Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

for

Synthesis of Polyethers from Epoxides via Binary Organocatalyst system

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Content

1. General Information.

All the synthesis of compounds, involving air and/or water-sensitive were carried out in glove box or with the standard Schlenk techniques under dry nitrogen. Epoxides were distilled over calciumhydride under nitrogen. Triphenylboroxin, 2,4,6-tris(4-fluorophenyl)boroxin and 2,4,6-tris(3,4-difluorophenyl)boroxin were purchased from TCI Shanghai and used as received. 2,4,6-tris(4-methoxyl)boroxin and 2,4,6-tris(3,4- methoxyl)boroxin were synthesized in laboratory.[1]

NMR. ^{1}H and ^{11}B NMR spectra were recorded on a Varian INOVA-400 MHz type spectrometer (^{1}H NMR, 400MHz and ^{11}B NMR, 128 MHz). The peak frequencies were referenced versus an internal standard $CHCl_3$ shift at 7.26 ppm for ^{1}H NMR.

Gel permeation chromatography (GPC). Molecular weights and molecular weight distributions of copolymers were measured by gel permeation chromatography (GPC) analysis at 30 ℃ and a flow rate of 1.0 mL/min, with THF as the eluent, on an Agilent 1260 instrument coupled with an Agilent RI detector and equipped with four PL gel columns. The sample concentration was about 1 mg/mL, and the injection volume was 100 μL. The curve was calibrated using monodisperse polystyrene standards covering the molecular weight rage from 580 to 460000 Da.

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS). MALDI-TOF mass spectrometry was performed on a Bruker ultrafleXetreme MALDI TOF/TOF mass spectrometer. Trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB) was used as a matrix. Sodium acetate (Aldrich, 98%) was added for ion formation.

Electrospray ionization mass spectrometry (ESI-MS). On-line monitoring of polymerization by ESI-MS in negative mode was carried out using the Waters Xevo G2-XS QTof instrument equipped with an orthogonal electrospray source (Z-spray) and referenced against the lock mass of m/z = 554.2615 (Sample cone = 10 V).

Gas chromatography-mass spectrometry (GC-MS). An Agilent 7890B-5977B instrument equipped with HP-5ms capillary chromatographic column (30 m*0.25 mm*0.25 μm) was employed for GC-MS experiments. The inlet temperature was set to 275 ℃ and the heating program was set to 35 ℃ (5 min), and then, the temperature was increased to 300 ℃ (2min) at a rate of 30 ℃/min.

General procedure for the ROP of epoxides. In a 10 mL flask equipped with a magnetic stirrer, catalysts and epoxides were refrigerated at −20 ℃ overnight and added in an argon atmosphere. Undergoing an appropriate time, a small amount of the resultant mixture was removed for ^{1}H NMR analysis to determine the PO conversion. The crude polymer was dissolved in 10 mL CH_2Cl_2, then, the solution was precipitated with excess hexane. This process was repeated 2−3 times and transparent polymer was obtained by vacuum-drying.

Synthesis of multi-block polyethers. In a 10 mL flask equipped with a magnetic stirrer, catalysts and epoxides were refrigerated at −20 ℃ overnight. For example, under the feed ratio of PO/TPBX/PPNCl = 50/1/0.5 as well as 2.5 mL THF added in an argon atmosphere, the polymerization was carried out under 0 ℃, and after the PO converted completely (comfirmed by ^{1}H NMR), 50 equiv of BO (refrigerated at −20 ℃ overnight) was directly added to the flask under the atmosphere of argon. Then a portion of the di-block copolymer was taken out for GPC experiment.

Synthesis of random copolyethers. In a 10 mL flask equipped with a magnetic stirrer, catalysts and PO and EO were refrigerated at −20 ℃ overnight were added in an argon atmosphere. Undergoing an appropriate time, a small amount of the resultant mixture was removed for ^{1}H NMR analysis to determine the PO and EO conversion. A portion of the random copolyether was taken out for GPC experiment.

2. ^{1}H NMR and ^{11}B NMR of PO and TPBX.

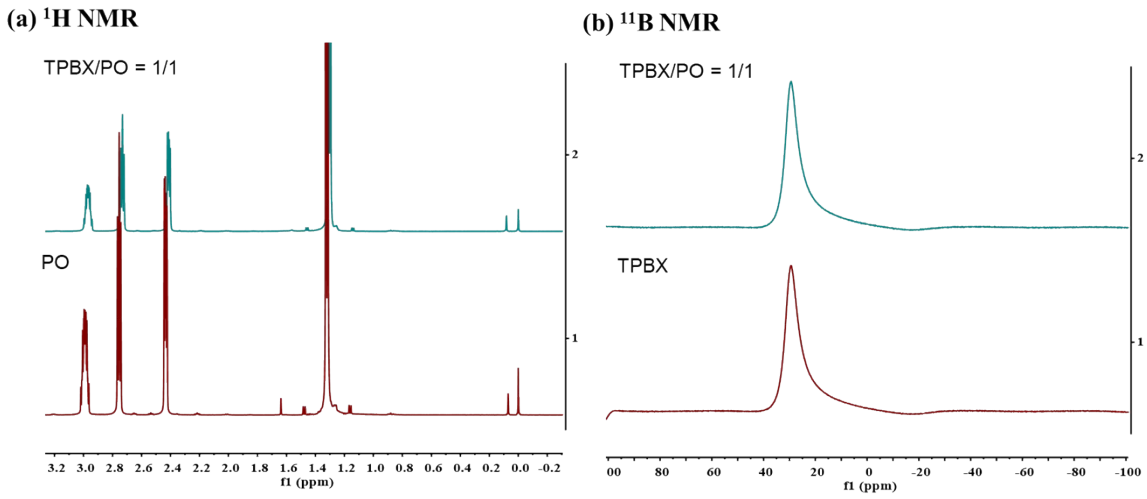
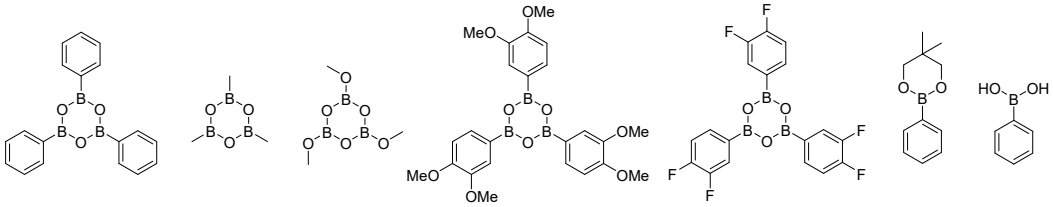


Fig. S1 (a) ^{1}H NMR spectra of PO and TPBX/PO (1/1) and (b) ^{11}B NMR spectra of TPBX and TPBX/PO (1/1).

