Electronic Supplementary Material (ESI) for Polymer Chemistry.

Borinane-based Organoboron Catalysts for Alternating Copolymerization of CO_2 with Cyclic Ethers: Improved Productivity and Facile Recovery

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Contents

Experimental section

Materials

All the reagents were purchased from Sigma-Aldrich and used as received unless otherwise stated. 1,4-Pentadiene, 9-Borabicyclo[3.3.1]nonane (9-BBN, 0.4 M in Hexane), borane dimethyl sulfide complex (BMS) and boron trifluoride diethyl etherate were used as received. Tetrabutylammonium chloride (TBACl) were dried under vacuum in the presence of P_2O_5 for 2 days. 5-bromo-1-pentene were purified by distillation. Propylene oxide (PO), 1-butylene oxide (BO), 1-ocene oxide (OO) and allyl glycidyl ether (AGE) were purified by distilling firstly over CaH_2 and then over n-butyl lithium for two times using standard Schlenk technique. Ethylene oxide (EO) were purified by distilling over sodium. The purified monomers were stored in Schlenk flasks and kept in glovebox. Propargyl alcohol (PA), 2-Hydroxyethyl acrylate (HEA), propylene glycol (PG) and pentaerythritol ethoxylate (PEG4OH, average Mn ~797) were degassed via three times of freeze-pump-thaw procedure. 1,4-Benzenedimethanol (DBzOH) was used as received. 1,4-diazabicyclo[2.2.2]octane (DABCO) was purified by two times of sublimation and stored in glove box.

Instruments

Nuclear magnetic resonance (NMR): ^{1}H, ^{11}B, ^{13}C and DOSY NMR spectra were recorded on a Bruker AVANCE III-400 or 600 MHz instrument in CDCl3.

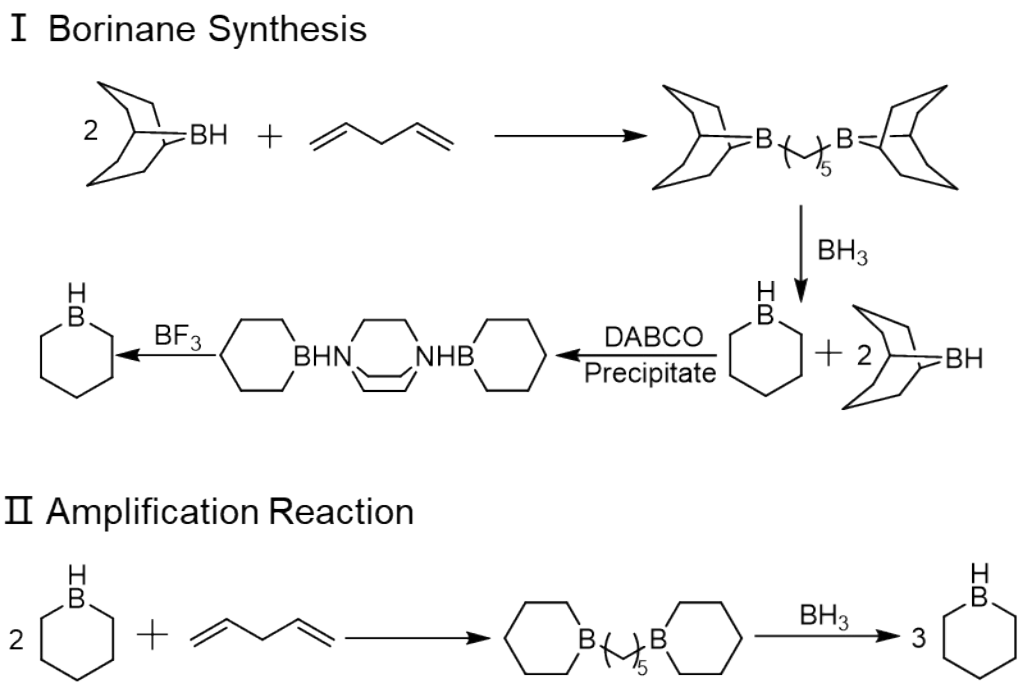
Gel permeation chromatography (GPC): GPC traces were acquired on a VISCOTEK VE2001 system equipped with the Styragel HR2 THF and Styragel HR4 THF using THF (1 mL/min) as the eluent. The relative molar masses and distributions were obtained at 35 ℃ using a RID detector and against linear polystyrene standards. DMF phase SEC was performed in DMF at a flow rate of 1.0 mL/min on an Agilent liquid chromatography system fitted with refractive index (RID) and

UV detectors, using two identical Aligent PLgel-M (5 μm) columns in connected series and an Agilent PLgel precolumn (10 μm). The column and flow path temperature were controlled at 35°C. Data analysis was performed using SEC-Addon for ChemStation software from Agilent.

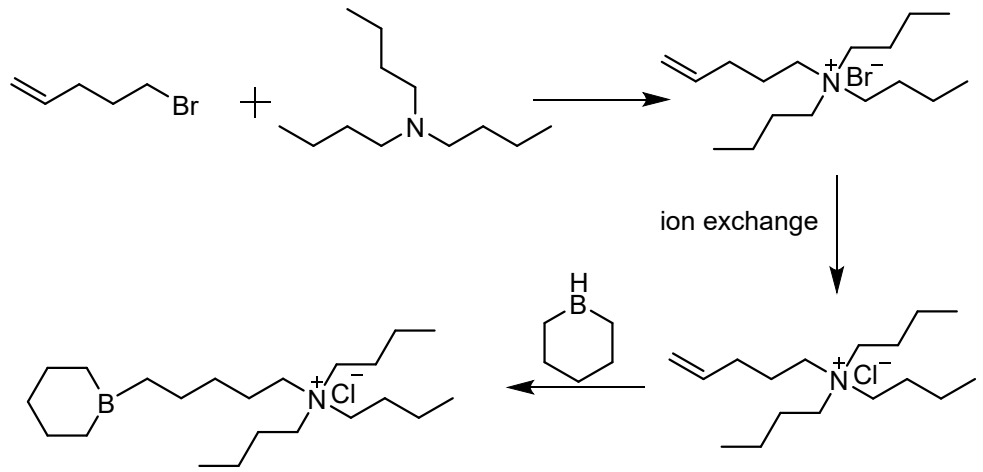
The matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectra were collected on an Autoflex (Bruker) mass spectrometer. The trans-2-[3-(4-t-butyl-phenyl)-2-methyl2-propenylidene] malononitrile (DCTB) was used as the matrix with a loading of 2:1 to sodium acetate which used as the ionizing agent.

Synthesis of borinane

Borinane was synthesized via Brown's method.[1] A round bottom flask was dried under 120 ℃ overnight and cooled under vacuum ahead of transferring to glove box. The flask was charged with 5 g 1,4 pentadiene (73.5 mmol) and 368 mL 9-BBN hexane solution. Reaction was monitored to the end of all the vinyl groups consumed. Subsequently, 7 mL BMS was added to form cyclic borinane. The reaction continued at room temperature for 24 h before anhydrous DABCO (4.1 g) THF solution was added to the above borinane and 9-BBN mixture solution. Borinane was immediately form complex with DABCO and precipitated. Interestingly, 9-BBN has no complexation with DABCO and could be recycled for further reaction. Borinane-DABCO adducts could be separated by simple filtration. The free borinane was obtained by reacting the above adducts with boron trifluoride. The above solution was concentrated under vacuum to yield pure borinane as white solid (5.7 g, 95% yield). Once the pure borinane was obtained, three moles of borinane could be easily generated from two moles of borinane (Scheme S1) without further separation or purification procedure. ^{1}H NMR ($CDCl_3$): δ 0.93 (brs, 4H), 1.47 (m, 2H), 1.52 (m, 4H) ppm. ^{13}C NMR ($CDCl_3$): δ 33.08, 28.97, 26.92 ppm. ^{11}B NMR ($CDCl_3$): δ 25.57 (brs) ppm.



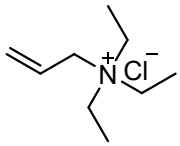
Scheme S1. The synthetic procedures and amplification reaction of borinane.



Scheme S2. The synthetic methodology for bifunctional catalysts.

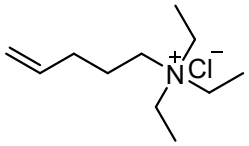
Synthesis of ammonium salts

N,N,N-triethylprop-2-en-1-aminium chloride



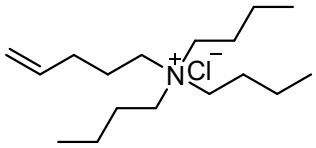
A flame dried flask charged with triethyl amine (10 mL, 71.9 mmol), allyl bromide (8.7 g) and 20 mL anhydrous acetonitrile then stirred overnight. The crude salt with slight yellow color was obtained after removal of solvent. The ammonium bromide salt was washed with ethyl acetate to afford pure salt as white solid (yield 98 %). The above bromide salt (1 g) dissolved in methanol passed through 10 g Amberlite IRA-402 (Cl form) ion-exchange resin at a drop rate of 1 mL/min. Solvent was removed and product was dried in vacuo at 50 °C to yield a white solid (0.8 g, 100% yield).

N,N,N-triethylpent-4-en-1-aminium chloride



A flame dried flask charged with triethyl amine (10 mL, 71.9 mmol), 5-bromo-1-pentene (10.7 g) and 20 mL anhydrous acetonitrile then stirred overnight. The crude salt with slight yellow color was obtained after removal of solvent. The ammonium bromide salt was washed with ethyl acetate to afford pure salt as white solid (yield 97 %). The above bromide salt (1 g) dissolved in methanol passed through 10 g Amberlite IRA-402 (Cl form) ion-exchange resin at a drop rate of 1 mL/min. Solvent was removed and product was dried in vacuo at 50 °C to yield a white solid (0.8 g, 100% yield).

N,N,N-tributylpent-4-en-1-aminium chloride

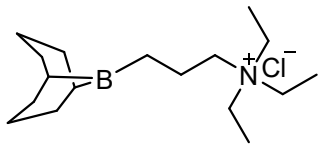


A flame dried flask charged with tributyl amine (10 mL, 42.2 mmol), 5-bromo-1-pentene (6.3 g) and 20 mL anhydrous acetonitrile then stirred overnight. The crude salt with slight yellow color was obtained after removal of solvent. The ammonium bromide salt was washed with cold diethyl ether to afford pure salt as white solid (yield 92 %). The above bromide salt (1 g) dissolved in methanol passed through 10 g Amberlite IRA-402 (Cl form) ion-exchange resin at a drop rate of 1 mL/min. Solvent was removed and product was dried in vacuo at 50 °C to yield a white solid (0.86 g, 100% yield).

Synthesis of bifunctional catalysts

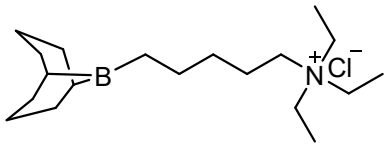
As shown in **Scheme 1**, all the bifunctional catalysts were synthesized via the direct hydroboration of borinane or 9-BBN with vinyl based ammonium salts. All the solvents utilized in this reaction were carefully dried to afford high yield and eliminate side reaction.

Catalyst 1



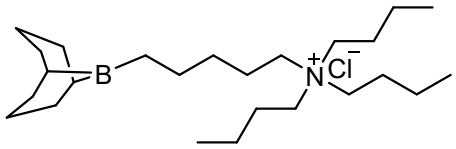
The fine dried ammonium salt, N,N,N-triethylprop-2-en-1-aminium chloride (1 g, 5.63 mmol), was charged in a flame dried Schlenk tube. An equivalent quantity of 9-BBN (11.3 mL, 5.63 mmol) THF solution was added and stirred overnight in glovebox. Solvent was removed under reduced pressure to afford crude products as white solid (catalyst **1**, 1.68 g, 100% yield).

Catalyst 2



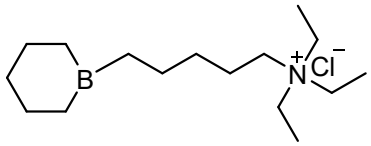
The fine dried ammonium salt, N,N,N-triethylpent-4-en-1-aminium chloride (1 g, 4.85 mmol), was charged in a flame dried Schlenk tube. An equivalent quantity of 9-BBN (9.7 mL, 4.85 mmol) THF solution was added and stirred overnight in glovebox. Solvent was removed under reduced pressure to afford crude products as white solid (catalyst **2**, 1.6 g, 100% yield).

Catalyst 3



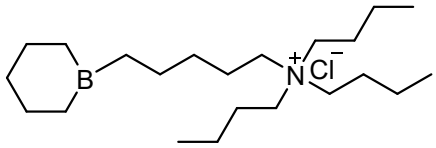
The fine dried ammonium salt, N,N,N-tributylpent-4-en-1-aminium chloride (1 g, 3.45 mmol), was charged in a flame dried Schlenk tube. An equivalent quantity of 9-BBN (6.9 mL, 3.45 mmol) THF solution was added and stirred overnight in glovebox. Solvent was removed under reduced pressure to afford crude products as white solid (catalyst **3**, 1.42 g, 100% yield).

Catalyst 4



The fine dried ammonium salt, N,N,N-triethylpent-4-en-1-aminium chloride (1 g, 4.85 mmol), was charged in a flame dried Schlenk tube. An equivalent quantity of borinane (398 mg, 4.85 mmol) with 1 mL anhydrous THF were added and stirred overnight in glovebox. Solvent was removed under reduced pressure to afford crude products as white solid (catalyst **4**, 1.40 g, 100% yield).

Catalyst 5



The fine dried ammonium salt, N,N,N-tributylpent-4-en-1-aminium chloride (1 g, 3.45 mmol), was charged in a flame dried Schlenk tube. An equivalent quantity of borinane (283 mg, 3.45 mmol) with 1 mL anhydrous THF were added and stirred overnight in glovebox. Solvent was removed under reduced pressure to afford crude products as white solid (catalyst **5**, 1.28 g, 100% yield).

Synthesis of poly(propylene carbonate) (PPC)

A typical polymerization procedure which corresponding to **Table 1**, entry 11 was described as follow: A 50 mL Parr reactor with a magnetic stir bar and a small glass vial inside was first dried in an oven at 120 °C overnight and then immediately transferred into glove box. After the reactor cool down, 1 eq. (74.4 mg) catalyst **5** and 100 eq. PO (1.4 mL) were added. Subsequently, the reactor was sealed and taken out from glove box. After charged with 10 bar CO_2, the reactor was heated at 60 °C for 12 h. The reactor was cooled, unreacted CO_2 was slowly released, and the polymerization was quenched by acid and samples were taken out for NMR and SEC analysis.

Catalyst recovery

Polymerization procedure is similar as above, the difference is adding toluene as solvent. Typically, 1 eq. (186 mg) catalyst **5**, 40 eq. PO (1.4 mL) and 2 mL toluene were added in a 50 mL Parr reactor. Subsequently, the reactor was sealed and taken out from glove box. After charged with 10 bar CO_2, the reactor was immersed in oil bath at 60 °C for 12 h. The reactor was transferred into glove box and polymerization was quenched by succinic acid (28.7 mg, 1 eq. to catalyst). The

above suspension was stirred overnight. Finally, recycled catalyst was obtained via filtration and washed with anhydrous hexane.

Computational Details

The reactant complexes and the intermediates and transition states were studied using density functional theory for geometric optimization and frequency calculations with M062X-D3/6-31G(d) level of theory[2-7]. The intrinsic reaction coordinate (IRC) scheme[8,9] was applied for the calculations of the reaction coordinates to confirm whether or not the transition states were directly connected to the reactants and products. The Shermo code[10] was used to derive the thermochemical corrections for the Gibbs free energies at 333.15 K. The single-point energy (SP) calculations were performed on the optimized geometries with the larger 6-311+G(d,p) basis set[7,11,12]. Approximate solvent effects of PO were taken into consideration based on the the integral equation formalism variant of polarizable continuum model (IEFPCM)[13] in SP calculations (ε = 16.0). All DFT calculations were carried out by the Gaussian 16 program package.[14]

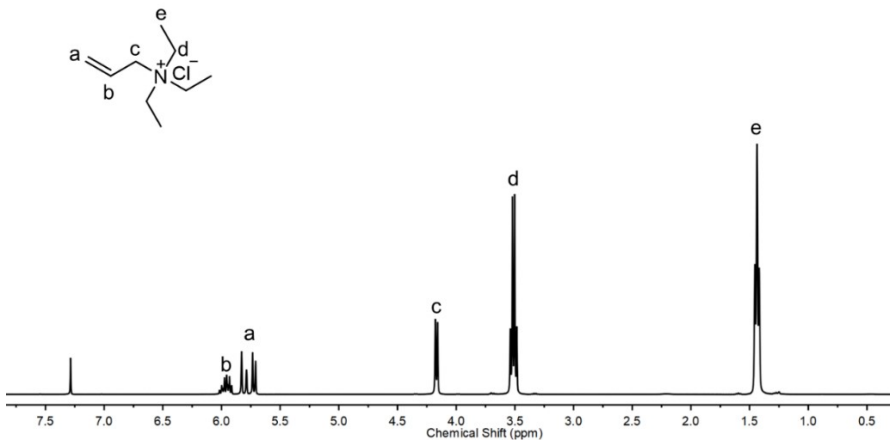


Figure S1. ^{1}H NMR of N,N,N-triethylprop-2-en-1-aminium chloride in $CDCl_3$.

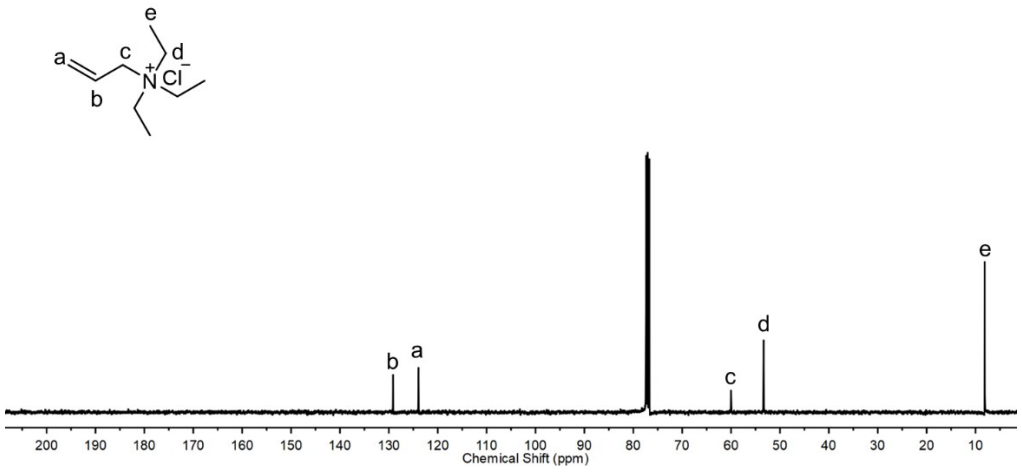


Figure S2. ^{13}C NMR of N,N,N-triethylprop-2-en-1-aminium chloride in $CDCl_3$.

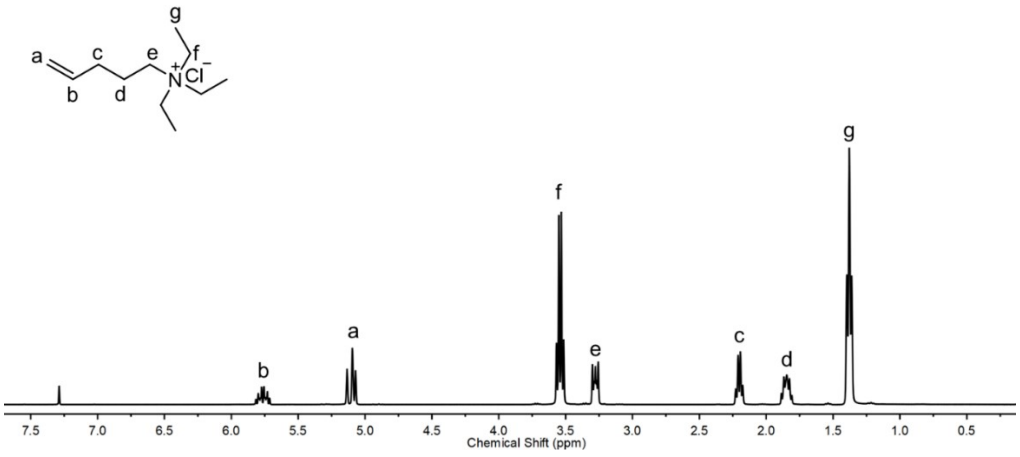


Figure S3. ^{1}H NMR of N,N,N-triethylpent-4-en-1-aminium chloride in $CDCl_3$.

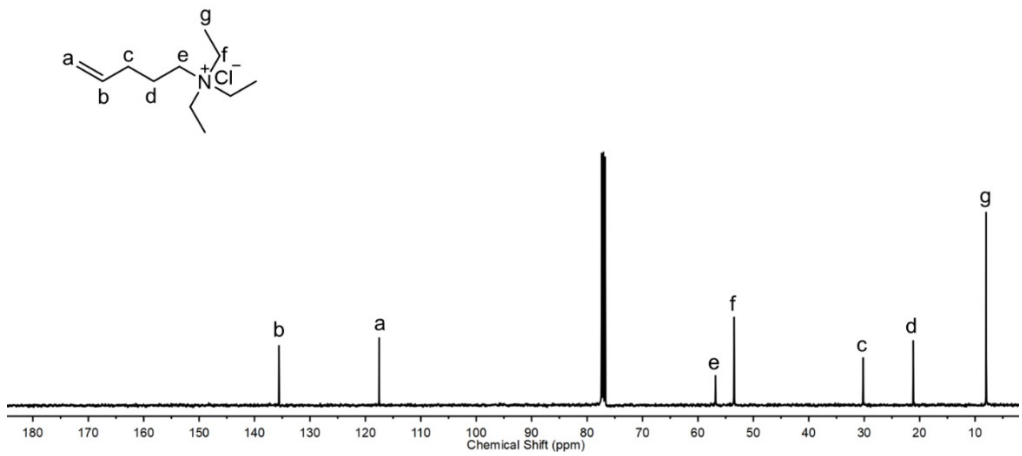


Figure S4. ^{13}C NMR of N,N,N-triethylpent-4-en-1-aminium chloride in $CDCl_3$.

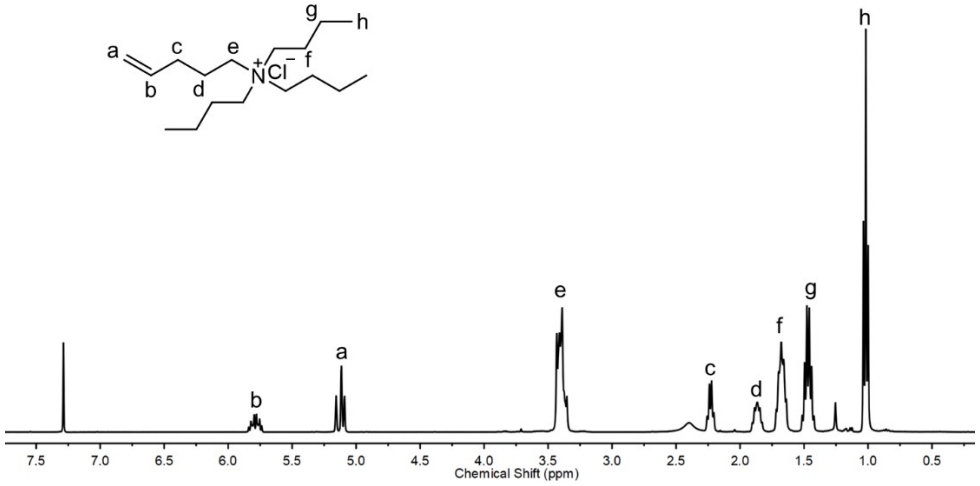


Figure S5. ^{1}H NMR of N,N,N-tributylpent-4-en-1-aminium chloride in $CDCl_3$.

