.880663000
H	2.534450000	1.353813000	-2.852808000
H	1.942869000	1.934924000	-1.264198000
H	2.819255000	0.366273000	-1.389066000
C	1.047180000	-0.836221000	-2.997913000
H	1.787618000	-1.489717000	-2.532818000
H	0.101832000	-1.367575000	-3.116244000
H	1.413391000	-0.492551000	-3.967090000
C	0.278237000	-0.164435000	-0.785313000
H	0.109591000	0.688491000	-0.137003000
H	-0.664262000	-0.671529000	-0.986470000
H	1.021008000	-0.848906000	-0.369777000
H	-2.538597000	3.289757000	-1.284593000
H	-2.754156000	2.130884000	-2.629289000
H	0.338299000	1.553055000	-3.741963000
H	-1.020194000	0.623343000	-3.065316000
H	-0.629113000	3.379666000	-2.776864000
C	-1.592155000	5.333852000	0.476597000
O	-1.541950000	5.253738000	-0.749154000
O	-1.477892000	6.143443000	1.369259000

Zero-point correction= 0.462598 (Hartree/Particle)
Thermal correction to Energy= 0.493310
Thermal correction to Enthalpy= 0.494254
Thermal correction to Gibbs Free Energy= 0.398627
Sum of electronic and zero-point Energies= -1446.439652
Sum of electronic and thermal Energies= -1446.408940
Sum of electronic and thermal Enthalpies= -1446.407996
Sum of electronic and thermal Free Energies= -1446.503623

C	-1.612180000	3.619492000	0.099808000
C	-0.261737000	3.404265000	-0.599687000
N	0.933408000	4.191806000	-0.049227000
O	-1.550503000	3.409639000	1.486541000
H	-1.168902000	2.505427000	1.631536000
C	0.686529000	5.665983000	-0.146003000
H	0.463687000	5.924625000	-1.183409000
H	-0.154986000	5.924545000	0.496244000
H	1.580288000	6.197188000	0.187366000
C	2.122175000	3.813146000	-0.893456000
H	2.989042000	4.388343000	-0.561976000
H	2.296271000	2.746273000	-0.753206000
H	1.905775000	4.031612000	-1.940760000
C	1.263607000	3.831047000	1.389493000
H	0.469030000	4.204952000	2.028214000
H	1.300696000	2.744573000	1.473963000
H	2.225091000	4.292329000	1.626118000
H	-3.581291000	2.794251000	-0.011416000
H	-2.831486000	2.978287000	-1.617984000
H	-0.337344000	3.683210000	-1.655554000
H	0.032071000	2.359131000	-0.522414000
H	-1.960463000	4.651047000	-0.048388000

Zero-point correction= 0.464481 (Hartree/Particle)
Thermal correction to Energy= 0.495075
Thermal correction to Enthalpy= 0.496019
Thermal correction to Gibbs Free Energy= 0.400749
Sum of electronic and zero-point Energies= -1446.459230
Sum of electronic and thermal Energies= -1446.428635
Sum of electronic and thermal Enthalpies= -1446.427691
Sum of electronic and thermal Free Energies= -1446.522961

TS3

56
7-Me-Br TS3 SCF Done: -1446.91350895 A.U.

O	-2.176855000	0.976206000	-0.121333000
O	-3.297725000	-0.936584000	2.033064000
H	-2.392210000	-0.551106000	2.203455000
C	-3.145144000	0.016757000	-0.216968000
O	-5.325076000	-2.532411000	0.615740000
C	-3.602422000	-0.808214000	0.742328000
O	-4.726491000	-1.345033000	-1.221518000
C	-4.639839000	-1.676770000	0.123964000
O	-3.809463000	2.009742000	-2.319087000
H	-4.281925000	2.523556000	-3.001278000
O	-5.953946000	1.689843000	-3.962760000
H	-6.760112000	1.898447000	-3.463932000
C	-3.825673000	-0.266627000	-1.522251000
H	-3.114757000	-0.598823000	-2.291689000
C	-4.661408000	0.893971000	-2.077195000
H	-5.419174000	1.145636000	-1.314055000
C	-5.369259000	0.517593000	-3.381709000
H	-4.631066000	0.166352000	-4.109769000
H	-6.104196000	-0.277404000	-3.212477000
O	-0.810892000	0.128013000	2.315196000
C	-0.145882000	-0.394906000	1.389612000
O	1.062982000	0.208737000	1.112907000
O	-0.462256000	-1.357299000	0.636047000
C	0.571570000	-0.691248000	-1.028667000
H	-0.271361000	-0.030263000	-1.122119000
H	0.518717000	-1.640869000	-1.540652000
C	1.683778000	-0.402571000	-0.037295000
H	2.358308000	0.360180000	-0.419717000
Br	1.439071000	0.483181000	-3.066579000
C	2.488498000	-1.643220000	0.336706000
H	3.018459000	-2.018978000	-0.545271000
H	3.224717000	-1.385176000	1.103686000

I4

56
7-Me-Br I4 SCF Done: -1446.95821699 A.U.

O	-2.222225000	0.990086000	0.222947000
O	-3.363248000	-1.361601000	1.794064000
H	-2.558641000	-0.907432000	2.125216000
C	-3.116364000	0.051317000	-0.187714000
O	-4.986928000	-2.857614000	-0.172086000
C	-3.568994000	-0.998684000	0.516726000
O	-4.334696000	-1.264561000	-1.651213000
C	-4.382687000	-1.841553000	-0.395613000
O	-3.875304000	2.345564000	-1.873644000
H	-4.256410000	2.923103000	-2.561817000
O	-5.470816000	2.109069000	-4.064995000
H	-6.386663000	2.052999000	-3.747793000
C	-3.562909000	-0.044675000	-1.616309000
H	-2.696497000	-0.131906000	-2.285570000
C	-4.484046000	1.080041000	-2.107615000
H	-5.427646000	1.002755000	-1.538617000
C	-4.775405000	0.943135000	-3.604246000
H	-3.829583000	0.926164000	-4.154331000
H	-5.327487000	0.018713000	-3.811737000
O	-0.727284000	-0.119418000	2.327054000
C	-0.138656000	-0.565404000	1.354542000
O	0.943910000	0.003447000	0.815783000
O	-0.508339000	-1.670400000	0.707993000
C	0.256044000	-1.770038000	-0.522816000
H	-0.361069000	-1.403295000	-1.346559000
H	0.525278000	-2.817490000	-0.665352000
C	1.456300000	-0.847738000	-0.263599000
H	1.625443000	-0.195373000	-1.121713000
Br	-0.024916000	0.950989000	-3.054075000
C	2.717524000	-1.545187000	0.212279000
H	3.133462000	-2.146559000	-0.603512000
H	3.469781000	-0.812759000	0.520142000

H	1.829591000	-2.425014000	0.720983000
C	-2.590218000	2.166396000	0.561598000
C	-1.387681000	3.104507000	0.668054000
C	-0.699343000	3.147933000	-0.711481000
N	0.585556000	3.975550000	-0.770455000
O	-0.499721000	2.809543000	1.720332000
H	-0.574753000	1.858427000	1.994511000
C	0.463704000	5.242473000	0.024468000
H	-0.424865000	5.784824000	-0.304829000
H	0.387186000	4.982759000	1.080015000
H	1.353909000	5.848679000	-0.153553000
C	0.856828000	4.300349000	-2.216823000
H	1.825995000	4.798696000	-2.286037000
H	0.876663000	3.364850000	-2.781682000
H	0.067795000	4.958480000	-2.585776000
C	1.748757000	3.160347000	-0.244402000
H	1.468428000	2.757513000	0.726644000
H	1.934670000	2.361119000	-0.962405000
H	2.619310000	3.816586000	-0.178139000
H	-2.945247000	1.925803000	1.570413000
H	-3.390646000	2.644300000	-0.013658000
H	-1.391987000	3.572371000	-1.443362000
H	-0.420382000	2.154888000	-1.056042000
H	-1.804065000	4.100367000	0.878097000

Zero-point correction=	0.464423 (Hartree/Particle)
Thermal correction to Energy=	0.494234
Thermal correction to Enthalpy=	0.495178
Thermal correction to Gibbs Free Energy=	0.403334
Sum of electronic and zero-point Energies=	-1446.449086
Sum of electronic and thermal Energies=	-1446.419275
Sum of electronic and thermal Enthalpies=	-1446.418330
Sum of electronic and thermal Free Energies=	-1446.510174

H	2.504207000	-2.206439000	1.060072000
C	-2.723781000	2.128222000	0.935639000
C	-1.565085000	3.121190000	1.008046000
C	-1.067332000	3.338121000	-0.435982000
N	0.266779000	4.065171000	-0.580251000
O	-0.546571000	2.719955000	1.908213000
H	-0.588434000	1.752557000	2.065256000
C	0.366491000	5.228629000	0.358879000
H	-0.499143000	5.877682000	0.209384000
H	0.390114000	4.851230000	1.380717000
H	1.283125000	5.778856000	0.136650000
C	0.363751000	4.544828000	-2.007873000
H	1.352094000	4.984439000	-2.158721000
H	0.222836000	3.681331000	-2.665731000
H	-0.411040000	5.294955000	-2.178761000
C	1.410864000	3.103909000	-0.332360000
H	1.290286000	2.686598000	0.663395000
H	1.346329000	2.321879000	-1.092645000
H	2.345094000	3.662770000	-0.425711000
H	-3.027898000	1.841333000	1.950460000
H	-3.570219000	2.560064000	0.394868000
H	-1.811327000	3.928409000	-0.976332000
H	-0.947149000	2.395878000	-0.972536000
H	-1.968459000	4.065478000	1.399283000

Zero-point correction=	0.466082 (Hartree/Particle)
Thermal correction to Energy=	0.496903
Thermal correction to Enthalpy=	0.497847
Thermal correction to Gibbs Free Energy=	0.402409
Sum of electronic and zero-point Energies=	-1446.492135
Sum of electronic and thermal Energies=	-1446.461314
Sum of electronic and thermal Enthalpies=	-1446.460370
Sum of electronic and thermal Free Energies=	-1446.555808

7-Me-I

I0			
43			
7-Me-I I0 SCF Done: -1063.23179249 A.U.			
O	-2.695780000	1.645015000	-1.430167000
O	-2.182010000	-1.320031000	-1.272304000
H	-1.409778000	-0.712272000	-1.201834000
C	-3.631849000	0.657417000	-1.498890000
O	-4.719141000	-2.618058000	-1.839159000
C	-3.321931000	-0.655870000	-1.475940000
O	-5.565343000	-0.525386000	-2.018571000
C	-4.544904000	-1.430511000	-1.780624000
O	-5.838948000	2.876383000	-0.819878000
H	-6.685990000	3.238291000	-0.495155000
O	-8.334910000	2.045625000	-0.333192000
H	-8.371396000	1.672786000	0.562320000
C	-5.098376000	0.824266000	-1.849032000
H	-5.221789000	1.364008000	-2.798424000
C	-6.033476000	1.470725000	-0.812338000
H	-5.793875000	1.046128000	0.178840000
C	-7.510546000	1.188426000	-1.133972000
H	-7.719319000	1.464012000	-2.172390000
H	-7.754595000	0.131321000	-0.996332000
C	-2.963380000	2.840369000	-0.690017000
C	-1.608723000	3.463725000	-0.339479000
C	-0.767492000	3.555088000	-1.621559000
N	0.516579000	4.389312000	-1.543210000
O	-0.951093000	2.763816000	0.690961000
H	-0.620704000	1.907509000	0.336145000
C	0.183105000	5.850618000	-1.527401000
H	-0.380982000	6.099511000	-2.428425000
H	-0.412781000	6.070342000	-0.641139000

I1			
53			
7-Me-I I1 SCF Done: -1256.37143642 A.U.			
O	-2.344312000	1.060045000	-0.328265000
O	-2.961947000	-1.510396000	1.127392000
H	-2.080212000	-1.074624000	1.195136000
C	-3.425573000	0.255928000	-0.495744000
O	-5.397734000	-2.571635000	-0.179915000
C	-3.648184000	-0.907461000	0.137991000
O	-5.252172000	-0.740656000	-1.514189000
C	-4.839319000	-1.546619000	-0.471854000
O	-4.501262000	2.826931000	-1.606516000
H	-5.083896000	3.505864000	-1.997128000
O	-6.915401000	2.956892000	-2.835903000
H	-7.605918000	2.952896000	-2.153662000
C	-4.396154000	0.416936000	-1.631198000
H	-3.855182000	0.381486000	-2.587360000
C	-5.303242000	1.649811000	-1.591911000
H	-5.896891000	1.602791000	-0.661423000
C	-6.250330000	1.687395000	-2.795222000
H	-5.665796000	1.629701000	-3.718403000
H	-6.953775000	0.847688000	-2.767184000
O	-0.366811000	-0.556224000	0.698100000
C	-0.245471000	-1.106468000	-0.649931000
H	0.153430000	-0.419423000	-1.391685000
H	-1.120100000	-1.661749000	-0.980530000
C	0.575667000	-1.641086000	0.442250000
H	1.612589000	-1.308743000	0.502953000
I	-1.008992000	0.756270000	-4.099101000
C	0.255100000	-2.951177000	1.112019000
H	0.820548000	-3.761372000	0.637562000

H	1.110120000	6.426339000	-1.498176000
C	1.320908000	4.062207000	-2.778868000
H	2.220388000	4.681124000	-2.786422000
H	1.581710000	3.000924000	-2.737787000
H	0.712064000	4.270683000	-3.660647000
C	1.370476000	4.062005000	-0.334067000
H	0.822701000	4.310535000	0.570881000
H	1.583970000	2.991223000	-0.347427000
H	2.288791000	4.647417000	-0.419139000
H	-3.493010000	2.619507000	0.240680000
H	-3.582211000	3.522698000	-1.282564000
H	-1.347509000	3.988167000	-2.441539000
H	-0.454337000	2.546481000	-1.898399000
H	-1.824039000	4.462456000	0.065210000
I	1.038197000	0.304249000	-1.152476000

Zero-point correction= 0.359243 (Hartree/Particle)
Thermal correction to Energy= 0.382588
Thermal correction to Enthalpy= 0.383532
Thermal correction to Gibbs Free Energy= 0.303389
Sum of electronic and zero-point Energies= -1062.872549
Sum of electronic and thermal Energies= -1062.849204
Sum of electronic and thermal Enthalpies= -1062.848260
Sum of electronic and thermal Free Energies= -1062.928404

H	0.525225000	-2.922397000	2.173542000
H	-0.813256000	-3.173590000	1.028286000
C	-2.434556000	2.192827000	0.542604000
C	-1.137663000	2.966079000	0.304686000
C	-1.078602000	3.293545000	-1.198311000
N	0.213824000	3.938815000	-1.696106000
O	-0.001621000	2.266454000	0.780517000
H	-0.140558000	1.297583000	0.676882000
C	0.656961000	5.044093000	-0.788284000
H	-0.166536000	5.749928000	-0.659374000
H	0.945279000	4.615454000	0.171614000
H	1.510884000	5.550160000	-1.243124000
C	-0.064887000	4.482473000	-3.076843000
H	0.864882000	4.882866000	-3.486384000
H	-0.432927000	3.657975000	-3.696500000
H	-0.813828000	5.272976000	-2.998325000
C	1.318935000	2.908775000	-1.815578000
H	1.492701000	2.493522000	-0.826255000
H	0.979096000	2.137450000	-2.513748000
H	2.207663000	3.413548000	-2.201184000
H	-2.479827000	1.868004000	1.590270000
H	-3.310622000	2.797964000	0.293325000
H	-1.888846000	3.986072000	-1.442425000
H	-1.214367000	2.397326000	-1.809062000
H	-1.193415000	3.893651000	0.889238000

Zero-point correction= 0.448762 (Hartree/Particle)
Thermal correction to Energy= 0.477642
Thermal correction to Enthalpy= 0.478586
Thermal correction to Gibbs Free Energy= 0.386528
Sum of electronic and zero-point Energies= -1255.922675
Sum of electronic and thermal Energies= -1255.893795
Sum of electronic and thermal Enthalpies= -1255.892850
Sum of electronic and thermal Free Energies= -1255.984908

TS1

53
7-Me-I TS1 SCF Done: -1256.34167228 A.U.

O	-2.691123000	1.054156000	-0.824612000
O	-3.165218000	-1.553060000	0.820988000
H	-2.236928000	-1.182998000	0.868264000
C	-3.795757000	0.252453000	-0.744408000
O	-5.807415000	-2.446935000	0.065938000
C	-3.933450000	-0.890099000	-0.037446000
O	-5.864242000	-0.649988000	-1.310807000
C	-5.269495000	-1.462993000	-0.365205000
O	-5.038088000	2.836844000	-1.905131000
H	-5.700858000	3.521984000	-2.116320000
O	-7.716413000	3.020959000	-2.184528000
H	-8.122304000	3.163090000	-1.314400000
C	-5.001160000	0.454252000	-1.629990000
H	-4.723126000	0.393093000	-2.691521000
C	-5.808700000	1.741304000	-1.426128000
H	-6.017277000	1.851559000	-0.346838000
C	-7.137724000	1.709609000	-2.191627000
H	-6.948180000	1.476343000	-3.244075000
H	-7.813364000	0.952787000	-1.780363000
O	-0.705012000	-0.566839000	0.928149000
C	-0.334316000	-0.871511000	-0.883018000
H	-0.691772000	0.072392000	-1.233677000
H	-0.907983000	-1.745394000	-1.169796000
C	0.512695000	-0.949401000	0.307767000
H	1.280592000	-0.168992000	0.379439000
I	1.223790000	-0.687209000	-3.240512000
C	1.048509000	-2.306162000	0.713285000
H	1.881445000	-2.593507000	0.062799000
H	1.397623000	-2.276223000	1.750714000
H	0.260013000	-3.062420000	0.636738000

I2

53
7-Me-I I2 SCF Done: -1256.35857289 A.U.