3. Evaluation of the Lewis acidity of boron compounds.

Gutmann-Beckett methods: The Lewis acid and the triethylphosphine oxide (Et_3PO) were placed together in 1:1 mole ratio in a small glass vial and dissolved in the minimum amount of dry C_6D_6. The solution was placed in an NMR tube, and the ^{31}P NMR chemical shift was recorded at room temperature.

Table S1. ^{31}P NMR data for Lewis acid-base adducts between **1**−**7** and Et_3PO.



	Et_3PO	Et_3PO
none	45.75	0
$B(Et)_3$	48.61	2.86
$B(OMe)_3$	46.99	1.24
$B(C_6F_5)_3$	75.83	30.08
1	69.32	23.57
2	57.64	11.89
3	67.12	21.37
4	53.05	7.30
5	68.62	22.87
6	46.28	0.53
7	55.03	9.28

[a]In C_6D_6 at room temperature.

4. Study for the mechanism of the catalyst deactivation.

The newly emerged peaks at δ 1.5 and 5.0 ppm in the ^{11}B NMR spectra (Fig. S2) and produced dioxaborolane species in the GC-MS spectrum (Fig. S3 a) indicated the structure of the catalyst has been changed.

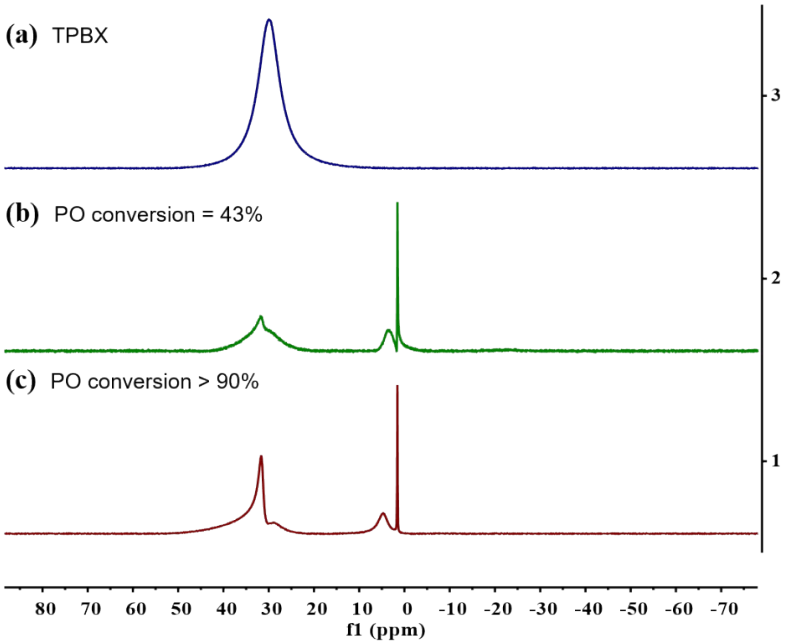


Fig. S2 ^{11}B NMR spectra of (a) TPBX; (b) reaction mixture at PO conversion of 43% and (c) reaction mixture at PO conversion of 90% in $CDCl_3$.

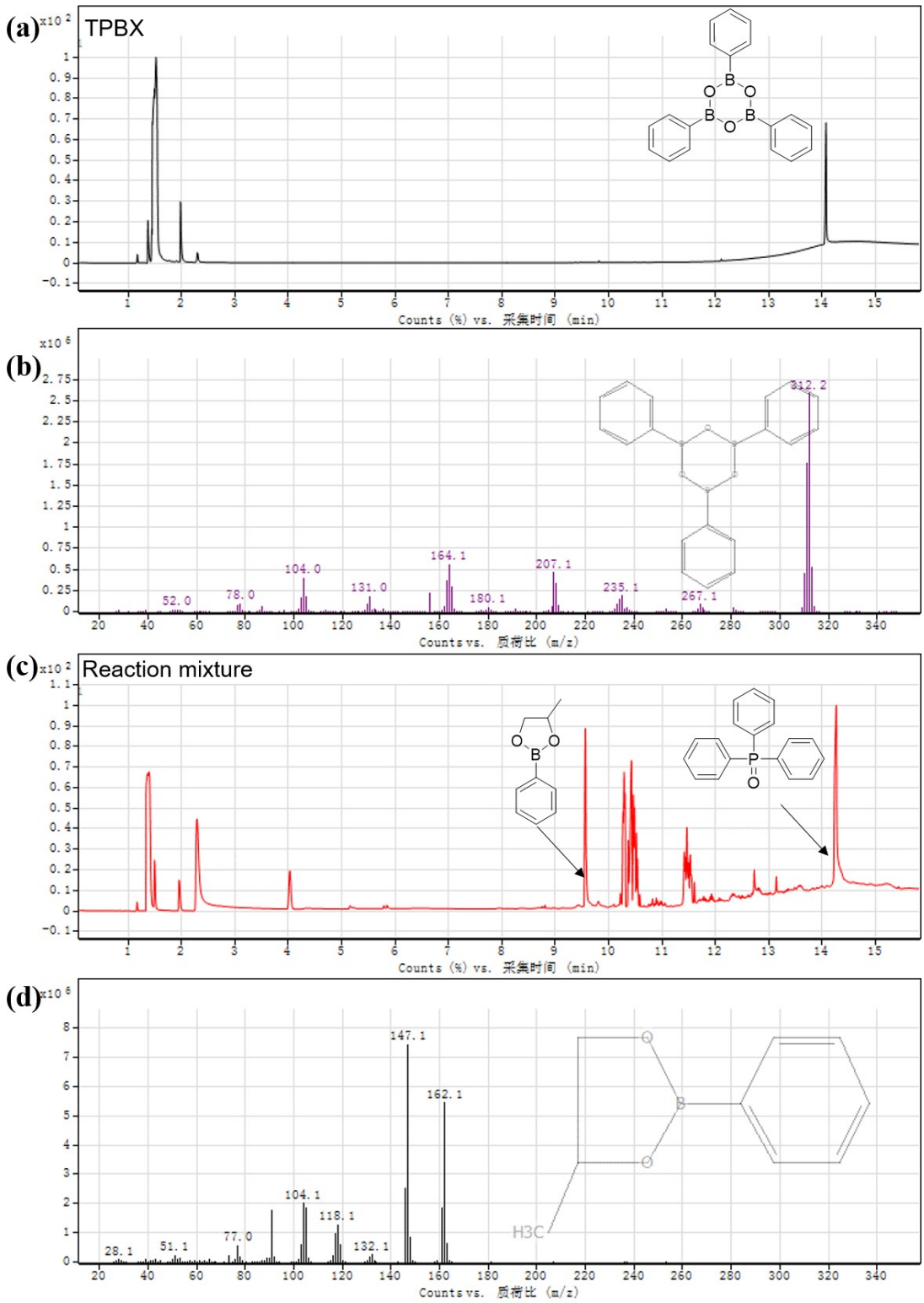


Fig. S3 GC-MS spectra of TPBX and reaction mixture: (a) Gas-phase chromatogram of TPBX (retention time = 14.076 min) and (b) mass spectrum of TPBX; (c) Gas-phase chromatogram of reaction mixture, in which 4-methyl-2-phenyl-1,3,2-dioxaborolane (retention time = 9.562 min) was detected and (d) mass spectrum of 4-methyl-2-phenyl-1,3,2-dioxaborolane.