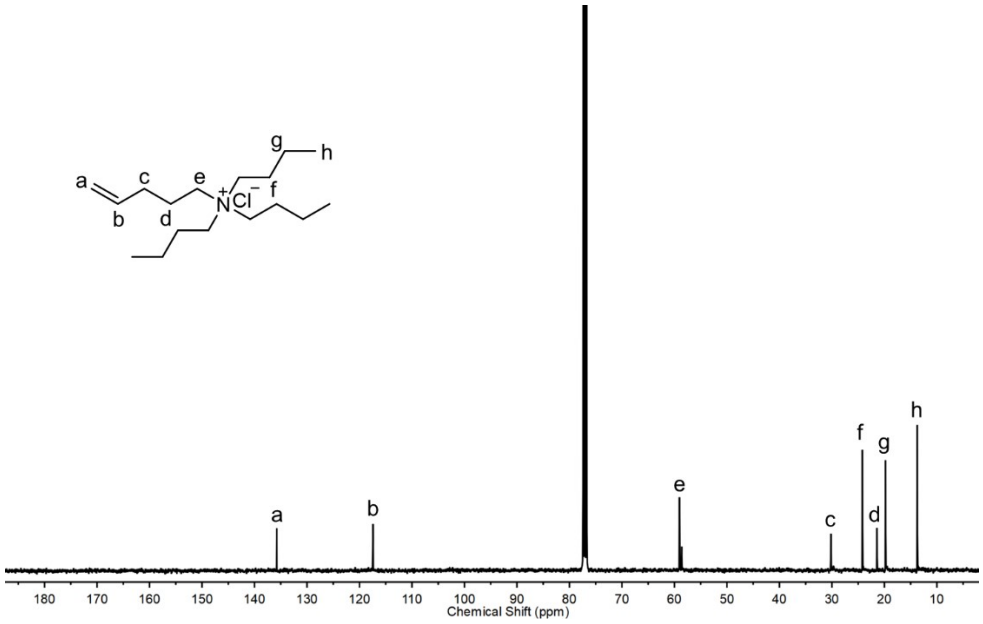


Figure S6. ^{13}C NMR of N,N,N-tributylpent-4-en-1-aminium chloride in $CDCl_3$.

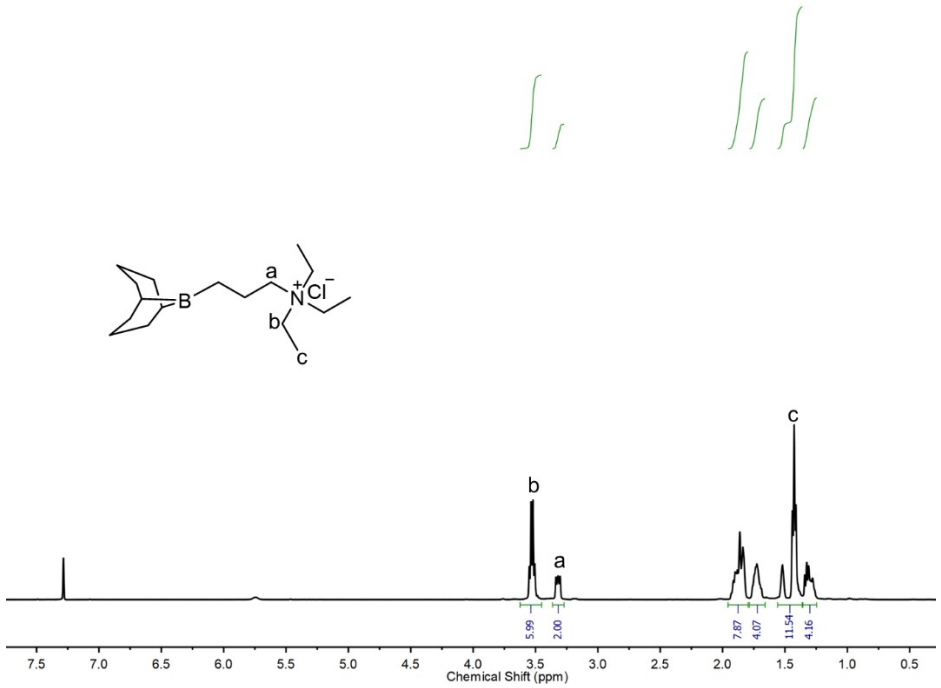


Figure S7. ^{1}H NMR of Catalyst **1** in $CDCl_3$.

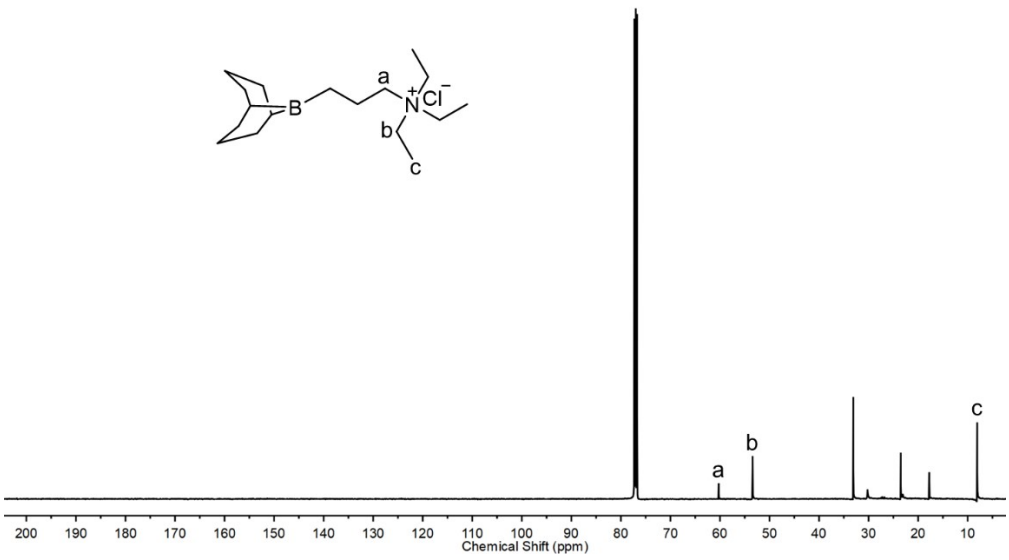


Figure S8. ^{13}C NMR of Catalyst **1** in $CDCl_3$.

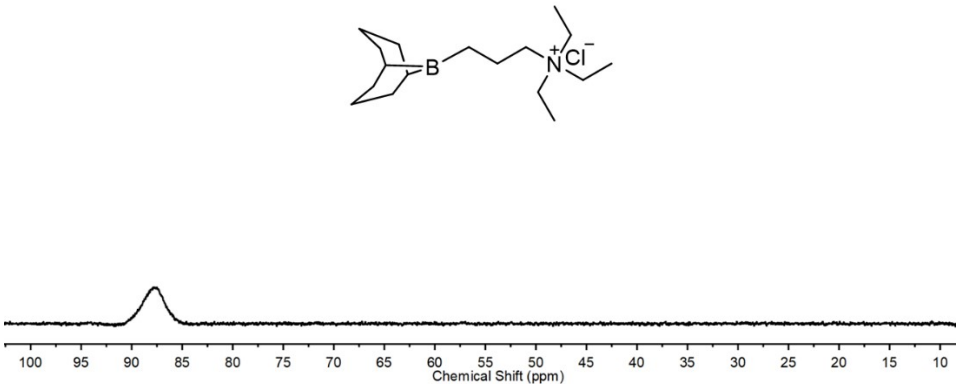


Figure S9. ^{11}B NMR of Catalyst **1** in $CDCl_3$.

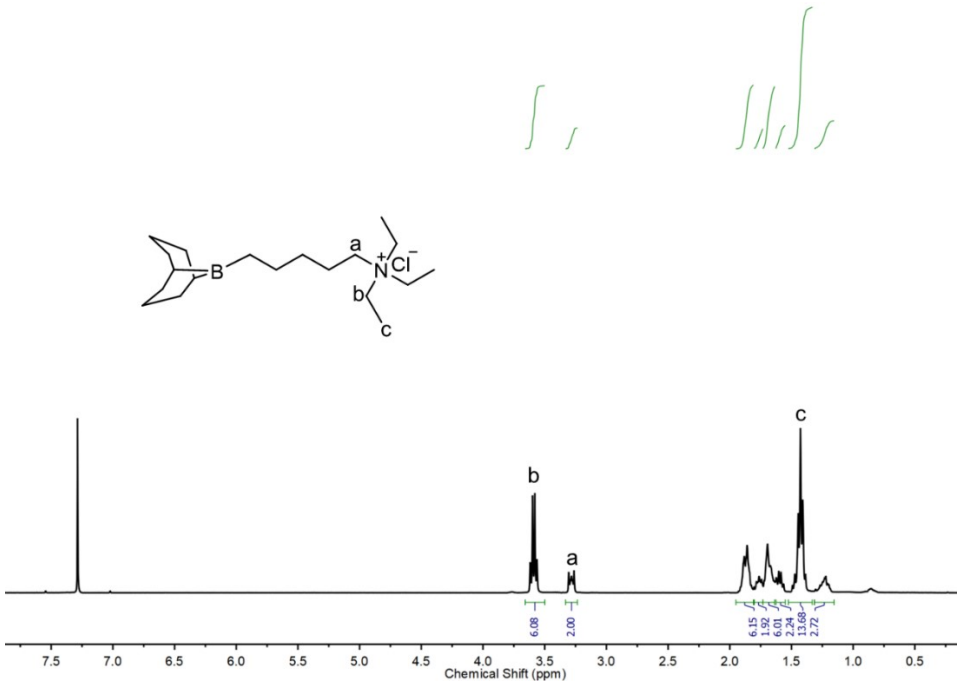


Figure S10. ^{1}H NMR of Catalyst **2** in $CDCl_3$.

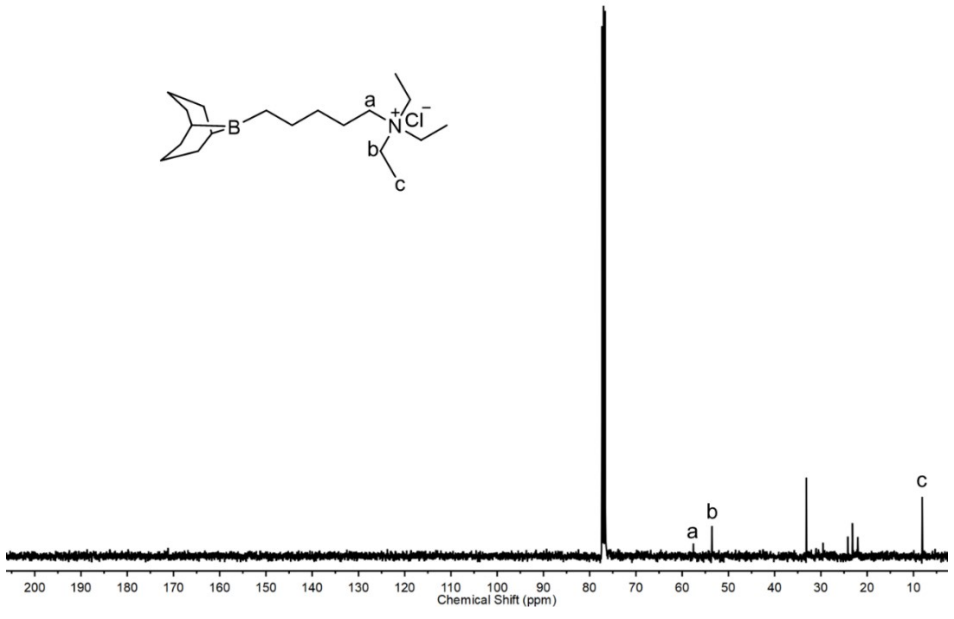


Figure S11. ^{13}C NMR of Catalyst **2** in $CDCl_3$.

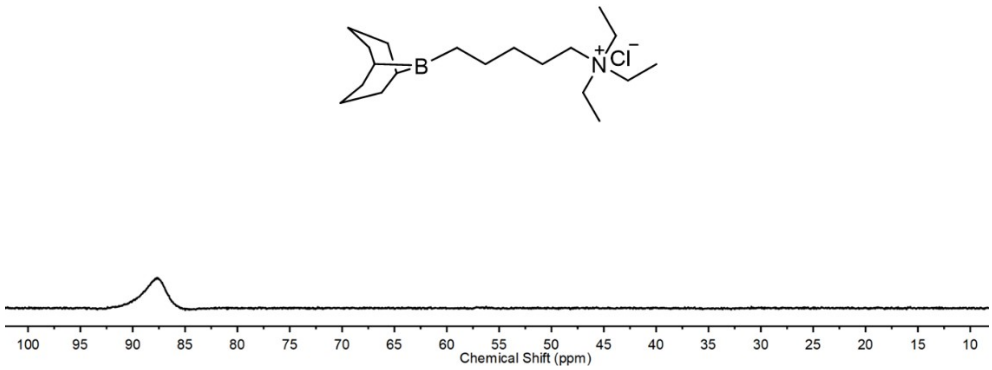


Figure S12. ^{11}B NMR of Catalyst **2** in $CDCl_3$.

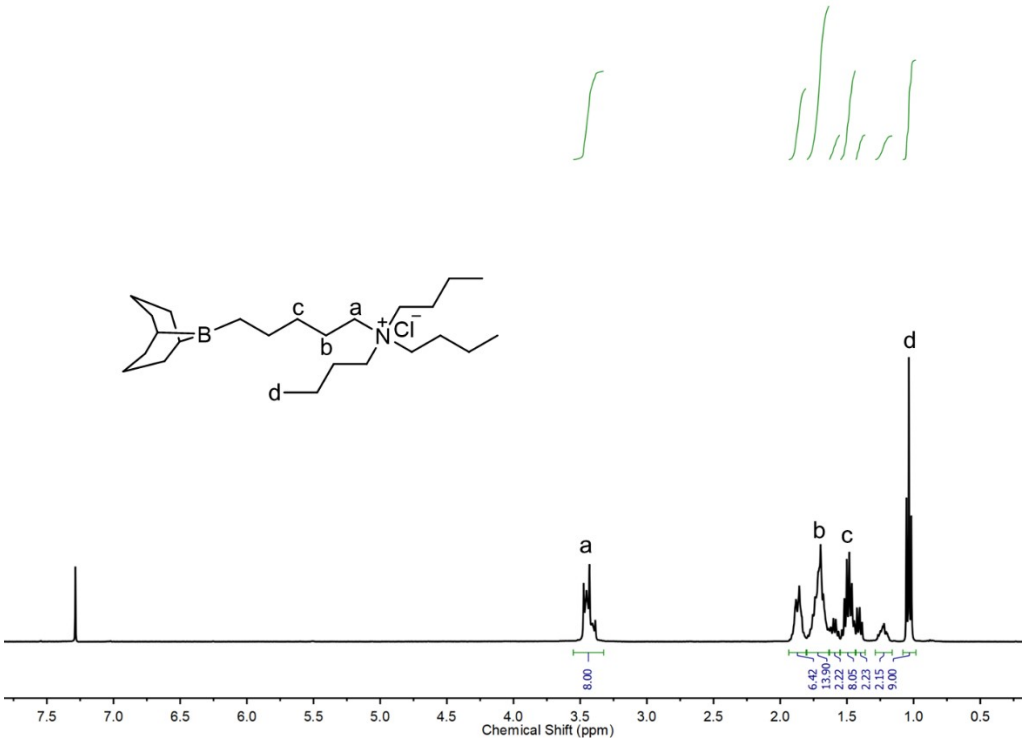


Figure S13. ^{1}H NMR of Catalyst **3** in $CDCl_3$.

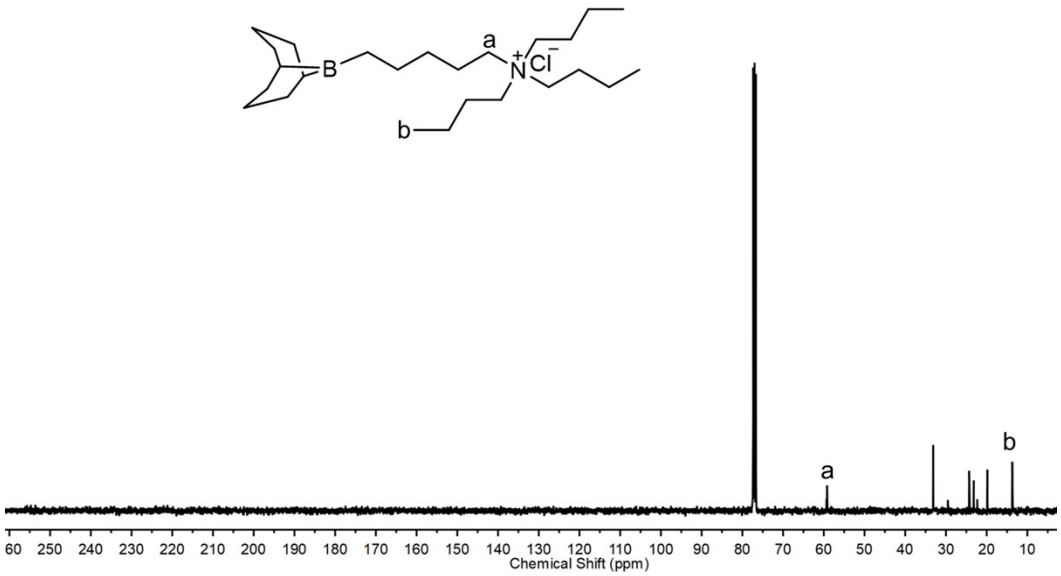


Figure S14. ^{13}C NMR of Catalyst **3** in $CDCl_3$.

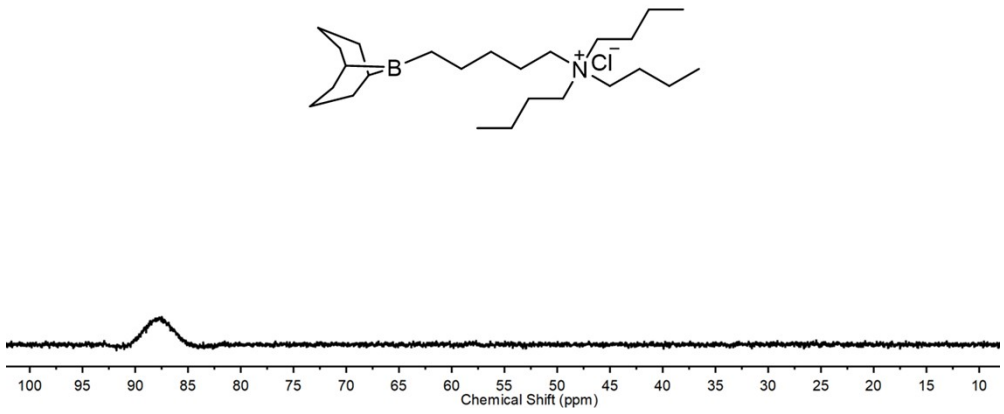


Figure S15. ^{11}B NMR of Catalyst **3** in $CDCl_3$.

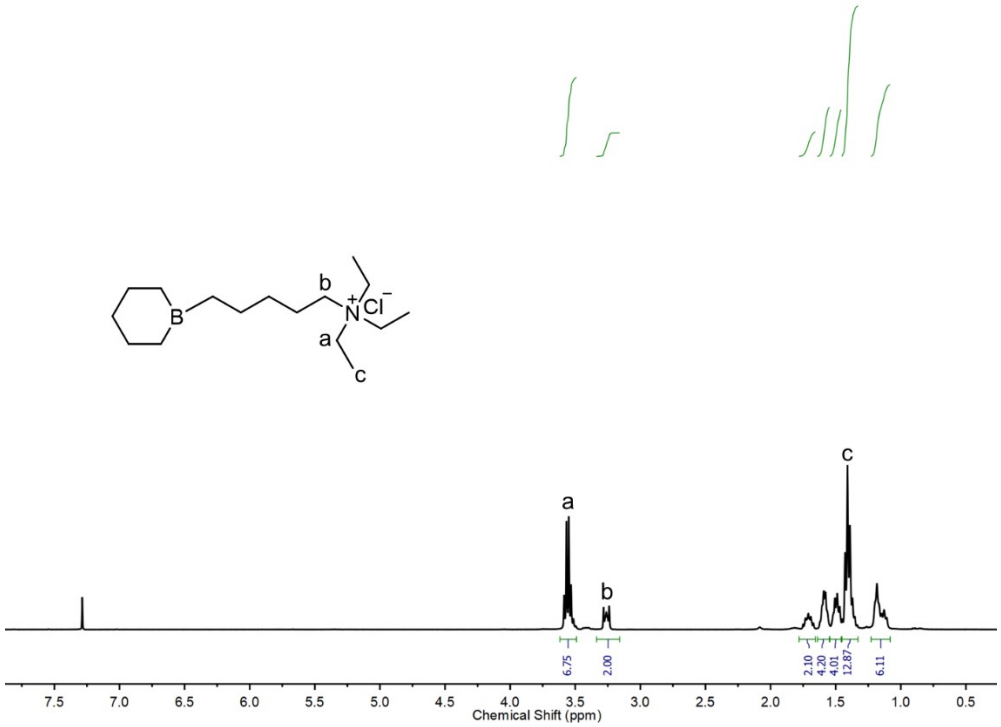


Figure S16. ^{1}H NMR of Catalyst **4** in $CDCl_3$.

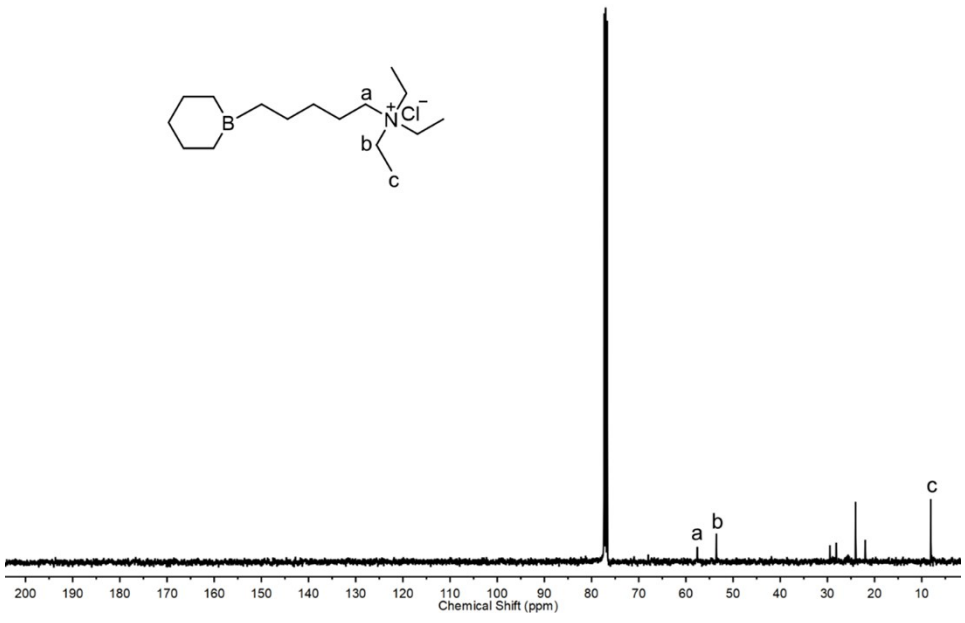


Figure S17. ^{13}C NMR of Catalyst **4** in $CDCl_3$.

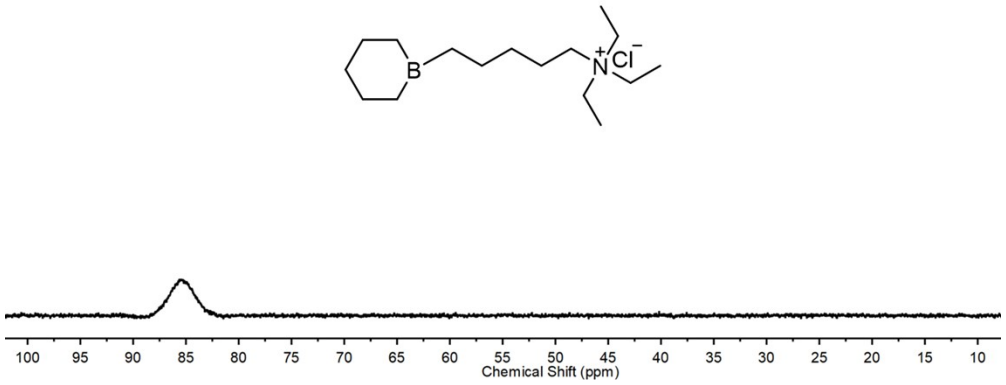


Figure S18. ^{11}B NMR of Catalyst **4** in $CDCl_3$.