O	-2.416267000	1.051299000	-0.765049000
O	-2.806279000	-1.475333000	0.939041000
H	-1.565384000	-0.768482000	1.254067000
C	-3.452198000	0.133630000	-0.765752000
O	-5.331502000	-2.683443000	-0.069746000
C	-3.544499000	-0.987454000	0.007582000
O	-5.376014000	-0.925664000	-1.490483000
C	-4.813352000	-1.668258000	-0.454987000
O	-4.731586000	2.643592000	-1.863802000
H	-5.409508000	3.306885000	-2.092673000
O	-7.386670000	2.685022000	-2.471482000
H	-7.878395000	2.719355000	-1.635210000
C	-4.577736000	0.243621000	-1.742090000
H	-4.237230000	0.217153000	-2.790155000
C	-5.489155000	1.466528000	-1.578245000
H	-5.842264000	1.479394000	-0.532084000
C	-6.697731000	1.425242000	-2.515010000
H	-6.357149000	1.314828000	-3.549647000
H	-7.354225000	0.583516000	-2.269118000
O	-0.603629000	-0.361735000	1.408151000
C	-0.120854000	-1.070769000	-0.811840000
H	-0.430035000	-0.064576000	-1.075404000
H	-0.914061000	-1.775370000	-1.056809000
C	0.312371000	-1.153853000	0.657378000
H	1.296762000	-0.683031000	0.773244000
I	1.540526000	-1.527167000	-2.246538000
C	0.345799000	-2.586610000	1.181099000
H	1.038038000	-3.205312000	0.599607000
H	0.660160000	-2.590058000	2.229103000
H	-0.661100000	-3.012662000	1.118460000

C	-2.680459000	2.250055000	-0.030520000
C	-1.237411000	2.762941000	0.032033000
C	-0.667669000	2.806689000	-1.404348000
N	0.748331000	3.370141000	-1.551685000
O	-0.429222000	2.060073000	0.936087000
H	-0.640547000	1.070620000	0.936765000
C	0.845347000	4.732627000	-0.934051000
H	0.052354000	5.366085000	-1.337330000
H	0.743650000	4.639747000	0.146971000
H	1.820789000	5.157700000	-1.176957000
C	1.044416000	3.454295000	-3.029638000
H	2.059782000	3.833971000	-3.159143000
H	0.968627000	2.448167000	-3.452505000
H	0.326428000	4.130062000	-3.498365000
C	1.787100000	2.461531000	-0.921564000
H	1.534989000	2.341361000	0.128843000
H	1.756547000	1.500072000	-1.441322000
H	2.763759000	2.929700000	-1.062245000
H	-3.005001000	2.030756000	0.994011000
H	-3.350942000	2.989714000	-0.479372000
H	-1.308012000	3.436331000	-2.030154000
H	-0.628593000	1.816916000	-1.855601000
H	-1.309850000	3.793873000	0.408107000

Zero-point correction= 0.446613 (Hartree/Particle)
Thermal correction to Energy= 0.474820
Thermal correction to Enthalpy= 0.475765
Thermal correction to Gibbs Free Energy= 0.385559
Sum of electronic and zero-point Energies= -1255.895059
Sum of electronic and thermal Energies= -1255.866852
Sum of electronic and thermal Enthalpies= -1255.865908
Sum of electronic and thermal Free Energies= -1255.956113

C	-2.487210000	2.056283000	0.243711000
C	-1.157647000	2.814055000	0.206824000
C	-0.950042000	3.280941000	-1.253809000
N	0.487633000	3.643548000	-1.633579000
O	-0.066109000	2.055765000	0.661298000
H	-0.359015000	1.138470000	0.993985000
C	1.139737000	4.470576000	-0.557760000
H	0.513392000	5.343340000	-0.362593000
H	1.228301000	3.853394000	0.335421000
H	2.122806000	4.787932000	-0.911433000
C	0.445444000	4.430002000	-2.912310000
H	1.467187000	4.618568000	-3.248037000
H	-0.091934000	3.848860000	-3.663480000
H	-0.070661000	5.375421000	-2.735795000
C	1.300509000	2.385161000	-1.868713000
H	1.277193000	1.805615000	-0.950001000
H	0.842348000	1.819061000	-2.680466000
H	2.316945000	2.677768000	-2.139902000
H	-2.613524000	1.602904000	1.234421000
H	-3.326538000	2.732840000	0.040720000
H	-1.558945000	4.169281000	-1.443714000
H	-1.257070000	2.493820000	-1.942373000
H	-1.264934000	3.707018000	0.845122000

Zero-point correction= 0.446688 (Hartree/Particle)
Thermal correction to Energy= 0.474791
Thermal correction to Enthalpy= 0.475736
Thermal correction to Gibbs Free Energy= 0.385237
Sum of electronic and zero-point Energies= -1255.911885
Sum of electronic and thermal Energies= -1255.883782
Sum of electronic and thermal Enthalpies= -1255.882837
Sum of electronic and thermal Free Energies= -1255.973336

TS2

56
7-Me-I TS2 SCF Done: -1444.94049563 A.U.

O	-2.230213000	1.265300000	-0.824887000
O	-4.399922000	3.019062000	0.578655000
H	-3.460763000	3.365289000	0.682423000
C	-3.457753000	0.953684000	-0.349926000
O	-6.633990000	1.137305000	0.997891000
C	-4.387994000	1.726116000	0.246326000
O	-5.270704000	-0.423947000	0.072669000
C	-5.571829000	0.867468000	0.508630000
O	-2.677693000	-1.129934000	-2.417855000
H	-2.779357000	-1.820686000	-3.102950000
O	-4.479222000	-2.928362000	-3.272499000
H	-5.103751000	-2.514707000	-3.889844000
C	-3.943600000	-0.458946000	-0.466009000
H	-3.337881000	-1.157477000	0.130532000
C	-4.008326000	-0.989597000	-1.903409000
H	-4.573351000	-0.264826000	-2.512413000
C	-4.694286000	-2.358579000	-1.974309000
H	-4.216992000	-3.045764000	-1.268336000
H	-5.756166000	-2.278419000	-1.720901000
O	-1.872372000	3.832480000	1.008266000
C	-1.248169000	2.086561000	2.366684000
H	-0.489640000	1.872700000	1.617730000
H	-2.132869000	1.472938000	2.195795000
C	-1.574309000	3.577463000	2.386034000
H	-0.684218000	4.154013000	2.661991000
I	-0.378316000	1.313486000	4.269874000
C	-2.732367000	3.965527000	3.298450000
H	-2.485973000	3.778674000	4.348569000
H	-2.929756000	5.031148000	3.163560000
H	-3.635811000	3.401411000	3.041685000
C	-2.167167000	2.372701000	-1.734966000

I3

56
7-Me-I I3 SCF Done: -1444.96154317 A.U.

O	-2.162227000	1.363923000	-0.510115000
O	-2.723466000	0.164494000	2.292963000
H	-1.781840000	0.482792000	2.189224000
C	-3.054500000	0.396448000	-0.132549000
O	-4.799949000	-1.842864000	1.843603000
C	-3.249443000	-0.109949000	1.101373000
O	-4.625723000	-1.299852000	-0.348438000
C	-4.286874000	-1.172255000	0.988478000
O	-4.145058000	1.341826000	-2.798924000
H	-4.750048000	1.529309000	-3.540854000
O	-6.506469000	0.379806000	-3.746424000
H	-7.223159000	0.804665000	-3.248370000
C	-3.873986000	-0.364439000	-1.138843000
H	-3.229204000	-0.922249000	-1.833162000
C	-4.873155000	0.455809000	-1.960421000
H	-5.511174000	1.019447000	-1.255243000
C	-5.763245000	-0.436373000	-2.832155000
H	-5.135097000	-1.079415000	-3.456804000
H	-6.410999000	-1.068611000	-2.215205000
O	-0.218016000	1.067739000	1.787172000
C	0.146063000	0.194478000	0.935311000
O	1.151419000	0.716522000	0.068514000
O	-0.249760000	-0.951507000	0.761036000
C	0.311806000	-0.498206000	-1.882137000
H	-0.468819000	0.259174000	-1.847454000
H	-0.092319000	-1.466462000	-1.606960000
C	1.545196000	-0.095795000	-1.060952000
H	2.145312000	0.602596000	-1.654640000
I	0.814743000	-0.677436000	-4.054553000
C	2.416453000	-1.276789000	-0.646778000
H	2.776032000	-1.807123000	-1.535162000

C	-0.694607000	2.542123000	-2.075295000
C	-0.174017000	1.270914000	-2.820193000
N	0.819275000	0.354904000	-2.102084000
O	0.071359000	2.802874000	-0.919353000
H	-0.456243000	3.437867000	-0.382401000
C	2.133919000	1.063180000	-1.883039000
H	2.534270000	1.356282000	-2.855943000
H	1.943779000	1.939997000	-1.267788000
H	2.820042000	0.371269000	-1.390653000
C	1.046651000	-0.833906000	-2.996586000
H	1.787482000	-1.486694000	-2.531128000
H	0.101110000	-1.365314000	-3.113145000
H	1.411983000	-0.491778000	-3.966640000
C	0.279790000	-0.158880000	-0.784348000
H	0.113159000	0.694953000	-0.136860000
H	-0.663432000	-0.665321000	-0.983670000
H	1.022446000	-0.843517000	-0.368925000
H	-2.537318000	3.295260000	-1.287258000
H	-2.753249000	2.141640000	-2.636251000
H	0.336870000	1.553518000	-3.744259000
H	-1.020850000	0.625507000	-3.063757000
H	-0.624826000	3.383739000	-2.779900000
C	-1.587359000	5.339447000	0.476139000
O	-1.536428000	5.261517000	-0.749572000
O	-1.468160000	6.145766000	1.371103000
H	3.281847000	-0.920268000	-0.078762000
H	1.839084000	-1.961815000	-0.023598000
C	-2.649262000	2.715520000	-0.557813000
C	-1.612504000	3.628068000	0.111136000
C	-0.264300000	3.408790000	-0.591562000
N	0.934244000	4.194158000	-0.045634000
O	-1.547155000	3.419781000	1.497895000
H	-1.166276000	2.515089000	1.642480000
C	0.691978000	5.668802000	-0.146004000
H	0.468898000	5.925415000	-1.183864000
H	-0.148133000	5.931638000	0.496360000
H	1.587701000	6.198111000	0.185119000
C	2.120092000	3.808985000	-0.891057000
H	2.989294000	4.383074000	-0.563793000
H	2.291409000	2.742162000	-0.746892000
H	1.901939000	4.023913000	-1.938736000
C	1.266244000	3.836046000	1.393322000
H	0.475204000	4.215763000	2.032986000
H	1.297882000	2.749588000	1.480887000
H	2.230623000	4.293200000	1.626180000
H	-3.581112000	2.799822000	0.010070000
H	-2.840907000	2.987633000	-1.600969000
H	-0.341840000	3.685831000	-1.647811000
H	0.027051000	2.363019000	-0.512425000
H	-1.959646000	4.659934000	-0.037528000

Zero-point correction=	0.462170 (Hartree/Particle)
Thermal correction to Energy=	0.493011
Thermal correction to Enthalpy=	0.493956
Thermal correction to Gibbs Free Energy=	0.397402
Sum of electronic and zero-point Energies=	-1444.478325
Sum of electronic and thermal Energies=	-1444.447484
Sum of electronic and thermal Enthalpies=	-1444.446540
Sum of electronic and thermal Free Energies=	-1444.543094

Zero-point correction=	0.464056 (Hartree/Particle)
Thermal correction to Energy=	0.494778
Thermal correction to Enthalpy=	0.495722
Thermal correction to Gibbs Free Energy=	0.399527
Sum of electronic and zero-point Energies=	-1444.497487
Sum of electronic and thermal Energies=	-1444.466765
Sum of electronic and thermal Enthalpies=	-1444.465821
Sum of electronic and thermal Free Energies=	-1444.562016

TS3

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7-Me-I TS3 SCF Done: -1444.95156612 A.U.

O	-2.169556000	0.986530000	-0.116886000
O	-3.300819000	-0.903696000	2.050955000
H	-2.394195000	-0.522129000	2.220934000
C	-3.134718000	0.023441000	-0.208804000
O	-5.316650000	-2.519329000	0.636987000
C	-3.597515000	-0.791236000	0.756413000
O	-4.706958000	-1.351161000	-1.209126000
C	-4.629349000	-1.668094000	0.140554000
O	-3.793858000	2.000587000	-2.319755000
H	-4.260368000	2.508154000	-3.010669000
O	-5.919200000	1.662759000	-3.985398000
H	-6.731583000	1.868700000	-3.495628000
C	-3.806908000	-0.273612000	-1.515118000
H	-3.091475000	-0.611284000	-2.277954000
C	-4.642246000	0.880944000	-2.083492000
H	-5.409333000	1.131040000	-1.329209000
C	-5.333935000	0.496022000	-3.394112000
H	-4.585997000	0.146632000	-4.113058000
H	-6.066000000	-0.302719000	-3.229783000
O	-0.803810000	0.157461000	2.320566000
C	-0.153120000	-0.386609000	1.396263000
O	1.046160000	0.216660000	1.078973000
O	-0.478076000	-1.372429000	0.679352000
C	0.536118000	-0.755296000	-1.030868000
H	-0.306001000	-0.094523000	-1.139670000
H	0.470407000	-1.728742000	-1.493585000
C	1.657246000	-0.424255000	-0.061380000
H	2.320836000	0.335140000	-0.469175000

I4

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7-Me-I I4 SCF Done: -1444.99662988 A.U.

O	-2.203134000	0.978055000	0.159323000
O	-3.377434000	-1.318331000	1.810250000
H	-2.558972000	-0.878348000	2.126455000
C	-3.113374000	0.036486000	-0.212392000
O	-5.062704000	-2.817305000	-0.094019000
C	-3.584227000	-0.981998000	0.525873000
O	-4.395574000	-1.277501000	-1.622280000
C	-4.436027000	-1.823715000	-0.352980000
O	-3.862411000	2.318981000	-1.896182000
H	-4.232853000	2.897453000	-2.589414000
O	-5.487683000	2.100340000	-4.068030000
H	-6.400464000	2.064527000	-3.739246000
C	-3.594725000	-0.077017000	-1.628006000
H	-2.749671000	-0.200024000	-2.318161000
C	-4.498330000	1.064321000	-2.116171000
H	-5.436099000	1.008479000	-1.535234000
C	-4.809453000	0.924205000	-3.608633000
H	-3.870546000	0.886229000	-4.169465000
H	-5.381328000	0.009074000	-3.803970000
O	-0.746146000	-0.112083000	2.312617000
C	-0.148848000	-0.571569000	1.350978000
O	0.934307000	-0.006470000	0.811132000
O	-0.509283000	-1.688688000	0.721733000
C	0.268819000	-1.811024000	-0.498148000
H	-0.344409000	-1.471878000	-1.336954000
H	0.546998000	-2.859279000	-0.614506000
C	1.460531000	-0.874574000	-0.248121000
H	1.634489000	-0.236140000	-1.116341000

I	1.421995000	0.385754000	-3.318895000
C	2.477912000	-1.645800000	0.339091000
H	3.001244000	-2.042889000	-0.537453000
H	3.220135000	-1.359262000	1.089945000
H	1.829795000	-2.421367000	0.753236000
C	-2.587938000	2.173972000	0.568279000
C	-1.391011000	3.118672000	0.675117000
C	-0.710511000	3.176909000	-0.707762000
N	0.580448000	3.996342000	-0.759151000
O	-0.493845000	2.821029000	1.718238000
H	-0.569675000	1.869569000	1.995028000
C	0.477982000	5.244373000	0.069213000
H	-0.407528000	5.803406000	-0.239617000
H	0.406915000	4.958394000	1.118207000
H	1.372860000	5.845715000	-0.101708000
C	0.840466000	4.358651000	-2.198233000
H	1.814088000	4.848617000	-2.264440000
H	0.844223000	3.440353000	-2.790955000
H	0.054578000	5.034506000	-2.540777000
C	1.740328000	3.157389000	-0.264806000
H	1.465885000	2.733832000	0.699073000
H	1.912075000	2.372739000	-1.002627000
H	2.618997000	3.801987000	-0.192453000
H	-2.940838000	1.930027000	1.576959000
H	-3.391619000	2.647974000	-0.005757000
H	-1.403280000	3.616588000	-1.430303000
H	-0.441875000	2.185383000	-1.066127000
H	-1.812451000	4.110637000	0.894204000

Zero-point correction= 0.464067 (Hartree/Particle)
Thermal correction to Energy= 0.493988
Thermal correction to Enthalpy= 0.494932
Thermal correction to Gibbs Free Energy= 0.402217
Sum of electronic and zero-point Energies= -1444.487499
Sum of electronic and thermal Energies= -1444.457578
Sum of electronic and thermal Enthalpies= -1444.456634
Sum of electronic and thermal Free Energies= -1444.549349