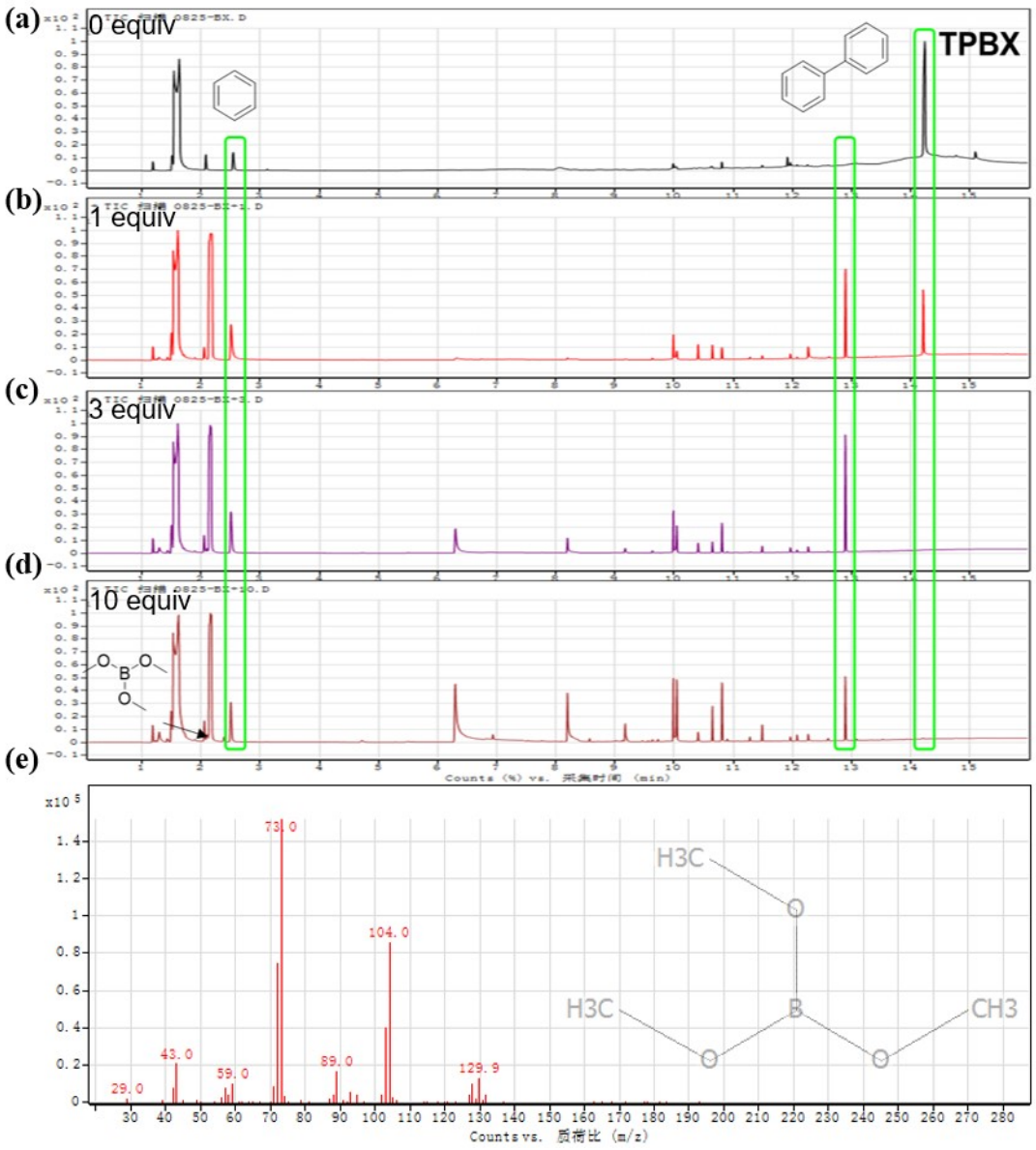
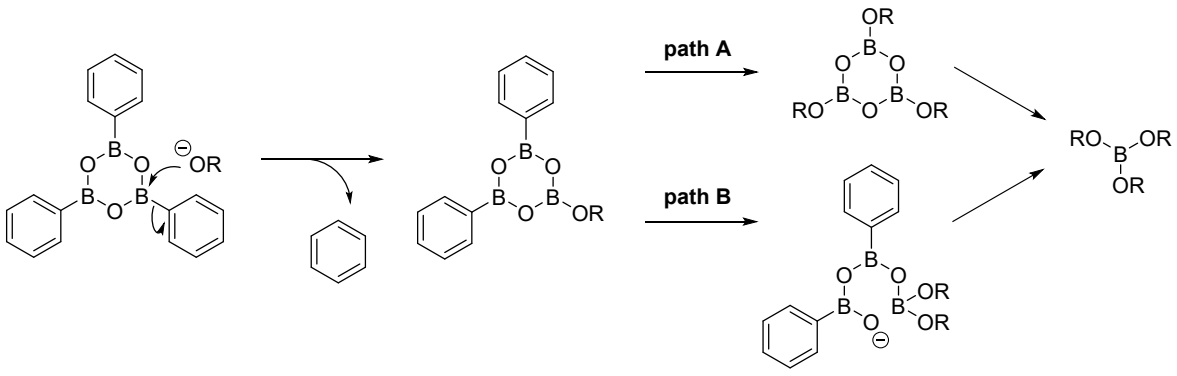


Fig. S4 Gas-phase chromatograms of TPBX with different equivs of NaOMe: (a) 0 equiv; (b) 1 equiv; (c) 3 equiv; (d) 10 equiv and (e) mass spectrum of trimethyl borate.



Scheme S1. Proposed mechanism for catalyst deactivation.

As shown, the structure of portion TPBX in the reaction mixture has been changed to the TPBX dimers at the beginning of the polymerization under 25 °C, while it remains as the original structure when the reaction was performed under 0 °C.