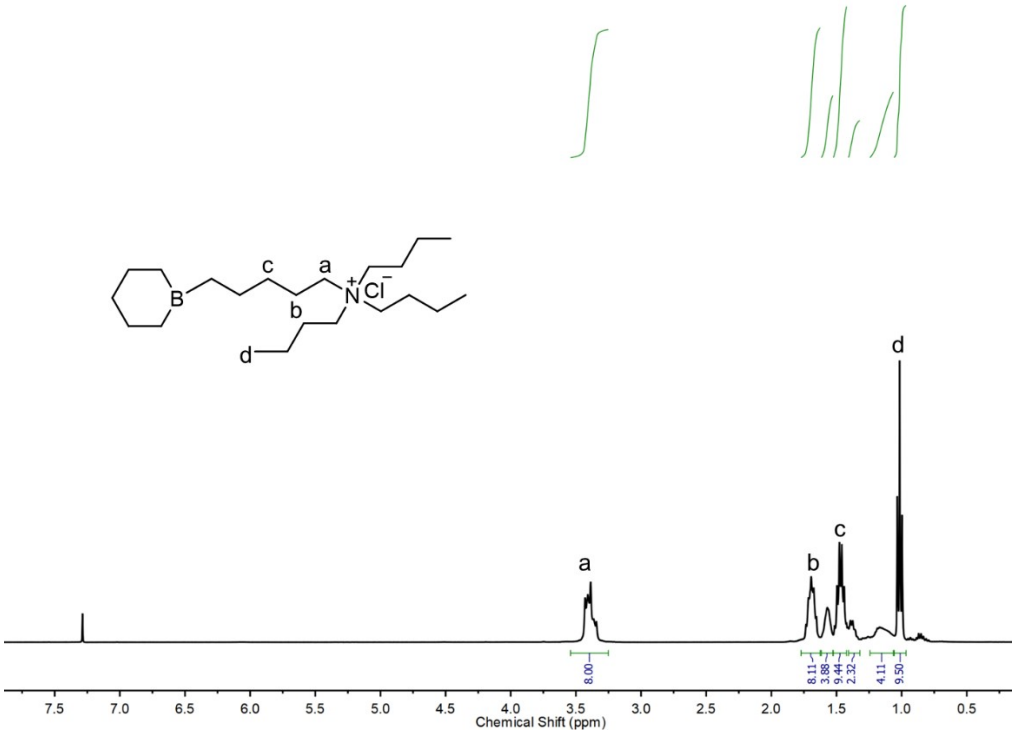


Figure S19. ^{1}H NMR of Catalyst **5** in $CDCl_3$.

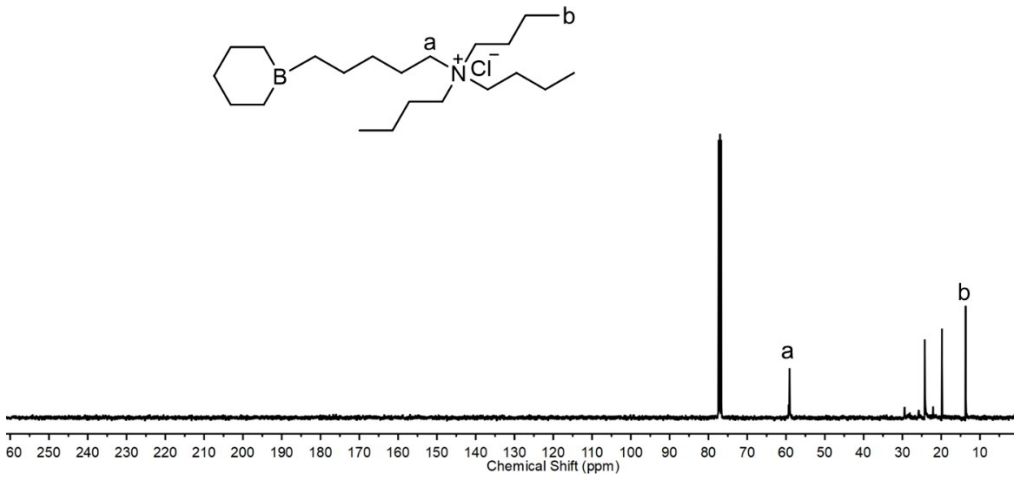


Figure S20. ^{13}C NMR of Catalyst **5** in $CDCl_3$.

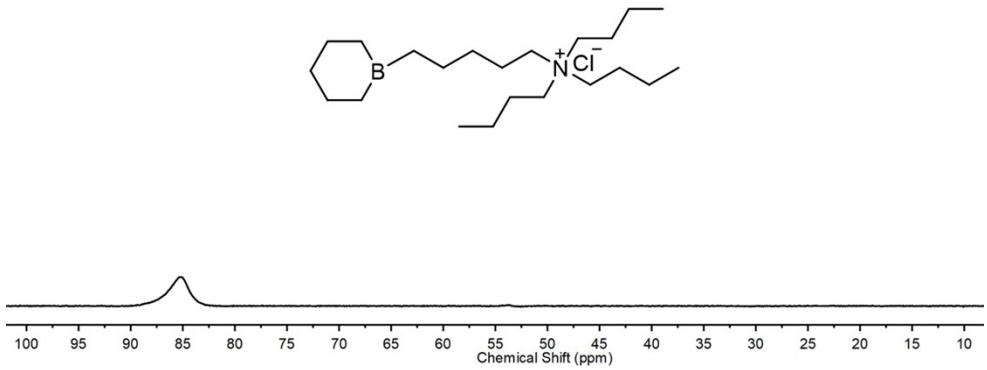
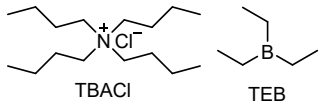
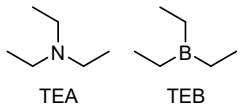
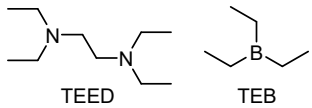
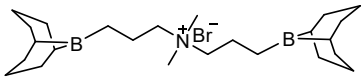
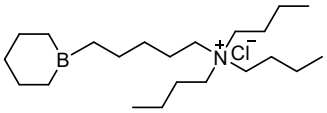


Figure S21. ^{11}B NMR of Catalyst **5** in $CDCl_3$.

Table S1. Comparison of the productivities of organocatalysts for the ROCOP of CO_2 and PO.

Entry	catalyst	Mw (g/mol)	T (°C)	Sel.[a]	CO_2 (%)[a]	Productivity (g / g)[b]
1[c]	 TBACl TEB	376	60	43	100	30
2[d,15]	 TEA TEB	199	60	99	100	171
3[d,15]	 TEED TEB	270	60	99	100	216
4[e,16]		450	25	99	95.2	146
5		372	60	90	100	271.5

[a] Polymer selectivity and the ratio of carbonate linkage were determined by ^{1}H NMR. [b] Productivity= (TON×102)/Mw of catalysts. [c] TBACl:TEB=1:1, refer to Table 1, entry 2. [d] TEA:TEB=1:1, TEED:TEB= 1:2. [e] The ratio of boron to cation N^+ is 2:1.

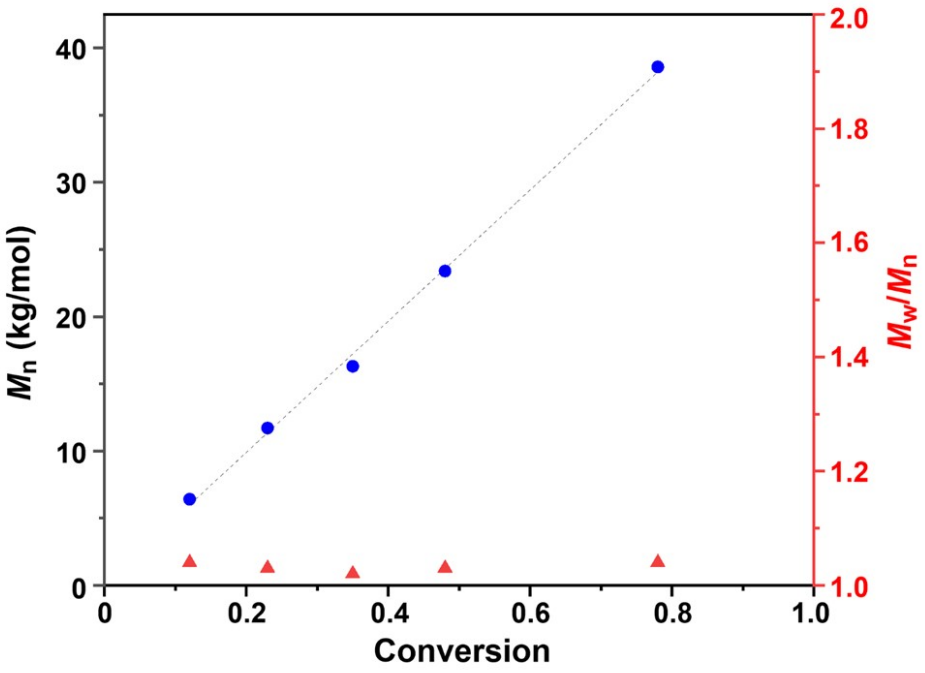


Figure S22. Linear plots of M_n versus PO conversion in the presence of catalyst **5**.

Table S2. ROCOP of CO_2 and PO in the presence of catalyst 5.[a]

Entry	Time (h)	Conv. (%)[b]	Sel.[b]	CO_2 (%)[b]	$M_{n,GPC}$ (kg mol^{-1})[c]	$Đ$[c]
1	2	12	97	100	6.4	1.04
2	4	23	98	100	11.7	1.03
3	6	35	96	100	16.3	1.02
4	8	48	96	100	23.4	1.03
5	15	78	96	100	38.6	1.04

[a] Polymerizations were run in neat condition, PO : **5** = 500 : 1 with 10 bar CO_2. [b] Conversion, polymer selectivity and the ratio of carbonate linkage were determined by ^{1}H NMR. [c] Determined by GPC in THF using standard PS as calibration.

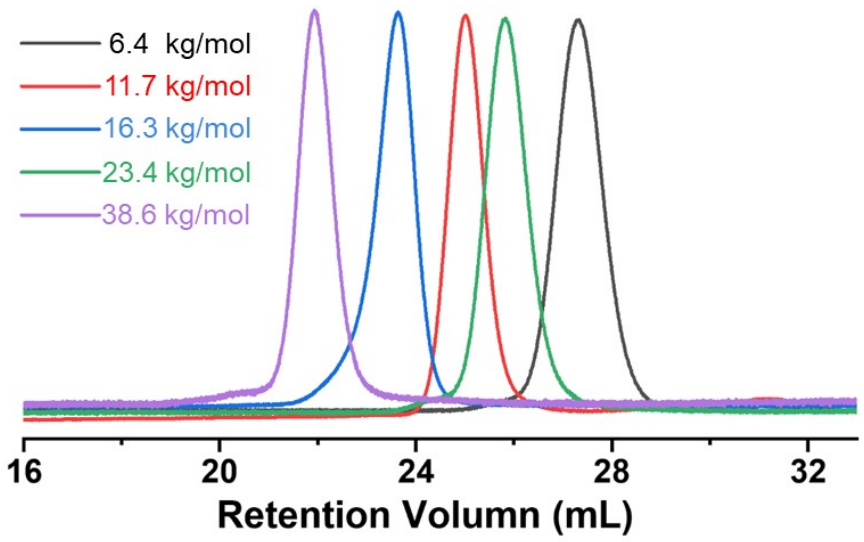


Figure S23. SEC traces of PPC samples from **Table S2**.

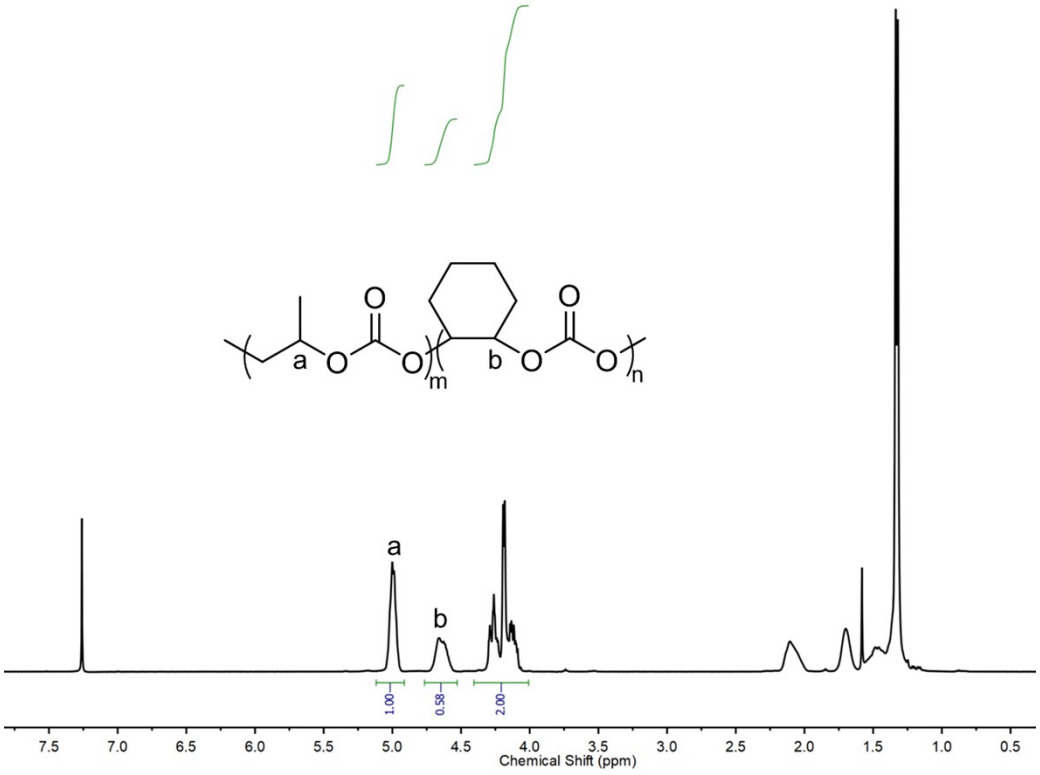


Figure S24. ^{1}H NMR spectrum of PPC-*b*-PCHC in $CDCl_3$.

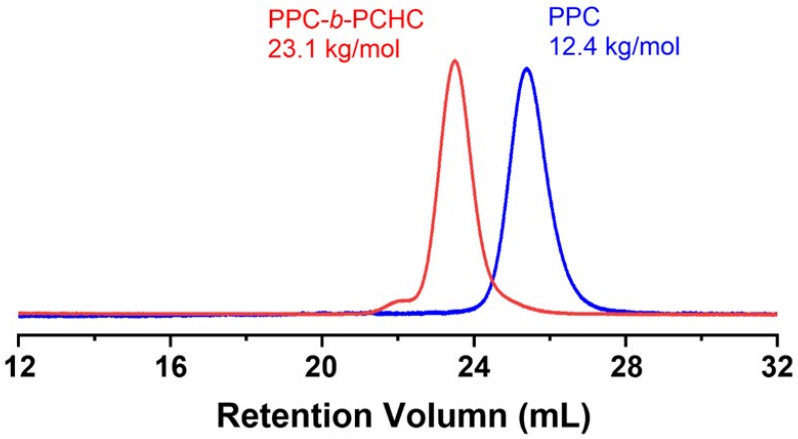


Figure S25. SEC traces of PPC and PPC-*b*-PCHC.

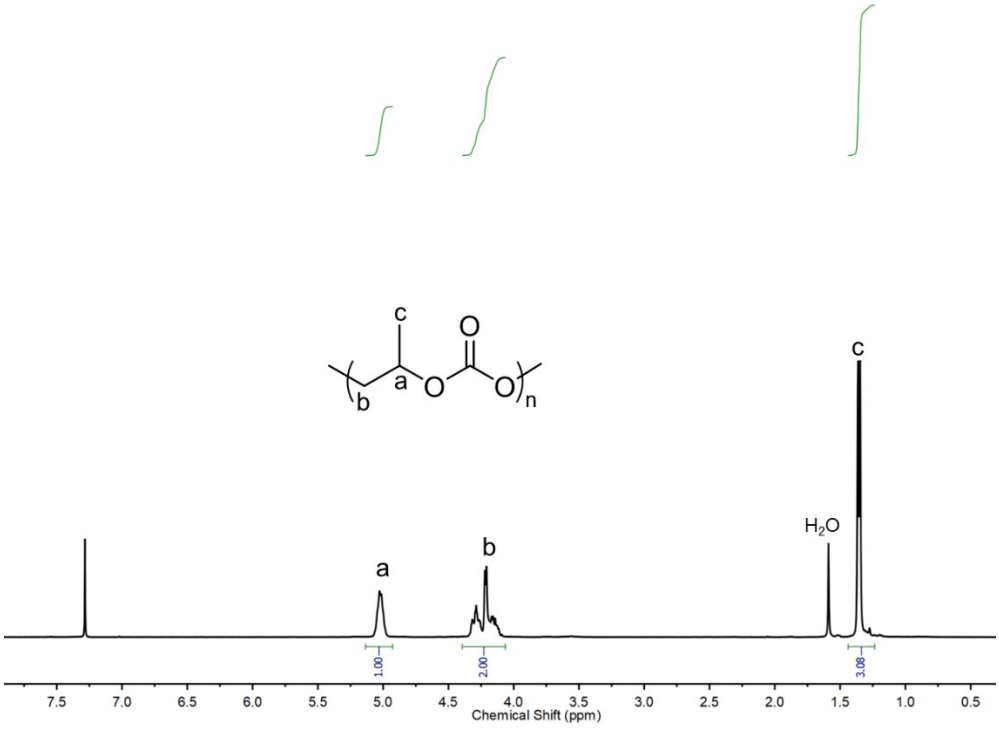


Figure S26. ^{1}H NMR spectrum of PPC sample, **Table 1**, entry 12.

Figure S27. Photograph of PPC-*b*-PCHC block copolymer powders.

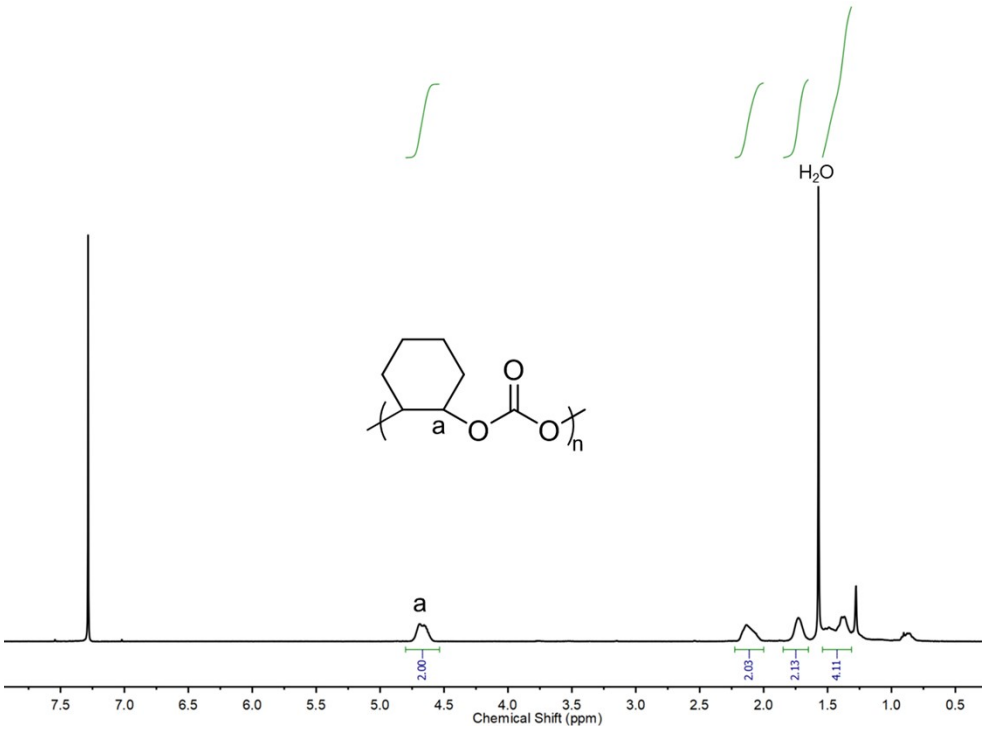


Figure S28. ^{1}H NMR spectrum of PCHC sample, **Table S3**, entry 1.

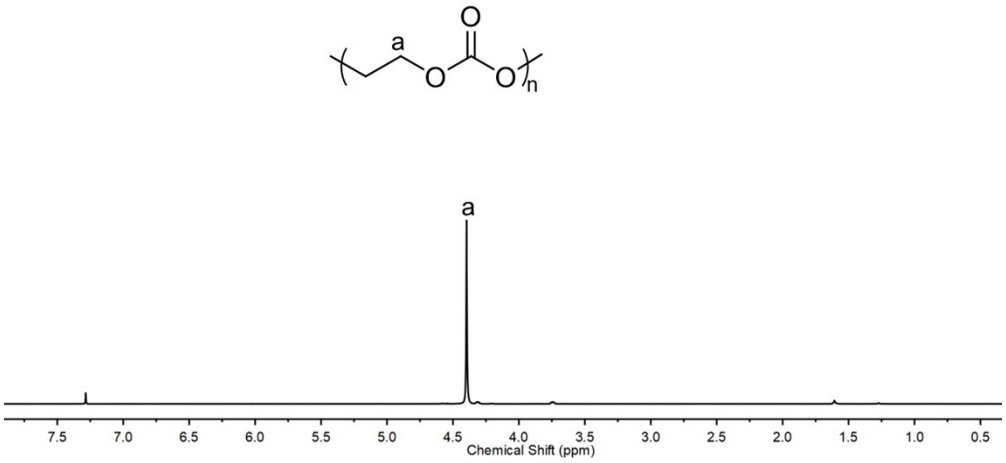


Figure S29. ^{1}H NMR spectrum of PEC sample, **Table S3**, entry 4.

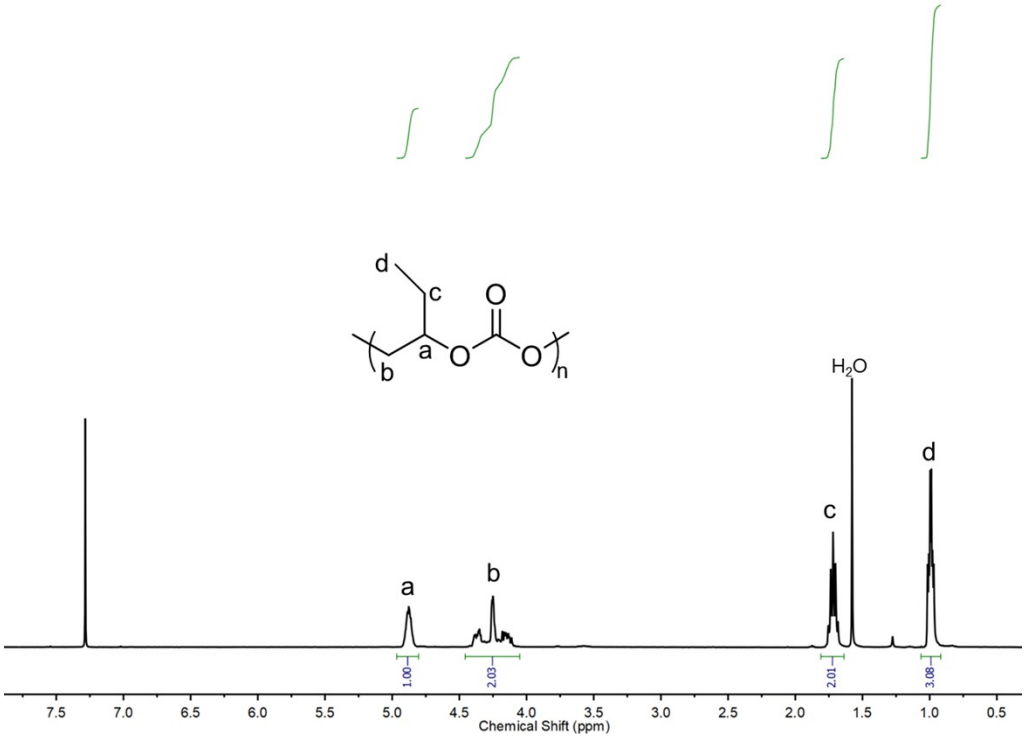


Figure S30. ^{1}H NMR spectrum of PBC sample, **Table S3**, entry 5.