I	0.039742000	0.913667000	-3.356324000
C	2.723960000	-1.553447000	0.247390000
H	3.148806000	-2.165587000	-0.555619000
H	3.468658000	-0.809545000	0.545718000
H	2.510947000	-2.201124000	1.105626000
C	-2.695545000	2.099140000	0.905695000
C	-1.545584000	3.100361000	0.990634000
C	-1.047523000	3.347811000	-0.448174000
N	0.276247000	4.099037000	-0.570397000
O	-0.518551000	2.699829000	1.880730000
H	-0.574930000	1.737036000	2.060541000
C	0.362164000	5.233442000	0.406520000
H	-0.512701000	5.874703000	0.279290000
H	0.394040000	4.824279000	1.415666000
H	1.270225000	5.802981000	0.198624000
C	0.366849000	4.630848000	-1.979621000
H	1.350746000	5.084598000	-2.116230000
H	0.234111000	3.792892000	-2.670957000
H	-0.415669000	5.378598000	-2.123088000
C	1.432076000	3.144370000	-0.353085000
H	1.309728000	2.685498000	0.624327000
H	1.387426000	2.391821000	-1.144418000
H	2.359583000	3.718069000	-0.417320000
H	-2.988536000	1.788295000	1.916702000
H	-3.550204000	2.539001000	0.384387000
H	-1.798851000	3.933771000	-0.982861000
H	-0.910719000	2.415687000	-0.997806000
H	-1.961485000	4.034503000	1.393721000

Zero-point correction= 0.465958 (Hartree/Particle)
Thermal correction to Energy= 0.496843
Thermal correction to Enthalpy= 0.497787
Thermal correction to Gibbs Free Energy= 0.401632
Sum of electronic and zero-point Energies= -1444.530672
Sum of electronic and thermal Energies= -1444.499787
Sum of electronic and thermal Enthalpies= -1444.498842
Sum of electronic and thermal Free Energies= -1444.594998

7-Me-I dimeric

I0			
86			
Dimer I0 SCF Done: -2126.54635114 A.U.			
O	-2.986011000	1.412160000	0.671919000
O	-3.943974000	-0.915440000	2.422992000
H	-2.969515000	-0.772202000	2.432700000
C	-4.115898000	0.672465000	0.545151000
O	-6.531420000	-1.684164000	1.318925000
C	-4.494142000	-0.350544000	1.335711000
O	-6.162485000	-0.098357000	-0.239814000
C	-5.807458000	-0.826621000	0.855267000
O	-4.880200000	3.186615000	-1.100431000
H	-5.440749000	3.949062000	-1.350360000
O	-7.482540000	3.740994000	-1.392758000
H	-7.814360000	4.008516000	-0.512866000
C	-5.152635000	0.895171000	-0.528709000
H	-4.758680000	0.705134000	-1.534124000
C	-5.803418000	2.283173000	-0.512525000
H	-6.001203000	2.561526000	0.533580000
C	-7.130559000	2.366414000	-1.279430000
H	-6.995243000	1.987120000	-2.298289000
H	-7.907294000	1.779134000	-0.778828000
I	-0.222439000	-0.777860000	2.540864000
C	-3.155844000	2.704094000	1.299426000
C	-1.928011000	2.967252000	2.155771000
C	-0.671240000	2.826201000	1.297599000

I1			
96			
Dimer I1 SCF Done: -2319.69218944 A.U.			
O	-2.811778000	1.308507000	1.473300000
O	-4.300243000	-0.695619000	3.207428000
H	-3.467519000	-0.273929000	3.540494000
C	-3.949200000	0.629883000	1.163783000
O	-6.578416000	-1.586405000	1.623287000
C	-4.558699000	-0.272579000	1.958125000
O	-5.799573000	-0.201693000	0.022951000
C	-5.741025000	-0.792401000	1.247659000
O	-4.357442000	2.915110000	-1.081418000
H	-4.876514000	3.655662000	-1.456125000
O	-6.937168000	3.477936000	-1.563574000
H	-7.331427000	3.855546000	-0.752440000
C	-4.727217000	0.758695000	-0.130805000
H	-4.134234000	0.467522000	-1.005358000
C	-5.340657000	2.143699000	-0.401279000
H	-5.594576000	2.615003000	0.558132000
C	-6.618781000	2.126475000	-1.251811000
H	-6.432565000	1.610996000	-2.199865000
H	-7.434217000	1.621874000	-0.724520000
O	-1.855653000	0.061470000	4.052594000
C	-1.068010000	-0.988930000	3.410952000
H	-0.120684000	-0.635204000	3.012404000
H	-1.666485000	-1.642028000	2.778232000

N	0.605809000	3.419577000	1.897086000
O	-1.893736000	2.097451000	3.282800000
H	-1.580832000	1.191968000	3.020301000
C	0.585539000	4.920382000	1.767828000
H	0.524729000	5.180925000	0.709614000
H	-0.278183000	5.325606000	2.302016000
H	1.507555000	5.318141000	2.196617000
C	1.761217000	2.848186000	1.116178000
H	2.686937000	3.307474000	1.468298000
H	1.781316000	1.767412000	1.276784000
H	1.612703000	3.069361000	0.057719000
C	0.793501000	3.051845000	3.351158000
H	0.013200000	3.527765000	3.941222000
H	0.731379000	1.966318000	3.447702000
H	1.777579000	3.415900000	3.654551000
H	-4.035167000	2.691644000	1.949021000
H	-3.301993000	3.466780000	0.530975000
H	-0.805656000	3.326679000	0.335624000
H	-0.475425000	1.766507000	1.123335000
H	-2.033065000	3.982772000	2.553142000
O	-5.586223000	3.290679000	5.211935000
O	-5.949073000	4.842412000	2.477749000
H	-5.232025000	5.196325000	3.046796000
C	-6.477006000	3.130005000	4.199010000
O	-8.301433000	3.639506000	1.301736000
C	-6.619515000	3.828967000	3.053716000
O	-8.310402000	2.248258000	3.075342000
C	-7.802166000	3.283211000	2.347191000
O	-5.926102000	0.399929000	5.108522000
H	-5.785940000	-0.569334000	5.079341000
O	-7.077687000	-1.755638000	4.052434000
H	-6.709234000	-1.948047000	3.164656000
C	-7.470185000	1.999705000	4.221357000
H	-8.093950000	1.995428000	5.122066000
C	-6.806801000	0.627657000	4.023354000
H	-6.246822000	0.688555000	3.076037000
C	-7.803100000	-0.539741000	3.941012000
H	-8.484579000	-0.495938000	4.799139000
H	-8.388975000	-0.485682000	3.016611000
I	-2.738764000	6.488536000	3.688650000
C	-4.240752000	2.896577000	4.885265000
C	-3.417501000	2.980228000	6.169421000
C	-3.625101000	4.384697000	6.756969000
N	-2.640690000	4.802607000	7.850451000
O	-2.048069000	2.722404000	5.915701000
H	-1.935634000	2.436548000	4.978214000
C	-2.430839000	3.693433000	8.841853000
H	-3.402192000	3.378134000	9.227805000
H	-1.937809000	2.865189000	8.333703000
H	-1.806998000	4.065951000	9.657002000
C	-3.224930000	6.003556000	8.542557000
H	-2.508164000	6.373135000	9.278704000
H	-3.422871000	6.770998000	7.792029000
H	-4.153886000	5.714193000	9.036906000
C	-1.311176000	5.206977000	7.247792000
H	-0.900652000	4.335649000	6.745629000
H	-1.492130000	5.997997000	6.516680000
H	-0.665395000	5.554545000	8.057469000
H	-3.823174000	3.587907000	4.147763000
H	-4.231230000	1.873941000	4.505614000
H	-4.622937000	4.437568000	7.196001000
H	-3.535336000	5.144795000	5.976772000
H	-3.805939000	2.227625000	6.870018000

C	-1.260528000	-1.018654000	4.862756000
H	-0.428566000	-0.640145000	5.455322000
I	1.696977000	1.440430000	4.423266000
C	-2.250820000	-1.915628000	5.552410000
H	-1.735792000	-2.793336000	5.958521000
H	-2.718068000	-1.372950000	6.381092000
H	-3.033670000	-2.250772000	4.865427000
C	-2.983122000	2.740505000	1.629189000
C	-1.789632000	3.335485000	2.348670000
C	-0.476206000	3.170629000	1.574647000
N	0.448744000	4.388043000	1.658720000
O	-1.657819000	2.874976000	3.684727000
H	-1.325346000	1.954296000	3.683979000
C	-0.099152000	5.513237000	0.821486000
H	-0.214885000	5.165605000	-0.207074000
H	-1.056900000	5.839671000	1.233020000
H	0.606373000	6.345150000	0.859001000
C	1.796695000	3.963316000	1.135758000
H	2.455789000	4.833204000	1.119894000
H	2.195242000	3.194844000	1.803958000
H	1.673464000	3.569507000	0.124703000
C	0.619197000	4.874917000	3.081579000
H	-0.328281000	5.284582000	3.433354000
H	0.948987000	4.030911000	3.690549000
H	1.375990000	5.662118000	3.067817000
H	-3.873743000	2.934963000	2.231095000
H	-3.121946000	3.206595000	0.649894000
H	-0.649601000	3.005354000	0.508332000
H	0.094805000	2.331917000	1.981004000
H	-2.050371000	4.395140000	2.445579000
O	-5.575572000	3.159780000	5.146933000
O	-5.632988000	4.650931000	2.416840000
H	-5.001561000	5.047501000	3.063194000
C	-6.469890000	3.059878000	4.124153000
O	-7.991024000	3.681516000	1.071145000
C	-6.468518000	3.758441000	2.970080000
O	-8.358445000	2.434526000	2.911344000
C	-7.651435000	3.342568000	2.184612000
O	-6.986517000	0.302856000	5.500376000
H	-7.077553000	-0.671590000	5.510122000
O	-8.126015000	-1.605254000	4.000715000
H	-7.503356000	-1.848998000	3.286247000
C	-7.678763000	2.148072000	4.154572000
H	-8.356345000	2.383226000	4.983477000
C	-7.358915000	0.648398000	4.174080000
H	-6.521342000	0.476187000	3.485346000
C	-8.516763000	-0.261037000	3.741011000
H	-9.400576000	-0.059109000	4.356054000
H	-8.769749000	-0.099923000	2.688090000
I	-2.971513000	6.679570000	3.689778000
C	-4.576470000	2.116517000	5.204283000
C	-3.665938000	2.388892000	6.400880000
C	-3.128902000	3.825191000	6.319249000
N	-1.954720000	4.147467000	7.244898000
O	-2.656560000	1.390564000	6.454606000
H	-2.270731000	1.281538000	5.567278000
C	-2.155118000	3.567650000	8.614774000
H	-3.115606000	3.909598000	9.005647000
H	-2.134576000	2.481353000	8.541459000
H	-1.346177000	3.916952000	9.259442000
C	-1.861723000	5.649708000	7.345828000
H	-0.968372000	5.905569000	7.919101000
H	-1.817556000	6.067948000	6.337248000
H	-2.753707000	6.024922000	7.850506000
C	-0.654219000	3.626427000	6.662678000
H	-0.674736000	2.541772000	6.653226000
H	-0.562874000	3.990072000	5.642125000

	H 0.168848000 3.985416000 7.282682000 H -3.973942000 2.138093000 4.290124000 H -5.045281000 1.139517000 5.329615000 H -3.934038000 4.517000000 6.571867000 H -2.787880000 4.064485000 5.313886000 H -4.247790000 2.264687000 7.319803000
Zero-point correction= 0.723947 (Hartree/Particle) Thermal correction to Energy= 0.771068 Thermal correction to Enthalpy= 0.772013 Thermal correction to Gibbs Free Energy= 0.638767 Sum of electronic and zero-point Energies= -2125.822404 Sum of electronic and thermal Energies= -2125.775283 Sum of electronic and thermal Enthalpies= -2125.774339 Sum of electronic and thermal Free Energies= -2125.907584	Zero-point correction= 0.813625 (Hartree/Particle) Thermal correction to Energy= 0.866353 Thermal correction to Enthalpy= 0.867297 Thermal correction to Gibbs Free Energy= 0.725055 Sum of electronic and zero-point Energies= -2318.878565 Sum of electronic and thermal Energies= -2318.825837 Sum of electronic and thermal Enthalpies= -2318.824893 Sum of electronic and thermal Free Energies= -2318.967134

TS1				**I2**			
96				96			
Dimer TS1 SCF Done: -2319.65863300 A.U.				Dimer I2 SCF Done: -2319.67926237 A.U.			
O	-3.140611000	0.543685000	-0.684206000	O	-2.951016000	1.161585000	1.031292000
O	-3.688941000	-1.066663000	1.933038000	O	-4.356112000	-1.129837000	2.558935000
H	-3.011591000	-0.335487000	2.023833000	H	-3.377291000	-0.517438000	3.354878000
C	-4.081878000	-0.408824000	-0.430514000	C	-4.083446000	0.443549000	0.699261000
O	-5.894581000	-2.779106000	1.324091000	O	-6.756991000	-1.717367000	1.030552000
C	-4.253301000	-1.091460000	0.723898000	C	-4.648863000	-0.553776000	1.435334000
O	-5.807315000	-1.939737000	-0.766040000	O	-6.012149000	-0.176493000	-0.438691000
C	-5.372147000	-2.036841000	0.517467000	C	-5.900240000	-0.921830000	0.698801000
O	-5.469444000	0.764091000	-3.121608000	O	-4.520215000	3.111428000	-0.849027000
H	-6.228732000	1.183459000	-3.575437000	H	-5.027986000	3.913859000	-1.087064000
O	-8.140642000	0.594106000	-3.097088000	O	-7.051395000	3.801539000	-1.383562000
H	-8.470596000	1.181257000	-2.388856000	H	-7.440468000	4.008598000	-0.510342000
C	-5.072519000	-0.909028000	-1.464245000	C	-4.929196000	0.781861000	-0.499938000
H	-4.570891000	-1.370913000	-2.322909000	H	-4.412548000	0.651081000	-1.459611000
C	-6.072744000	0.130864000	-1.998918000	C	-5.537445000	2.191786000	-0.464099000
H	-6.275532000	0.869940000	-1.210700000	H	-5.857047000	2.388131000	0.570417000
C	-7.425183000	-0.447282000	-2.439981000	C	-6.755542000	2.406177000	-1.369264000
H	-7.271236000	-1.245123000	-3.173846000	H	-6.513694000	2.123817000	-2.399797000
H	-7.976599000	-0.850007000	-1.584935000	H	-7.604094000	1.805478000	-1.025135000
O	-2.005264000	0.928337000	2.133242000	O	-2.565361000	-0.173489000	3.962527000
C	-0.533678000	0.280465000	1.233113000	C	-1.181790000	-1.215094000	2.326209000
H	-0.530524000	-0.797275000	1.346803000	H	-1.206224000	-0.238873000	1.850483000
C	-0.621359000	1.123820000	2.423271000	H	-1.847703000	-1.893654000	1.795118000
H	-0.315585000	2.164400000	2.279479000	C	-1.508249000	-1.121937000	3.822606000
I	2.086934000	0.613133000	0.123018000	H	-0.645606000	-0.707867000	4.360058000
C	-0.155569000	0.564239000	3.747520000	I	0.885882000	-1.969695000	1.935598000
H	0.937421000	0.596961000	3.804946000	C	-1.911607000	-2.463929000	4.424736000
H	-0.575755000	1.157107000	4.566783000	H	-1.111405000	-3.203754000	4.315849000
H	-0.487006000	-0.473112000	3.864416000	H	-2.138146000	-2.339530000	5.487972000
C	-3.639391000	1.867291000	-0.988380000	H	-2.810860000	-2.829649000	3.917832000
C	-2.498324000	2.856764000	-0.824482000	C	-3.233019000	2.357204000	1.780185000
C	-1.342113000	2.506319000	-1.771171000	C	-1.953449000	2.856706000	2.438420000
N	-0.345585000	3.637850000	-2.028793000	C	-0.885327000	2.975946000	1.345540000
O	-2.053352000	2.946849000	0.518120000	N	0.517494000	3.330131000	1.845257000
H	-2.180834000	2.079684000	1.024916000	O	-1.509138000	2.072594000	3.539707000
C	-1.007695000	4.768648000	-2.772126000	H	-1.996557000	1.162743000	3.600460000
H	-1.442179000	4.376179000	-3.693591000	C	0.462466000	4.372379000	2.934661000
H	-1.785253000	5.222162000	-2.153367000	H	-0.143486000	5.218211000	2.603664000
H	-0.246588000	5.514433000	-3.008559000	H	0.003542000	3.928014000	3.815832000
C	0.771857000	3.066455000	-2.868692000	H	1.484174000	4.689735000	3.153615000
H	1.475472000	3.867879000	-3.101455000	C	1.297401000	3.875862000	0.682518000
H	1.271990000	2.280017000	-2.295660000	H	2.332303000	4.034747000	0.992142000
H	0.346571000	2.663420000	-3.789702000	H	1.259458000	3.154456000	-0.135618000
C	0.251681000	4.164579000	-0.743851000	H	0.851062000	4.821093000	0.369344000
H	-0.536041000	4.624369000	-0.152338000	C	1.209688000	2.090097000	2.362115000
H	0.704639000	3.329557000	-0.204950000	H	0.592184000	1.675064000	3.155161000
H	1.013383000	4.898943000	-1.013800000	H	1.303431000	1.368760000	1.548643000
H	-4.436465000	2.130759000	-0.287430000	H	2.198319000	2.373946000	2.728976000