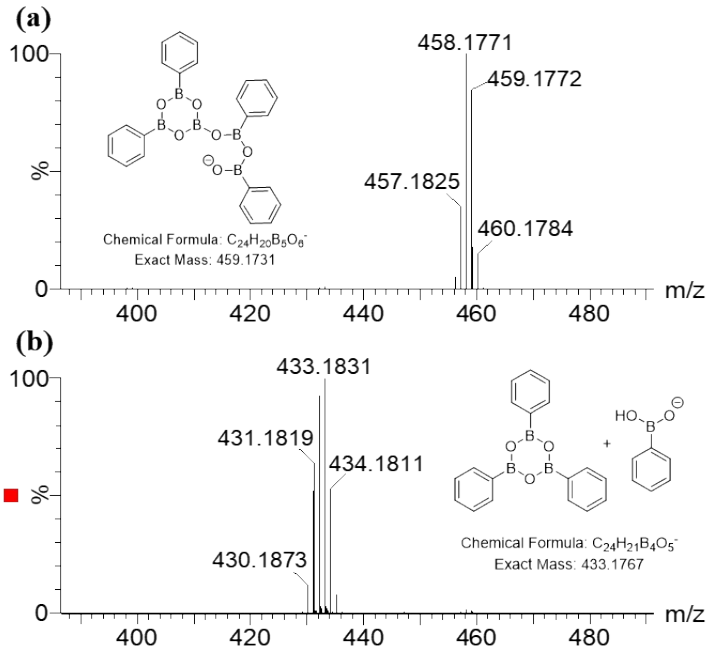


Fig. S5 ESI mass spectra of the catalyst at the beginning of the polymerization under (a) 25 ℃ and (b) 0 ℃ in negative mode.

5. Synthesis of PO/EO multi-block and random copolymers.

Table S2. Polymerization of PO and EO to produce multi-block copolymers.[a]

Entry	Mon.	Mon./cat. (mole ratio)	Time (h)	Conv.[b] (%)	M_n(theo)[c] (kg/mol)	M_n(GPC)[d] (kg/mol)	$Đ$[d]
1	PO	50/1/0.5	19	>99	5.8	8.0	1.21
2	EO	60/-/-	45	>99	11.1	12.5	1.25
3	PO	50/-/-	27.3	>99	16.9	18.1	1.30
4	EO	60/-/-	23	>99	22.2	17.1	1.27
5	PO	50/-/-	24.3	-	-	21.5	1.29

[a]Reactions carried out in 2.5 mL THF at 0 ℃ and PO was refrigerated at −20 ℃ overnight. [b]Obtained by using ^{1}H NMR spectroscopy. [c]Theoretical molecular weights. [d]Determined by gel permeation chromatography in THF, calibrated with PS standards.

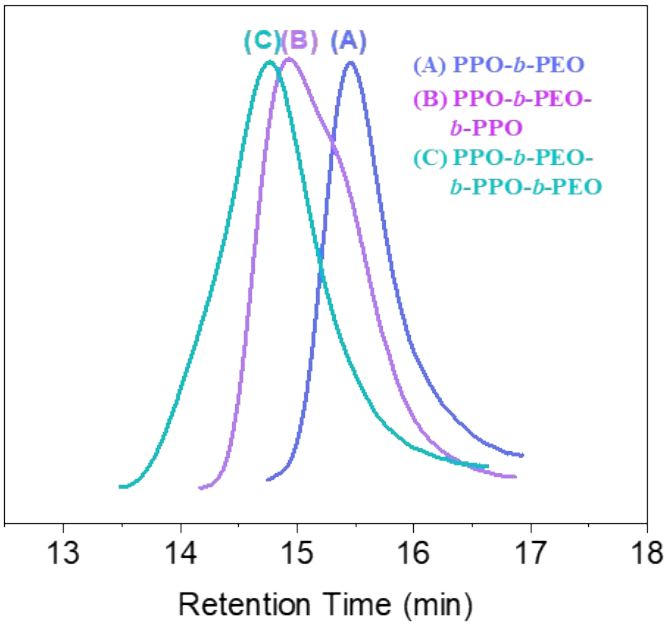
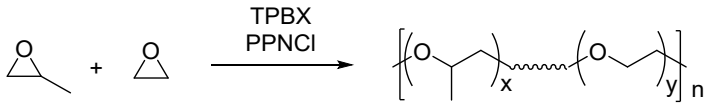


Fig. S6 GPC traces of the resultant PPO-*b*-PEO, PPO-*b*-PEO-*b*-PPO and PPO-*b*-PEO-*b*-PPO-*b*-PEO.

Table S3. Polymerization of PO and EO to produce random copolymers.[a]



PO EO PPO-*r*-PEO

Entry	PO/EO/cat. (mole ratio)	Time (min)	Conv.[b] (%)		PPO/PEO	M_n[c] (kg/mol)	$Đ$[c]
			PO	EO			
1	0/500/1/0.5	25	-	50	-	17.9	1.12
2	100/150/1/0.5	35	87	84	1/2.14	21.2	1.38
3	200/240/1/0.5	15	43	66	1/1.63	21.6	1.24
4	200/240/1/0.5	80	71	89	1/1.56	29.4	1.26

[a]Reactions were performed in neat epoxides at 0 °C and PO was refrigerated at −20 °C overnight. [b]Obtained by using ^{1}H NMR spectroscopy. [c]Determined by gel permeation chromatography in THF, calibrated with PS standards.