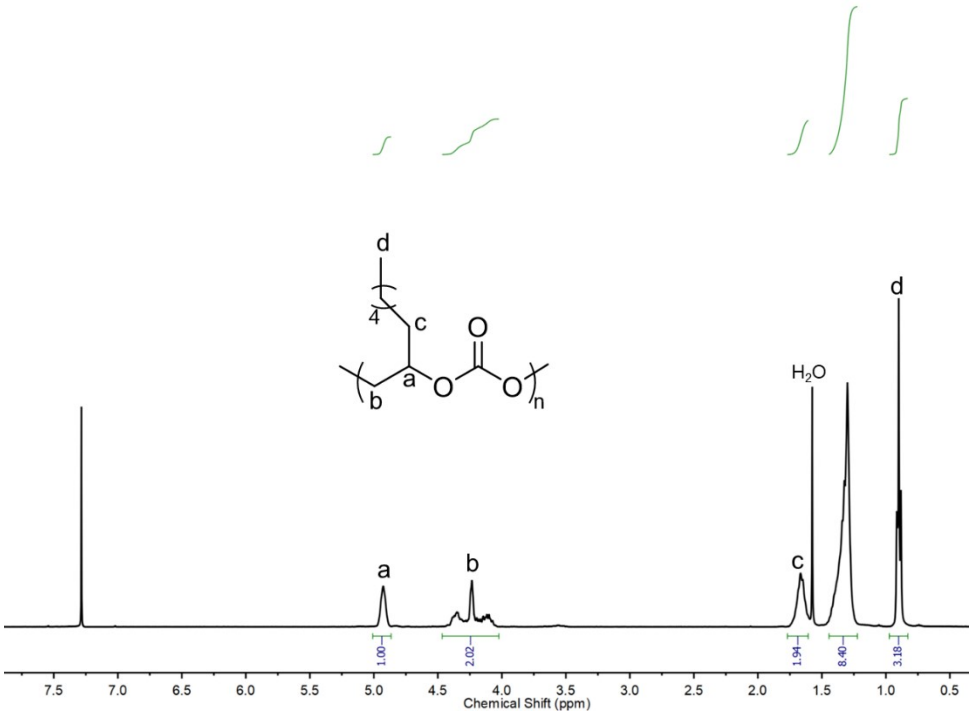


Figure S31. [1]H NMR spectrum of POC sample, **Table S3**, entry 6.

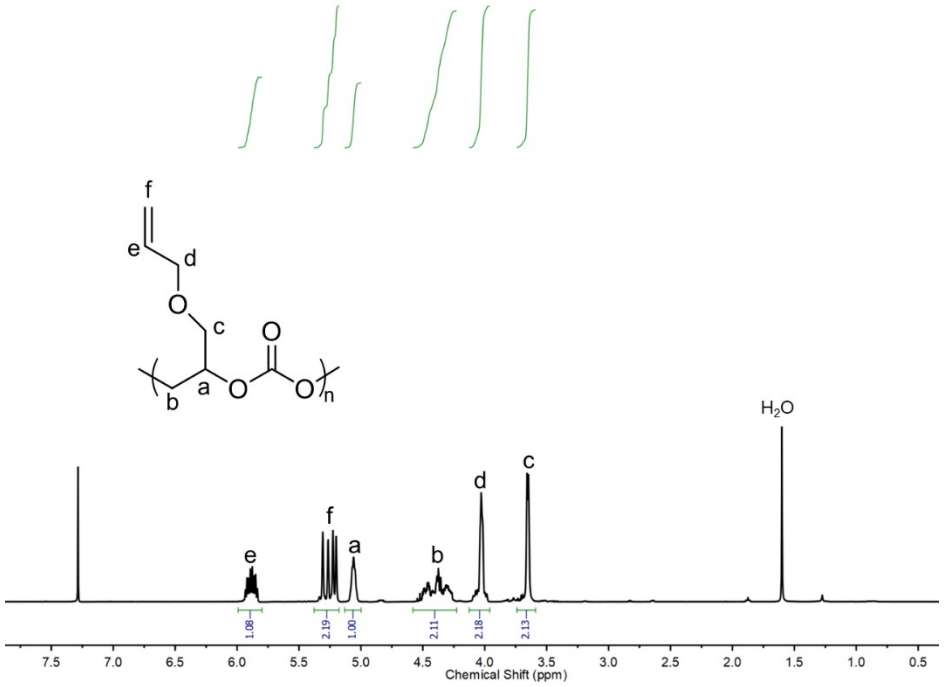


Figure S32. [1]H NMR spectrum of PAGEC sample, **Table S3**, entry 7.

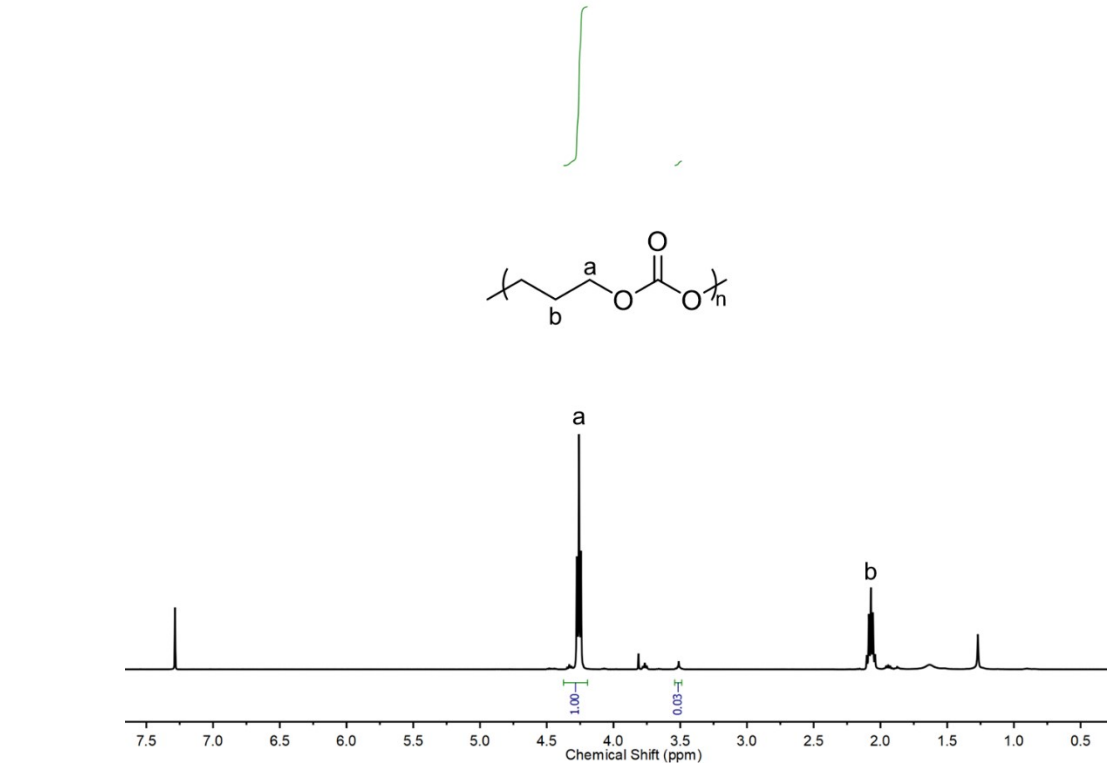


Figure S33. ^{1}H NMR spectrum of poly(oxetane carbonate) sample, **Table S3**, entry 10.

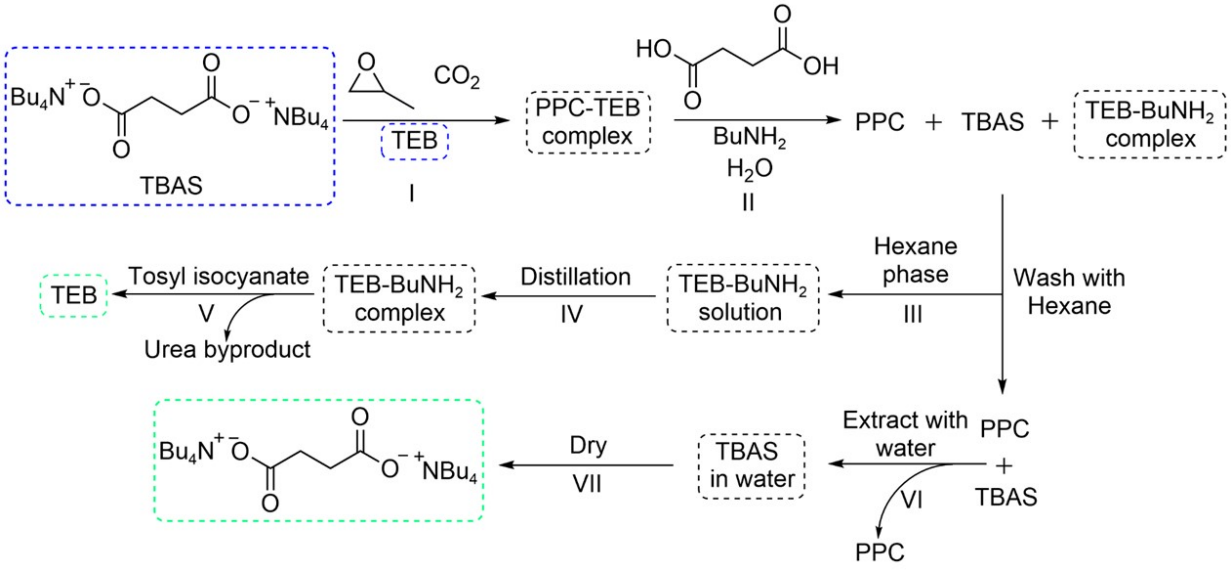


Figure S34. Procedures for TEB and ammonium salts recycling.

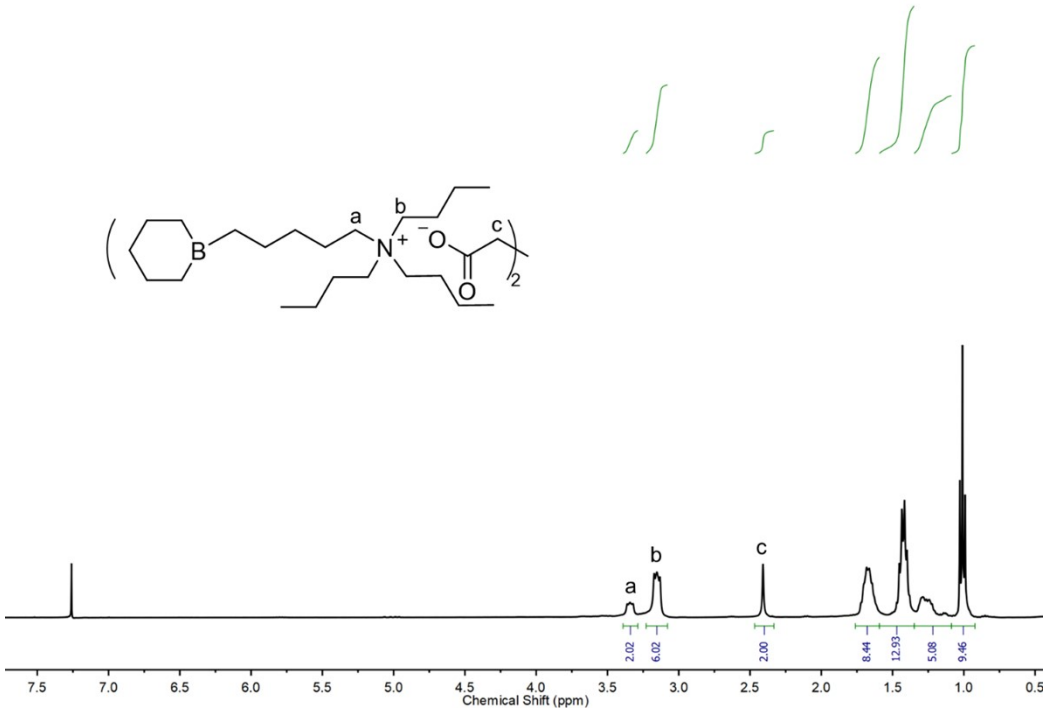


Figure S35. ^{1}H NMR spectrum of recycled catalyst **5**.

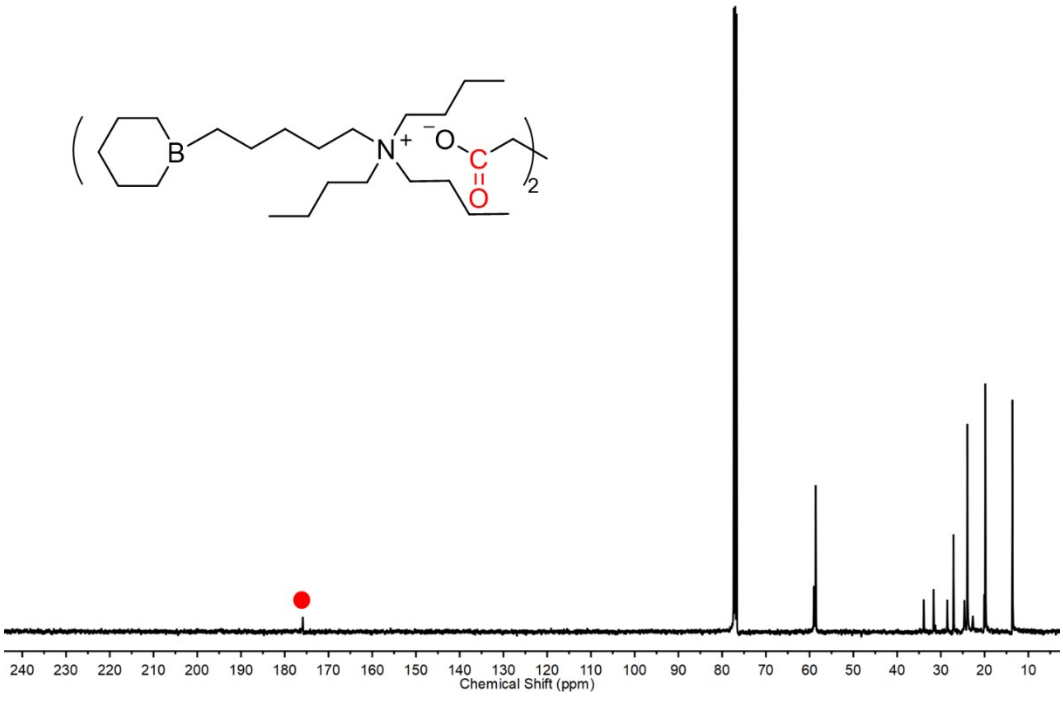


Figure S36. ^{13}C NMR spectrum of recycled catalyst **5**.

Figure S37. ^{11}B NMR spectrum of recycled catalyst **5**.

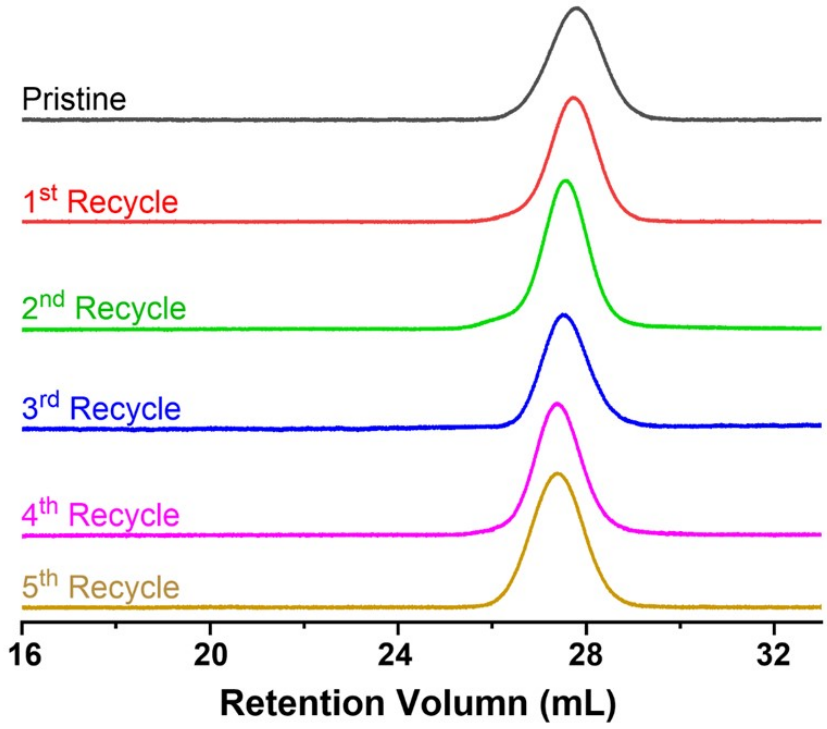


Figure S38. SEC traces of PPC obtained by recycled catalysts **5**.

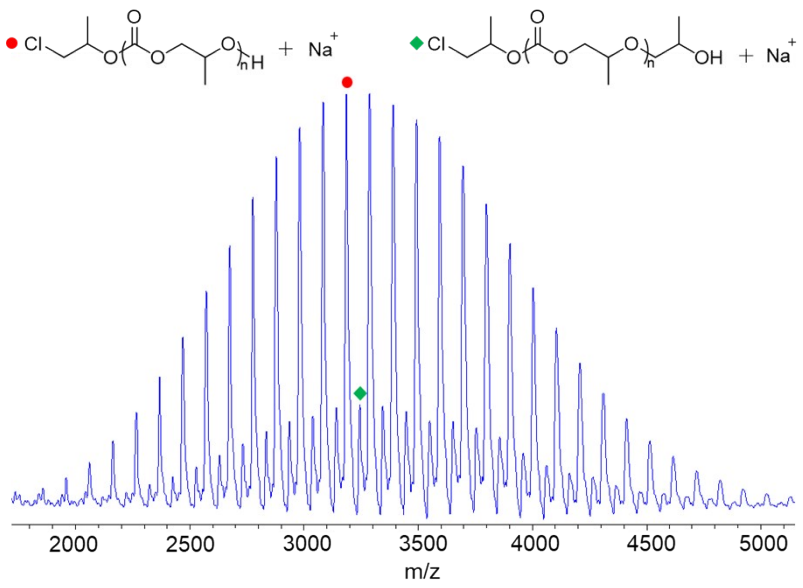


Figure S39. MALDI-TOF MS spectrum of pristine PPC catalyzed by **5**.

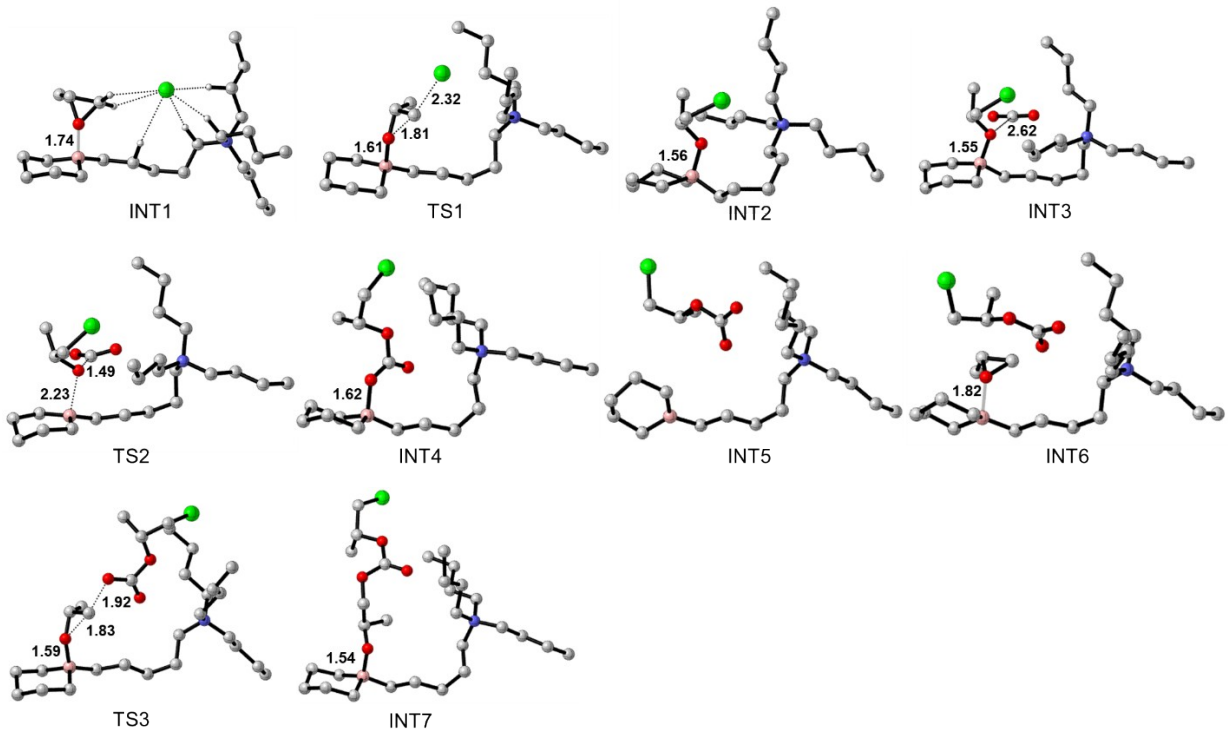


Figure S40. DFT computation optimized structures of intermediates and transition states for catalyst **5** mediated ROCOP.

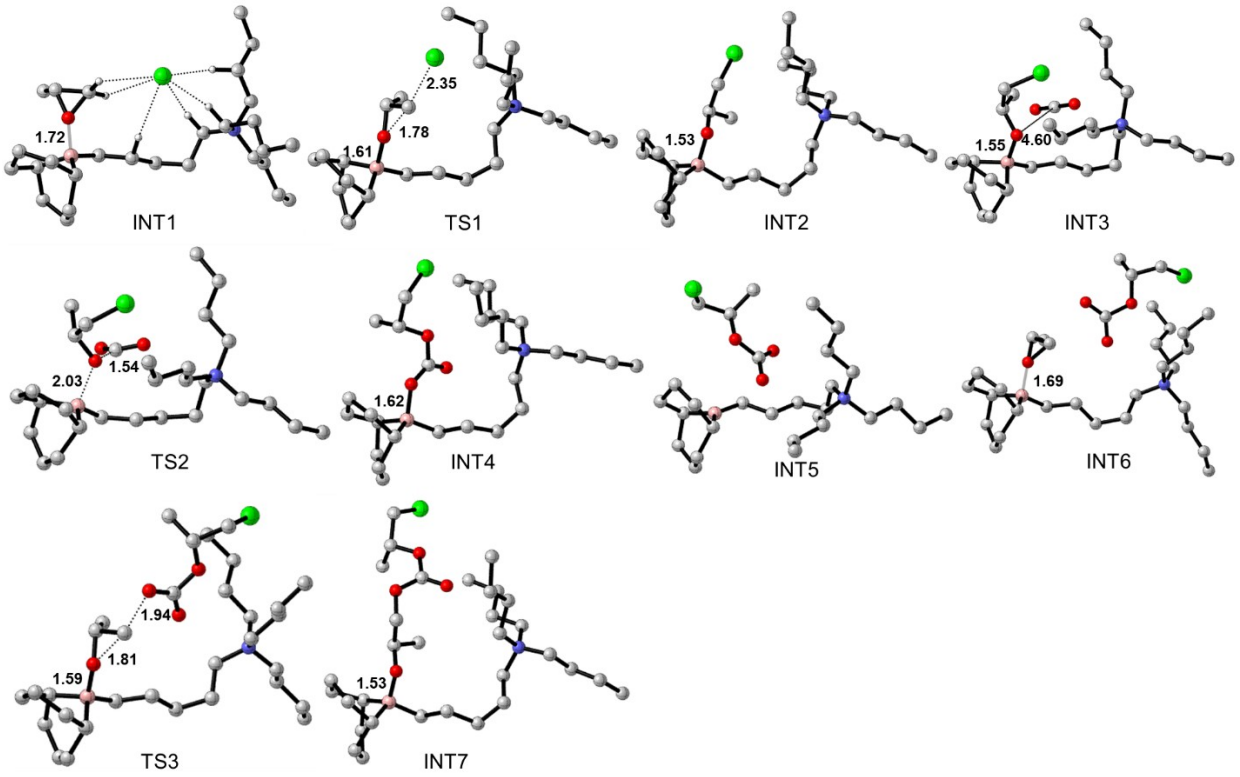


Figure S41. DFT computation optimized structures of intermediates and transition states for catalyst **3** mediated ROCOP.

REFERENCES

(1) Brown, H. C. a. P., G.G. Organoboranes: XXVIII. Convenient procedures for the synthesis of borinane. *J. Organomet. Chem.* **1983**, *250*, 13-22.

(2) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, *120*, 215-241.

(3) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104.

(4) Hehre, W. J.; Ditchfield, R.; Pople, J. A. Self—Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian—Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972**, *56*, 2257-2261.

(5) Dill, J. D.; Pople, J. A. Self-consistent molecular orbital methods. XV. Extended Gaussian-type basis sets for lithium, beryllium, and boron. *J. Chem. Phys.* **1975**, *62*, 2921-2923.

(6) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. Self-consistent molecular orbital methods. XXIII. A polarization-type basis set for second-row elements. *J. Chem. Phys.* **1982**, *77*, 3654-3665.

(7) Timothy Clark, J. C., Gunther W. Spitznagel, and Paul von Rague Schleyer. Efficient Diffuse Function- Augmented Basis Sets for Anion Calculations. III.* The 3-21+G Basis Set for First-Row Elements, Li-F. *J. Comput. Chem.* **1983**, *4*, 294-301.