H	-4.050070000	1.893186000	-2.001040000
H	-1.728535000	2.227082000	-2.755265000
H	-0.750260000	1.677275000	-1.382086000
H	-2.920790000	3.833099000	-1.084613000
H	-0.777783000	0.669509000	0.266499000
O	-5.805367000	3.488401000	2.804346000
O	-6.611719000	3.613747000	-0.274249000
H	-6.023463000	4.354566000	-0.010496000
C	-6.688134000	2.766894000	2.066769000
O	-8.700533000	1.645983000	-0.519557000
C	-7.030320000	2.865690000	0.764274000
O	-8.367905000	1.206593000	1.667770000
C	-8.104100000	1.877500000	0.510121000
O	-5.475050000	0.801398000	3.826437000
H	-5.104156000	-0.053329000	4.127330000
O	-6.234145000	-1.761765000	3.933740000
H	-5.908541000	-2.228023000	3.135188000
C	-7.424279000	1.606885000	2.683015000
H	-7.973488000	1.876584000	3.591410000
C	-6.497809000	0.406312000	2.932723000
H	-6.074154000	0.151149000	1.949735000
C	-7.213125000	-0.829035000	3.502502000
H	-7.786783000	-0.538427000	4.390915000
H	-7.899235000	-1.253601000	2.759893000
I	-4.103375000	6.350383000	-0.462279000
C	-4.424686000	3.312308000	2.434561000
C	-3.579329000	4.217509000	3.331265000
C	-4.175938000	5.633357000	3.261353000
N	-3.319988000	6.752046000	3.856910000
O	-2.217814000	4.166169000	2.945850000
H	-2.165719000	3.946785000	1.986222000
C	-2.797824000	6.367170000	5.210523000
H	-3.637172000	6.068816000	5.841893000
H	-2.100792000	5.538411000	5.089811000
H	-2.287481000	7.227807000	5.647795000
C	-4.199854000	7.967849000	3.971483000
H	-3.601695000	8.805915000	4.334933000
H	-4.602932000	8.193266000	2.982224000
H	-5.011975000	7.756575000	4.669265000
C	-2.158904000	7.099110000	2.947317000
H	-1.517258000	6.224961000	2.882303000
H	-2.558041000	7.339834000	1.959380000
H	-1.635755000	7.954077000	3.381655000
H	-4.279061000	3.618961000	1.394911000
H	-4.125558000	2.271409000	2.576890000
H	-5.124270000	5.645161000	3.802158000
H	-4.353687000	5.924201000	2.222865000
H	-3.638047000	3.842427000	4.359638000

Zero-point correction= 0.811500 (Hartree/Particle)
Thermal correction to Energy= 0.863522
Thermal correction to Enthalpy= 0.864466
Thermal correction to Gibbs Free Energy= 0.721498
Sum of electronic and zero-point Energies= -2318.847133
Sum of electronic and thermal Energies= -2318.795111
Sum of electronic and thermal Enthalpies= -2318.794167
Sum of electronic and thermal Free Energies= -2318.937135

H	-3.980746000	2.134060000	2.544782000
H	-3.627231000	3.129744000	1.113171000
H	-1.186937000	3.771694000	0.659369000
H	-0.786199000	2.046122000	0.784022000
H	-2.169598000	3.863944000	2.813849000
O	-5.523226000	3.227405000	5.292044000
O	-5.748628000	4.784060000	2.514199000
H	-5.049270000	5.150665000	3.096464000
C	-6.350949000	3.069368000	4.220016000
O	-8.075673000	3.648627000	1.271872000
C	-6.443466000	3.779434000	3.074846000
O	-8.198619000	2.269649000	3.051800000
C	-7.624449000	3.272991000	2.332679000
O	-5.754176000	0.319480000	4.885574000
H	-5.500533000	-0.608112000	4.704759000
O	-7.074125000	-1.808066000	3.863400000
H	-6.734893000	-1.951539000	2.954363000
C	-7.365827000	1.955482000	4.189081000
H	-7.992227000	1.925131000	5.087152000
C	-6.734763000	0.582881000	3.899855000
H	-6.265920000	0.675876000	2.909626000
C	-7.755209000	-0.568503000	3.868778000
H	-8.352246000	-0.540002000	4.789355000
H	-8.427135000	-0.452615000	3.008518000
I	-2.718830000	6.603266000	3.615997000
C	-4.150864000	2.869701000	5.065247000
C	-3.358239000	3.149399000	6.339291000
C	-3.626805000	4.608940000	6.731568000
N	-2.705151000	5.202558000	7.797464000
O	-1.979123000	2.899315000	6.129851000
H	-1.820122000	2.606704000	5.197811000
C	-2.542556000	4.258484000	8.952589000
H	-3.530823000	3.986900000	9.328911000
H	-2.014557000	3.371924000	8.601962000
H	-1.967583000	4.757087000	9.735734000
C	-3.336113000	6.486715000	8.264093000
H	-2.666124000	6.972891000	8.976220000
H	-3.491296000	7.127396000	7.393702000
H	-4.291636000	6.262191000	8.741267000
C	-1.346199000	5.532711000	7.215468000
H	-0.901588000	4.602939000	6.871711000
H	-1.493100000	6.205655000	6.367274000
H	-0.750901000	6.006859000	7.999301000
H	-3.739921000	3.496176000	4.268169000
H	-4.084475000	1.808974000	4.813282000
H	-4.644531000	4.686563000	7.119179000
H	-3.524659000	5.265013000	5.863208000
H	-3.723273000	2.480221000	7.130620000

Zero-point correction= 0.811113 (Hartree/Particle)
Thermal correction to Energy= 0.863002
Thermal correction to Enthalpy= 0.863947
Thermal correction to Gibbs Free Energy= 0.720662
Sum of electronic and zero-point Energies= -2318.868150
Sum of electronic and thermal Energies= -2318.816260
Sum of electronic and thermal Enthalpies= -2318.815316
Sum of electronic and thermal Free Energies= -2318.958601

TS2

99

Dimer TS2 SCF Done: -2508.27215629 A.U.

O	-2.756881000	0.935684000	1.233905000
O	-4.299509000	-1.443284000	2.502093000
H	-3.404610000	-1.181498000	2.980673000
C	-3.888822000	0.305851000	0.818915000
O	-6.656076000	-1.760578000	0.856906000
C	-4.533150000	-0.724748000	1.400370000

I3

99

Dimer I3 SCF Done: -2508.27195727 A.U.

O	-2.742770000	0.681940000	1.456529000
O	-4.412262000	-1.144927000	3.253996000
H	-2.927990000	-0.984170000	3.780749000
C	-3.939048000	0.065693000	1.196267000
O	-6.870170000	-1.702785000	1.653052000
C	-4.650048000	-0.728350000	2.042833000

O	-5.801450000	-0.101022000	-0.438222000	O	-5.910519000	-0.402921000	0.083574000
C	-5.771987000	-0.971144000	0.625995000	C	-5.916045000	-1.036654000	1.300954000
O	-4.189963000	3.142826000	0.005247000	O	-4.042212000	2.735708000	-0.066254000
H	-4.625912000	4.007738000	-0.141393000	H	-4.424359000	3.589213000	-0.357343000
O	-6.498769000	4.088121000	-0.958946000	O	-6.288042000	3.703039000	-1.133758000
H	-7.110867000	4.146279000	-0.197312000	H	-6.860427000	3.934944000	-0.373530000
C	-4.692352000	0.817184000	-0.346448000	C	-4.731782000	0.425039000	-0.020017000
H	-4.141738000	0.803151000	-1.294679000	H	-4.234306000	0.205063000	-0.973258000
C	-5.264664000	2.218888000	-0.091361000	C	-5.188242000	1.892918000	0.004484000
H	-5.804433000	2.156888000	0.865910000	H	-5.703008000	2.034654000	0.967407000
C	-6.242621000	2.704448000	-1.169630000	C	-6.151312000	2.283924000	-1.122844000
H	-5.772548000	2.618690000	-2.156258000	H	-5.720058000	2.004203000	-2.091040000
H	-7.157434000	2.101760000	-1.156298000	H	-7.112964000	1.772645000	-1.000895000
O	-2.119394000	-0.887791000	3.686646000	O	-1.949453000	-0.959177000	4.083284000
C	-0.934778000	-1.803821000	1.904582000	C	-1.348239000	-2.147477000	2.116204000
H	-0.691335000	-0.775823000	1.648797000	H	-0.975258000	-1.195934000	1.745314000
H	-1.766348000	-2.158758000	1.295269000	H	-2.333430000	-2.347859000	1.696611000
C	-1.216762000	-1.947563000	3.405932000	C	-1.351234000	-2.187405000	3.647404000
H	-0.277912000	-1.780701000	3.958515000	H	-0.318705000	-2.165425000	4.014053000
I	0.835709000	-2.979172000	1.205578000	I	-0.000185000	-3.673826000	1.210341000
C	-1.791943000	-3.313692000	3.778831000	C	-2.105527000	-3.378083000	4.230587000
H	-1.089623000	-4.116708000	3.533087000	H	-1.659589000	-4.326024000	3.914165000
H	-2.011696000	-3.349476000	4.848525000	H	-2.086402000	-3.324938000	5.323656000
H	-2.728226000	-3.485104000	3.236203000	H	-3.149801000	-3.341512000	3.902097000
C	-2.966566000	1.730277000	2.413843000	C	-2.835563000	1.604206000	2.542344000
C	-1.615807000	2.278728000	2.848567000	C	-1.425754000	2.114657000	2.806840000
C	-1.097222000	3.154050000	1.708624000	C	-1.024473000	2.951414000	1.593039000
N	0.316896000	3.701178000	1.922488000	N	0.454029000	3.346438000	1.538760000
O	-0.691221000	1.268206000	3.179414000	O	-0.502952000	1.066161000	3.019013000
H	-1.219491000	0.448391000	3.450736000	H	-0.993147000	0.314739000	3.452109000
C	0.537110000	4.096249000	3.360106000	C	0.991429000	3.673464000	2.910006000
H	-0.250128000	4.797585000	3.645158000	H	0.365168000	4.454449000	3.344531000
H	0.500838000	3.193794000	3.969855000	H	0.962560000	2.766188000	3.512851000
H	1.517573000	4.572080000	3.432996000	H	2.016995000	4.030774000	2.794511000
C	0.474022000	4.917843000	1.050824000	C	0.567629000	4.566571000	0.666677000
H	1.506775000	5.267391000	1.116487000	H	1.624121000	4.809275000	0.533367000
H	0.237350000	4.639389000	0.022315000	H	0.108160000	4.347677000	-0.298954000
H	-0.218563000	5.687693000	1.399178000	H	0.042345000	5.391663000	1.152886000
C	1.332665000	2.658418000	1.529252000	C	1.257807000	2.218903000	0.941881000
H	1.121257000	1.757410000	2.103123000	H	1.071737000	1.328195000	1.539423000
H	1.226219000	2.459272000	0.461421000	H	0.922379000	2.062323000	-0.084823000
H	2.331003000	3.048981000	1.738865000	H	2.313339000	2.499529000	0.953445000
H	-3.383974000	1.110511000	3.209893000	H	-3.236212000	1.104346000	3.426862000
H	-3.652254000	2.549698000	2.178531000	H	-3.498834000	2.433195000	2.268641000
H	-1.756414000	4.016795000	1.601006000	H	-1.596406000	3.879691000	1.609755000
H	-1.076209000	2.594492000	0.772981000	H	-1.243342000	2.411818000	0.670671000
H	-1.803337000	2.921317000	3.721564000	H	-1.468776000	2.769750000	3.690641000
O	-5.619316000	3.529486000	5.229422000	O	-5.581376000	3.509551000	5.277418000
O	-6.055174000	4.892563000	2.421232000	O	-5.577527000	4.760216000	2.347970000
H	-5.255840000	5.220315000	2.887088000	H	-4.822895000	5.042670000	2.899388000
C	-6.400447000	3.163386000	4.173025000	C	-6.351659000	3.263517000	4.183643000
O	-8.172414000	3.382055000	1.207425000	O	-7.952935000	3.666580000	1.143044000
C	-6.587632000	3.806415000	3.002271000	C	-6.358156000	3.851126000	2.970052000
O	-8.070063000	2.031724000	3.012984000	O	-8.226941000	2.490828000	3.050580000
C	-7.671336000	3.103429000	2.276105000	C	-7.556690000	3.361834000	2.249364000
O	-5.642607000	0.445842000	5.214300000	O	-5.747246000	0.621654000	4.908154000
H	-5.531621000	-0.527538000	5.292196000	H	-5.303694000	-0.189851000	4.555369000
O	-6.573453000	-1.797116000	4.196002000	O	-7.430537000	-1.577387000	4.415480000
H	-5.947382000	-1.942700000	3.457151000	H	-7.142298000	-1.790243000	3.503258000
C	-7.244244000	1.912005000	4.193274000	C	-7.433931000	2.221518000	4.231085000
H	-7.894888000	1.860485000	5.073368000	H	-8.079316000	2.328939000	5.110045000
C	-6.445406000	0.604747000	4.056144000	C	-6.888372000	0.780821000	4.090571000
H	-5.814300000	0.711909000	3.160607000	H	-6.605681000	0.696505000	3.032554000
C	-7.340783000	-0.640958000	3.896657000	C	-7.959096000	-0.274894000	4.413802000
H	-8.148234000	-0.607452000	4.637552000	H	-8.328722000	-0.088279000	5.431107000
H	-7.777655000	-0.677674000	2.894051000	H	-8.803716000	-0.152085000	3.714724000
I	-2.750588000	6.436349000	3.187107000	I	-2.116623000	6.146650000	3.624531000

C	-4.246382000	3.106848000	5.155264000
C	-3.541709000	3.549509000	6.436193000
C	-3.740165000	5.059834000	6.567101000
N	-2.842327000	5.788466000	7.565084000
O	-2.158778000	3.242916000	6.347414000
H	-2.073391000	2.278165000	6.201817000
C	-2.757253000	5.040299000	8.863590000
H	-3.768148000	4.869652000	9.238970000
H	-2.255018000	4.091698000	8.676397000
H	-2.188605000	5.638972000	9.578075000
C	-3.444330000	7.149872000	7.791058000
H	-2.781729000	7.727135000	8.438902000
H	-3.550014000	7.643070000	6.822649000
H	-4.421676000	7.033772000	8.262603000
C	-1.453503000	5.979992000	6.990510000
H	-1.026877000	4.997011000	6.811367000
H	-1.549068000	6.518644000	6.044838000
H	-0.865672000	6.550843000	7.712745000
H	-3.757909000	3.593188000	4.305373000
H	-4.197212000	2.021238000	5.072483000
H	-4.771378000	5.244306000	6.872352000
H	-3.563880000	5.551407000	5.606839000
H	-4.000407000	3.031951000	7.292290000
C	-2.723837000	-0.537788000	5.649176000
O	-3.393669000	-1.472257000	5.908752000
O	-2.187416000	0.511528000	5.832524000

Zero-point correction= 0.825694 (Hartree/Particle)
Thermal correction to Energy= 0.880313
Thermal correction to Enthalpy= 0.881257
Thermal correction to Gibbs Free Energy= 0.732900
Sum of electronic and zero-point Energies= -2507.446462
Sum of electronic and thermal Energies= -2507.391843
Sum of electronic and thermal Enthalpies= -2507.390899
Sum of electronic and thermal Free Energies= -2507.539256

C	-4.191593000	3.167352000	5.172864000
C	-3.474357000	3.666309000	6.430906000
C	-4.002417000	5.062207000	6.791361000
N	-3.311941000	5.753018000	7.972503000
O	-2.068813000	3.630948000	6.223513000
H	-1.873934000	4.208235000	5.448810000
C	-3.217034000	4.828011000	9.153118000
H	-4.210101000	4.433154000	9.375905000
H	-2.534864000	4.015233000	8.907132000
H	-2.835340000	5.390128000	10.007615000
C	-4.149445000	6.949425000	8.337502000
H	-3.660429000	7.492506000	9.148532000
H	-4.239422000	7.590375000	7.458946000
H	-5.136951000	6.610955000	8.655256000
C	-1.925093000	6.238421000	7.605528000
H	-1.304500000	5.369387000	7.405495000
H	-1.993902000	6.847436000	6.702351000
H	-1.537957000	6.820203000	8.444778000
H	-3.745906000	3.658255000	4.302383000
H	-4.098656000	2.085866000	5.094000000
H	-5.057954000	4.980999000	7.054572000
H	-3.895289000	5.741215000	5.942717000
H	-3.672743000	2.964461000	7.244627000
C	-1.503603000	0.703485000	6.291014000
O	-2.632344000	0.640931000	6.595281000
O	-0.368669000	0.791346000	6.026527000

Zero-point correction= 0.826351 (Hartree/Particle)
Thermal correction to Energy= 0.882192
Thermal correction to Enthalpy= 0.883136
Thermal correction to Gibbs Free Energy= 0.730490
Sum of electronic and zero-point Energies= -2507.445606
Sum of electronic and thermal Energies= -2507.389765
Sum of electronic and thermal Enthalpies= -2507.388821
Sum of electronic and thermal Free Energies= -2507.541467

TS3

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Dimer TS3 SCF Done: -2508.26748556 A.U.