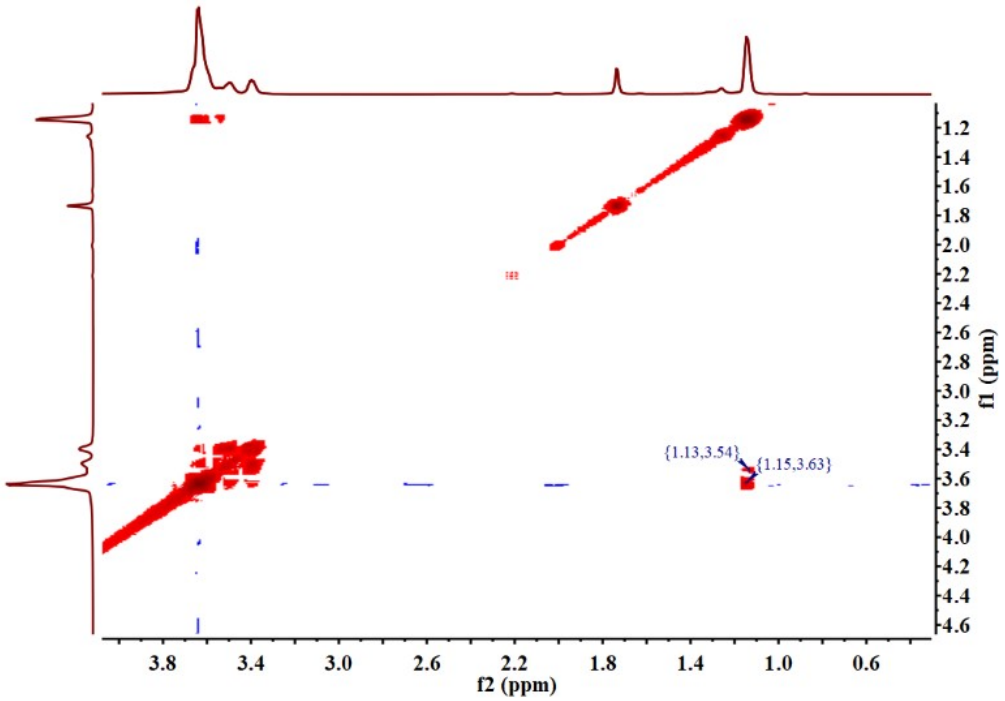


Fig. S7 ^{1}H-^{1}H COSY NMR spectrum of PPO-*r*-PEO copolymer.

6. *Kinetics studies for the ROP of PO.*

The *in-suit* IR experiments were carried out in a neat Schlenk strip bottle equipped with a magnetic stirrer and charged with chloroform solution of TPBX/PPNCl at 0 ℃. The order in catalyst was determined by applying five TPBX concentrations (0.045 M, 0.049 M, 0.078 M, 0.107 M and 0.192 M). Then, cold PO was added before the reaction mixture was stirred, and the FTIR probe began collecting scans. The infrared spectrometer was set up to collect one spectrum every 30 s over a certain period. The intensity of the peak at 1104 cm^{-1} (stretch vibration of C−O−C in PO) was monitored to determine the initial rate coefficient (k_{obs}).

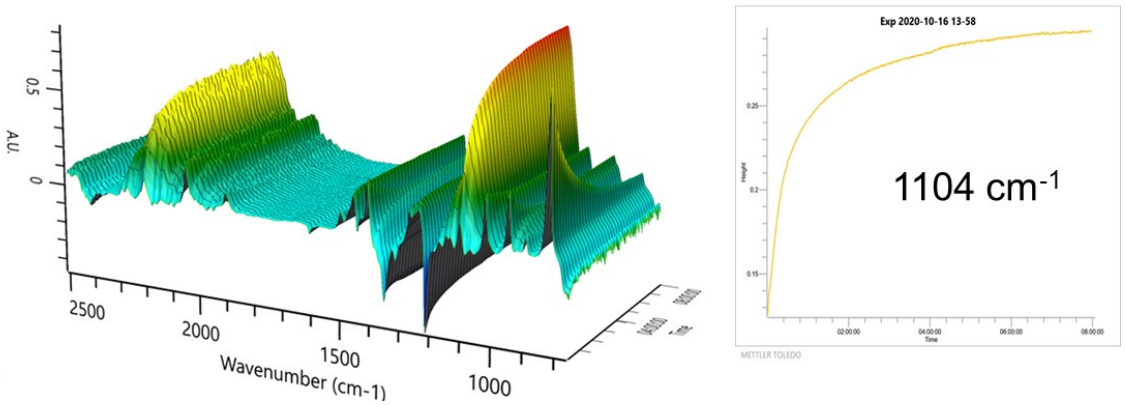


Fig. S8 Three-dimensional stack plot of the infrared spectrum of the ROP of PO catalyzed by TPBX/PPNCl and the *in-situ* IR trace of 1104 cm^{-1} (stretch vibration of C−O−C in PO).

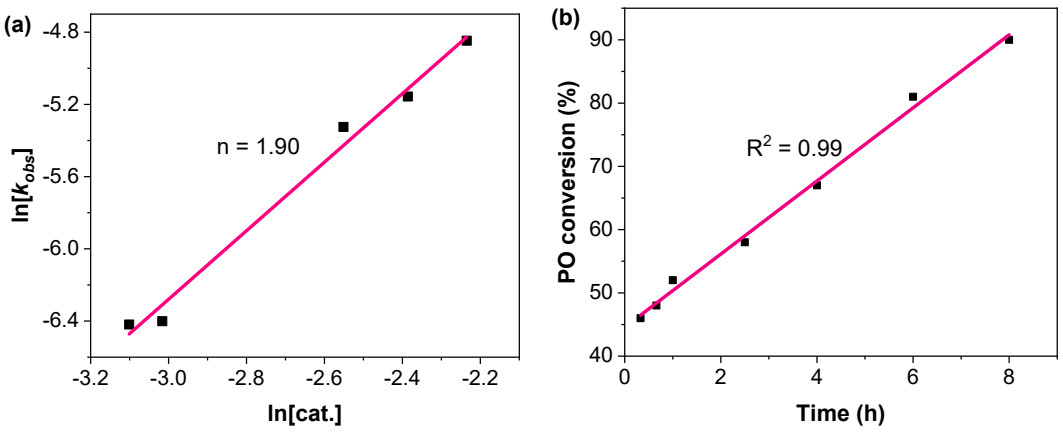
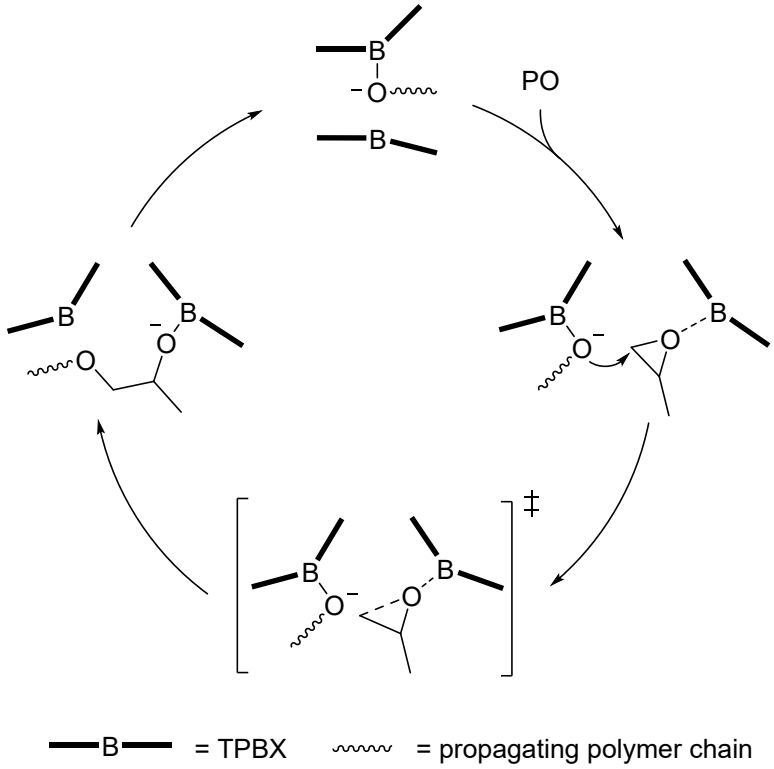


Fig. S9 Reaction kinetic analysis to determine order in (a) catalyst TPBX (second order) and (b) PO (quasi-zero-order).