(8) Fukui, K. A Formulation of the Reaction Coordinate. *J. Chem. Phys.* **1970**, *74*, 4161-4163.

(9) Fukui, K. The Path of Chemical Reactions — The IRC Approach. *Acc. Chem. Res.* **1981**, *14*, 363-368.

(10) Lu, T.; Chen, Q. Shermo: A general code for calculating molecular thermochemistry properties. *Comput. Theor. Chem.* **2021**, *1200*.

(11) McLean, A. D.; Chandler, G. S. Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11–18. *J. Chem. Phys.* **1980**, *72*, 5639-5648.

(12) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions. *J. Chem. Phys.* **1980**, *72*, 650-654.

(13) Jacopo Tomasi, B. M., and Roberto Cammi. Quantum Mechanical Continuum Solvation Models. *Chem. Rev.* **2005**, *105*, 2999−3093.

(14) Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. . Gaussian 16, Revision C.01. . *In Gaussian, Inc., Wallingford CT: 2016*.

(15) Wang, Y.; Zhang, J.-Y.; Yang, J.-L.; Zhang, H.-K.; Kiriratnikom, J.; Zhang, C.-J.; Chen, K.-L.; Cao, X.-H.; Hu, L.-F.; Zhang, X.-H.; Tang, B. Z. Highly Selective and Productive Synthesis of a Carbon Dioxide-Based Copolymer upon Zwitterionic Growth. *Macromolecules* **2021**, *54*, 2178-2186.
(16) Yang, G.-W.; Xu, C.-K.; Xie, R.; Zhang, Y.-Y.; Lu, C.; Qi, H.; Yang, L.; Wang, Y.; Wu, G.-P. Precision copolymerization of CO2 and epoxides enabled by organoboron catalysts. *Nat. Synth.* **2022**.

Cartesian coordinates for the optimized structures

PO

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CO_2

C	0.00000000	-0.00156000	0.00000000
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Catalyst 5

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B	3.01263300	-0.27745100	-0.48007400
Cl	1.74047500	0.73030200	-1.77078000

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H	1.50605600	-2.52906200	-1.06295300
H	0.76672400	-1.88497600	0.40316300
C	-0.47744000	-1.67296600	-1.33826300
H	-0.43565700	-1.06234100	-2.25154200
H	-0.73588400	-2.68733900	-1.66422000
C	-1.58432900	-1.15296900	-0.41749200
H	-1.65338900	-1.83304600	0.44273700
H	-1.29169300	-0.17343900	-0.01074300
C	-2.94680500	-1.08532700	-1.11514500
H	-3.12232200	-2.05869800	-1.60394800
H	-2.88964400	-0.36938400	-1.95231100

C	-5.66677500	-1.06856200	-0.93384100
C	-4.24130400	-1.52138500	1.27280600
C	-6.86634400	-0.74522100	-0.03369300
H	-5.70998900	-2.14316300	-1.17659500
H	-5.75138600	-0.55613700	-1.90121900
C	-5.51756200	-1.21811300	2.07223000
H	-4.15422300	-2.61273400	1.13759500
H	-3.36232200	-1.22205800	1.86159800
C	-6.79223200	-1.52910800	1.28103600
H	-7.81773000	-0.95911600	-0.53861300
H	-6.87933200	0.33117000	0.20276500
H	-5.53281000	-1.76888700	3.02204700
H	-5.52623700	-0.15074600	2.33430700
H	-7.67572200	-1.31813800	1.89666000
H	-6.81904700	-2.60446400	1.04974900
B	-4.25177000	-0.84448900	-0.19199300
Cl	-0.08375200	2.39546800	0.32427600
C	-4.62382200	2.05422700	-0.37002200
C	-3.24254800	1.81368700	0.07356400
O	-4.26841700	0.82327200	0.29118200
H	-5.26231900	2.65462900	0.27497700
H	-2.84447100	2.24542900	0.98450000
H	-2.49560900	1.54337400	-0.66547900
C	-5.00259000	2.02238300	-1.82217500
H	-6.03934700	1.70350400	-1.95367600
H	-4.89410900	3.03187700	-2.23099200
H	-4.35069000	1.34668200	-2.37974000

TS1

N	2.62099700	-0.34985900	0.03283800

C	3.82326900	-1.02535000	0.64492900
H	4.44562600	-0.22845800	1.06015800
H	3.44070800	-1.61946300	1.47911400
C	4.64741400	-1.90964900	-0.28205400
H	4.00948700	-2.63598200	-0.79903900
H	5.15146600	-1.31266000	-1.04944200
C	5.70295500	-2.66777500	0.52893000
H	5.20128400	-3.29289700	1.27787000
H	6.32120300	-1.95070200	1.08305100
C	6.58870000	-3.53571900	-0.36026600
H	7.12346700	-2.92611700	-1.09536200
H	7.33113100	-4.07600300	0.23192300
H	5.99199100	-4.27351100	-0.90587000
C	3.05878900	0.56451700	-1.09291700
H	3.61156500	-0.06075400	-1.79773800
H	3.76033500	1.27581300	-0.64873100
C	1.91681000	1.28765200	-1.79623000
H	1.40885200	0.60587900	-2.48896100
H	1.16646800	1.65077300	-1.08305600
C	2.43518000	2.50107300	-2.57068200
H	3.20799600	2.19531300	-3.28862400
H	2.91159800	3.19284900	-1.86384600
C	1.29135400	3.21497900	-3.28584500
H	1.64996300	4.09557600	-3.82514200
H	0.80864400	2.54939000	-4.00969200
H	0.53843600	3.53562700	-2.55835000
C	1.91387300	0.44647800	1.12559000
H	0.90765500	0.67311800	0.76295700
H	1.83302000	-0.22910200	1.98057500
C	2.57399500	1.75478300	1.53368400

H	2.41303700	2.50098700	0.74764300
H	3.65456400	1.64637300	1.69551100
C	1.91660800	2.26204400	2.82135300
H	2.20546400	1.61197200	3.65743800
H	0.82939400	2.19799700	2.70636600
C	2.29633100	3.71071100	3.10569500
H	1.87070200	4.04968400	4.05352000
H	3.38368500	3.83650700	3.15877800
H	1.90860800	4.35501200	2.31088400
C	1.65325600	-1.37039400	-0.52823200
H	2.10677500	-1.76781700	-1.44078700
H	0.77417000	-0.79554400	-0.82285100
C	1.24641200	-2.50758300	0.40523000
H	2.01715300	-3.28762000	0.40630900
H	1.13378200	-2.15838400	1.43809900
C	-0.11459100	-3.04268600	-0.07082800
H	-0.09947300	-3.13610100	-1.16612200
H	-0.27359300	-4.05302900	0.31860100
C	-1.26633800	-2.11766700	0.35416500
H	-1.54881200	-2.35344100	1.38839800
H	-0.88248000	-1.08710300	0.39524600
C	-2.49658000	-2.15267500	-0.54981400
H	-2.88734200	-3.18279700	-0.55352900
H	-2.17376500	-1.97109500	-1.58769800
C	-4.91558900	-1.16565700	-1.25066700
C	-4.36875100	-1.60675000	1.33592300
C	-6.15928300	-0.39654800	-0.78774300
H	-5.20959600	-2.20361000	-1.47996700
H	-4.55305600	-0.74754200	-2.20427100
C	-5.64250900	-0.81760300	1.66668300

H	-4.61326400	-2.68207100	1.32977600
H	-3.63534100	-1.46948700	2.14703300
C	-6.68468000	-0.92975200	0.54922100
H	-6.96099300	-0.43201200	-1.53863800
H	-5.90013500	0.66449900	-0.65721100
H	-6.08681700	-1.14555700	2.61704200
H	-5.38335500	0.24323500	1.79157500
H	-7.60062500	-0.39529900	0.83365100
H	-6.96342000	-1.98753300	0.42540700
B	-3.75342000	-1.19935300	-0.11204400
Cl	-0.36261000	3.05103000	0.30250600
C	-2.68198800	1.24616900	-0.71545300
C	-2.03349700	1.47034700	0.58202300
O	-3.37119200	0.34309700	0.11358700
H	-3.32921900	2.06691300	-1.04231200
H	-2.54345400	2.06457100	1.32527000
H	-1.31003100	0.74564900	0.92017200
C	-1.82969900	0.73534000	-1.85372200
H	-2.44763100	0.27407100	-2.62784400
H	-1.28179000	1.58208800	-2.27996000
H	-1.10866100	-0.00842700	-1.50210800

INT2

N	2.10377100	-0.08574700	-0.21204400
C	3.54928200	-0.45229600	-0.00969800
H	4.13599400	0.25930000	-0.59670200
H	3.76961900	-0.27388700	1.04653000
C	3.92644100	-1.87630400	-0.39509000
H	3.33659900	-2.60070900	0.17706800
H	3.72246400	-2.05744700	-1.45662100

C	5.41356600	-2.11783500	-0.12293500
H	5.61974800	-1.93887600	0.93974200
H	6.01166300	-1.38938300	-0.68459200
C	5.83733800	-3.53486400	-0.49908300
H	5.66347300	-3.72572600	-1.56278700
H	6.89923100	-3.69596900	-0.29748400
H	5.26956400	-4.27650600	0.07135900
C	1.78105800	-0.10329000	-1.69454800
H	1.77725800	-1.15665100	-1.98495900
H	2.61963600	0.38189000	-2.20469800
C	0.45839200	0.54313600	-2.08714100
H	-0.36264200	0.22848400	-1.42813600
H	0.53063600	1.63533600	-2.00218700
C	0.11665600	0.17841000	-3.53367000
H	-0.00626100	-0.90928600	-3.60751900
H	0.94844500	0.45184700	-4.19764200
C	-1.16753800	0.86354800	-3.98983900
H	-1.40833300	0.60520500	-5.02454900
H	-2.00614800	0.55418600	-3.35845600
H	-1.07423500	1.95331200	-3.92550200
C	1.84497300	1.28194900	0.37139900
H	0.76706600	1.43498600	0.28889200
H	2.07262700	1.20747400	1.43698300
C	2.62333800	2.43341600	-0.24775200
H	2.49647000	2.45986700	-1.33665300
H	3.69752300	2.33684500	-0.04847400
C	2.12408900	3.75551700	0.34398000
H	2.21873600	3.72288500	1.43619400
H	1.05280200	3.86066900	0.13497000
C	2.88700200	4.95424800	-0.21142000

H	2.51643000	5.88899600	0.21645000
H	3.95554100	4.88043400	0.01634400
H	2.77958500	5.01711000	-1.29923900
C	1.16707700	-1.07174300	0.48095500
H	1.23611200	-1.99696900	-0.09480100
H	0.15896900	-0.65908700	0.36455300
C	1.44818700	-1.33175400	1.95470600
H	2.48086500	-1.66786300	2.11567100
H	1.29889400	-0.41089700	2.52982300
C	0.47810500	-2.39200300	2.50883100
H	0.69368500	-3.36453300	2.04541100
H	0.70395000	-2.49514700	3.57676900
C	-1.00018500	-2.02847100	2.28974900
H	-1.59722500	-2.49761300	3.08008800
H	-1.09403800	-0.94335100	2.44436500
C	-1.57043200	-2.40770800	0.90734800
H	-2.12835000	-3.35005900	1.00053100
H	-0.74627800	-2.66559700	0.22339000
C	-2.73639700	-1.63525700	-1.38514600
C	-4.02545100	-1.27554700	0.94094300
C	-3.89903700	-0.86779000	-2.02127900
H	-2.92845900	-2.71302700	-1.51988500
H	-1.79759800	-1.43536200	-1.93379300
C	-5.22278900	-0.73231700	0.13568800
H	-4.24788800	-2.33521000	1.14441000
H	-4.01960500	-0.80292400	1.93824700
C	-5.21593400	-1.21180400	-1.31841200
H	-3.99249800	-1.06146900	-3.10050100
H	-3.72863300	0.21839600	-1.91668200
H	-6.17342000	-1.01766400	0.60863700

H	-5.22755600	0.36771500	0.11805500
H	-6.06801600	-0.77760700	-1.85769200
H	-5.34938500	-2.30346300	-1.34265100
B	-2.54668400	-1.28157300	0.20357200
Cl	-0.58959900	1.99096700	2.60741700
C	-2.43866700	1.24643800	0.63622000
C	-2.29344300	1.58271900	2.12154300
O	-1.78429200	0.07676000	0.28910900
H	-3.52675200	1.13782800	0.51971000
H	-2.89140900	2.45262600	2.40045600
H	-2.57134500	0.72283500	2.73032400
C	-2.00377000	2.40328300	-0.26140400
H	-2.20838200	2.14613200	-1.30527500
H	-2.53586200	3.32839600	-0.01412000
H	-0.92988700	2.59500700	-0.15954900

INT3

N	2.64126500	-0.08927800	0.09285000
C	3.89804000	-0.56162600	0.78640200
H	4.23365400	0.27114100	1.40929100
H	3.60216700	-1.37556000	1.45385800
C	5.03354300	-1.02164900	-0.11905800
H	4.74050500	-1.92047600	-0.67149800
H	5.28988200	-0.25447500	-0.85939900
C	6.27506200	-1.33443500	0.72126400
H	6.01914700	-2.08322700	1.48099700
H	6.58511400	-0.43251300	1.26312900
C	7.42867300	-1.84486600	-0.13754900
H	7.71562500	-1.10263600	-0.88926800
H	8.30835300	-2.06181300	0.47324400

H	7.14864300	-2.76338600	-0.66268000
C	2.88309000	1.30159600	-0.45642100
H	3.82804000	1.25767900	-1.00449700
H	3.03426300	1.94376300	0.41455500
C	1.77690200	1.85395700	-1.35015700
H	1.85299200	1.42705100	-2.35574900
H	0.78185800	1.59100300	-0.97544300
C	1.88196300	3.37835200	-1.42810400
H	2.88349900	3.66628700	-1.77512700
H	1.76490900	3.79493700	-0.41885300
C	0.81676200	3.96744700	-2.34714200
H	0.91686700	5.05336200	-2.42218500
H	0.89319300	3.54843900	-3.35573400
H	-0.18212600	3.74457600	-1.96027400
C	1.50254300	-0.05624500	1.10365100
H	0.60205900	0.26316200	0.57352300
H	1.34501100	-1.09338900	1.40771000
C	1.71046700	0.82892700	2.32397800
H	1.68374700	1.88655900	2.03920600
H	2.66778400	0.63711800	2.82301500
C	0.57207100	0.56590600	3.31591100
H	0.66903800	-0.45041700	3.71695600
H	-0.38207000	0.59669200	2.77886700
C	0.55835800	1.58745700	4.44746000
H	-0.23418100	1.36517700	5.16625500
H	1.51154700	1.59551200	4.98756100
H	0.38248700	2.59261400	4.05099700
C	2.27378500	-1.00345200	-1.06606500
H	3.06242000	-0.85368600	-1.80817200
H	1.35107900	-0.59416800	-1.47575200

C	2.08545100	-2.49360200	-0.73136000
H	2.87091200	-3.07200700	-1.23022400
H	2.20482400	-2.68404000	0.34229600
C	0.69116600	-2.97562400	-1.16619500
H	0.56145400	-2.76183500	-2.23633400
H	0.63292300	-4.06435200	-1.05478600
C	-0.41561500	-2.28662500	-0.37279900
H	-0.32640100	-2.57582600	0.68664600
H	-0.25015200	-1.20684900	-0.40907700
C	-1.85486700	-2.48430100	-0.83166600
H	-2.19296200	-3.50325600	-0.59195800
H	-1.89840700	-2.41707300	-1.93306400
C	-4.37898300	-1.56114500	-0.69762500
C	-2.79566300	-1.56306100	1.51533300
C	-5.54682800	-1.20148300	0.23958800
H	-4.49518400	-2.62954000	-0.94298800
H	-4.50190400	-1.03639600	-1.65828900
C	-4.04568100	-1.09549700	2.27613600
H	-2.68338200	-2.63904000	1.73480600
H	-1.89058000	-1.09436300	1.94565000
C	-5.31509000	-1.69936200	1.66849900
H	-6.49554500	-1.60897400	-0.13850600
H	-5.69766900	-0.11201600	0.28656700
H	-3.98880700	-1.35123900	3.34455100
H	-4.14889000	0.00163600	2.23767200
H	-6.18547500	-1.46678300	2.29643000
H	-5.21551100	-2.79520700	1.65795200
B	-2.84316000	-1.37040400	-0.12794600
Cl	-0.84495100	2.66593800	0.85661500
C	-2.93860200	1.14280800	-0.24716900

C	-2.45566400	1.82405900	1.03591000
O	-2.22608300	-0.00737600	-0.54434400
H	-3.98971500	0.90542900	-0.01521700
H	-3.14216300	2.60810500	1.36097700
H	-2.31674200	1.08964500	1.82838000
C	-2.93150300	2.10582100	-1.43283800
H	-3.51576700	1.68205500	-2.25225400
H	-3.34474900	3.08652900	-1.17189100
H	-1.89949700	2.24662100	-1.77511500
C	-1.49676800	-0.22457500	-3.05426800
O	-0.36997000	-0.09236000	-2.77027300
O	-2.57278000	-0.34866800	-3.46834800

TS2

N	2.71069000	-0.15650800	0.03045500
C	3.85492200	-0.78706900	0.78646600
H	4.19372500	-0.04550500	1.51353100
H	3.44001700	-1.62910000	1.34560900
C	5.03334700	-1.25683800	-0.05729100
H	4.71762000	-2.04388900	-0.74992100
H	5.44121200	-0.43713100	-0.65971300
C	6.13990000	-1.80418300	0.84856700
H	5.73518600	-2.61654000	1.46486400
H	6.46615700	-1.01892600	1.54166000
C	7.33347500	-2.31250900	0.04474000
H	7.76799000	-1.51026500	-0.56015600
H	8.11610300	-2.69945100	0.70197600
H	7.03379500	-3.11824300	-0.63269900
C	3.14852100	1.21769700	-0.43600100
H	4.01720200	1.05857000	-1.08065800

H	3.48970100	1.74136900	0.46264500
C	2.09548200	2.03996300	-1.16113500
H	1.79109200	1.55969300	-2.09467000
H	1.17820600	2.11639400	-0.56990600
C	2.63271800	3.44404600	-1.44336200
H	3.54103000	3.38412000	-2.05768600
H	2.92515200	3.92443900	-0.49973400
C	1.58148400	4.29651000	-2.15009700
H	1.95409100	5.30486600	-2.34949300
H	1.29147000	3.84290000	-3.10244100
H	0.67838800	4.37871100	-1.53700300
C	1.50167700	-0.03642300	0.94305700
H	0.66762300	0.28728200	0.30777200
H	1.29021400	-1.05503600	1.28095300
C	1.66166300	0.89137400	2.13904200
H	1.60691300	1.93696600	1.81316200
H	2.62090400	0.75447300	2.65357400
C	0.52828500	0.61399300	3.13134600
H	0.67439900	-0.38075600	3.57099100
H	-0.41913000	0.57645200	2.58191300
C	0.44950700	1.67134800	4.22641600
H	-0.33901900	1.43612900	4.94609500
H	1.39526800	1.74269500	4.77484000
H	0.23083000	2.65232100	3.79345800
C	2.30880900	-0.99282500	-1.17855700
H	3.12060800	-0.86658000	-1.89989500
H	1.40857700	-0.51237000	-1.57454400
C	2.03867000	-2.48607800	-0.90523400
H	2.82394700	-3.08156400	-1.38387400
H	2.09290100	-2.72370800	0.16430000

C	0.65600500	-2.91052500	-1.42448200
H	0.50423200	-2.48420700	-2.42453600
H	0.62971200	-4.00073300	-1.53976500
C	-0.47930100	-2.45009300	-0.51064200
H	-0.42418100	-3.00451300	0.43932600
H	-0.32924200	-1.39668600	-0.26866300
C	-1.87469000	-2.57737100	-1.12239600
H	-2.16063100	-3.64097600	-1.18066600
H	-1.86032700	-2.22137500	-2.16123300
C	-4.44175200	-1.69613100	-1.04719300
C	-2.99542700	-1.86992100	1.27799300
C	-5.65313400	-1.34901600	-0.16119400
H	-4.62210500	-2.68187500	-1.50670600
H	-4.34155600	-1.00842000	-1.89747300
C	-4.27887700	-1.38429900	1.96800500
H	-2.85442500	-2.93305400	1.54120400
H	-2.10231700	-1.36305400	1.67203900
C	-5.52596000	-1.91910600	1.25549500
H	-6.58248300	-1.70747900	-0.62087500
H	-5.77199300	-0.26000700	-0.07591200
H	-4.29273000	-1.68041300	3.02478900
H	-4.32909000	-0.28504400	1.96244100
H	-6.42478900	-1.68174000	1.83743200
H	-5.46402100	-3.01656300	1.20409100
B	-3.03256200	-1.83433200	-0.31833000
Cl	-1.09073100	2.77340200	0.96489400
C	-3.07751500	1.25678500	-0.24666100
C	-2.63052500	1.83405100	1.09086900
O	-2.18359100	0.20954100	-0.58673600
H	-4.05849500	0.80707000	-0.04189500

H	-3.37547800	2.52310600	1.49351500
H	-2.44265000	1.03052300	1.80494500
C	-3.26370600	2.33759900	-1.30557400
H	-3.72685200	1.92170100	-2.19861100
H	-3.89509400	3.13175700	-0.89302000
H	-2.30060100	2.77201400	-1.58971000
C	-1.49938000	0.30691200	-1.90182700
O	-0.27294900	0.44441700	-1.75545500
O	-2.22619000	0.20525500	-2.87437300

INT4

N	2.67379200	-0.28014700	0.03159200
C	3.94526700	-0.60371500	0.77231500
H	4.22144000	0.29609700	1.32817700
H	3.68663100	-1.37874700	1.49784000
C	5.11569600	-1.06912300	-0.08456400
H	4.81254100	-1.89441100	-0.73875600
H	5.47744700	-0.25853500	-0.72641700
C	6.26287600	-1.54243900	0.81263800
H	5.91309900	-2.37610300	1.43390700
H	6.54490800	-0.73587800	1.50094500
C	7.47931300	-1.97744000	0.00040900
H	7.86351200	-1.14954500	-0.60384800
H	8.28634600	-2.32053500	0.65234600
H	7.22323000	-2.79736500	-0.67799300
C	2.92991400	0.86588600	-0.92496000
H	3.68558400	0.50970800	-1.62954100
H	3.38066200	1.66266800	-0.32371100
C	1.71174700	1.37891400	-1.67978600
H	1.34662200	0.62291800	-2.38046900

H	0.86971300	1.58518300	-1.01167900
C	2.06500200	2.66317000	-2.43221500
H	2.93431600	2.49771700	-3.08292800
H	2.35541200	3.43768900	-1.70953700
C	0.87737700	3.15004100	-3.25863000
H	1.10293300	4.09356300	-3.76271900
H	0.60666800	2.41182300	-4.01964900
H	0.00426500	3.30100900	-2.61601800
C	1.59939400	0.10368500	1.03209400
H	0.65959700	0.08511700	0.47951600
H	1.57364000	-0.70110400	1.77105300
C	1.75346300	1.45098900	1.72128800
H	1.60294400	2.26603300	1.00325500
H	2.74401100	1.58140600	2.17495100
C	0.67965900	1.55106600	2.80864200
H	0.86928000	0.79456000	3.57997200
H	-0.28663100	1.29635900	2.35563600
C	0.62581600	2.93896900	3.43929700
H	-0.15145000	2.99382000	4.20678000
H	1.58036100	3.19089700	3.91336900
H	0.41584500	3.70317400	2.68316900
C	2.16338600	-1.48754700	-0.74654700
H	2.81588600	-1.58890800	-1.61819800
H	1.16719600	-1.20348600	-1.09573300
C	2.09550300	-2.80630600	0.03479200
H	3.03269600	-3.36336100	-0.08650300
H	1.96788500	-2.63657600	1.11017300
C	0.87464300	-3.60445300	-0.45545800
H	0.82116800	-3.53513400	-1.54994800
H	1.01036200	-4.66548600	-0.22121000