O	-2.681262000	0.837038000	0.152752000
O	-4.123799000	-1.694625000	1.228886000
H	-3.178420000	-1.581935000	1.560982000
C	-3.681997000	0.098644000	-0.393209000
O	-6.177954000	-2.261002000	-0.763308000
C	-4.282434000	-1.004182000	0.096635000
O	-5.236206000	-0.598729000	-1.974357000
C	-5.325583000	-1.403856000	-0.869489000
O	-4.307361000	2.880583000	-1.336763000
H	-4.576224000	3.574540000	-1.978586000
O	-6.258540000	3.410188000	-3.014970000
H	-6.977651000	3.472660000	-2.350249000
C	-4.283797000	0.459386000	-1.723234000
H	-3.547551000	0.480992000	-2.535318000
C	-5.116331000	1.749849000	-1.696060000
H	-5.869993000	1.596627000	-0.918809000
C	-5.828764000	2.054085000	-3.024239000
H	-5.125290000	1.958552000	-3.859198000
H	-6.652417000	1.348169000	-3.174769000
O	-1.609192000	-1.298055000	1.943203000
C	-0.916464000	-1.374234000	0.899193000
O	0.356444000	-0.877225000	0.988935000
O	-1.266405000	-1.794673000	-0.241751000
C	-0.043188000	-0.602092000	-1.337028000
H	-0.769255000	0.171693000	-1.158218000
H	-0.147441000	-1.196421000	-2.231838000
C	1.016337000	-0.922984000	-0.298868000

I4

99
Dimer I4 SCF Done: -2508.31443586 A.U.

O	-2.569095000	0.587021000	0.515175000
O	-4.045469000	-1.947267000	1.409562000
H	-3.110689000	-1.877188000	1.710964000
C	-3.560771000	-0.086578000	-0.116264000
O	-6.108495000	-2.362329000	-0.638274000
C	-4.193320000	-1.199617000	0.297632000
O	-5.106384000	-0.662977000	-1.750264000
C	-5.232114000	-1.522527000	-0.696123000
O	-3.970865000	2.691273000	-0.802569000
H	-3.185210000	2.861346000	-1.370085000
O	-5.881784000	3.456297000	-2.720499000
H	-6.719102000	3.354785000	-2.227490000
C	-4.091854000	0.330782000	-1.460394000
H	-3.326210000	0.296240000	-2.242928000
C	-4.786113000	1.707188000	-1.440600000
H	-5.654153000	1.587941000	-0.789737000
C	-5.260927000	2.190610000	-2.815212000
H	-4.389594000	2.311963000	-3.469435000
H	-5.915769000	1.422202000	-3.254013000
O	-1.257671000	-1.579109000	1.839926000
C	-0.744425000	-1.528605000	0.732359000
O	0.363552000	-0.837124000	0.462435000
O	-1.231982000	-2.152406000	-0.339960000
C	-0.520777000	-1.690384000	-1.517550000
H	-1.146770000	-0.961767000	-2.038733000
H	-0.320038000	-2.556372000	-2.149903000
C	0.745054000	-1.037205000	-0.937344000

H	1.765963000	-0.137984000	-0.242028000	H	0.890775000	-0.043301000	-1.365349000
I	1.226668000	1.372616000	-2.764280000	I	-0.837719000	2.128703000	-2.646631000
C	1.694841000	-2.266520000	-0.536712000	C	1.999102000	-1.889014000	-0.995737000
H	2.259112000	-2.232552000	-1.474708000	H	2.315621000	-2.003432000	-2.038205000
H	2.387796000	-2.480222000	0.282235000	H	2.811977000	-1.415002000	-0.437763000
H	0.950608000	-3.064788000	-0.593575000	H	1.816626000	-2.883813000	-0.573590000
C	-3.055199000	1.604187000	1.317009000	C	-2.970884000	1.268382000	1.729376000
C	-1.794683000	2.188205000	1.952344000	C	-1.735982000	1.971942000	2.282544000
C	-0.951237000	2.836459000	0.839601000	C	-1.194987000	2.902072000	1.175061000
N	0.403587000	3.383642000	1.289839000	N	0.230750000	3.410407000	1.353348000
O	-1.072115000	1.289768000	2.765134000	O	-0.770409000	1.073580000	2.803574000
H	-1.242440000	0.351017000	2.508551000	H	-0.945493000	0.160337000	2.500429000
C	0.339854000	4.009216000	2.657580000	C	0.490111000	3.852999000	2.767081000
H	-0.445905000	4.766306000	2.658620000	H	-0.261082000	4.597221000	3.038994000
H	0.137842000	3.223963000	3.385075000	H	0.441596000	2.980335000	3.417074000
H	1.307357000	4.473802000	2.858389000	H	1.485218000	4.301175000	2.805713000
C	0.824696000	4.425519000	0.282733000	C	0.410296000	4.584435000	0.416785000
H	1.837263000	4.752759000	0.528372000	H	1.455844000	4.896944000	0.461669000
H	0.811681000	3.968275000	-0.709509000	H	0.153980000	4.256863000	-0.593513000
H	0.125632000	5.262622000	0.337565000	H	-0.243881000	5.394660000	0.742116000
C	1.422466000	2.271098000	1.294430000	C	1.212936000	2.337006000	0.954769000
H	1.025770000	1.448026000	1.885826000	H	1.031080000	1.460848000	1.570887000
H	1.586298000	1.967027000	0.259231000	H	1.043677000	2.109740000	-0.099937000
H	2.351088000	2.659018000	1.718793000	H	2.221708000	2.728946000	1.103548000
H	-3.587408000	0.973900000	2.039198000	H	-3.378985000	0.557246000	2.455042000
H	-3.711555000	2.415248000	0.989168000	H	-3.743532000	1.996087000	1.472184000
H	-1.513381000	3.679336000	0.432907000	H	-1.832870000	3.788496000	1.130817000
H	-0.728569000	2.139143000	0.033801000	H	-1.206287000	2.411254000	0.202438000
H	-2.143936000	2.995904000	2.609293000	H	-2.073858000	2.594016000	3.122762000
O	-6.074904000	2.737803000	3.377670000	O	-5.846691000	2.773817000	3.300088000
O	-5.875226000	4.178284000	0.567641000	O	-5.801712000	4.250721000	0.491124000
H	-5.211415000	3.806401000	-0.066894000	H	-5.152374000	3.906664000	-0.176552000
C	-6.707168000	2.552406000	2.219810000	C	-6.535588000	2.601919000	2.170567000
O	-8.125945000	2.927363000	-0.920682000	O	-8.058119000	2.914893000	-0.926172000
C	-6.672353000	3.164280000	1.010168000	C	-6.554490000	3.217373000	0.961927000
O	-8.423603000	1.654831000	0.925372000	O	-8.292806000	1.681133000	0.951327000
C	-7.777102000	2.620943000	0.204343000	C	-7.676723000	2.643034000	0.194195000
O	-5.959483000	-0.068887000	2.943728000	O	-5.905656000	-0.096635000	3.027122000
H	-5.641430000	-0.988761000	2.844806000	H	-5.719367000	-1.057297000	2.996808000
O	-7.112761000	-2.340492000	1.949029000	O	-7.118953000	-2.299049000	2.039352000
H	-6.733686000	-2.490971000	1.058291000	H	-6.738088000	-2.514466000	1.162745000
C	-7.679484000	1.404809000	2.137680000	C	-7.521146000	1.461568000	2.149233000
H	-8.372953000	1.362903000	2.982728000	H	-8.189093000	1.465743000	3.016531000
C	-6.935614000	0.067535000	1.936114000	C	-6.830590000	0.096014000	1.979748000
H	-6.456785000	0.156730000	0.948344000	H	-6.309342000	0.156310000	1.012056000
C	-7.874636000	-1.150438000	1.920396000	C	-7.827165000	-1.076486000	1.932776000
H	-8.480201000	-1.145705000	2.835135000	H	-8.487641000	-1.021426000	2.806852000
H	-8.547585000	-1.092452000	1.053619000	H	-8.439323000	-1.016705000	1.024279000
I	-2.682157000	6.310212000	1.518847000	I	-2.391747000	6.628099000	2.413201000
C	-4.970457000	3.656263000	3.484145000	C	-4.913282000	3.860637000	3.444249000
C	-5.420714000	5.005294000	4.079486000	C	-5.609592000	5.128169000	3.999391000
C	-6.219402000	5.781364000	3.022157000	C	-6.183711000	5.947418000	2.832251000
N	-6.674652000	7.188740000	3.416515000	N	-6.779300000	7.311148000	3.196607000
O	-4.311674000	5.718001000	4.582052000	O	-4.751307000	5.871640000	4.836699000
H	-3.684678000	5.874456000	3.831814000	H	-3.938077000	6.094427000	4.316435000
C	-7.333664000	7.185608000	4.764949000	C	-7.674579000	7.204946000	4.396783000
H	-8.129678000	6.438257000	4.770271000	H	-8.421015000	6.429061000	4.214970000
H	-6.583765000	6.947154000	5.518555000	H	-7.062603000	6.951433000	5.261840000
H	-7.749939000	8.176926000	4.954327000	H	-8.166694000	8.166976000	4.552861000
C	-7.661604000	7.636106000	2.370276000	C	-7.578745000	7.768343000	2.004701000
H	-7.959160000	8.665303000	2.579630000	H	-7.960220000	8.772896000	2.197149000
H	-7.180899000	7.573494000	1.392776000	H	-6.925769000	7.772756000	1.130603000
H	-8.533545000	6.980372000	2.396837000	H	-8.406534000	7.076332000	1.841490000
C	-5.518707000	8.168834000	3.427861000	C	-5.700355000	8.339058000	3.467855000
H	-4.827802000	7.869985000	4.211024000	H	-5.154208000	8.032360000	4.354825000
H	-5.007479000	8.120844000	2.465150000	H	-5.015715000	8.364173000	2.619314000
H	-5.925926000	9.165477000	3.611419000	H	-6.186687000	9.306285000	3.612673000

H	-4.476773000	3.806835000	2.524233000
H	-4.275406000	3.199550000	4.191014000
H	-7.131118000	5.229641000	2.780028000
H	-5.632906000	5.893922000	2.109992000
H	-6.056051000	4.778247000	4.942759000

Zero-point correction=	0.828795 (Hartree/Particle)
Thermal correction to Energy=	0.882367
Thermal correction to Enthalpy=	0.883311
Thermal correction to Gibbs Free Energy=	0.737992
Sum of electronic and zero-point Energies=	-2507.438690
Sum of electronic and thermal Energies=	-2507.385119
Sum of electronic and thermal Enthalpies=	-2507.384174
Sum of electronic and thermal Free Energies=	-2507.529494

H	-4.382714000	4.059310000	2.512034000
H	-4.208162000	3.526018000	4.206636000
H	-6.991635000	5.387359000	2.358895000
H	-5.415902000	6.142583000	2.083699000
H	-6.421912000	4.773534000	4.643387000

Zero-point correction=	0.830327 (Hartree/Particle)
Thermal correction to Energy=	0.884786
Thermal correction to Enthalpy=	0.885730
Thermal correction to Gibbs Free Energy=	0.738351
Sum of electronic and zero-point Energies=	-2507.484109
Sum of electronic and thermal Energies=	-2507.429650
Sum of electronic and thermal Enthalpies=	-2507.428705
Sum of electronic and thermal Free Energies=	-2507.576085

7b-I dimeric

I0			
104			
INT0dREALet SCF Done: -2362.44944248 A.U.			
O	-2.956287	1.291052	0.667314
O	-3.934603	-0.917560	2.574955
H	-2.952944	-0.817535	2.560256
C	-4.099460	0.562271	0.606598
O	-6.533578	-1.713269	1.547747
C	-4.483045	-0.406251	1.461280
O	-6.169494	-0.223338	-0.105585
C	-5.808263	-0.891423	1.024860
O	-4.884310	3.023052	-1.102292
H	-5.444850	3.785819	-1.350929
O	-7.494386	3.575437	-1.361952
H	-7.830077	3.849590	-0.484958
C	-5.156424	0.747307	-0.455937
H	-4.785737	0.513515	-1.460855
C	-5.801507	2.138443	-0.477455
H	-5.986952	2.447244	0.562505
C	-7.136784	2.203805	-1.231244
H	-7.009260	1.808505	-2.245190
H	-7.906509	1.622833	-0.713276
I	-0.290588	-0.928068	2.602625
C	-3.093219	2.608354	1.245600
C	-1.856079	2.888204	2.081827
C	-0.598163	2.733417	1.221114
N	0.645588	3.449173	1.741242
O	-1.815996	2.050562	3.232069
H	-1.512509	1.134940	2.992961
C	0.413386	4.963819	1.818870
H	-0.250570	5.142910	2.667469
H	1.387042	5.398800	2.050607
C	1.786804	3.168581	0.762244
H	2.590785	3.859376	1.025906
H	1.411083	3.460745	-0.219903
C	0.984287	2.929824	3.142617
H	0.140597	3.206197	3.772588
H	0.985110	1.839182	3.074766
H	-3.968322	2.640124	1.900124
H	-3.232395	3.343846	0.449481
H	-0.776206	3.119695	0.217690
H	-0.356489	1.673330	1.142231
H	-1.966827	3.913002	2.451323
O	-5.485769	3.473918	5.100624
O	-6.023779	4.797209	2.270307
H	-5.278429	5.205805	2.766450
C	-6.411973	3.210206	4.142683
O	-8.382765	3.442133	1.306058
C	-6.629529	3.814405	2.955656
O	-8.272217	2.197992	3.182252

I1			
114			
INT0dREALetINT1 SCF Done: -2555.60332299 A.U.			
O	-2.936280	1.409490	0.948644
O	-3.965371	-1.180556	2.116765
H	-3.182898	-0.724786	2.524317
C	-4.036161	0.712757	0.557953
O	-6.443282	-1.768673	0.722997
C	-4.448318	-0.445661	1.105513
O	-5.987092	0.059611	-0.529358
C	-5.706328	-0.842349	0.453504
O	-4.807466	3.466620	-0.855368
H	-5.390372	4.248228	-0.948305
O	-7.435619	3.977430	-0.943127
H	-7.736398	4.094136	-0.018809
C	-4.992356	1.112562	-0.547091
H	-4.512872	1.109672	-1.533232
C	-5.690109	2.466721	-0.354800
H	-5.865795	2.619083	0.718201
C	-7.043835	2.614621	-1.061126
H	-6.937273	2.400819	-2.129983
H	-7.783535	1.931460	-0.631365
O	-1.844009	-0.168489	3.447614
C	-0.753060	-1.133657	3.549328
H	0.229868	-0.673041	3.622183
H	-0.858873	-1.981224	2.873695
C	-1.687780	-0.982995	4.666506
H	-1.346522	-0.378376	5.500549
I	1.065574	1.646979	5.666827
C	-2.794715	-1.957424	4.957770
H	-2.478989	-2.626725	5.765948
H	-3.689112	-1.419582	5.286006
H	-3.051735	-2.558469	4.080653
C	-3.231130	2.666347	1.617630
C	-1.971155	3.212848	2.258947
C	-0.778971	3.100344	1.294462
N	0.222427	4.240730	1.394213
O	-1.664744	2.646598	3.515949
H	-1.531509	1.676929	3.440047
C	-0.404225	5.557465	0.907144
H	-1.058964	5.909475	1.708310
H	0.426826	6.260167	0.824962
C	1.418799	3.907135	0.510202
H	2.034768	4.807587	0.481650
H	1.018514	3.749228	-0.493584
C	0.643788	4.416141	2.860995
H	-0.253241	4.747897	3.383514
H	0.889323	3.426632	3.248573
H	-3.978628	2.497198	2.397235
H	-3.625385	3.376935	0.888989

C	-7.826675	3.183381	2.352169
O	-5.749290	0.555745	5.226574
H	-5.565977	-0.406469	5.233403
O	-6.882457	-1.690780	4.325544
H	-6.559839	-1.914333	3.427333
C	-7.369462	2.059147	4.299225
H	-7.948070	2.106790	5.228500
C	-6.679644	0.692984	4.166230
H	-6.159372	0.703447	3.195380
C	-7.646297	-0.500175	4.198299
H	-8.279274	-0.429775	5.091254
H	-8.283964	-0.506423	3.307362
I	-2.927325	6.537113	3.280326
C	-4.144265	3.067190	4.771305
C	-3.317422	3.141796	6.055620
C	-3.413911	4.567925	6.592897
N	-2.636264	4.896346	7.870738
O	-1.964314	2.798326	5.813395
H	-1.876725	2.427920	4.903489
C	-3.007406	3.912783	8.988445
H	-2.908546	4.460616	9.926609
H	-4.068325	3.698133	8.838553
C	-3.129166	6.290902	8.274076
H	-3.117330	6.890780	7.361945
H	-4.174242	6.153956	8.564842
C	-1.123469	4.899292	7.646250
H	-0.874720	3.893843	7.321162
H	-0.681638	5.083648	8.628662
H	-3.727839	3.744611	4.021649
H	-4.143853	2.038060	4.410415
H	-4.460114	4.784449	6.817678
H	-3.082597	5.270059	5.825966
H	-3.770438	2.432613	6.762216
C	2.297388	1.731145	0.732896
H	1.514023	0.994778	0.539995
H	3.032378	1.661853	-0.076047
H	2.795968	1.443618	1.661291
C	-0.181144	5.614082	0.576896
H	0.414857	5.448906	-0.326003
H	-1.213143	5.303113	0.401245
H	-0.219500	6.690244	0.768624
C	2.285126	3.457600	3.735423
H	2.401647	2.986833	4.717078
H	3.167587	3.193828	3.146284
H	2.274458	4.540485	3.890287
C	-0.623068	5.897774	6.610883
H	0.466801	5.792573	6.564968
H	-1.022941	5.697537	5.614177
H	-0.841910	6.939636	6.859464
C	-2.350322	6.987689	9.384112
H	-2.873413	7.921782	9.612875
H	-2.303342	6.406656	10.309952
H	-1.332753	7.247848	9.083757
C	-2.191652	2.623050	9.069965
H	-1.182909	2.805551	9.450069
H	-2.697345	1.964124	9.783484
H	-2.110697	2.098917	8.116986