Scheme S2. Proposed mechanism for the ROP of PO by using TPBX/PPNCl.

7. Computational Details.

All calculations were performed with Gaussian 16 suite of the programs.[2] The DFT method of M062X was used for single point energy calculations, geometry optimizations and frequency analyses. The 6-31G(d) all election basis set was used for all atoms. SMD model was used, in which PO was simulated with THF. Frequency calculations were performed to identify the geometrically optimized stationary points (no imaginary frequencies for minima and one imaginary frequency for

transition-state structures), and to obtain the thermodynamic data. To improve the accuracy of the energy, the single point energy of each optimized structure was calculated with 6-311+G(d,p) for all atoms. The relative free energy was obtained by combining the single-point energy with Gibbs free energy correction. To increase computational efficiency, the propagating polymer chain was simplified as 1-chloro-2-propanol anion.

PO

Charge = 0 Multiplicity = 1

C	1.04178	0.61009	-0.05142
C	-0.14877	-0.05467	0.49323
O	0.81367	-0.77567	-0.25829
H	0.93691	1.23646	-0.9358
H	1.87657	0.85402	0.60205
H	-0.14747	-0.29405	1.5573
C	-1.50082	0.10692	-0.14601
H	-2.07448	-0.82032	-0.06917
H	-2.06907	0.90347	0.34165
H	-1.38501	0.35175	-1.20447

PPN^+

Charge = 1 Multiplicity = 1

N	0.	-0.00014	-0.75845
P	1.51299	-0.01196	-0.26191
P	-1.51296	0.01189	-0.26193
C	-1.72027	0.07293	1.53354
C	-2.28202	-0.9938	2.23861
C	-1.22945	1.1914	2.22093
C	-2.35272	-0.94008	3.62939
H	-2.66278	-1.86094	1.70761
C	-1.29309	1.2334	3.60694
H	-0.79289	2.02287	1.67128
C	-1.85677	0.1671	4.30989
H	-2.79599	-1.76404	4.17817
H	-0.90538	2.09455	4.14049
H	-1.91054	0.20455	5.39308
C	-2.35161	-1.47255	-0.85264
C	-3.7403	-1.4906	-1.0164
C	-1.59703	-2.62505	-1.08698
C	-4.37084	-2.66673	-1.40807
H	-4.32483	-0.58992	-0.8497
C	-2.23521	-3.79784	-1.47931
H	-0.51623	-2.5951	-0.97668
C	-3.61906	-3.81787	-1.63741

H	-5.44698	-2.68358	-1.54148
H	-1.65232	-4.69322	-1.6664
H	-4.11424	-4.73235	-1.94653
C	-2.35953	1.45109	-0.94859
C	-1.94116	1.93154	-2.19465
C	-3.43728	2.0484	-0.28704
C	-2.60264	3.00818	-2.77491
H	-1.09503	1.46616	-2.69269
C	-4.09641	3.12332	-0.87725
H	-3.75301	1.68479	0.68708
C	-3.67964	3.60085	-2.11753
H	-2.27981	3.3843	-3.73966
H	-4.93037	3.59122	-0.36556
H	-4.19426	4.44053	-2.57263
C	1.72024	-0.07317	1.53355
C	2.28178	0.99354	2.23881
C	1.22946	-1.19178	2.22074
C	2.35233	0.93966	3.62958
H	2.66248	1.86079	1.70794
C	1.29296	-1.23395	3.60675
H	0.79297	-2.02319	1.67093
C	1.85645	-0.16768	4.30989
H	2.79542	1.76361	4.17853
H	0.90527	-2.09521	4.14015
H	1.91012	-0.20525	5.39309
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C	3.74021	1.49085	-1.01596
C	1.59682	2.62509	-1.08673
C	4.37068	2.66708	-1.40741
H	4.32479	0.5902	-0.84928
C	2.23495	3.79799	-1.47884
H	0.51601	2.59503	-0.97659
C	3.61881	3.81818	-1.63673
H	5.44684	2.68405	-1.54064
H	1.65199	4.69333	-1.6659
H	4.11396	4.73274	-1.94565
C	2.35973	-1.451	-0.94868
C	3.43753	-2.04824	-0.28714
C	1.94148	-1.93134	-2.19482
C	4.09681	-3.12301	-0.87744
H	3.75317	-1.6847	0.68704
C	2.60313	-3.00784	-2.77516
H	1.09531	-1.46601	-2.69283
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H	4.93081	-3.59086	-0.36576
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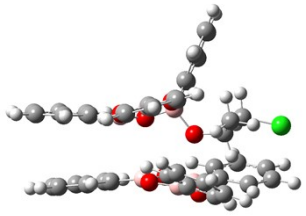
H	4.19491	-4.44001	-2.57297

Path A:

I



Charge = −1 Multiplicity = 1

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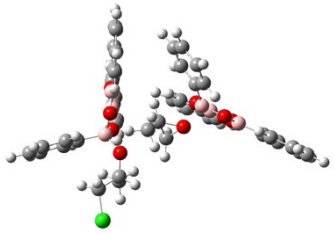
B	2.15537	-0.2389	0.89956
O	0.85997	-0.59257	0.93205
C	-0.88033	-0.00757	2.67274
C	-1.05008	0.89973	3.72322
C	-1.35617	-1.31283	2.86716
C	-1.68849	0.53488	4.90982
H	-0.67752	1.91437	3.59717
C	-1.99297	-1.69134	4.04496
H	-1.23063	-2.03592	2.06209
C	-2.16648	-0.76251	5.07174
H	-1.81454	1.26225	5.70814
H	-2.36031	-2.70733	4.1665
H	-2.66842	-1.05082	5.9915
C	3.30531	-1.3057	1.07357
C	3.00615	-2.63326	1.40204
C	4.65032	-0.94679	0.93202
C	4.01466	-3.57662	1.56824
H	1.96222	-2.91634	1.51126
C	5.66775	-1.88416	1.09476
H	4.89045	0.08513	0.68914
C	5.34885	-3.20252	1.41143
H	3.76412	-4.60636	1.80745
H	6.70732	-1.59	0.97646
H	6.13832	-3.93935	1.53486
C	2.02545	3.57036	0.73947
C	3.30232	3.90653	0.27671