C	-0.43228400	-3.06813100	0.16205800
H	-0.62140900	-3.60029100	1.10390600
H	-0.26922900	-2.02142000	0.45516800
C	-1.66496200	-3.13237500	-0.74418600
H	-2.00378800	-4.17786700	-0.81284900
H	-1.36503500	-2.84114800	-1.75930500
C	-4.14742200	-2.18418000	-1.31907900
C	-3.46346300	-2.61197100	1.23842700
C	-5.35914200	-1.40617800	-0.78805700
H	-4.46706000	-3.21441600	-1.54514500
H	-3.81653000	-1.75580500	-2.27853500
C	-4.71347900	-1.81515600	1.63379300
H	-3.71442800	-3.68542400	1.25586800
H	-2.68233200	-2.47339200	2.00302100
C	-5.81622400	-1.93162800	0.57674800
H	-6.20141700	-1.42939500	-1.49380600
H	-5.08678000	-0.34557600	-0.66762300
H	-5.10535600	-2.12830700	2.61209100
H	-4.44618300	-0.75150800	1.73514700
H	-6.71557200	-1.39489200	0.90723400
H	-6.10092700	-2.98975900	0.47437600
B	-2.92790400	-2.23230200	-0.24955100
Cl	-0.93760600	4.17525500	0.14817600
C	-2.57668800	1.94297000	0.19274000
C	-2.14218100	3.14787900	1.00951600
O	-1.39660300	1.25678900	-0.20736900
H	-3.16231600	1.30079800	0.86179500
H	-2.99986500	3.78444300	1.23153900
H	-1.66768700	2.84403000	1.94268900
C	-3.40130900	2.30309600	-1.03288900

H	-3.67710400	1.38888300	-1.56604100
H	-4.32144000	2.81991900	-0.74378300
H	-2.82314900	2.94546600	-1.70331200
C	-1.53426200	-0.06368200	-0.62163000
O	-0.68025900	-0.45587800	-1.40372500
O	-2.49739600	-0.67712900	-0.06660500

INT5

N	-3.01021600	0.12286000	0.02896100
C	-4.36293100	0.70272200	0.34375500
H	-4.88805400	-0.04824600	0.94022800
H	-4.18231600	1.56699400	0.98729800
C	-5.21097400	1.11462400	-0.85376400
H	-4.62045700	1.70420400	-1.56538300
H	-5.57795100	0.23359600	-1.39107900
C	-6.40695700	1.94882400	-0.38749100
H	-6.04032700	2.85529000	0.11045700
H	-6.97211900	1.38616800	0.36611800
C	-7.32545100	2.32951400	-1.54499700
H	-7.72993900	1.43746000	-2.03357400
H	-8.16741900	2.93406800	-1.19881400
H	-6.78332100	2.90817300	-2.29977100
C	-3.18934700	-1.11427900	-0.82545000
H	-3.70717900	-0.78751200	-1.73105600
H	-3.86461500	-1.77083600	-0.26780200
C	-1.89331300	-1.82881800	-1.16394600
H	-1.30863800	-1.24172600	-1.88071600
H	-1.27684100	-1.94070200	-0.26823800
C	-2.15123600	-3.22468800	-1.73065000
H	-2.77144400	-3.17375400	-2.63572800

H	-2.71552600	-3.81154100	-0.99345200
C	-0.82326000	-3.91822400	-2.02956300
H	-0.97285600	-4.95163000	-2.35361400
H	-0.28118500	-3.39014100	-2.82087400
H	-0.18784100	-3.91980400	-1.13695100
C	-2.30614200	-0.21232900	1.34528200
H	-1.23976400	-0.31205700	1.12030900
H	-2.45943600	0.66192400	1.98450400
C	-2.77831100	-1.47246600	2.05224700
H	-2.48837100	-2.35318700	1.46998100
H	-3.86808400	-1.49358600	2.19430100
C	-2.07916100	-1.56097800	3.41153300
H	-2.39132600	-0.71729500	4.04141800
H	-1.00249600	-1.47694400	3.23476600
C	-2.38114600	-2.88146800	4.11240900
H	-1.89883500	-2.92677000	5.09243300
H	-3.45827200	-3.02106600	4.25974800
H	-2.00581200	-3.71879800	3.51628500
C	-2.13261900	1.10988100	-0.72265100
H	-2.48564200	1.12015400	-1.75872400
H	-1.12717900	0.67484200	-0.69610800
C	-2.13032300	2.52821700	-0.15829100
H	-3.06687800	3.04048800	-0.41140200
H	-2.05383500	2.51427500	0.93563100
C	-0.92180400	3.29715900	-0.71192300
H	-0.80317900	3.07038500	-1.78119600
H	-1.11388200	4.37453400	-0.64801800
C	0.36780500	2.95138600	0.03573000
H	0.28146700	3.33281600	1.06365000
H	0.46977200	1.86329900	0.11910200

C	1.62537000	3.51923800	-0.62169800
H	1.54259800	4.60686100	-0.77016800
H	1.70576700	3.10898600	-1.64570100
C	4.28321000	4.02199700	-0.26655300
C	3.13957700	1.97630200	1.09366100
C	5.62815200	3.32107400	-0.02539700
H	4.19251100	4.86370200	0.44571300
H	4.24090300	4.49134200	-1.25794500
C	4.56083200	1.41486200	1.25100200
H	2.83870400	2.45349000	2.04696500
H	2.40161900	1.17840700	0.93887300
C	5.62141300	2.51851400	1.27862900
H	6.45049500	4.04613900	-0.01984000
H	5.83287300	2.63053600	-0.85521400
H	4.63526500	0.79111000	2.14951300
H	4.78204100	0.75319100	0.40081300
H	6.61154200	2.08231000	1.45369500
H	5.42133700	3.19579200	2.12215000
B	3.00654500	3.14548900	0.04608300
Cl	4.56417200	-3.64541400	-0.91203200
C	2.91018000	-1.41666800	-0.79897100
C	4.33091700	-1.89676000	-0.55864700
O	2.09459100	-2.03931700	0.17210100
H	2.91887500	-0.33181300	-0.62797500
H	5.03133400	-1.35327000	-1.19620900
H	4.59642500	-1.75375100	0.48935400
C	2.39590100	-1.68904900	-2.20532800
H	1.40201100	-1.24578400	-2.30159300
H	3.05719500	-1.24746900	-2.95863900
H	2.33247000	-2.76635300	-2.37938300

C	0.88560500	-1.42367200	0.47245400
O	0.16272500	-2.07706500	1.24052600
O	0.65240400	-0.31254400	-0.07200600

INT6

N	-3.40088100	-0.25037600	-0.08148200
C	-4.69094700	-0.91545000	-0.48275700
H	-5.38752300	-0.10968800	-0.72867700
H	-4.47998100	-1.45999300	-1.40593300
C	-5.31215300	-1.85239000	0.54624400
H	-4.56247800	-2.54492100	0.94722300
H	-5.71476000	-1.28658300	1.39328500
C	-6.44281200	-2.66045000	-0.09613100
H	-6.03277700	-3.26268000	-0.91663800
H	-7.17087600	-1.97430700	-0.54667500
C	-7.14204200	-3.56724200	0.91238300
H	-7.58750600	-2.98127300	1.72253700
H	-7.93902500	-4.14509800	0.43798100
H	-6.43456900	-4.27316500	1.35910700
C	-3.64775500	0.59217300	1.15124400
H	-3.99969700	-0.09605000	1.92443700
H	-4.47425300	1.26279000	0.89572300
C	-2.44086800	1.37872000	1.63291400
H	-1.69015900	0.70543000	2.05973700
H	-1.95206400	1.88864000	0.79669300
C	-2.84814700	2.42360100	2.67174500
H	-3.33765100	1.94855300	3.53279400
H	-3.58586300	3.10539800	2.22764100
C	-1.62795100	3.22062300	3.12799200
H	-1.90421900	4.01497500	3.82657100

H	-0.90342300	2.56835400	3.62654800
H	-1.12850500	3.67416300	2.26549600
C	-2.91700700	0.60838500	-1.24805100
H	-1.86481100	0.84085400	-1.06283600
H	-3.00139100	-0.02942700	-2.13213700
C	-3.65789300	1.91785500	-1.46690900
H	-3.44128100	2.60573000	-0.64253800
H	-4.74699300	1.78241800	-1.52579300
C	-3.14936800	2.55994300	-2.76094100
H	-3.37947100	1.90337800	-3.61055100
H	-2.06114300	2.64684200	-2.68346700
C	-3.76504800	3.93756200	-2.98388400
H	-3.40946300	4.38078200	-3.91772000
H	-4.85885600	3.88540800	-3.03026800
H	-3.49063300	4.61364600	-2.16834300
C	-2.30969900	-1.26403900	0.22587000
H	-2.53754100	-1.67937100	1.21325900
H	-1.38525400	-0.67728100	0.29265800
C	-2.18206000	-2.38974100	-0.79555200
H	-3.06595500	-3.03856400	-0.75915000
H	-2.11469100	-1.98452800	-1.81211900
C	-0.92083100	-3.21939900	-0.52104800
H	-0.87988300	-3.47508300	0.54907400
H	-1.00429800	-4.17459600	-1.05324200
C	0.37546700	-2.52362200	-0.93603500
H	0.33009600	-2.30753300	-2.01245000
H	0.44868800	-1.53740600	-0.45753400
C	1.62814200	-3.36144600	-0.65119000
H	1.66931700	-4.19742200	-1.36632800
H	1.53509900	-3.85385100	0.33255800

Cl	4.01331300	4.34818600	0.09141100
C	2.53158600	2.01809900	0.39152900
C	3.79787000	2.58960400	-0.22256800
O	1.43734000	2.62683200	-0.25990100
H	2.54471600	0.94330700	0.16259000
H	4.67929500	2.08931400	0.18317300
H	3.77219700	2.46486400	-1.30538900
C	2.43543200	2.22996600	1.89754600
H	1.50493100	1.78801500	2.26395900
H	3.28232500	1.77169600	2.42150500
H	2.42477600	3.29938700	2.12315200
C	0.23520700	1.93580000	-0.27263700
O	-0.70779000	2.58256200	-0.75610300
O	0.22342700	0.76771500	0.19978900
B	3.01442500	-2.55565700	-0.75532300
C	4.37047700	-3.39280900	-0.56248100
C	3.13273400	-1.40949900	-1.87434800
O	2.94467500	-1.45016000	0.69141400
C	5.62364500	-2.50745200	-0.52703100
H	4.44127900	-4.03902900	-1.45332500
H	4.35138100	-4.08577700	0.28905700
C	4.45844000	-0.63980100	-1.78853500
H	3.06788700	-1.89675600	-2.86167000
H	2.28962900	-0.70455800	-1.82886100
C	3.29103500	-1.51825200	2.08501400
C	1.89566600	-1.31824200	1.66155300
C	5.67385800	-1.57017500	-1.73809600
H	6.53929000	-3.11127500	-0.48343000
H	5.62001400	-1.88820700	0.38487200
H	4.56461100	0.06769700	-2.62132200

H	4.45759200	-0.03700700	-0.86828500
H	3.85968100	-0.63919200	2.38374000
C	3.75559600	-2.83392700	2.64061400
H	1.41282900	-0.34560300	1.62813700
H	1.23924900	-2.18526700	1.71142100
H	6.59810600	-0.97984700	-1.71861900
H	5.70519200	-2.17618500	-2.65546100
H	4.79557800	-3.03132600	2.36940900
H	3.68110500	-2.80554300	3.73216700
H	3.13519600	-3.65146100	2.26495800

TS3

N	2.28418900	1.81882900	-0.07608600
C	3.00473000	3.02242100	-0.62680400
H	3.95951200	2.65960400	-1.01680400
H	2.40892100	3.36951000	-1.47454200
C	3.23957000	4.16790400	0.34980100
H	2.31207000	4.43471800	0.86931100
H	3.97066400	3.88345500	1.11443000
C	3.75756000	5.39674700	-0.40297100
H	3.00981700	5.70503300	-1.14428500
H	4.66153500	5.12751700	-0.96360300
C	4.05992500	6.55760300	0.54011900
H	4.82776000	6.28036000	1.26930000
H	4.41915700	7.42991300	-0.01123800
H	3.16340200	6.85492400	1.09318500
C	3.09565500	1.22956200	1.05615300
H	3.15358700	2.00647100	1.82269000
H	4.10456900	1.07505700	0.66034000
C	2.54733500	-0.05592300	1.65798600

H	1.58831400	0.13207100	2.15176700
H	2.34734600	-0.81182200	0.89265600
C	3.54680300	-0.62310300	2.66796000
H	3.81600600	0.14171100	3.40879800
H	4.47280400	-0.89534900	2.14416200
C	2.97368400	-1.85095800	3.36936500
H	3.70042900	-2.29652400	4.05365100
H	2.07977500	-1.58844800	3.94387700
H	2.68916600	-2.60563300	2.62991500
C	2.10614500	0.80481200	-1.19621300
H	1.34864700	0.09984100	-0.84346300
H	1.69089400	1.36571800	-2.03774400
C	3.35712400	0.05452000	-1.63268400
H	3.75811400	-0.54705900	-0.80870400
H	4.15211000	0.73066000	-1.97271900
C	2.97847600	-0.89811700	-2.77054400
H	2.56193900	-0.32655100	-3.60930500
H	2.17870500	-1.55521700	-2.40687600
C	4.16945600	-1.72558400	-3.24520300
H	3.87906000	-2.41344300	-4.04460100
H	4.96513600	-1.08150600	-3.63404200
H	4.58775100	-2.31412100	-2.42146300
C	0.90251400	2.19248200	0.45239100
H	1.06815400	2.70557900	1.40432700
H	0.40190800	1.24273300	0.64967000
C	0.05328300	3.06273000	-0.46769700
H	0.48554700	4.06811100	-0.54668000
H	0.01133400	2.64119200	-1.47956900
C	-1.38017900	3.13541600	0.08989000
H	-1.33682900	3.27365600	1.18025600

H	-1.87366900	4.02911100	-0.30767500
C	-2.22736900	1.89854600	-0.23400700
H	-2.42918900	1.89192700	-1.31539500
H	-1.62594500	1.00378600	-0.03208500
C	-3.54536600	1.84123200	0.54331700
H	-4.03709800	2.82210900	0.42927500
H	-3.31433500	1.77191400	1.61836200
Cl	3.87289700	-3.63312100	0.05712000
C	1.16380700	-3.95571800	-0.38398300
C	2.53104500	-4.22569800	-0.98962100
O	1.09822700	-2.55145100	-0.16699800
H	0.41748400	-4.23603000	-1.13701500
H	2.68631700	-5.29665500	-1.12737300
H	2.64279400	-3.71337700	-1.94644200
C	0.89997800	-4.72208200	0.90179900
H	-0.09797300	-4.47425200	1.26843900
H	0.94629000	-5.80032000	0.72059800
H	1.64085200	-4.46243600	1.66263000
C	-0.14599300	-1.96525500	-0.03482000
O	-0.11505100	-0.76527200	0.24810100
O	-1.15019300	-2.70413400	-0.24582400
B	-4.70302700	0.77329700	0.07809700
C	-5.95954400	0.79641500	1.11793600
C	-5.21844000	1.06008300	-1.44104600
O	-4.28045400	-0.75751400	-0.00614700
C	-7.13573300	-0.05358300	0.62207000
H	-6.30531600	1.83697700	1.23723300
H	-5.66329800	0.46731300	2.12772300
C	-6.43380100	0.19882900	-1.80996500
H	-5.50133200	2.12210300	-1.53280900

H	-4.41881200	0.89607300	-2.18236000
C	-3.45559400	-1.52702400	0.83771300
C	-2.72968100	-1.63433700	-0.43490800
C	-7.56747700	0.35400500	-0.79073900
H	-7.99842500	0.00752000	1.30101900
H	-6.83090300	-1.10997200	0.59721600
H	-6.81060500	0.43537300	-2.81567000
H	-6.13003900	-0.85748300	-1.82954100
H	-3.97128500	-2.44725000	1.13510900
C	-2.76957300	-0.89149600	2.02551000
H	-3.12819600	-2.30267700	-1.18409700
H	-2.16287500	-0.77214100	-0.74901700
H	-8.43911600	-0.23633300	-1.10390000
H	-7.89025000	1.40650500	-0.77403800
H	-3.51337400	-0.52303600	2.73703900
H	-2.15529400	-1.65342800	2.51784500
H	-2.11742100	-0.07230100	1.72542300

INT7

N	3.10044400	-0.37431900	-0.03766700
C	4.53156700	-0.38300800	-0.51665300
H	4.62822500	-1.23399400	-1.19481900
H	4.65764700	0.52970100	-1.10394700
C	5.59839400	-0.45698300	0.56905300
H	5.41031300	0.28275400	1.35561500
H	5.60239500	-1.44418500	1.04373800
C	6.97808800	-0.19162200	-0.04042100
H	6.98898700	0.81408800	-0.47845300
H	7.15449000	-0.89409800	-0.86458200
C	8.09206100	-0.31802500	0.99467400

H	8.11788400	-1.32550000	1.42176200
H	9.06878800	-0.11718600	0.54799400
H	7.94531800	0.39123300	1.81533500
C	2.82623200	-1.64013500	0.74465800
H	3.52249300	-1.63423600	1.58685800
H	3.09823900	-2.47084500	0.08643400
C	1.39658400	-1.79143600	1.24077000
H	1.16560800	-1.02455900	1.98925700
H	0.68115500	-1.67223400	0.42140000
C	1.18781300	-3.17522200	1.86070100
H	1.85445000	-3.30600900	2.72281900
H	1.46180700	-3.94527000	1.12808200
C	-0.26787300	-3.36859600	2.27803500
H	-0.42397500	-4.34683800	2.74019400
H	-0.57248300	-2.60001200	2.99712900
H	-0.92574300	-3.30225700	1.40518500
C	2.18267900	-0.27761800	-1.25069500
H	1.18700900	-0.01702400	-0.88241500
H	2.55358000	0.56673200	-1.83731200
C	2.07737700	-1.53031700	-2.10847000
H	1.52645700	-2.30547700	-1.56633500
H	3.06108500	-1.93480800	-2.37800300
C	1.30471900	-1.19514400	-3.38852400
H	1.91908100	-0.54855800	-4.02721300
H	0.40667900	-0.62988700	-3.11965100
C	0.89609900	-2.45808200	-4.13880300
H	0.38059300	-2.21360700	-5.07107100
H	1.76726100	-3.07419700	-4.38719100
H	0.21851100	-3.05507300	-3.52075900
C	2.84278500	0.82631400	0.85856300

H	3.28297600	0.59042100	1.83148100
H	1.75993400	0.87177300	0.98594200
C	3.35778200	2.17148300	0.35485800
H	4.42877600	2.27081000	0.57093700
H	3.23111100	2.27037500	-0.72974000
C	2.51575000	3.26663000	1.03037300
H	2.38771600	3.01416900	2.09296500
H	3.05886400	4.21668400	1.00746200
C	1.14257500	3.40361300	0.35233900
H	1.24224100	4.08863500	-0.50018300
H	0.85588500	2.44171700	-0.10224200
C	-0.01091300	3.84958500	1.24568600
H	0.20161300	4.85630200	1.63923200
H	-0.02922200	3.19018700	2.13312300
Cl	-3.35247700	-5.38824400	1.04454100
C	-3.87935200	-2.90795800	-0.05369400
C	-4.26213100	-4.37557400	-0.12253900
O	-2.50999700	-2.84925100	-0.49130600
H	-4.50293500	-2.38265300	-0.78527400
H	-5.32239100	-4.49174200	0.10639400
H	-4.05396700	-4.77339900	-1.11601100
C	-4.04407100	-2.28492800	1.32183700
H	-3.85650800	-1.21055300	1.27626000
H	-5.06544300	-2.44186900	1.68148500
H	-3.35178600	-2.74631100	2.03081500
C	-1.97863500	-1.69086100	-0.89697700
O	-0.80167100	-1.62421200	-1.17992100
O	-2.86217000	-0.71113100	-0.95743800
B	-1.45479300	3.86214300	0.43756300
C	-2.72221300	4.00901900	1.46399200

C	-1.49962800	5.08904400	-0.64560200
O	-1.57307400	2.59702000	-0.42419400
C	-4.05220000	4.21422600	0.72431900
H	-2.54810000	4.88878300	2.10535300
H	-2.81505200	3.16068100	2.16509300
C	-2.88096700	5.20744900	-1.29890900
H	-1.26253100	6.04558300	-0.14987800
H	-0.74044600	4.95667300	-1.43342600
C	-2.12852500	1.43006500	0.04705700
C	-2.36398800	0.62318800	-1.22973700
C	-3.98234700	5.39403500	-0.25099000
H	-4.89242300	4.36123600	1.41947100
H	-4.29468600	3.31313400	0.13784800
H	-2.92811000	6.02923700	-2.02904200
H	-3.08654400	4.28037000	-1.85510600
H	-3.10468600	1.58729300	0.54049500
C	-1.22974700	0.68073900	1.03737300
H	-3.12890600	1.10308500	-1.84014700
H	-1.43090700	0.55260400	-1.79155000
H	-4.95612800	5.53501400	-0.74027000
H	-3.78015200	6.31432600	0.31818000
H	-1.07391400	1.30203000	1.92273100
H	-1.64996100	-0.28259600	1.35915000
H	-0.25938400	0.49031100	0.56629400

Catalyst 3

N	-2.23777500	0.01532600	0.01562000
C	-3.61696800	-0.58696400	-0.00053600
H	-4.30886000	0.22321700	0.24989300
H	-3.81538700	-0.88403700	-1.03403800
C	-3.83241700	-1.76912100	0.93397200
H	-3.19590900	-2.61018700	0.63673200
H	-3.56605700	-1.50715500	1.96469000
C	-5.29711700	-2.21300000	0.89207700
H	-5.57267700	-2.45515600	-0.14194000
H	-5.93978100	-1.37876900	1.19967700
C	-5.55136900	-3.42060400	1.78987000
H	-5.30442900	-3.19248100	2.83156400
H	-6.59976700	-3.72639100	1.75196400
H	-4.94005300	-4.27369300	1.47961000
C	-1.96158100	0.63116800	1.37880400
H	-1.75001100	-0.20867500	2.04501000
H	-2.89206000	1.09515500	1.71933600
C	-0.80863400	1.62669900	1.41391700
H	0.05645200	1.26220200	0.84763000
H	-1.11312200	2.57043200	0.94449800
C	-0.37227800	1.89469000	2.85540700
H	-0.00565200	0.95867100	3.29514000
H	-1.23035900	2.21703100	3.46082400
C	0.73197700	2.94730200	2.90240600
H	1.08364800	3.10720700	3.92485600
H	1.58447200	2.63175300	2.29219400
H	0.37495400	3.90588600	2.51203400
C	-2.13697600	1.05656800	-1.08323800

H	-1.08415200	1.34672400	-1.11663900
H	-2.35377400	0.52311300	-2.01162000
C	-3.08314500	2.25483500	-0.93296000
H	-2.50503900	3.16033900	-1.14882400
H	-3.42339000	2.37030600	0.10356600
C	-4.29479900	2.21639000	-1.86846400
H	-4.88223700	1.30605200	-1.69348800
H	-3.93843900	2.15619800	-2.90381600
C	-5.18521500	3.44355900	-1.69861100
H	-6.03596200	3.41575700	-2.38403100
H	-5.57715600	3.50612000	-0.67782400
H	-4.62351100	4.36199800	-1.89623200
C	-1.15809000	-1.03605400	-0.21643000
H	-1.21083500	-1.71339700	0.63923100
H	-0.21760000	-0.48884000	-0.18174500
C	-1.23895500	-1.81053900	-1.52184000
H	-2.22544000	-2.27994400	-1.63850000
H	-1.08103000	-1.13335400	-2.36819000
C	-0.15236400	-2.90197600	-1.58610700
H	-0.25303500	-3.56981800	-0.71836300
H	-0.37651600	-3.50894900	-2.47135700
C	1.28616500	-2.36726900	-1.67609300
H	1.90905200	-3.16699900	-2.09311100
H	1.30097300	-1.55798500	-2.41569900
C	1.90403300	-1.88469900	-0.34393600
H	2.56541700	-2.68038700	0.01951800
H	1.13105900	-1.82671400	0.43788600
Cl	1.40842900	0.84378400	-1.33719900
B	2.75272300	-0.49234100	-0.38091500
C	4.13416200	-0.45918300	-1.21781600

C	3.11703700	0.12923200	1.06863800
C	4.52960800	0.99757800	-1.54636400
C	5.26823800	-1.10068900	-0.34206800
H	4.06974600	-1.01496000	-2.16392400
C	4.08296600	1.34994200	0.98887900
C	3.82094600	-1.01295100	1.83923800
H	2.21622400	0.41249000	1.63985900
H	5.59880500	1.03368200	-1.80097700
H	3.98746200	1.32816100	-2.43837300
C	4.22866300	1.99529400	-0.39873800
H	5.83121200	-1.82995000	-0.93847800
H	5.99466200	-0.31789400	-0.09152900
C	4.84331100	-1.79569000	0.96762800
H	5.07638600	1.03562000	1.33599800
H	3.77407000	2.12762400	1.70186100
H	3.07224500	-1.72117000	2.21729300
H	4.32445400	-0.60221600	2.72556000
H	3.29944800	2.52286400	-0.62831800
H	5.01541300	2.75909400	-0.35190600
H	5.74492800	-2.00854800	1.55476900
H	4.42548900	-2.77702800	0.71953000