H	-1.097063	3.048473	0.253792
H	-0.242345	2.181510	1.525406
H	-2.204104	4.259920	2.476525
O	-4.954354	2.960139	5.200768
O	-5.730366	4.608581	2.748001
H	-4.976840	4.963968	3.275598
C	-5.953583	2.705883	4.320981
O	-8.161095	3.425698	1.739432
C	-6.290795	3.518926	3.293979
O	-7.938091	1.914492	3.392612
C	-7.537156	3.012938	2.695488
O	-5.951284	-0.450899	5.244795
H	-5.992483	-1.408254	5.039747
O	-7.062874	-2.095485	3.487355
H	-6.628532	-2.216288	2.618846
C	-6.962093	1.569675	4.404380
H	-7.470227	1.537101	5.374837
C	-6.457462	0.152550	4.061927
H	-5.663857	0.235612	3.306446
C	-7.566998	-0.765875	3.512374
H	-8.420996	-0.751625	4.198907
H	-7.904580	-0.438549	2.525996
I	-2.987574	6.660544	3.722285
C	-4.015918	1.907358	5.537378
C	-3.171467	2.395003	6.719229
C	-2.413713	3.682258	6.375358
N	-1.994139	4.526098	7.582525
O	-2.322120	1.337910	7.140750
H	-1.454473	1.411311	6.684886
C	-3.216684	4.966454	8.386915
H	-3.541495	4.093355	8.956983
H	-2.851140	5.705059	9.102029
C	-1.288193	5.783493	7.064175
H	-1.221170	6.467769	7.912802
H	-1.954024	6.219609	6.318628
C	-1.062113	3.706773	8.477356
H	-1.627926	2.825524	8.778852
H	-0.255695	3.352602	7.831303
H	-3.383053	1.704824	4.672952
H	-4.540768	1.000546	5.837899
H	-3.010783	4.328789	5.733984
H	-1.509286	3.427172	5.824174
H	-3.871356	2.570684	7.544160
C	-0.510373	4.444937	9.690641
H	-1.286803	4.737651	10.403638
H	0.164660	3.755141	10.207314
H	0.073371	5.329970	9.422952
C	-4.369435	5.539865	7.567610
H	-4.858421	4.782027	6.951272
H	-5.110332	5.933206	8.271831
H	-4.059796	6.358137	6.911986
C	0.084666	5.552045	6.448718
H	0.851928	5.308301	7.188135
H	0.082608	4.754686	5.703768
H	0.370015	6.482544	5.947281
C	1.778416	5.403298	3.094298
H	1.974501	5.403218	4.170436
H	2.712113	5.116061	2.602404
H	1.518811	6.425872	2.805629
C	-1.178953	5.489531	-0.404277
H	-0.590547	5.096431	-1.239717
H	-2.106707	4.916908	-0.321787
H	-1.462848	6.516122	-0.657113
C	2.253821	2.706745	0.947948
H	1.703062	1.764767	0.893184
H	3.103030	2.628030	0.261131
H	2.650395	2.812269	1.960468

Zero-point correction= 0.896504 (Hartree/Particle) Thermal correction to Energy= 0.951554 Thermal correction to Enthalpy= 0.952498 Thermal correction to Gibbs Free Energy= 0.802302 Sum of electronic and zero-point Energies= -2361.552939 Sum of electronic and thermal Energies= -2361.497889 Sum of electronic and thermal Enthalpies= -2361.496944 Sum of electronic and thermal Free Energies= -2361.647141	Zero-point correction= 0.986129 (Hartree/Particle) Thermal correction to Energy= 1.046849 Thermal correction to Enthalpy= 1.047793 Thermal correction to Gibbs Free Energy= 0.887943 Sum of electronic and zero-point Energies= -2554.617194 Sum of electronic and thermal Energies= -2554.556474 Sum of electronic and thermal Enthalpies= -2554.555530 Sum of electronic and thermal Free Energies= -2554.715380

TS1				**I2**			
114				114			
INT0dREALetTS1 SCF Done: -2555.56323015 A.U.				INT0dREALetINT2 SCF Done: -2555.58496790 A.U.			
O	-3.147602	0.590832	-0.762862	O	-2.997551	1.205427	1.049988
O	-3.472769	-1.114473	1.818757	O	-4.311567	-0.980991	2.796532
H	-2.816475	-0.356318	1.877523	H	-3.287209	-0.271172	3.511417
C	-4.046410	-0.395002	-0.485437	C	-4.151688	0.480609	0.835586
O	-5.670080	-2.874628	1.303496	O	-6.771709	-1.700098	1.395628
C	-4.120378	-1.121605	0.652524	C	-4.666988	-0.478092	1.657636
O	-5.748399	-1.964569	-0.758294	O	-6.113811	-0.233223	-0.180015
C	-5.224252	-2.091316	0.489535	C	-5.941301	-0.908367	0.992899
O	-5.644668	0.828727	-3.031986	O	-4.673254	2.996306	-0.995228
H	-6.442327	1.248748	-3.413348	H	-5.204162	3.770122	-1.273354
O	-8.305123	0.574274	-2.834130	O	-7.249387	3.637078	-1.369865
H	-8.610226	1.111520	-2.076634	H	-7.561027	3.933149	-0.491643
C	-5.091347	-0.889435	-1.467640	C	-5.040700	0.721254	-0.354640
H	-4.637174	-1.307934	-2.373826	H	-4.555879	0.513408	-1.317746
C	-6.154748	0.135726	-1.897932	C	-5.650189	2.130259	-0.421391
H	-6.328473	0.838975	-1.071044	H	-5.879720	2.447816	0.606130
C	-7.514030	-0.469890	-2.275389	C	-6.942731	2.249836	-1.235866
H	-7.383198	-1.227996	-3.054623	H	-6.789404	1.860219	-2.248079
H	-7.993807	-0.929307	-1.406080	H	-7.754423	1.690716	-0.758799
O	-1.852721	0.919662	1.907420	O	-2.472794	0.152444	4.036137
C	-0.230850	0.507945	1.207851	C	-1.148768	-1.039576	2.448488
H	-0.199823	-0.570849	1.134822	H	-1.350743	-0.164047	1.839230
C	-0.561338	1.140784	2.481865	H	-1.733080	-1.881758	2.080388
H	-0.322543	2.205333	2.554843	C	-1.379205	-0.753342	3.940088
I	2.582334	0.836658	0.723702	H	-0.509907	-0.226944	4.351879
C	-0.293681	0.393074	3.766117	I	0.983796	-1.552674	1.985786
H	0.768753	0.459356	4.021484	C	-1.655404	-2.023373	4.738754
H	-0.887194	0.826054	4.578349	H	-0.822254	-2.730692	4.658768
H	-0.566788	-0.662367	3.659698	H	-1.809654	-1.773247	5.792736
C	-3.697957	1.908708	-0.995216	H	-2.565919	-2.497932	4.356885
C	-2.574878	2.927170	-0.877469	C	-3.205983	2.507868	1.627695
C	-1.477455	2.596092	-1.899360	C	-1.875689	3.026896	2.161900
N	-0.401632	3.661130	-2.104523	C	-0.832464	2.832088	1.051670
O	-2.062565	3.015707	0.440973	N	0.534516	3.479218	1.273810
H	-2.079836	2.116807	0.913464	O	-1.466978	2.415415	3.377969
C	-1.035161	5.031506	-2.363651	H	-1.919906	1.514244	3.515682
H	-1.518039	5.334514	-1.432064	C	0.384077	4.954247	1.662307
H	-0.201276	5.710422	-2.548773	H	-0.108880	4.974107	2.636443
C	0.440137	3.259778	-3.315377	H	1.399476	5.334912	1.786079
H	1.118645	4.094956	-3.498742	C	1.322228	3.387450	-0.029874
H	-0.250644	3.204792	-4.158331	H	2.229704	3.976517	0.119857
C	0.480479	3.754123	-0.847792	H	0.719430	3.896939	-0.782348
H	-0.187454	4.070103	-0.050328	C	1.260168	2.733390	2.401159
H	0.810490	2.741115	-0.613284	H	0.647470	2.883594	3.287136
H	-4.456855	2.130739	-0.239705	H	1.195375	1.672010	2.154898
H	-4.173903	1.951080	-1.978565	H	-3.932258	2.437651	2.441080
H	-1.932653	2.428300	-2.877600	H	-3.593697	3.191831	0.867363
H	-0.967569	1.679809	-1.607473	H	-1.221791	3.234398	0.114659
H	-3.035575	3.893657	-1.101843	H	-0.652455	1.769127	0.910573
H	-0.276723	1.078226	0.300388	H	-2.024670	4.091142	2.371327
O	-5.713057	3.353041	2.956854	O	-5.374363	3.369885	5.355642
O	-6.760910	3.460313	-0.055960	O	-5.606064	4.880184	2.563866
H	-6.167145	4.215186	0.152264	H	-4.911352	5.255127	3.148011
C	-6.606312	2.588682	2.275128	C	-6.239805	3.229922	4.316361
O	-8.765830	1.407291	-0.161896	O	-7.996314	3.779617	1.382919

C	-7.053520	2.685477	1.004389
O	-8.239680	0.955333	1.983769
C	-8.098841	1.651539	0.820631
O	-5.185675	0.635773	3.924698
H	-4.758883	-0.210552	4.170316
O	-5.821320	-1.965097	3.976292
H	-5.536816	-2.388057	3.138956
C	-7.236126	1.385297	2.927322
H	-7.721924	1.616049	3.881403
C	-6.243316	0.222614	3.080457
H	-5.869667	0.016605	2.066451
C	-6.866375	-1.061606	3.649876
H	-7.388052	-0.827948	4.585881
H	-7.583788	-1.489612	2.939913
I	-4.475557	6.299717	-0.571564
C	-4.344172	3.221018	2.527581
C	-3.486614	4.203560	3.332821
C	-4.055472	5.603911	3.080967
N	-3.425439	6.789874	3.805994
O	-2.130066	4.073520	2.949995
H	-2.099479	3.904552	1.981433
C	-3.668233	6.626349	5.301749
H	-4.726251	6.381765	5.412223
H	-3.094986	5.746643	5.600216
C	-4.082294	8.058029	3.250556
H	-3.506709	8.896224	3.650735
H	-3.934465	8.015842	2.169378
C	-1.913479	6.880955	3.562664
H	-1.493735	5.959944	3.961487
H	-1.569674	7.728650	4.158592
H	-4.264537	3.474405	1.466783
H	-3.990316	2.202174	2.701612
H	-5.108470	5.600840	3.360284
H	-4.000566	5.828118	2.013914
H	-3.550879	3.928980	4.391624
C	1.212984	1.952057	-3.173397
H	1.889667	1.933134	-2.314232
H	0.552925	1.083612	-3.104224
H	1.817267	1.828958	-4.078354
C	1.700363	4.657745	-0.954061
H	2.223230	4.576549	0.004098
H	2.408837	4.329782	-1.719345
H	1.452161	5.710755	-1.117703
C	-2.039068	5.103822	-3.507994
H	-1.592488	4.892695	-4.483977
H	-2.903656	4.454515	-3.354942
H	-2.429252	6.125565	-3.524053
C	-5.568671	8.220744	3.545207
H	-6.171015	7.443882	3.068996
H	-5.800037	8.254559	4.613813
H	-5.880474	9.175174	3.109188
C	-1.489449	7.053695	2.109422
H	-0.398235	6.960619	2.083112
H	-1.910116	6.288453	1.456014
H	-1.751450	8.032619	1.701036
C	-3.304028	7.819405	6.179766
H	-3.879832	8.715385	5.933691
H	-3.541478	7.551147	7.214296
H	-2.239530	8.064497	6.145487

Zero-point correction=	0.983392 (Hartree/Particle)
Thermal correction to Energy=	1.043811
Thermal correction to Enthalpy=	1.044756
Thermal correction to Gibbs Free Energy=	0.882277
Sum of electronic and zero-point Energies=	-2554.579838
Sum of electronic and thermal Energies=	-2554.519419
Sum of electronic and thermal Enthalpies=	-2554.518475
Sum of electronic and thermal Free Energies=	-2554.680953

C	-6.331548	3.913433	3.155234
O	-8.125641	2.450021	3.200834
C	-7.536789	3.421211	2.446379
O	-5.692425	0.518958	5.074458
H	-5.418958	-0.402554	4.894478
O	-7.085408	-1.631565	4.192223
H	-6.776082	-1.822839	3.280650
C	-7.289500	2.151284	4.339232
H	-7.906788	2.175655	5.244305
C	-6.696281	0.751468	4.103972
H	-6.253843	0.785631	3.098670
C	-7.738931	-0.378310	4.161183
H	-8.303614	-0.292620	5.098728
H	-8.439031	-0.287098	3.319670
I	-2.541767	6.618466	3.768828
C	-4.007737	3.028064	5.056319
C	-3.183730	3.187505	6.332412
C	-3.391863	4.613897	6.846135
N	-2.832741	4.939098	8.227601
O	-1.818268	2.911866	6.079439
H	-1.660467	2.903063	5.107008
C	-3.395865	3.987069	9.277823
H	-2.944325	3.015719	9.068632
H	-3.006733	4.325662	10.239974
C	-3.242991	6.384263	8.503457
H	-2.893563	6.958582	7.643481
H	-4.333375	6.399531	8.473391
C	-1.307313	4.785206	8.263771
H	-1.113827	3.756223	7.966223
H	-1.020756	4.918718	9.310063
H	-3.614243	3.705807	4.293100
H	-3.957814	1.988307	4.732189
H	-4.457358	4.836286	6.888231
H	-2.940388	5.314191	6.142028
H	-3.555752	2.448897	7.053920
C	-0.536856	5.729854	7.352697
H	0.521352	5.456995	7.427932
H	-0.834090	5.631604	6.305956
H	-0.627064	6.780103	7.644295
C	-2.733725	6.984092	9.807909
H	-3.107229	8.011518	9.864849
H	-3.101408	6.455388	10.692299
H	-1.642507	7.031291	9.852793
C	-4.915602	3.868036	9.317141
H	-5.328946	3.460598	8.391083
H	-5.171266	3.176017	10.126053
H	-5.408079	4.820157	9.535522
C	-0.388332	5.822750	0.677456
H	0.118333	5.932888	-0.285920
H	-1.409476	5.471082	0.515992
H	-0.482022	6.811643	1.134635
C	2.709777	3.138856	2.637172
H	2.820811	4.186925	2.928711
H	3.079351	2.529874	3.468749
H	3.358669	2.939786	1.779423
C	1.661386	1.976310	-0.499617
H	2.281750	1.425707	0.211457
H	0.771931	1.378715	-0.711653
H	2.225796	2.067068	-1.433508

Zero-point correction=	0.983936 (Hartree/Particle)
Thermal correction to Energy=	1.044173
Thermal correction to Enthalpy=	1.045117
Thermal correction to Gibbs Free Energy=	0.882881
Sum of electronic and zero-point Energies=	-2554.601032
Sum of electronic and thermal Energies=	-2554.540795
Sum of electronic and thermal Enthalpies=	-2554.539851
Sum of electronic and thermal Free Energies=	-2554.702087