C	1.09238	4.59931	0.91467
C	3.6387	5.22769	-0.01338
H	4.0296	3.11153	0.13198
C	1.41857	5.92217	0.63078
H	0.0942	4.33774	1.25686
C	2.69344	6.23728	0.1614
H	4.63236	5.4721	-0.37887
H	0.67999	6.70778	0.76323
H	2.94971	7.26796	-0.06854
O	-1.19644	0.30365	0.13665
C	-2.3839	1.06828	0.11391
H	-2.7664	0.98383	-0.91273
C	-3.45065	0.43161	1.01908
H	-3.29966	0.65474	2.07447
H	-3.49288	-0.64768	0.86803
C	-2.20391	2.55389	0.42088
H	-1.95096	2.70744	1.47387
H	-1.39666	2.96634	-0.18942
H	-3.13408	3.0831	0.19503
Cl	-5.09681	1.07545	0.60032
B	-0.46092	0.18607	-2.27556
O	-1.66457	-0.48784	-2.42551
B	-1.79142	-1.65776	-1.71177
O	-0.67151	-2.38222	-1.37226
B	0.57481	-1.84976	-1.63192
O	0.68935	-0.53752	-2.02922
C	1.81229	-2.79994	-1.65407
C	3.0946	-2.3131	-1.93334
C	1.65668	-4.17019	-1.41464
C	4.19388	-3.16458	-1.95614
H	3.22494	-1.24795	-2.10735
C	2.74892	-5.03156	-1.44724
H	0.66338	-4.5535	-1.19667
C	4.01931	-4.52561	-1.714
H	5.18743	-2.76802	-2.14127
H	2.6154	-6.09246	-1.25554
H	4.87829	-5.19107	-1.72133
C	-3.20517	-2.21782	-1.35691
C	-3.33771	-3.41695	-0.64412
C	-4.3639	-1.50643	-1.68869
C	-4.591	-3.89323	-0.27429
H	-2.43985	-3.96553	-0.37259
C	-5.62131	-1.97452	-1.31805
H	-4.26894	-0.56333	-2.221

C	-5.73401	-3.16925	-0.61148
H	-4.68051	-4.82011	0.28458
H	-6.50858	-1.39796	-1.55985
H	-6.71335	-3.53205	-0.31272
C	-0.39405	1.71964	-2.54998
C	-1.50814	2.40698	-3.04775
C	0.74852	2.45422	-2.21165
C	-1.48432	3.78961	-3.20217
H	-2.40485	1.84431	-3.29619
C	0.77676	3.83971	-2.35112
H	1.61283	1.93119	-1.8065
C	-0.34206	4.50581	-2.84706
H	-2.35811	4.31184	-3.5811
H	1.65689	4.40006	-2.04643
H	-0.32626	5.58777	-2.9447

II



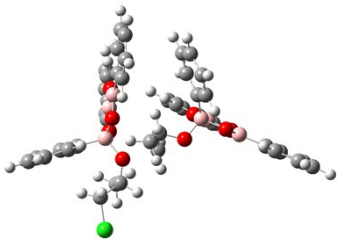
Charge = −1 Multiplicity = 1

B	-2.53081	-1.03335	-1.20193
O	-2.56476	-1.07449	0.1356
O	-2.41415	0.16201	-1.90388
B	-2.79466	0.15849	0.93724
B	-2.24214	1.32925	-1.16729
O	-2.33673	1.35097	0.16934
C	-4.38778	0.31091	1.25334
C	-5.30763	-0.728	1.07018
C	-4.88438	1.51799	1.76806
C	-6.6532	-0.58737	1.41351
H	-4.95458	-1.66764	0.64828
C	-6.22319	1.67467	2.11356
H	-4.19328	2.34915	1.89924
C	-7.11382	0.61432	1.94368
H	-7.34292	-1.41449	1.26573
H	-6.57805	2.62068	2.5148
H	-8.15952	0.72854	2.21579
C	-1.91015	2.6524	-1.96315
C	-1.6977	3.85668	-1.28102

C	-1.86842	2.67207	-3.36298
C	-1.46034	5.0439	-1.96816
H	-1.73316	3.84957	-0.19431
C	-1.64714	3.85707	-4.06068
H	-2.02892	1.74173	-3.90138
C	-1.44468	5.04633	-3.36143
H	-1.28972	5.96695	-1.4218
H	-1.63043	3.85677	-5.14709
H	-1.26767	5.97212	-3.90219
C	-2.62932	-2.36615	-2.04082
C	-2.69557	-2.35118	-3.43922
C	-2.67042	-3.6048	-1.38915
C	-2.80252	-3.5345	-4.16745
H	-2.66167	-1.39358	-3.95208
C	-2.76655	-4.79332	-2.10766
H	-2.62038	-3.61824	-0.30307
C	-2.83448	-4.75835	-3.49998
H	-2.85468	-3.50664	-5.25216
H	-2.78713	-5.74661	-1.58749
H	-2.91166	-5.6835	-4.06449
O	-1.96299	0.16066	2.14746
C	-2.14884	-0.70458	3.22953
H	-1.23017	-0.64241	3.83629
C	-3.27935	-0.18575	4.13154
H	-4.26917	-0.43557	3.75052
H	-3.19288	0.89443	4.2488
C	-2.35867	-2.16702	2.8456
H	-3.30291	-2.2905	2.30852
H	-1.55385	-2.49458	2.18365
H	-2.37217	-2.79258	3.74254
Cl	-3.16761	-0.90624	5.79096
B	3.06136	-1.34213	-0.73636
O	4.27811	-1.46573	-0.0825
B	4.79864	-0.37297	0.59258
O	4.14378	0.80733	0.6276
B	2.88725	0.99562	-0.04587
O	2.41355	-0.15082	-0.77168
C	2.73206	2.3855	-0.81345
C	1.92147	2.49775	-1.94923
C	3.34065	3.54846	-0.32679
C	1.71035	3.72505	-2.57186
H	1.43802	1.60604	-2.34334
C	3.1392	4.7814	-0.94309
H	3.98081	3.47823	0.54984