INT1

N	3.26583600	-0.17450000	-0.08525800
C	3.98235600	-1.49291400	0.01678400
H	4.80394000	-1.34625800	0.72364200
H	3.27835400	-2.19611100	0.46876600
C	4.52181200	-2.04361100	-1.29812200
H	3.75612700	-2.00362800	-2.08147800
H	5.36878400	-1.44149300	-1.64583600

C	4.97603600	-3.49366600	-1.11570100
H	4.11631500	-4.10235900	-0.80870400
H	5.70483600	-3.54767400	-0.29706400
C	5.58708700	-4.06669300	-2.39105700
H	6.46682500	-3.49147300	-2.69666400
H	5.89693800	-5.10492400	-2.24880100
H	4.86665800	-4.04044000	-3.21477200
C	4.22333200	0.84559100	-0.67356600
H	4.31383500	0.58902400	-1.73250800
H	5.19969500	0.66544900	-0.21193400
C	3.80582600	2.29640900	-0.51340900
H	2.75239400	2.44163800	-0.77926200
H	3.88599900	2.59708900	0.53858000
C	4.69168600	3.20482700	-1.36676500
H	4.57068200	2.93809200	-2.42465500
H	5.75126600	3.04496800	-1.12346900
C	4.32419700	4.67230900	-1.16077300
H	4.91376000	5.32577000	-1.80955300
H	3.26323400	4.83396000	-1.37286400
H	4.50121500	4.97376700	-0.12369000
C	2.77838500	0.25432400	1.29099700
H	2.17835800	1.15655200	1.12321100
H	2.08771800	-0.53171400	1.60961500
C	3.87514000	0.45664000	2.34193400
H	3.64883500	1.38906800	2.87148100
H	4.85496000	0.62154100	1.87570200
C	3.97799100	-0.67421500	3.36917200
H	4.16833800	-1.63098400	2.86579600
H	3.00840200	-0.78153100	3.86991400
C	5.06784000	-0.41063100	4.40370600

H	5.11614200	-1.21219700	5.14517400
H	6.05109200	-0.33271000	3.92727300
H	4.88039800	0.52817800	4.93445000
C	2.02798800	-0.27539800	-0.97975900
H	2.38446900	-0.21343600	-2.01150700
H	1.42725800	0.61967600	-0.76280400
C	1.20122000	-1.54454300	-0.79839900
H	1.72913200	-2.40589300	-1.22562200
H	1.03773900	-1.76543000	0.26338200
C	-0.17512000	-1.36698800	-1.46405100
H	-0.08598800	-0.69461500	-2.32918600
H	-0.51089400	-2.33217400	-1.86165400
C	-1.23701000	-0.83513100	-0.49895500
H	-1.34912200	-1.56971300	0.31190000
H	-0.87808600	0.09305600	-0.02771100
C	-2.59656500	-0.61797000	-1.16907300
H	-2.83497400	-1.51949400	-1.75076800
H	-2.48422000	0.16219100	-1.93893400
Cl	0.48527400	2.60569500	0.17166400
C	-4.08980100	2.56565400	-0.66431500
C	-2.70163900	2.32701200	-0.23609600
O	-3.75046000	1.40106300	0.11232700
H	-4.68310100	3.25590100	-0.06708300
H	-2.26874100	2.83498800	0.61794500
H	-1.97748100	1.95586400	-0.95334900
C	-4.54018400	2.38289300	-2.08502300
H	-5.59518700	2.10144200	-2.12620600
H	-4.41374600	3.33077000	-2.61728200
H	-3.95201500	1.61463900	-2.59011100
B	-3.84297200	-0.29689900	-0.17366500

C	-3.82873000	-0.85729800	1.34973000
C	-5.31778700	-0.65695100	-0.73860000
C	-4.77808000	-0.01310200	2.23522700
C	-4.30272000	-2.34697900	1.34329300
H	-2.83170200	-0.81490300	1.80766800
C	-6.44962500	-0.36945100	0.29621100
C	-5.26561900	-2.18179100	-1.04163100
H	-5.56653300	-0.15599900	-1.68313100
H	-5.08160500	-0.60975600	3.10669200
H	-4.23783600	0.85262700	2.63406300
C	-6.03695600	0.49694700	1.49425000
H	-3.64075000	-2.95843700	1.96993300
H	-5.29160400	-2.41226500	1.81559800
C	-4.38780900	-2.98316800	-0.05017900
H	-6.83730000	-1.32231300	0.67965000
H	-7.30450000	0.10646700	-0.20229100
H	-4.88817200	-2.34896000	-2.05765600
H	-6.28781000	-2.58329400	-1.03151000
H	-5.85998200	1.51909100	1.14179100
H	-6.87863000	0.56796700	2.19391200
H	-4.76591100	-4.00931700	0.03320900
H	-3.36927100	-3.07226000	-0.44804100

TS1

N	3.01492800	0.49785300	-0.04368400
C	4.13620500	1.29026700	-0.66919400
H	4.87098600	0.56009800	-1.01825400
H	3.70511600	1.77657100	-1.54835700
C	4.80649200	2.33029900	0.21928000
H	4.06209100	2.99288800	0.67599000

H	5.36164800	1.85224400	1.03331100
C	5.77589600	3.17500500	-0.61330000
H	5.21813000	3.68348800	-1.40937900
H	6.49943500	2.51638700	-1.10948200
C	6.51274500	4.20303400	0.24041800
H	7.10169100	3.71327800	1.02223000
H	7.19415500	4.80299100	-0.36744700
H	5.80810800	4.88440900	0.72758700
C	3.53340900	-0.28058700	1.14826700
H	3.97449400	0.45428100	1.82558000
H	4.33779400	-0.91562500	0.76731600
C	2.47518900	-1.10825600	1.86749900
H	1.85955400	-0.46120300	2.50395000
H	1.80200800	-1.61036600	1.16125500
C	3.12447700	-2.19347700	2.72860100
H	3.82541200	-1.74491500	3.44530000
H	3.71201900	-2.85463200	2.07838200
C	2.06254800	-3.01231100	3.45752100
H	2.51704000	-3.80348300	4.05949500
H	1.47160000	-2.37693300	4.12613500
H	1.38376200	-3.47345200	2.73255100
C	2.45574700	-0.45075100	-1.09905000
H	1.47925500	-0.78918900	-0.74426500
H	2.31226600	0.15477800	-1.99727200
C	3.29350800	-1.68271900	-1.40634800
H	3.20660800	-2.39393900	-0.57728100
H	4.35518200	-1.44294300	-1.55082700
C	2.74663100	-2.35111200	-2.67203000
H	2.97350700	-1.72208000	-3.54261900
H	1.65738900	-2.42413500	-2.58436800

C	3.31932100	-3.75230300	-2.85172400
H	2.97162000	-4.20205200	-3.78512500
H	4.41495200	-3.73775600	-2.87051900
H	2.99233100	-4.39121200	-2.02588100
C	1.90282200	1.41108900	0.42852700
H	2.26993300	1.91798000	1.32555800
H	1.09807600	0.74232900	0.73622600
C	1.37878300	2.42820600	-0.58094100
H	2.05924700	3.28618200	-0.63916700
H	1.30945400	1.99603600	-1.58601100
C	-0.03395100	2.84720100	-0.13748400
H	-0.03231900	3.01583500	0.94900600
H	-0.29537400	3.80719200	-0.59337900
C	-1.08243500	1.78171100	-0.49314200
H	-1.37972000	1.90802100	-1.54295900
H	-0.60069100	0.79571100	-0.45422700
C	-2.31755000	1.76417200	0.40611800
H	-2.76738800	2.76529400	0.36723200
H	-1.98038500	1.64701800	1.45004800
Cl	0.48831400	-3.27349300	-0.16745200
C	-2.02675900	-1.60558600	0.66313500
C	-1.30509500	-1.82313800	-0.59701400
O	-2.69431400	-0.76846200	-0.24518900
H	-2.64999900	-2.45011900	0.97958600
H	-1.72663600	-2.48741000	-1.33724800
H	-0.59491600	-1.08126200	-0.92184400
C	-1.27304000	-1.00478400	1.82647500
H	-1.96275000	-0.60020500	2.57089200
H	-0.65977000	-1.78882400	2.28253200
H	-0.61840100	-0.19431600	1.49232000

B	-3.43891800	0.63702400	0.00541000
C	-4.27908700	0.91006000	-1.36295100
C	-4.58344800	0.36855600	1.12992900
C	-4.88249300	-0.42631000	-1.85228100
C	-5.44150800	1.92264400	-1.09792000
H	-3.65573300	1.31211300	-2.17657900
C	-5.70992500	-0.57564700	0.60766800
C	-5.18381500	1.74568000	1.48997100
H	-4.17127200	-0.06165500	2.05654700
H	-5.69843000	-0.22261300	-2.56083800
H	-4.12579400	-0.98806100	-2.41275000
C	-5.40009100	-1.32539000	-0.70008800
H	-5.47218600	2.67905600	-1.89314500
H	-6.39634600	1.38820600	-1.18008400
C	-5.41895700	2.65661700	0.25471900
H	-6.62811500	0.00920800	0.46425300
H	-5.96600300	-1.31844300	1.37512700
H	-4.51287800	2.26778100	2.18445600
H	-6.12977000	1.60541300	2.03179600
H	-4.64827600	-2.09206500	-0.48640800
H	-6.30041500	-1.86463400	-1.02066800
H	-6.36109600	3.20620700	0.37165000
H	-4.64061700	3.42648600	0.21905300

INT2

N	2.92679900	0.46062900	-0.03360800
C	4.07586900	1.13456900	-0.74477600
H	4.69482400	0.33722700	-1.16347100
H	3.63079000	1.68678300	-1.57604800
C	4.92947500	2.07046200	0.10144500

H	4.30360900	2.79552100	0.63411400
H	5.49640600	1.51119100	0.85360000
C	5.91086300	2.82996300	-0.79672700
H	5.34544700	3.41849500	-1.52959400
H	6.51307400	2.11261400	-1.36805500
C	6.82587800	3.74741700	0.00920000
H	7.42207100	3.17493300	0.72670600
H	7.51462400	4.28779900	-0.64447200
H	6.24407300	4.48633300	0.56905600
C	3.45922700	-0.38458900	1.10286600
H	3.98477200	0.29928400	1.77322400
H	4.19931100	-1.05867000	0.66117900
C	2.40474400	-1.16640900	1.87427200
H	1.77450400	-0.48612900	2.45765400
H	1.73719600	-1.71625100	1.20171000
C	3.06758000	-2.17156200	2.81881600
H	3.75214500	-1.65084500	3.50075200
H	3.67813600	-2.86934600	2.23096900
C	2.01993900	-2.94621800	3.61415700
H	2.48793800	-3.67849500	4.27674500
H	1.41763500	-2.26911900	4.22798300
H	1.34060300	-3.47772000	2.94002100
C	2.17684100	-0.40687500	-1.03611100
H	1.20574400	-0.63359400	-0.58813100
H	1.99473600	0.22764400	-1.90687500
C	2.87347200	-1.69825400	-1.44774800
H	2.85331400	-2.41670300	-0.61990600
H	3.92471700	-1.52986900	-1.71352100
C	2.15395900	-2.31600900	-2.65080400
H	2.26145000	-1.65201800	-3.51721600

H	1.08289700	-2.38744300	-2.43432000
C	2.69449500	-3.70470200	-2.97483900
H	2.19994300	-4.12112100	-3.85554100
H	3.77125300	-3.67511400	-3.17400400
H	2.51872500	-4.38671000	-2.13722700
C	1.96428100	1.49620700	0.52734100
H	2.44743300	1.92384600	1.41008100
H	1.09468300	0.93213600	0.86552100
C	1.51744500	2.59980800	-0.42925200
H	2.25743000	3.40950200	-0.44118000
H	1.42203400	2.22924400	-1.45658200
C	0.12643000	3.07264300	0.02936100
H	0.12944800	3.18256600	1.12335300
H	-0.07500400	4.06928400	-0.37548600
C	-0.96090100	2.07087300	-0.39858500
H	-1.30394100	2.33475100	-1.40838200
H	-0.51285300	1.07279900	-0.51847900
C	-2.16050800	1.93575000	0.53860900
H	-2.64158800	2.91989000	0.61894400
H	-1.77053700	1.72422700	1.55132300
Cl	-0.04055900	-3.54139300	0.00574700
C	-1.96366300	-1.44411900	0.31917100
C	-1.19175900	-2.31231400	-0.68829900
O	-2.36054300	-0.40094100	-0.49013000
H	-2.82118300	-2.02953700	0.70161200
H	-1.87468100	-2.86266000	-1.33531000
H	-0.58956000	-1.63894900	-1.30013600
C	-1.12238700	-1.02592600	1.52475600
H	-1.72010000	-0.38848700	2.17784100
H	-0.76101900	-1.88806800	2.09557700

H	-0.25986100	-0.44091800	1.18480300
B	-3.21919600	0.76363000	0.01368100
C	-4.14390000	1.24190300	-1.26028900
C	-4.33606100	0.29705100	1.11953100
C	-4.68503800	-0.02567900	-1.95382900
C	-5.34938000	2.12767300	-0.81576000
H	-3.56427700	1.80693600	-2.00798000
C	-5.41463400	-0.62886200	0.47264100
C	-5.00176500	1.56502600	1.69436100
H	-3.90210700	-0.24382000	1.97649800
H	-5.54037000	0.23173800	-2.59739400
H	-3.91409100	-0.43933300	-2.61387800
C	-5.09938700	-1.13030300	-0.94933500
H	-5.46074700	2.99025100	-1.48754400
H	-6.27714600	1.55342000	-0.94160500
C	-5.30688900	2.64971900	0.62889500
H	-6.37771400	-0.10060000	0.44883600
H	-5.59154000	-1.50820200	1.10879600
H	-4.34442100	2.00510700	2.45644600
H	-5.93051200	1.29394500	2.21857700
H	-4.28687700	-1.86198400	-0.88277800
H	-5.96877800	-1.68226900	-1.33082300
H	-6.26185100	3.13988900	0.85904400
H	-4.55333700	3.44182200	0.69076900

INT3

N	2.86258900	-0.36118600	0.19930900
C	3.83274300	-1.31857000	0.85033000
H	4.20208000	-0.81137300	1.74566700
H	3.24840100	-2.18189000	1.17984100

C	4.99833100	-1.78269500	-0.01314800
H	4.63207000	-2.38678100	-0.85062900
H	5.54336100	-0.93226100	-0.44052500
C	5.96682700	-2.62374400	0.82325000
H	5.42196800	-3.46201900	1.27447700
H	6.35167700	-2.01825200	1.65293400
C	7.12783600	-3.15378100	-0.01341900
H	7.69944800	-2.33151300	-0.45559200
H	7.81231300	-3.74928500	0.59550000
H	6.76510200	-3.78720000	-0.82896000
C	3.48444400	1.01924100	0.16711900
H	4.49813600	0.89765800	-0.22418400
H	3.56338000	1.33433100	1.21041400
C	2.71703500	2.05253300	-0.65213000
H	2.91811000	1.91632900	-1.72027800
H	1.63658300	1.93973400	-0.51358700
C	3.10275900	3.47270200	-0.23660300
H	4.18868200	3.60868600	-0.32594700
H	2.85071500	3.61534300	0.82214400
C	2.36923000	4.51000200	-1.08151600
H	2.63058300	5.52616300	-0.77576000
H	2.62007400	4.39927400	-2.14157600
H	1.28663800	4.38934400	-0.97247500
C	1.58276700	-0.33797000	1.02308500
H	0.87073800	0.31509700	0.51741700
H	1.18184700	-1.34976600	0.96325700
C	1.67607600	0.08791600	2.47841900
H	1.91851300	1.15339900	2.55871200
H	2.42866200	-0.47627700	3.04271900
C	0.28051700	-0.15084200	3.07925800

H	0.13466700	-1.22944100	3.22115000
H	-0.48041600	0.15963900	2.35005000
C	0.07925900	0.58614800	4.39772500
H	-0.91010900	0.37165800	4.81134800
H	0.82765100	0.29289000	5.14263000
H	0.15680300	1.66835300	4.24661300
C	2.54460900	-0.77475800	-1.23114200
H	3.48227600	-0.64823800	-1.77845900
H	1.84533200	-0.02633000	-1.59827700
C	1.94837000	-2.17937900	-1.43406000
H	2.63069300	-2.75895700	-2.06571200
H	1.88022000	-2.72522300	-0.48515100
C	0.54412300	-2.11797800	-2.06706200
H	0.61444500	-1.62878500	-3.04824700
H	0.19934300	-3.14163600	-2.25293800
C	-0.44295900	-1.38469600	-1.16232900
H	-0.41373700	-1.87299200	-0.17741900
H	-0.09006600	-0.36228100	-0.99843200
C	-1.90613100	-1.26855400	-1.56308400
H	-2.25995700	-2.24739700	-1.90967200
H	-1.99817500	-0.59678900	-2.43625400
Cl	-0.00394100	2.88041200	1.36147300
C	-2.27847700	1.73128000	0.16464900
C	-1.80794800	2.61592500	1.31466800
O	-1.93704400	0.41577700	0.40323100
H	-3.37543200	1.87358200	0.19395100
H	-2.23278600	3.61901000	1.25605300
H	-2.05354900	2.15048200	2.27044300
C	-1.79696700	2.23750700	-1.19563500
H	-2.30295800	1.66693800	-1.97941500

H	-2.01096400	3.30307600	-1.34138700
H	-0.71421800	2.08285900	-1.28100900
C	-0.32990200	1.12298800	-3.84345000
O	0.68066700	1.03065600	-3.26632600
O	-1.31390400	1.22906100	-4.44678500
B	-2.76739400	-0.72369700	-0.24497500
C	-4.31025500	-0.30226100	-0.60268600
C	-2.97002600	-1.87792700	0.91500800
C	-4.92692500	-1.44621500	-1.43655700
C	-5.16647000	-0.06841000	0.68242700
H	-4.37829700	0.60033000	-1.23163900
C	-4.08389600	-2.90694400	0.54159300
C	-3.37997400	-1.18068500	2.22872800
H	-2.04375400	-2.44080400	1.12244600
H	-6.01794700	-1.31669400	-1.48797900
H	-4.56675700	-1.37065100	-2.47058300
C	-4.59948000	-2.86663400	-0.90583000
H	-5.73703500	0.86786400	0.59736000
H	-5.92927600	-0.85563300	0.75358300
C	-4.38987200	-0.02564800	2.01274700
H	-4.94241800	-2.75100700	1.20850100
H	-3.74739600	-3.93089900	0.75558500
H	-2.49322200	-0.76767300	2.72549000
H	-3.80440400	-1.91793400	2.92705200
H	-3.85504500	-3.33645800	-1.55670000
H	-5.48879800	-3.50563200	-0.97904300
H	-5.10994200	0.00531100	2.84083500
H	-3.84963400	0.92526000	2.06325600

TS2

N	3.01611200	-0.32902200	0.07749500
C	3.95456200	-1.22897200	0.84164300
H	4.30643300	-0.64737400	1.69840300
H	3.35408900	-2.05394100	1.23191000
C	5.13571100	-1.78267100	0.05561600
H	4.77915500	-2.42455300	-0.75768900
H	5.72463600	-0.97785200	-0.39934200
C	6.04274000	-2.60202300	0.97770200
H	5.45477600	-3.39929500	1.44897800
H	6.40982600	-1.96269900	1.79003000
C	7.22255000	-3.20876400	0.22341000
H	7.83726400	-2.42772400	-0.23532100
H	7.86189800	-3.79001000	0.89240400
H	6.87618500	-3.87413200	-0.57361900
C	3.69355900	1.00891200	-0.12906600
H	4.62347900	0.80517100	-0.66694100
H	3.95772100	1.36606900	0.87079000
C	2.87013100	2.05508200	-0.86685600
H	2.75492100	1.78374200	-1.92097000
H	1.85268400	2.11565000	-0.47030500
C	3.54469400	3.42354100	-0.75517600
H	4.58038200	3.36665200	-1.11657000
H	3.59867100	3.71445700	0.30262800
C	2.77693300	4.48297200	-1.54143900
H	3.23872100	5.46830400	-1.43624400
H	2.74915100	4.23147500	-2.60604300
H	1.74225200	4.54856400	-1.19084900
C	1.73732600	-0.14965500	0.87371700
H	1.02133200	0.32412600	0.19429200
H	1.38429700	-1.16255600	1.08548900

C	1.81454900	0.65363100	2.16103700
H	2.00425000	1.71131400	1.93986500
H	2.59859300	0.30404400	2.84520000
C	0.43861700	0.52743500	2.82758600
H	0.31313200	-0.49404800	3.20869700
H	-0.32398700	0.65726000	2.04903000
C	0.21943900	1.54005800	3.94471400
H	-0.76271300	1.40281800	4.40656100
H	0.97677600	1.43679800	4.72944700
H	0.27046500	2.56049800	3.55187300
C	2.64743100	-0.90559200	-1.28585300
H	3.56131300	-0.82923100	-1.88099700
H	1.90018400	-0.21841500	-1.69124000
C	2.09289400	-2.34569200	-1.30009500
H	2.76844700	-2.95550300	-1.91027600
H	2.10929100	-2.79905300	-0.30070700
C	0.65985100	-2.43575300	-1.86123200
H	0.55946700	-1.74858200	-2.71150000
H	0.49622900	-3.44628700	-2.25478800
C	-0.41480000	-2.11310800	-0.82412900
H	-0.37013700	-2.87161200	-0.02749900
H	-0.16823100	-1.16395200	-0.34961700
C	-1.84744600	-2.00696500	-1.37030700
H	-2.25539800	-3.02015200	-1.46764300
H	-1.83586200	-1.59854300	-2.38440000
Cl	-0.41850600	3.22551500	0.65187400
C	-2.58280400	1.86150300	-0.47642200
C	-2.09663900	2.57099300	0.78461600
O	-1.86682700	0.63878500	-0.66593500
H	-3.62268400	1.58787100	-0.27393000

H	-2.73867800	3.42622500	1.00602400
H	-2.08411600	1.89761000	1.63912200
C	-2.59865700	2.81376800	-1.67091400
H	-3.06709400	2.34227800	-2.53306600
H	-3.16605700	3.70609900	-1.38580200
H	-1.58799800	3.12314500	-1.95173100
C	-0.96041400	0.69295600	-1.91275700
O	0.21853800	0.87854500	-1.59248900
O	-1.55353700	0.55422400	-2.95926800
B	-2.79820600	-1.13938600	-0.39768500
C	-4.32280700	-0.84495400	-0.78360500
C	-2.79193800	-1.59191000	1.14703000
C	-4.86373000	-2.26113900	-1.11055700
C	-5.19913100	-0.24163500	0.36523800
H	-4.41759000	-0.23214400	-1.68874800
C	-3.82985600	-2.77696600	1.24236000
C	-3.25600200	-0.51597800	2.13512200
H	-1.81373300	-1.95857700	1.48756900
H	-5.95885100	-2.22635700	-1.17845100
H	-4.50389800	-2.56544400	-2.09962600
C	-4.43012400	-3.33146800	-0.06716900
H	-5.79684800	0.59062800	-0.02924400
H	-5.93915700	-0.99824100	0.65395800
C	-4.52012900	0.25330100	1.67059200
H	-4.66099800	-2.43727200	1.87299700
H	-3.37823500	-3.61357000	1.78942800
H	-2.43585500	0.18759600	2.31550500
H	-3.44944000	-0.98222200	3.11137900
H	-3.70453700	-4.00998800	-0.52586100
H	-5.28657900	-3.96251900	0.19715300

H	-5.27602800	0.22608100	2.46350500
H	-4.27291800	1.31583600	1.57358800

INT4

N	2.94611600	-0.65569900	0.02742800
C	4.14711400	-1.22184800	0.74042900
H	4.65492200	-0.37894400	1.21634700
H	3.75591200	-1.86653700	1.53129400
C	5.12869600	-2.00315000	-0.12376700
H	4.60759300	-2.77597400	-0.70011200
H	5.63063900	-1.34346700	-0.83977700
C	6.18495000	-2.67112200	0.76124300
H	5.68860100	-3.35660100	1.45916100
H	6.68408500	-1.90892600	1.37259500
C	7.21998200	-3.43181500	-0.06264900
H	7.74899800	-2.75902100	-0.74499400
H	7.96245200	-3.90943300	0.58126400
H	6.74358700	-4.21277500	-0.66365200
C	3.40702700	0.33241200	-1.02385100
H	4.02109600	-0.23646700	-1.72634600
H	4.06079900	1.03997700	-0.50285700
C	2.30005800	1.06366200	-1.77015300
H	1.74322200	0.37111600	-2.40723700
H	1.55744300	1.49218200	-1.08970600
C	2.89538900	2.19005200	-2.61697100
H	3.67948000	1.79701500	-3.27820400
H	3.37860800	2.92253300	-1.95627200
C	1.81099800	2.87772500	-3.44255500
H	2.21773100	3.71484300	-4.01614200
H	1.35288000	2.17323500	-4.14338900