TS2				**I3**			
117				117			
INT0dREALetTS2 SCF Done: -2744.17437977 A.U.				INT0dREALetINT3 SCF Done: -2744.17336580 A.U.			
O	-2.730922	0.867311	1.224629	O	-2.520521	0.918890	1.630999
O	-4.241954	-1.478534	2.562840	O	-4.234597	-1.003794	3.297468
H	-3.326401	-1.213891	3.006209	H	-2.797435	-0.780949	3.913394
C	-3.872224	0.237640	0.842125	C	-3.658726	0.236181	1.283234
O	-6.659670	-1.796763	0.982736	O	-6.552915	-1.632746	1.526006
C	-4.509272	-0.778377	1.455584	C	-4.397506	-0.588877	2.075241
O	-5.822498	-0.161522	-0.353901	O	-5.527561	-0.298225	0.030615
C	-5.772418	-1.021424	0.720439	C	-5.597786	-0.936853	1.244256
O	-4.147524	3.070268	-0.025834	O	-3.654231	2.835140	-0.199597
H	-4.581492	3.937385	-0.165908	H	-4.030602	3.674464	-0.537885
O	-6.482916	4.023908	-0.923874	O	-5.906194	3.763293	-1.279552
H	-7.077360	4.097270	-0.149773	H	-6.474047	4.019204	-0.523068
C	-4.697907	0.740779	-0.309840	C	-4.357236	0.544256	-0.002866
H	-4.173348	0.700053	-1.272200	H	-3.784458	0.299860	-0.907729
C	-5.238267	2.157701	-0.067141	C	-4.811673	2.008609	-0.069004
H	-5.746702	2.127545	0.908432	H	-5.321243	2.226160	0.880434
C	-6.244618	2.635094	-1.121983	C	-5.771999	2.344876	-1.213959
H	-5.805781	2.530315	-2.121133	H	-5.341491	2.024039	-2.169524
H	-7.163378	2.040751	-1.070735	H	-6.733959	1.841575	-1.068541
O	-2.023309	-0.909118	3.667388	O	-1.838068	-0.698808	4.262220
C	-0.876750	-1.871200	1.888536	C	-1.110846	-1.863939	2.324211
H	-0.623760	-0.852271	1.606311	H	-0.849713	-0.879459	1.947716
H	-1.724417	-2.227299	1.302436	H	-2.057602	-2.183661	1.890658
C	-1.132645	-1.980108	3.397364	C	-1.137648	-1.879247	3.855675
H	-0.182801	-1.806947	3.929033	H	-0.117733	-1.769950	4.240741
I	0.864094	-3.086757	1.179486	I	0.425226	-3.222869	1.455187
C	-1.709995	-3.333031	3.813071	C	-1.805194	-3.121019	4.437657
H	-1.014841	-4.146801	3.582732	H	-1.282781	-4.033520	4.133092
H	-1.918601	-3.336438	4.885711	H	-1.806835	-3.061445	5.530465
H	-2.653011	-3.514522	3.285379	H	-2.844031	-3.167737	4.092827
C	-2.917485	1.663988	2.407368	C	-2.732582	1.845191	2.702274
C	-1.564680	2.248338	2.786970	C	-1.370311	2.444874	3.016917
C	-1.152985	3.152186	1.621763	C	-0.976828	3.328455	1.791910
N	0.237746	3.783872	1.709198	N	0.407615	3.164647	1.182439
O	-0.603091	1.254659	3.059699	O	-0.428307	1.433279	3.322148
H	-1.104484	0.436107	3.367913	H	-0.922409	0.662630	3.710822
C	0.468867	4.222991	3.160480	C	1.503945	3.297416	2.241185
H	0.714454	3.307247	3.701265	H	1.324251	2.479167	2.936460
H	-0.501648	4.581538	3.507151	H	2.447523	3.113719	1.722655
C	0.248548	5.007823	0.795828	C	0.526761	4.261145	0.131315
H	1.266796	5.398239	0.809896	H	-0.311144	4.113446	-0.551522
H	-0.411362	5.734640	1.277402	H	0.355507	5.204923	0.651267
C	1.240392	2.718762	1.259185	C	0.542444	1.771527	0.543943
H	0.989434	1.836120	1.847899	H	0.284283	1.086175	1.347795
H	0.988250	2.505607	0.219107	H	1.602260	1.651519	0.306905
H	-3.292390	1.039419	3.219680	H	-3.149996	1.324144	3.565825
H	-3.631955	2.464162	2.193565	H	-3.432986	2.629246	2.388256
H	-1.865878	3.976418	1.565586	H	-1.069270	4.375940	2.080551
H	-1.189569	2.585814	0.693444	H	-1.680406	3.151290	0.979189
H	-1.728974	2.864437	3.680337	H	-1.478896	3.117088	3.879673
O	-5.469289	3.591674	5.223337	O	-5.637810	3.524125	5.333707
O	-6.012138	4.894052	2.386767	O	-5.329832	4.794578	2.413698
H	-5.208719	5.260765	2.819337	H	-4.671064	5.132209	3.053915
C	-6.286641	3.211181	4.199461	C	-6.294273	3.302956	4.165705
O	-8.131922	3.327146	1.274399	O	-7.586329	3.728673	0.982732
C	-6.512241	3.821790	3.017745	C	-6.177464	3.896254	2.958962
O	-7.975317	2.031183	3.116768	O	-8.052788	2.544917	2.846457
C	-7.605255	3.084989	2.339631	C	-7.301398	3.417505	2.121845
O	-5.455024	0.550532	5.288443	O	-5.746330	0.664975	4.900713
H	-5.340007	-0.418695	5.405516	H	-5.254573	-0.123716	4.564236
O	-6.389885	-1.741263	4.395760	O	-7.361868	-1.539571	4.230656
H	-5.777305	-1.903977	3.647825	H	-6.993803	-1.732906	3.343637
C	-7.116471	1.953723	4.275969	C	-7.378525	2.263917	4.095464
H	-7.742225	1.918013	5.174879	H	-8.106648	2.359678	4.908444

C	-6.301691	0.654887	4.155249
H	-5.704562	0.740464	3.234387
C	-7.182038	-0.609142	4.070796
H	-7.970576	-0.556971	4.830889
H	-7.644714	-0.692502	3.082459
I	-2.797005	6.534607	3.041804
C	-4.083660	3.236927	5.060600
C	-3.331651	3.656195	6.324322
C	-3.491936	5.162166	6.465715
N	-2.951876	5.825192	7.726889
O	-1.953949	3.342972	6.185142
H	-1.874563	2.374589	6.068360
C	-3.511551	5.155137	8.976643
H	-3.072214	4.155950	8.995838
H	-3.106553	5.704821	9.828453
C	-3.382354	7.288977	7.629086
H	-3.032010	7.635115	6.654530
H	-4.472420	7.280943	7.588494
C	-1.424125	5.707161	7.806574
H	-1.220225	4.638266	7.779077
H	-1.146219	6.102645	8.786474
H	-3.663669	3.765514	4.199612
H	-3.995543	2.157080	4.945208
H	-4.552747	5.403923	6.416199
H	-3.014103	5.651353	5.615672
H	-3.778764	3.117754	7.173183
C	-2.554927	-0.474475	5.638256
O	-3.213850	-1.397583	5.960711
O	-2.014089	0.581214	5.757409
C	2.716944	3.066231	1.385981
H	3.038532	3.133149	2.428093
H	3.281508	2.248800	0.925184
H	2.993949	3.988765	0.866228
C	-0.208659	4.760912	-0.638725
H	0.421991	4.043550	-1.172568
H	-1.249064	4.432227	-0.697289
H	-0.137322	5.716723	-1.168014
C	1.483427	5.337267	3.403791
H	2.476892	5.143511	2.997533
H	1.124458	6.298731	3.027894
H	1.584263	5.435620	4.490385
C	-0.657058	6.406727	6.692839
H	0.402336	6.165686	6.832494
H	-0.951568	6.059252	5.699964
H	-0.753398	7.495671	6.721091
C	-2.893635	8.198324	8.748532
H	-3.263862	7.897583	9.733164
H	-1.803645	8.271908	8.788097
H	-3.280785	9.202433	8.548357
C	-5.031873	5.074152	9.058249
H	-5.467659	4.493265	8.241407
H	-5.285516	4.567650	9.995014
H	-5.505272	6.059806	9.083082
Zero-point correction=			0.998579 (Hartree/Particle)
Thermal correction to Energy=			1.061218
Thermal correction to Enthalpy=			1.062162
Thermal correction to Gibbs Free Energy=			0.896198
Sum of electronic and zero-point Energies=			-2743.175801
Sum of electronic and thermal Energies=			-2743.113162
Sum of electronic and thermal Enthalpies=			-2743.112218
Sum of electronic and thermal Free Energies=			-2743.278182

C	-6.813829	0.826722	3.990490
H	-6.439905	0.756031	2.960020
C	-7.899186	-0.240186	4.207723
H	-8.351819	-0.073791	5.194340
H	-8.685375	-0.111501	3.444250
I	-2.237209	6.323826	4.024376
C	-4.234217	3.218533	5.347440
C	-3.642705	3.671593	6.685669
C	-4.232521	5.038930	7.061213
N	-3.646761	5.725631	8.304196
O	-2.224414	3.670306	6.598461
H	-1.970248	4.283924	5.873796
C	-3.611591	4.694424	9.429367
H	-4.618862	4.268755	9.465686
H	-2.927056	3.916995	9.090332
C	-4.596369	6.859899	8.671673
H	-4.148375	7.383837	9.514419
H	-5.512946	6.380444	9.027830
C	-2.231164	6.257662	7.985799
H	-1.574724	5.396283	8.093832
H	-2.238420	6.518884	6.926094
H	-3.725459	3.756404	4.542849
H	-4.108473	2.143499	5.234997
H	-5.301118	4.917826	7.246632
H	-4.094085	5.731658	6.231891
H	-3.892661	2.922861	7.439803
C	-1.577072	0.782680	6.575400
O	-2.717727	0.678505	6.819464
O	-0.431806	0.901444	6.377112
C	-3.191174	5.181846	10.810949
H	-3.812917	5.995876	11.192635
H	-3.303977	4.336700	11.497933
H	-2.143246	5.486267	10.841838
C	-4.901877	7.830487	7.532474
H	-3.999975	8.185900	7.027066
H	-5.558283	7.392999	6.777632
H	-5.415410	8.698393	7.958218
C	-1.738514	7.452752	8.795745
H	-2.294998	8.368246	8.579582
H	-1.732213	7.293065	9.875506
H	-0.703889	7.629422	8.482848
C	-0.321177	1.526087	-0.687238
H	-0.232205	0.461179	-0.927936
H	-1.378972	1.730162	-0.508874
H	0.016168	2.089698	-1.562937
C	1.847191	4.295974	-0.627480
H	2.696691	4.526956	0.021404
H	2.052675	3.361930	-1.157350
H	1.781126	5.091862	-1.376233
C	1.536795	4.634165	2.971654
H	0.591017	4.872552	3.466322
H	2.306058	4.562475	3.747872
H	1.805496	5.472034	2.320915
Zero-point correction=			0.999380 (Hartree/Particle)
Thermal correction to Energy=			1.063164
Thermal correction to Enthalpy=			1.064108
Thermal correction to Gibbs Free Energy=			0.894151
Sum of electronic and zero-point Energies=			-2743.173986
Sum of electronic and thermal Energies=			-2743.110202
Sum of electronic and thermal Enthalpies=			-2743.109258
Sum of electronic and thermal Free Energies=			-2743.279215

TS3			
117			
INT0dREALetTS3 SCF Done: -2744.12783185 A.U.			
O	-3.003588	1.332642	0.225353
O	-4.680831	-0.489223	2.077597

I4			
117			
INT0dREALetINT4 SCF Done: -2744.21786791 A.U.			
O	-2.479384	0.416195	0.608759
O	-4.073153	-2.071816	1.407646

H	-3.887409	-0.028950	2.463613
C	-3.999721	0.454729	-0.086939
O	-6.279473	-2.119382	0.282247
C	-4.675994	-0.352806	0.751940
O	-5.350101	-0.912708	-1.393225
C	-5.535484	-1.236078	-0.071018
O	-3.906938	2.224942	-2.553804
H	-4.175559	2.686042	-3.372226
O	-5.662346	1.888376	-4.571550
H	-6.538155	2.237281	-4.341082
C	-4.348369	0.115447	-1.511330
H	-3.480134	-0.304919	-2.037400
C	-4.927632	1.248608	-2.361353
H	-5.784293	1.684255	-1.818245
C	-5.398114	0.756369	-3.735381
H	-4.586743	0.208688	-4.225226
H	-6.263331	0.091618	-3.641932
O	-2.388247	0.621058	2.991626
C	-1.518401	-0.077039	2.416242
O	-0.219517	0.148443	2.792119
O	-1.680846	-0.926120	1.495672
C	0.155971	-0.958245	0.717729
H	-0.160625	-0.112676	0.134823
H	0.042961	-1.935554	0.273311
C	0.674451	-0.795676	2.135143
H	1.641671	-0.297404	2.147699
I	2.488324	-0.537053	-0.696571
C	0.726130	-2.108336	2.908079
H	1.405556	-2.805122	2.406732
H	1.104030	-1.927094	3.919089
H	-0.270163	-2.555381	2.982040
C	-3.364828	2.704769	0.436541
C	-2.087012	3.428814	0.876771
C	-0.984835	3.055882	-0.135448
N	0.420821	3.613866	0.070113
O	-1.749411	3.171231	2.223450
H	-2.040498	2.262126	2.480626
C	0.407644	5.129916	0.268314
H	-0.358417	5.509565	-0.411107
H	1.372811	5.490236	-0.094222
C	1.237550	3.283095	-1.192160
H	2.244784	3.647314	-0.989148
H	1.290311	2.191662	-1.242599
C	1.072996	2.874639	1.247954
H	0.446262	3.086812	2.109113
H	0.965238	1.815563	1.014098
H	-4.111059	2.787518	1.236245
H	-3.758735	3.131405	-0.491096
H	-1.320707	3.387434	-1.118076
H	-0.873278	1.974205	-0.173498
H	-2.292959	4.504025	0.802522
O	-2.792565	-1.904362	6.408354
O	-4.342111	-3.270080	8.636862
H	-3.658919	-2.608069	8.893258
C	-3.467508	-3.084643	6.356640
O	-5.468024	-5.703144	7.417439
C	-4.141831	-3.655899	7.370570
O	-4.358663	-5.067330	5.544837
C	-4.747515	-4.913961	6.865781
O	-2.809999	-2.586008	3.396906
H	-2.953854	-2.449429	2.440710
O	-4.248118	-3.818498	1.474397
H	-5.103805	-3.360230	1.386903
C	-3.464648	-4.007209	5.164277
H	-2.465360	-4.439411	5.007491
C	-3.897013	-3.399393	3.828459
H	-4.800693	-2.785298	3.972217

H	-3.139256	-2.053513	1.717418
C	-3.496744	-0.185808	-0.052118
O	-6.158414	-2.305774	-0.653709
C	-4.186574	-1.278069	0.322318
O	-5.091861	-0.593385	-1.683891
C	-5.245605	-1.503324	-0.675118
O	-3.786072	2.658206	-0.578614
H	-2.980983	2.761523	-1.132521
O	-5.925994	3.481031	-2.381760
H	-6.868469	3.230045	-2.287206
C	-4.027303	0.335060	-1.356567
H	-3.278892	0.314506	-2.156232
C	-4.651442	1.745212	-1.228570
H	-5.508053	1.629353	-0.561131
C	-5.145332	2.294326	-2.570233
H	-4.281374	2.566146	-3.185950
H	-5.725222	1.527315	-3.097392
O	-1.263874	-1.767426	1.977283
C	-0.723811	-1.681792	0.884035
O	0.397575	-0.994893	0.665391
O	-1.192493	-2.262318	-0.220351
C	-0.452740	-1.766871	-1.366232
H	-1.070453	-1.032627	-1.889217
H	-0.226536	-2.616641	-2.012179
C	0.792747	-1.114790	-0.739131
H	0.917383	-0.096831	-1.114879
I	-0.715007	2.027216	-2.510057
C	2.068534	-1.930017	-0.830361
H	2.393929	-1.983779	-1.874988
H	2.865453	-1.462723	-0.244113
H	1.910527	-2.948925	-0.458878
C	-2.866613	0.979894	1.883200
C	-1.671863	1.744409	2.441692
C	-1.221380	2.753444	1.365180
N	0.138269	3.417408	1.550191
O	-0.627172	0.897677	2.893939
H	-0.832285	-0.036755	2.692933
C	0.367824	3.838290	2.990635
H	0.373690	2.913741	3.570251
H	1.369491	4.265306	3.032148
C	0.111842	4.620276	0.594345
H	-0.154774	4.202538	-0.380297
H	-0.711651	5.257774	0.917016
C	1.199751	2.394792	1.087055
H	0.812264	1.422930	1.380697
H	1.187471	2.457959	-0.003439
H	-3.172484	0.189319	2.575384
H	-3.714110	1.645656	1.719576
H	-1.967140	3.548098	1.303837
H	-1.172072	2.274352	0.387975
H	-2.040571	2.295307	3.318307
O	-6.004535	2.976248	2.928999
O	-6.240652	4.399646	0.138055
H	-5.915111	4.188150	-0.783581
C	-6.754285	2.723439	1.848616
O	-8.375738	2.801287	-1.210750
C	-6.885908	3.318111	0.638363
O	-8.495485	1.652437	0.732998
C	-7.967810	2.618042	-0.078945
O	-5.983889	0.072595	2.825124
H	-5.809045	-0.890605	2.868103
O	-7.163583	-2.206569	2.016654
H	-6.788185	-2.462992	1.148729
C	-7.680073	1.536338	1.917422
H	-8.325690	1.553600	2.802166
C	-6.944672	0.188070	1.798062
H	-6.455462	0.207359	0.812578

C	-4.180582	-4.451531	2.749583
H	-3.341913	-5.154442	2.697102
H	-5.089654	-5.015609	2.989165
I	-1.499476	-1.156052	9.847817
C	-3.473248	-0.776074	5.823415
C	-2.750715	0.500553	6.271061
C	-1.247051	0.211061	6.182111
N	-0.261488	1.379594	6.316856
O	-3.165750	0.952842	7.539119
H	-2.868842	0.307688	8.226179
C	-0.637249	2.457022	5.315925
H	-0.850543	1.936783	4.384115
H	-1.568630	2.893386	5.671535
C	1.107799	0.812058	5.934617
H	1.824303	1.620215	6.090992
H	1.051017	0.601677	4.863856
C	-0.168856	1.916890	7.764371
H	-0.357908	1.057560	8.413269
H	0.871578	2.224688	7.893989
H	-4.508329	-0.729038	6.180310
H	-3.448696	-0.866418	4.736131
H	-1.029945	-0.240008	5.213515
H	-0.997048	-0.493775	6.972891
H	-3.046061	1.276856	5.557984
C	0.731522	3.873464	-2.503159
H	1.471580	3.619733	-3.269019
H	-0.220821	3.448354	-2.829445
H	0.647672	4.964107	-2.479000
C	2.545443	3.187110	1.486311
H	2.810742	2.769744	2.463507
H	3.193160	2.705623	0.749764
H	2.765359	4.258390	1.519658
C	0.172567	5.640725	1.688737
H	-0.728412	5.240084	2.151834
H	1.016550	5.420396	2.346378
H	0.078063	6.730127	1.629410
C	1.537607	-0.428756	6.713678
H	0.970675	-1.317391	6.429037
H	2.592486	-0.615082	6.485077
H	1.441165	-0.306327	7.795620
C	-1.102731	3.059081	8.140267
H	-0.874611	3.995762	7.621730
H	-2.145343	2.777921	7.990269
H	-0.960221	3.230559	9.212785
C	0.408325	3.545580	5.096687
H	0.746360	4.004612	6.029978
H	1.284755	3.178654	4.553973
H	-0.056106	4.325326	4.485486
Zero-point correction=			0.998967 (Hartree/Particle)
Thermal correction to Energy=			1.061748
Thermal correction to Enthalpy=			1.062692
Thermal correction to Gibbs Free Energy=			0.895725
Sum of electronic and zero-point Energies=			-2743.128864
Sum of electronic and thermal Energies=			-2743.066084
Sum of electronic and thermal Enthalpies=			-2743.065139
Sum of electronic and thermal Free Energies=			-2743.232107

C	-7.908365	-1.013033	1.844147
H	-8.556154	-0.921025	2.724650
H	-8.535932	-1.029389	0.944957
I	-2.717933	7.318413	1.039939
C	-4.851282	3.840979	2.841975
C	-5.150101	5.177649	3.545657
C	-6.043363	6.003499	2.614255
N	-6.670006	7.272849	3.175720
O	-3.955903	5.820151	3.931209
H	-3.512806	6.194790	3.125218
C	-7.423773	6.988630	4.469449
H	-6.658714	6.800790	5.225398
H	-7.931871	7.917536	4.735404
C	-7.650709	7.798789	2.125925
H	-8.090022	8.703219	2.550812
H	-8.440610	7.050289	2.046974
C	-5.564940	8.304111	3.459477
H	-4.973330	7.873302	4.266353
H	-4.918841	8.312335	2.579388
H	-4.531662	3.976086	1.805191
H	-4.067179	3.342698	3.414939
H	-6.873397	5.394416	2.262791
H	-5.455164	6.297220	1.745757
H	-5.669151	4.922601	4.475974
C	-7.046218	8.058868	0.749301
H	-6.166817	8.706867	0.782976
H	-6.771299	7.130845	0.242370
H	-7.811075	8.556704	0.144052
C	-0.637040	4.845374	3.539928
H	-0.602449	5.805810	3.020286
H	-1.671061	4.495760	3.511693
H	-0.385289	5.022817	4.591108
C	1.392679	5.431345	0.491669
H	1.743722	5.805292	1.458869
H	2.200943	4.885499	-0.001470
H	1.157474	6.304451	-0.125343
C	2.606919	2.555106	1.651688
H	2.649611	2.328905	2.720796
H	3.236752	1.818342	1.140403
H	3.048610	3.538400	1.479425
C	-8.422045	5.833468	4.426739
H	-9.224308	5.990093	3.700913
H	-7.946656	4.871297	4.221278
H	-8.887931	5.766417	5.415318
C	-6.043669	9.709859	3.794174
H	-6.526090	10.205615	2.947085
H	-6.711603	9.753581	4.660427
H	-5.152171	10.295328	4.041108
Zero-point correction=			1.003542 (Hartree/Particle)
Thermal correction to Energy=			1.065868
Thermal correction to Enthalpy=			1.066813
Thermal correction to Gibbs Free Energy=			0.902150
Sum of electronic and zero-point Energies=			-2743.214326
Sum of electronic and thermal Energies=			-2743.151999
Sum of electronic and thermal Enthalpies=			-2743.151055
Sum of electronic and thermal Free Energies=			-2743.315718

I0 (isomer plane)			
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INT0det SCF Done: -2362.43479391 A.U.			
O	-3.823625	1.629528	0.986012
O	-3.665590	-1.228977	1.931523
H	-3.283197	-0.521836	2.512106
C	-4.368737	0.549654	0.384653
O	-5.113219	-2.804100	-0.047625
C	-4.319187	-0.702856	0.873395
O	-5.566592	-0.831651	-1.054413

C	-5.018724	-1.596202	-0.055344
O	-6.024755	2.762283	-0.827486
H	-6.788736	3.271618	-1.156834
O	-8.355734	2.196478	-2.107144
H	-9.034100	1.976305	-1.448665
C	-5.191083	0.544280	-0.885050
H	-4.601399	0.826825	-1.766886
C	-6.451865	1.410925	-0.845938
H	-7.014084	1.161295	0.070894
C	-7.350623	1.179632	-2.066943
H	-6.764661	1.306328	-2.983002
H	-7.774942	0.169415	-2.060487
I	-1.701558	0.564216	4.151088
C	-3.203026	2.649442	0.186500
C	-1.674048	2.599247	0.336496
C	-1.157094	1.216603	-0.095039
N	0.363318	0.983585	-0.169156
O	-1.256306	3.001011	1.619233
H	-1.615608	2.389771	2.303731
C	1.082000	2.159895	-0.823433
H	0.427681	2.471478	-1.642856
H	1.984313	1.747668	-1.276300
C	0.503087	-0.240973	-1.094135
H	-0.284523	-0.928029	-0.778097
H	0.238968	0.132863	-2.088976
C	0.861291	0.673304	1.251189
H	0.416479	1.447862	1.869497
H	0.378742	-0.271736	1.512254
H	-3.552003	3.606137	0.578436
H	-3.510482	2.576392	-0.859243
H	-1.540650	0.997201	-1.094605
H	-1.538703	0.451124	0.580646
H	-1.293514	3.363951	-0.352238
O	-0.553221	-3.045230	1.949998
O	1.006122	-5.691515	2.352942
H	1.888788	-5.224473	2.367438
C	-0.260269	-4.038200	1.073537
O	0.727360	-7.065270	-0.292265
C	0.363122	-5.213871	1.246398
O	-0.318997	-5.162982	-0.961907
C	0.322231	-5.965062	-0.030315
O	-2.051380	-1.999127	-0.289097
H	-2.208107	-1.972921	0.671232
O	-3.544124	-2.803892	-2.531150
H	-4.239920	-3.115538	-1.925665
C	-0.594580	-3.877391	-0.387662
H	0.105059	-3.161538	-0.839940
C	-2.010223	-3.368154	-0.693149
H	-2.761215	-3.944469	-0.136221
C	-2.328594	-3.436462	-2.188714
H	-1.542172	-2.908798	-2.744132
H	-2.296933	-4.491988	-2.497116
I	3.519077	-3.301465	2.010111
C	-1.402722	-3.372846	3.088942
C	-0.658430	-3.646042	4.407781
C	0.559646	-2.716844	4.468084
N	1.224252	-2.528699	5.833146
O	-0.363361	-5.007635	4.634678
H	0.140840	-5.354089	3.864488
C	0.234409	-1.828786	6.764314
H	-0.188149	-0.996385	6.198192
H	-0.568802	-2.546896	6.937363
C	2.480439	-1.681914	5.611665
H	3.039383	-1.720297	6.550002
H	3.056541	-2.199267	4.841386
C	1.633988	-3.860267	6.469180
H	0.713802	-4.431521	6.581774

H	2.024007	-3.604620	7.456240
H	-2.023866	-4.240309	2.846232
H	-2.032175	-2.492130	3.209772
H	0.251506	-1.720679	4.150673
H	1.332467	-3.064991	3.781461
H	-1.382618	-3.376134	5.185338
C	2.235306	-0.241900	5.177410
H	3.217509	0.215167	5.017540
H	1.686981	-0.179626	4.236374
H	1.698514	0.355033	5.918394
C	0.792787	-1.346334	8.099166
H	-0.029061	-0.857393	8.632357
H	1.156853	-2.158471	8.734467
H	1.589125	-0.606942	7.983546
C	2.656667	-4.680183	5.696182
H	2.793552	-5.620358	6.241061
H	2.314471	-4.927593	4.693021
H	3.630608	-4.193780	5.613484
C	1.848111	-0.952916	-1.127719
H	2.085890	-1.475049	-0.197837
H	1.777732	-1.714933	-1.912205
H	2.686920	-0.302413	-1.391740
C	2.382788	0.595893	1.462870
H	2.656607	1.225107	2.314656
H	2.704548	-0.426158	1.677167
H	2.967603	0.940529	0.608747
C	1.448630	3.343056	0.072553
H	0.628135	3.681427	0.703978
H	2.293130	3.108352	0.722561
H	1.754595	4.166591	-0.581726

Zero-point correction= 0.894898 (Hartree/Particle)
Thermal correction to Energy= 0.950630
Thermal correction to Enthalpy= 0.951574
Thermal correction to Gibbs Free Energy= 0.801640
Sum of electronic and zero-point Energies= -2361.539896
Sum of electronic and thermal Energies= -2361.484164
Sum of electronic and thermal Enthalpies= -2361.483220
Sum of electronic and thermal Free Energies= -2361.633154

7-Me-I tetramer

I1

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INT1q SCF Done: -4253.14559194 A.U.

O	-3.543811	-0.226755	2.811847
O	-2.749782	-2.990270	1.838715
H	-2.457175	-2.736483	2.754666
C	-3.966953	-0.849487	1.690493
O	-4.142175	-3.360704	-0.686738
C	-3.632425	-2.103259	1.327649
O	-5.078837	-1.341821	-0.294658
C	-4.275797	-2.401700	0.041481
O	-6.147499	1.208016	2.057004
H	-7.029974	1.621057	2.105394
O	-8.495308	0.977856	0.709087
H	-9.024594	0.268435	1.107685
C	-4.943242	-0.293354	0.677447
H	-4.543875	0.583282	0.150957
C	-6.322428	0.066595	1.235489
H	-6.692814	-0.791103	1.823551
C	-7.329970	0.390103	0.125043
H	-6.912733	1.155319	-0.537532
H	-7.561650	-0.499633	-0.471073
I	-1.228267	-2.552519	4.935514
C	-3.211690	1.172497	2.772675
C	-1.687601	1.343261	2.714423
C	-1.147447	0.782477	1.377872

N	0.361613	0.579131	1.294832
O	-1.055702	0.828881	3.861849
H	-1.397763	-0.067891	4.086199
C	1.123261	1.714744	1.917247
H	0.799808	2.650660	1.456220
H	0.922538	1.722042	2.987446
H	2.185181	1.551899	1.723962
C	0.735791	0.473171	-0.165687
H	1.775867	0.142940	-0.236268
H	0.073078	-0.262747	-0.618596
H	0.603372	1.451784	-0.631992
C	0.754468	-0.715380	1.972860
H	0.460217	-0.663511	3.016720
H	0.242242	-1.531008	1.466647
H	1.830943	-0.847565	1.849966
H	-3.571896	1.590863	3.713890
H	-3.722021	1.683832	1.953266
H	-1.411336	1.478875	0.575631
H	-1.576187	-0.186731	1.126176
H	-1.491386	2.423637	2.734926
O	0.332825	-3.956472	0.800269
O	2.456199	-5.986849	-0.351474
H	3.396141	-5.768764	-0.619587
C	0.824020	-4.152240	-0.432468
O	2.281728	-5.497905	-3.260203
C	1.678721	-5.048662	-0.959849
O	0.891806	-3.791032	-2.731756
C	1.690242	-4.851754	-2.415599
O	-1.342873	-2.048181	-0.402653
H	-1.477291	-2.631102	0.368289
O	-2.853613	-1.641722	-2.727729
H	-3.422632	-2.359509	-2.396864
C	0.400992	-3.194312	-1.514228
H	0.948873	-2.253151	-1.380664
C	-1.099239	-2.873895	-1.541126
H	-1.693844	-3.793624	-1.463603
C	-1.523026	-2.109664	-2.796055
H	-0.887995	-1.221640	-2.912317
H	-1.343756	-2.756018	-3.668832
I	4.039842	-2.033845	0.330256
C	0.127851	-5.074803	1.707055
C	1.257251	-5.273632	2.733655
C	1.838198	-3.896267	3.059898
N	2.859395	-3.864276	4.190661
O	2.225712	-6.229306	2.370590
H	2.445379	-6.118628	1.420856
C	2.408319	-4.684970	5.369347
H	1.389447	-4.388277	5.629587
H	2.471237	-5.741624	5.108293
H	3.088277	-4.484884	6.199338
C	2.997989	-2.425564	4.609226
H	3.777770	-2.359158	5.370727
H	3.285374	-1.844109	3.730058
H	2.040164	-2.084077	5.009001
C	4.199473	-4.360165	3.705714
H	4.059467	-5.365008	3.316535
H	4.542488	-3.683032	2.921869
H	4.894630	-4.366955	4.544771
H	-0.017741	-5.994636	1.132980
H	-0.796285	-4.808019	2.223575
H	1.021173	-3.244819	3.375406
H	2.340453	-3.465604	2.190700
H	0.759600	-5.678648	3.621281
O	5.510456	-6.658314	1.102591
O	5.303359	-9.606592	1.748373
H	5.054935	-8.967195	2.457776
C	5.636971	-7.692386	0.234474

O	5.798957	-11.006762	-0.757923
C	5.481007	-8.989010	0.557735
O	5.970672	-8.957183	-1.692614
C	5.735609	-9.802791	-0.641401
O	4.838274	-5.520651	-1.438702
H	4.757926	-4.858970	-2.161939
O	4.908880	-5.360844	-4.051614
H	3.936770	-5.457778	-4.111119
C	5.963041	-7.595708	-1.241923
H	6.976515	-7.201913	-1.398079
C	4.973271	-6.789443	-2.085544
H	4.003263	-7.301946	-2.083257
C	5.454360	-6.564641	-3.535922
H	6.541474	-6.428922	-3.553416
H	5.209738	-7.441724	-4.147894
I	4.789461	-8.053604	4.940003
C	6.402839	-5.526788	1.001475
C	7.469901	-5.620343	2.097930
C	8.413558	-6.806171	1.803346
N	9.358138	-7.221435	2.928502
O	6.904643	-5.643312	3.391982
H	6.221796	-6.347420	3.460303
C	9.965084	-6.034793	3.620622
H	10.448874	-5.399769	2.875322
H	9.173808	-5.491141	4.134729
H	10.704435	-6.402298	4.334559
C	10.455278	-8.061012	2.316688
H	11.030470	-8.526207	3.121438
H	9.975702	-8.822481	1.702487
H	11.091036	-7.417733	1.704854
C	8.635639	-8.076896	3.946390
H	7.840829	-7.491051	4.397276
H	8.230137	-8.946934	3.433751
H	9.362871	-8.415301	4.687658
H	5.790445	-4.635138	1.147102
H	6.846359	-5.455076	0.007205
H	9.046746	-6.541356	0.950956
H	7.869856	-7.713058	1.538603
H	8.048776	-4.689766	2.053638
O	7.787340	-11.301407	3.508622
O	9.288176	-13.615693	4.971888
H	9.912694	-13.070182	5.511137
C	8.810045	-12.093974	3.115118
O	11.086893	-14.681882	2.822109
C	9.416574	-13.141893	3.691537
O	10.335018	-12.932644	1.577528
C	10.380011	-13.716026	2.721910
O	8.116818	-10.058480	1.017815
H	7.374033	-10.194717	1.632191
O	8.606080	-10.646830	-1.683509
H	7.717025	-11.043922	-1.686389
C	9.522510	-11.776918	1.826788
H	10.207915	-10.938769	2.011965
C	8.616222	-11.355758	0.665373
H	7.775312	-12.051021	0.545087
C	9.371212	-11.242856	-0.658319
H	10.251519	-10.601951	-0.518017
H	9.737302	-12.246034	-0.925843
I	11.057376	-10.533385	5.875961
C	6.561788	-11.907987	4.005934
C	6.450934	-11.960931	5.541764
C	7.221351	-10.764554	6.099547
N	7.114071	-10.535960	7.604423
O	6.812524	-13.201928	6.113017
H	7.692937	-13.460604	5.758482
C	5.685610	-10.599076	8.067346
H	5.085577	-9.934458	7.441014

H	5.335468	-11.628032	7.986742
H	5.648467	-10.277560	9.110161
C	7.661743	-9.154898	7.867853
H	7.659225	-8.979507	8.945784
H	8.683231	-9.118309	7.480516
H	7.022659	-8.429398	7.358990
C	7.947219	-11.542191	8.361772
H	7.575936	-12.535649	8.118566
H	8.985951	-11.432109	8.040908
H	7.852161	-11.329398	9.428913
H	6.460908	-12.919029	3.599796
H	5.777717	-11.266887	3.599373
H	6.833272	-9.856895	5.634210
H	8.289164	-10.847474	5.889788
H	5.382072	-11.844346	5.751656

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