H	1.01991900	3.25828800	-2.78877600
C	2.05001200	0.03546900	1.03800400
H	1.09800900	0.20044000	0.53226000
H	1.88702100	-0.68741400	1.84106500
C	2.55093200	1.35390900	1.60857000
H	2.52306900	2.13563600	0.84004100
H	3.58046900	1.28728200	1.98218800
C	1.62115800	1.75694300	2.75669900
H	1.71597200	1.03138900	3.57396400
H	0.58677000	1.68510200	2.39809200
C	1.91371400	3.16344700	3.26945600
H	1.23564200	3.43614500	4.08302500
H	2.93786400	3.23549100	3.65057300
H	1.80284400	3.90169500	2.46794800
C	2.12705800	-1.75774800	-0.63275800
H	2.69205900	-2.07586100	-1.51335500
H	1.20967600	-1.27071500	-0.97455100
C	1.79300500	-2.96014700	0.25860700
H	2.57808200	-3.72158100	0.17240800
H	1.74126000	-2.68005500	1.31701400
C	0.41173900	-3.50179600	-0.14588400
H	0.34917300	-3.53033600	-1.24174000
H	0.31102100	-4.53787500	0.19375800
C	-0.72937400	-2.62708500	0.41347000
H	-1.04002100	-3.02987200	1.38674800
H	-0.32513900	-1.63005800	0.63589500
C	-1.93952500	-2.48545100	-0.51422700
H	-2.44099800	-3.46045600	-0.55770500
H	-1.56724300	-2.29545800	-1.52969700
Cl	0.46046100	4.43822500	-0.04518100

C	-1.63296900	2.64824500	0.25077400
C	-0.89037700	3.77577300	0.94730100
O	-0.66425800	1.68197500	-0.13587700
H	-2.30891300	2.20947200	0.99613700
H	-1.56907500	4.60492000	1.15210100
H	-0.44162000	3.43851800	1.88156200
C	-2.42301300	3.10589500	-0.96571600
H	-2.92352800	2.24706600	-1.42281800
H	-3.19015700	3.83131000	-0.67804300
H	-1.75375600	3.56074300	-1.70175100
C	-1.13449300	0.43287300	-0.53252900
O	-0.43735000	-0.14983200	-1.34877200
O	-2.19144100	0.06951300	0.07419900
B	-3.00546200	-1.31713900	-0.10083400
C	-4.18361900	-1.06144000	-1.19198700
C	-3.80483500	-1.50344400	1.30970900
C	-4.83572500	-2.43230300	-1.47332200
C	-5.27319800	-0.07118400	-0.67557300
H	-3.77702100	-0.67865900	-2.14078300
C	-5.00554900	-2.48880100	1.12904100
C	-4.35492200	-0.13386900	1.76373100
H	-3.16300700	-1.88750400	2.11733700
H	-5.79708800	-2.28951300	-1.98719600
H	-4.20451500	-3.00293300	-2.16598200
C	-5.05079100	-3.28096200	-0.19014400
H	-5.53291100	0.65196100	-1.46126200
H	-6.20178800	-0.62593900	-0.48740300
C	-4.91430700	0.71932800	0.59577500
H	-5.94174300	-1.92293700	1.22058200
H	-5.03000000	-3.20928200	1.95736400

H	-3.55757300	0.43599600	2.25895500
H	-5.13692700	-0.28139800	2.52282500
H	-4.29012900	-4.06735900	-0.14391500
H	-6.01027500	-3.80984800	-0.24911200
H	-5.79759800	1.27958300	0.92837600
H	-4.16963200	1.47236800	0.32140100

INT5

N	3.19129100	-0.12148600	0.06995900
C	4.48863300	-0.87706700	0.17553400
H	4.89009600	-0.66148400	1.16999200
H	4.23015100	-1.93827600	0.14683100
C	5.53175000	-0.57531100	-0.89274600
H	5.10614100	-0.71002000	-1.89382700
H	5.87960300	0.46100900	-0.82205500
C	6.73217300	-1.51231700	-0.73214800
H	6.39374100	-2.55168600	-0.82424600
H	7.14458800	-1.40638800	0.27900200
C	7.81894100	-1.22929600	-1.76546400
H	8.19228000	-0.20470000	-1.67048200
H	8.66635900	-1.90844300	-1.64343500
H	7.43268500	-1.35223200	-2.78225600
C	3.46258400	1.35649300	0.24321200
H	4.12749600	1.64234000	-0.57564600
H	4.02284700	1.45697100	1.17814500
C	2.22621600	2.24361400	0.24707000
H	1.76746000	2.26246400	-0.74783500
H	1.45398600	1.85179200	0.91730500
C	2.59587600	3.66363500	0.67870500
H	3.42330200	4.04569700	0.06543100

H	2.95938100	3.64385700	1.71498300
C	1.39316500	4.59724100	0.56622600
H	1.61878300	5.59057600	0.96335100
H	1.09027000	4.70937000	-0.47909900
H	0.53510100	4.19250300	1.11330500
C	2.23289500	-0.62225000	1.14048900
H	1.24014800	-0.23286000	0.88094200
H	2.21412600	-1.71108600	1.03936100
C	2.54755200	-0.23551600	2.57740200
H	2.59909300	0.85451100	2.68334800
H	3.50260400	-0.64805000	2.92947900
C	1.39993900	-0.74250000	3.45956000
H	1.32458400	-1.83345600	3.36616600
H	0.46243200	-0.32590800	3.07240700
C	1.59136000	-0.36039300	4.92383200
H	0.76461500	-0.72822000	5.53683600
H	2.52096400	-0.77828100	5.32553500
H	1.63395200	0.72743800	5.03984500
C	2.51507000	-0.32635600	-1.27656600
H	3.10139000	0.24598100	-2.00111900
H	1.52814500	0.14872100	-1.19607800
C	2.36467700	-1.78438600	-1.73160900
H	3.15310800	-2.03397200	-2.45127300
H	2.47728800	-2.48649500	-0.89726600
C	0.96550400	-1.99416900	-2.32969300
H	0.70258900	-1.13250600	-2.95652400
H	0.96710500	-2.87788800	-2.97874300
C	-0.08616500	-2.15019300	-1.23174900
H	0.09421100	-3.09948900	-0.70250800
H	0.02844600	-1.35046900	-0.49218700

C	-1.52295800	-2.09278000	-1.74228900
H	-1.69029000	-2.80384500	-2.56661300
H	-1.67975800	-1.09269200	-2.18761700
Cl	-3.97516800	4.30817900	0.14085800
C	-2.40894300	2.57699200	-1.35986300
C	-3.84175900	3.01424400	-1.10277300
O	-1.95247600	1.95056800	-0.17520400
H	-2.44844000	1.83291800	-2.16800800
H	-4.28591700	3.41244700	-2.01682200
H	-4.43458100	2.17678500	-0.73607300
C	-1.50217400	3.72398400	-1.78407100
H	-0.51782600	3.32293900	-2.03063400
H	-1.91073600	4.23403800	-2.66312100
H	-1.41269600	4.44859300	-0.97047900
C	-0.83181700	1.13377200	-0.28351000
O	-0.47907100	0.63886700	0.80766300
O	-0.31915600	0.99247600	-1.41571600
B	-2.65184100	-2.22976900	-0.65895800
C	-2.49769600	-2.05994500	0.90714100
C	-4.13603400	-2.64753600	-1.01829300
C	-3.34085000	-0.81877000	1.32636000
C	-3.04481900	-3.38220300	1.54222100
H	-1.46548700	-1.89786900	1.23506200
C	-5.13346900	-1.75717100	-0.22137300
C	-4.20946800	-4.14987800	-0.60281000
H	-4.36003600	-2.57004300	-2.08858900
H	-3.79790100	-1.00724700	2.30768500
H	-2.68197200	0.04667700	1.43142100
C	-4.44314200	-0.49452200	0.30614700
H	-2.37618900	-3.71273600	2.34544500

H	-4.01756900	-3.19671300	2.01512100
C	-3.20275400	-4.50825800	0.51120900
H	-5.55264800	-2.31468700	0.62679800
H	-5.98518100	-1.48874000	-0.85714900
H	-4.01762700	-4.78839200	-1.47221500
H	-5.22841300	-4.38056400	-0.26580500
H	-3.98277400	0.02793600	-0.54861600
H	-5.16762400	0.20400200	0.74223600
H	-3.50064700	-5.44433700	0.99743100
H	-2.21686500	-4.69983400	0.05850100

INT6

N	2.41121800	1.95942600	-0.08580700
C	2.88911300	3.26540200	-0.66466600
H	3.87190700	3.06946000	-1.10087900
H	2.20505700	3.50261600	-1.48300200
C	2.97286500	4.43846500	0.30488000
H	2.05522300	4.52258900	0.89858600
H	3.80160500	4.30164800	1.00797800
C	3.18561400	5.74206700	-0.46943800
H	2.33381700	5.90304400	-1.14210100
H	4.07352000	5.64704300	-1.10710100
C	3.34334800	6.94054500	0.46176400
H	4.20919100	6.81418700	1.11939200
H	3.48319000	7.86459400	-0.10454300
H	2.45763300	7.06355200	1.09308300
C	3.36098000	1.53041400	1.00799300
H	3.34058900	2.32900500	1.75423200
H	4.35937800	1.51763400	0.55932600
C	3.04795500	0.19673900	1.66728300

H	2.09657100	0.25248300	2.20749300
H	2.93481100	-0.60776000	0.93320400
C	4.17493700	-0.15551100	2.64101900
H	4.36158500	0.68357500	3.32551500
H	5.10154200	-0.31268400	2.07357500
C	3.84313300	-1.41233000	3.43755800
H	4.66993500	-1.70220900	4.09144100
H	2.95431800	-1.25801100	4.05760300
H	3.63652000	-2.24106100	2.75529300
C	2.35847700	0.92128600	-1.19942500
H	1.74688200	0.09524100	-0.81735700
H	1.81674300	1.40328000	-2.01857900
C	3.70240700	0.40493500	-1.68964200
H	4.21104000	-0.15602500	-0.89712600
H	4.37083100	1.21382100	-2.01379000
C	3.46127300	-0.54931100	-2.86205300
H	2.92054500	-0.02691100	-3.66147700
H	2.80495900	-1.35410000	-2.50945600
C	4.76815200	-1.11777200	-3.40827700
H	4.58360000	-1.84037600	-4.20841600
H	5.39980000	-0.32183200	-3.81691000
H	5.33728800	-1.61837100	-2.61731900
C	1.01389900	2.08732000	0.50645200
H	1.13254400	2.59512800	1.46863400
H	0.68187400	1.06098900	0.68559100
C	0.00434200	2.83819200	-0.35325500
H	0.27694500	3.89816600	-0.42702000
H	-0.02082400	2.43290900	-1.37233000
C	-1.39440400	2.69298500	0.26668300
H	-1.32291000	2.80634600	1.35830700

H	-2.02835100	3.51652400	-0.08117100
C	-2.07342400	1.36132300	-0.06678900
H	-2.28892800	1.35078900	-1.14573700
H	-1.36260000	0.54524300	0.10880200
C	-3.36370100	1.13950700	0.73251300
H	-3.86357800	2.11451400	0.82219200
H	-3.09818900	0.86742700	1.76625000
Cl	5.07214800	-2.77634900	0.04825000
C	2.49362000	-3.72771700	-0.28928200
C	3.86818200	-3.70017300	-0.93338400
O	2.07748900	-2.38180600	-0.14815200
H	1.82319500	-4.23471800	-0.99551700
H	4.26757900	-4.70981300	-1.04009500
H	3.83726500	-3.21238700	-1.90814200
C	2.47061100	-4.48404400	1.03123200
H	1.45962700	-4.45098500	1.43836900
H	2.75249000	-5.53061200	0.87496400
H	3.17004700	-4.04183700	1.74520500
C	0.68450300	-2.17915400	0.04414000
O	0.41390300	-0.96708000	0.21169900
O	-0.04298900	-3.17150500	0.00386300
O	-3.69819100	-1.37044600	-0.13808600
C	-2.96412300	-2.32407700	0.65644500
C	-2.49536700	-1.94590200	-0.68239600
H	-3.52951500	-3.25001000	0.74721900
C	-2.25563400	-1.85096500	1.88952400
H	-2.68977300	-2.59779900	-1.52893100
H	-1.63997200	-1.28295800	-0.74084000
H	-2.96905200	-1.59375500	2.67772000
H	-1.61151600	-2.66579000	2.23106000

H	-1.61139100	-0.99960000	1.66399900
B	-4.45520800	0.11665500	0.10839800
C	-5.10459900	0.46271300	-1.33595100
C	-5.70739700	-0.26541300	1.05391200
C	-5.63582900	-0.83203200	-1.99346600
C	-6.30170300	1.45329100	-1.13664400
H	-4.39168700	0.92498300	-2.03427800
C	-6.75992900	-1.16231200	0.33073300
C	-6.36026500	1.08100500	1.44397100
H	-5.39166200	-0.76552700	1.98218200
H	-6.34690800	-0.56754200	-2.78843200
H	-4.81283100	-1.35814300	-2.49371700
C	-6.30722500	-1.80804800	-0.99166600
H	-6.24007900	2.26596200	-1.87144100
H	-7.23338700	0.92506400	-1.37380700
C	-6.44664000	2.08350400	0.26037500
H	-7.65829200	-0.56368800	0.13232000
H	-7.09674800	-1.96182500	1.00323200
H	-5.78646100	1.54655800	2.25487100
H	-7.36453700	0.89720400	1.84902700
H	-5.60807100	-2.61830500	-0.75959900
H	-7.17364500	-2.28786600	-1.46286800
H	-7.39738100	2.62818900	0.30256200
H	-5.67109400	2.84850100	0.37572500

TS3

N	2.48015500	2.00140800	-0.08979100
C	3.04174500	3.28447200	-0.64704400
H	4.05373800	3.05468600	-0.99124100
H	2.43758600	3.52263100	-1.52588700

C	3.07040700	4.47427200	0.30375800
H	2.08891200	4.62801900	0.76654100
H	3.79000300	4.30936000	1.11310400
C	3.46201100	5.74218200	-0.46061300
H	2.72355800	5.92785100	-1.25048700
H	4.42447700	5.58343000	-0.96296600
C	3.55210400	6.95694600	0.45849700
H	4.30631200	6.80435100	1.23695900
H	3.82379400	7.85515100	-0.10130700
H	2.59343500	7.14514800	0.95195100
C	3.33250200	1.55288400	1.07713700
H	3.25658500	2.34285400	1.82854800
H	4.36435600	1.53783800	0.71190700
C	2.95571000	0.21177000	1.68987500
H	1.97340000	0.27349200	2.16948000
H	2.86901100	-0.57312200	0.93278500
C	4.00875900	-0.20441800	2.71869000
H	4.16259100	0.59708000	3.45364600
H	4.96987500	-0.35454600	2.20902200
C	3.59702200	-1.49157700	3.42729000
H	4.36920200	-1.82947300	4.12334000
H	2.66987100	-1.34572000	3.99042800
H	3.42404600	-2.28461100	2.69334000
C	2.48247200	0.95317200	-1.19217200
H	1.81981000	0.15568400	-0.84633100
H	2.02165300	1.43594300	-2.05811900
C	3.83955200	0.37726000	-1.57361800
H	4.29088700	-0.15065000	-0.72550200
H	4.54481700	1.15222500	-1.90047100
C	3.63582400	-0.63521300	-2.70449800

H	3.17704100	-0.13834700	-3.56843700
H	2.91990300	-1.38984700	-2.35555900
C	4.94446100	-1.30030800	-3.12107000
H	4.77972700	-2.03110100	-3.91813600
H	5.66068400	-0.55980300	-3.49232400
H	5.40598500	-1.81681700	-2.27255400
C	1.04462300	2.18639400	0.39310600
H	1.10918000	2.74785000	1.32986800
H	0.68059300	1.18080500	0.61143200
C	0.10432100	2.89526000	-0.57567200
H	0.41029000	3.94045000	-0.70841000
H	0.12452000	2.41693500	-1.56262300
C	-1.33344000	2.82873900	-0.02747400
H	-1.31708400	3.03496000	1.05283700
H	-1.92345300	3.63442300	-0.47803700
C	-2.03281900	1.48666100	-0.27702100
H	-2.23206300	1.39237600	-1.35543200
H	-1.33317000	0.68114400	-0.02666000
C	-3.33653200	1.33070600	0.51391800
H	-3.87862500	2.28157900	0.41715400
H	-3.08148100	1.26397700	1.58466300
Cl	4.78563100	-3.23924100	0.17748000
C	2.14900900	-3.88741000	-0.34103100
C	3.55663600	-3.99249800	-0.90354500
O	1.90618500	-2.50099400	-0.13760400
H	1.46548300	-4.26053300	-1.11315100
H	3.84365300	-5.03736900	-1.02968100
H	3.63429500	-3.47347900	-1.86014600
C	1.94008800	-4.67068600	0.94456500
H	0.90613600	-4.54917200	1.27364700

H	2.12989900	-5.73577600	0.78001200
H	2.61376900	-4.31044000	1.72672300
C	0.59588600	-2.07098200	-0.05229600
O	0.47403900	-0.87759600	0.24031600
O	-0.30538900	-2.91777700	-0.31162000
O	-3.58870900	-1.22866000	-0.22050800
C	-2.77901900	-1.97914000	0.65287800
C	-1.98140800	-1.97933800	-0.58205200
H	-3.24882200	-2.94300000	0.88457400
C	-2.20090200	-1.34946600	1.90043600
H	-2.27553900	-2.65718900	-1.37085800
H	-1.44983200	-1.07761200	-0.83213800
H	-2.99819900	-1.10221100	2.60546500
H	-1.52700400	-2.07568500	2.36805000
H	-1.62635100	-0.45225900	1.67342800
B	-4.35998500	0.13336300	0.04100800
C	-5.15268600	0.42249600	-1.35817000
C	-5.55994200	-0.18526800	1.10229600
C	-5.69443900	-0.91752800	-1.90699200
C	-6.35602700	1.39613700	-1.13119900
H	-4.50213700	0.85963300	-2.13218300
C	-6.63797200	-1.14028600	0.50179700
C	-6.22043900	1.15975400	1.47005200
H	-5.18349700	-0.63214100	2.03618900
H	-6.48041900	-0.72051000	-2.65114900
H	-4.89543100	-1.44618800	-2.44029700
C	-6.24296700	-1.85603000	-0.80121400
H	-6.35563700	2.18197900	-1.89850200
H	-7.28781800	0.84127500	-1.29976100
C	-6.45666100	2.08463400	0.24421400

H	-7.55830700	-0.56924500	0.31873100
H	-6.92210500	-1.90289100	1.23978800
H	-5.58815500	1.69334000	2.19142700
H	-7.17519200	0.97620800	1.98354700
H	-5.47889500	-2.60238000	-0.56266200
H	-7.11050700	-2.41336000	-1.17793900
H	-7.44273100	2.55976700	0.32086200
H	-5.73978300	2.91213200	0.27420700

INT7

N	2.91020400	1.67659500	-0.02247300
C	4.01497500	2.61113900	-0.45193100
H	4.74710800	2.00263800	-0.98777800
H	3.56309500	3.30071600	-1.16914800
C	4.70101000	3.39272000	0.66174200
H	3.96440400	3.87773200	1.31230000
H	5.30394200	2.72802800	1.28988200
C	5.61032200	4.46642100	0.05673400
H	5.00171200	5.15725100	-0.53974000
H	6.31981100	3.99626500	-0.63567400
C	6.37031400	5.24022200	1.13003500
H	7.00920600	4.57243200	1.71647000
H	7.00661100	6.00869900	0.68462800
H	5.67839600	5.73440600	1.81930300
C	3.46893800	0.64236300	0.93102200
H	3.86534600	1.19731100	1.78475900
H	4.31029700	0.17347400	0.41190500
C	2.46926700	-0.40619700	1.39481000
H	1.70814100	0.04711800	2.04031500
H	1.94824600	-0.85482100	0.54381200

C	3.17549100	-1.52673900	2.16180400
H	3.65557000	-1.12347800	3.06258300
H	3.97464700	-1.94544600	1.53653300
C	2.19027500	-2.63323200	2.53150500
H	2.67895600	-3.42918000	3.09942500
H	1.36864500	-2.23698600	3.13845600
H	1.76389800	-3.08044800	1.62711500
C	2.33050800	1.01001700	-1.26417500
H	1.38208900	0.55106500	-0.97171800
H	2.11028000	1.82225900	-1.96128900
C	3.20740900	-0.04439300	-1.92428100
H	3.25228100	-0.93723800	-1.29282900
H	4.23267300	0.31048200	-2.08804000
C	2.59141000	-0.43497800	-3.27188000
H	2.70056200	0.39753500	-3.97798200
H	1.51928700	-0.60655500	-3.13244000
C	3.23314700	-1.69998000	-3.83124700
H	2.81988300	-1.95221800	-4.81116800
H	4.31651200	-1.58165800	-3.94298900
H	3.04784000	-2.54092600	-3.15596200
C	1.80064100	2.44570800	0.67489600
H	2.16562200	2.68149300	1.67849100
H	0.97286900	1.74225100	0.77989800
C	1.31484500	3.71163200	-0.02378700
H	2.01331100	4.53736600	0.16100800
H	1.24961200	3.57199600	-1.10917400
C	-0.09654400	4.01427000	0.50402500
H	-0.09651500	3.90376400	1.59795300
H	-0.34233800	5.06229700	0.30604200
C	-1.14665000	3.07450900	-0.11690300

H	-1.56165500	3.54971500	-1.01576500
H	-0.65883700	2.16201100	-0.49191500
C	-2.27949100	2.65573500	0.81850700
H	-2.76880400	3.56784200	1.18672700
H	-1.81752000	2.20023800	1.71519300
Cl	1.41897700	-6.33673100	1.35198200
C	-0.50127500	-4.92340600	-0.04262200
C	0.20774000	-6.26383000	0.03224700
O	0.51725900	-3.97441300	-0.40807400
H	-1.22559900	-4.99158600	-0.86164400
H	-0.51923400	-7.05615100	0.21593100
H	0.74068900	-6.46140400	-0.89807800
C	-1.19784100	-4.51519700	1.24418200
H	-1.78337200	-3.60718100	1.08864500
H	-1.87528900	-5.31077900	1.56862800
H	-0.46152600	-4.34348300	2.03370200
C	0.18221300	-2.77657400	-0.89633400
O	1.03585400	-1.94195400	-1.10767200
O	-1.11389500	-2.65123000	-1.11684600
O	-2.51071600	0.63447900	-0.73505500
C	-2.13759500	-0.58904900	-0.23032600
C	-1.61119300	-1.33302900	-1.45713100
H	-2.99446200	-1.16357600	0.17253400
C	-1.07951100	-0.49713100	0.87464900
H	-2.41807600	-1.49826400	-2.17155000
H	-0.81372300	-0.75391600	-1.92706600
H	-1.49762500	0.03283600	1.73340000
H	-0.72103400	-1.47860800	1.21500100
H	-0.22139200	0.07028100	0.49726500
B	-3.34841100	1.62254800	0.08484600

C	-4.37210800	2.36174800	-0.97108600
C	-4.37464800	0.87892200	1.12556200
C	-4.94577400	1.27802400	-1.90644100
C	-5.55654800	3.07703200	-0.25002700
H	-3.85756900	3.10464400	-1.60134400
C	-5.48891100	0.09696100	0.36023700
C	-5.01098300	1.95888300	2.02637800
H	-3.86597900	0.17192600	1.80250200
H	-5.83951600	1.65926300	-2.42386000
H	-4.21228100	1.04309100	-2.68599400
C	-5.29376200	-0.03773800	-1.16323200
H	-5.73517300	4.06697500	-0.69258900
H	-6.48029200	2.51441300	-0.44189900
C	-5.41454800	3.25078100	1.26971700
H	-6.45869200	0.57958500	0.54359200
H	-5.59738600	-0.91640000	0.77460900
H	-4.30263400	2.23040300	2.82057700
H	-5.89199900	1.54390100	2.53885200
H	-4.49116800	-0.76163300	-1.34206200
H	-6.19793500	-0.48795000	-1.59445300
H	-6.35792700	3.64019100	1.67425600
H	-4.67272400	4.03279100	1.46252900