C	2.31704	4.87145	-2.06494
H	1.05532	3.7885	-3.43509
H	3.61792	5.67331	-0.54751
H	2.14356	5.833	-2.54059
C	6.17946	-0.53476	1.32288
C	6.75055	0.54361	2.00928
C	6.87005	-1.75216	1.30629
C	7.97371	0.41309	2.66002
H	6.2177	1.4905	2.0246
C	8.094	-1.89201	1.95457
H	6.43278	-2.59371	0.77567
C	8.64645	-0.80724	2.63246
H	8.40456	1.25834	3.18871
H	8.61815	-2.84304	1.93356
H	9.60126	-0.91283	3.13982
C	2.43256	-2.60853	-1.40578
C	3.09359	-3.84311	-1.36566
C	1.18512	-2.54095	-2.04008
C	2.52888	-4.97721	-1.94064
H	4.05992	-3.90345	-0.87184
C	0.61349	-3.67003	-2.62
H	0.65771	-1.58981	-2.07694
C	1.28692	-4.88837	-2.56732
H	3.0511	-5.92891	-1.89877
H	-0.35431	-3.60332	-3.10531
H	0.83534	-5.7705	-3.01313
O	1.83124	1.13945	1.23757
C	0.45052	1.58641	1.00945
C	0.70293	0.22729	1.45882
H	0.24717	1.72559	-0.0482
H	0.64409	-0.58513	0.74276
H	0.57792	-0.01436	2.50761
C	-0.02038	2.66094	1.93461
H	-1.1122	2.64129	1.9219
H	0.33058	2.46641	2.95112
H	0.34744	3.63532	1.60187

TS1



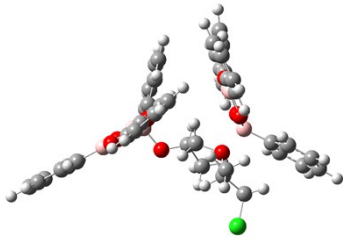
Charge = −1 Multiplicity = 1

B	-2.58414	-0.94988	-1.27445
O	-2.56891	-1.02359	0.06801
O	-2.4164	0.25485	-1.94148
B	-2.65443	0.19176	0.89233
B	-2.13758	1.39071	-1.18973
O	-2.17594	1.37142	0.15636
C	-4.17572	0.43837	1.40303
C	-5.18305	-0.52496	1.28008
C	-4.52148	1.6551	2.00862
C	-6.46957	-0.30589	1.77436
H	-4.94764	-1.4653	0.78461
C	-5.79984	1.88807	2.5063
H	-3.76183	2.43082	2.08872
C	-6.77837	0.89971	2.39806
H	-7.23137	-1.07408	1.67136
H	-6.03899	2.83774	2.97751
H	-7.77693	1.07394	2.78879
C	-1.76707	2.7113	-1.9602
C	-1.42223	3.87457	-1.26132
C	-1.79837	2.76569	-3.35905
C	-1.11846	5.05492	-1.93233
H	-1.39605	3.84152	-0.17498
C	-1.51225	3.9464	-4.03915
H	-2.06008	1.8664	-3.91025
C	-1.17018	5.09275	-3.32398
H	-0.83418	5.94247	-1.37497
H	-1.54815	3.97423	-5.12471
H	-0.93504	6.01309	-3.85166
C	-2.80314	-2.24986	-2.1338
C	-2.85431	-2.20231	-3.53191
C	-2.94837	-3.49275	-1.50582
C	-3.04309	-3.36007	-4.2834
H	-2.73751	-1.2415	-4.02607
C	-3.13168	-4.65592	-2.24781
H	-2.90419	-3.5329	-0.4202

C	-3.17873	-4.58938	-3.63968
H	-3.07752	-3.30874	-5.3678
H	-3.23193	-5.6142	-1.74667
H	-3.31909	-5.4952	-4.22284
O	-1.70408	0.06951	2.06444
C	-1.91015	-0.84327	3.12652
H	-0.95508	-0.89394	3.66925
C	-2.92251	-0.26334	4.1231
H	-3.95559	-0.42384	3.81859
H	-2.74054	0.8022	4.26309
C	-2.27107	-2.25556	2.68264
H	-3.25546	-2.27282	2.20977
H	-1.5413	-2.61833	1.95583
H	-2.27907	-2.91782	3.55246
Cl	-2.73009	-1.05407	5.73815
B	2.79233	-1.40276	-0.61661
O	4.05518	-1.54665	-0.05851
B	4.6278	-0.45736	0.58475
O	3.99762	0.72316	0.67751
B	2.66561	0.94712	0.12732
O	2.12313	-0.2338	-0.55403
C	2.5921	2.26594	-0.79716
C	1.94015	2.27359	-2.03534
C	3.14024	3.47498	-0.34783
C	1.8375	3.43501	-2.79878
H	1.49829	1.3486	-2.39992
C	3.04123	4.64373	-1.09906
H	3.65566	3.49091	0.6107
C	2.38582	4.62513	-2.32929
H	1.30784	3.41739	-3.7468
H	3.47318	5.56991	-0.72798
H	2.29364	5.53598	-2.91531
C	6.06123	-0.64294	1.21184
C	6.68935	0.42361	1.86603
C	6.74015	-1.86437	1.13527
C	7.95459	0.27802	2.42722
H	6.16471	1.37335	1.92611
C	8.00611	-2.02019	1.69387
H	6.25958	-2.69685	0.62802
C	8.61451	-0.94679	2.34127
H	8.42887	1.11531	2.93137
H	8.52005	-2.97492	1.62616
H	9.60227	-1.06446	2.77839
C	2.15482	-2.65709	-1.31742

C	2.81563	-3.89218	-1.30671
C	0.91834	-2.57319	-1.9704
C	2.26174	-5.01016	-1.92317
H	3.77665	-3.96416	-0.80424
C	0.36006	-3.68374	-2.59862
H	0.39485	-1.61897	-1.99061
C	1.03232	-4.90367	-2.57078
H	2.78528	-5.96205	-1.90158
H	-0.59542	-3.60164	-3.1062
H	0.59243	-5.77156	-3.05484
O	1.79556	1.19832	1.37974
C	0.46315	1.67697	1.18422
C	0.24628	0.31778	1.66325
H	0.2325	1.83894	0.13251
H	0.28883	-0.49376	0.94717
H	0.42091	0.12385	2.71201
C	0.09579	2.83915	2.06407
H	-0.98967	2.96657	2.04407
H	0.4212	2.65285	3.09139
H	0.58133	3.74724	1.6964

III



Charge = −1 Multiplicity = 1

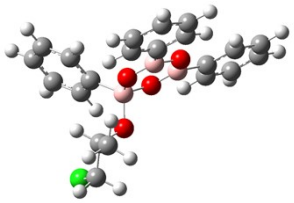
B	2.68317	-0.33405	1.61539
O	2.93096	-0.7742	0.3571
O	2.26867	0.96288	1.84915
B	2.79048	0.08675	-0.78383
B	2.11882	1.83828	0.78014
O	2.32431	1.40888	-0.49226
C	4.04306	0.05527	-1.77748
C	5.07302	-0.88114	-1.63741
C	4.13456	0.9761	-2.82894
C	6.13079	-0.936	-2.54412
H	5.03603	-1.57767	-0.80261
C	5.18406	0.92988	-3.74198
H	3.36324	1.73719	-2.92606
C	6.17955	-0.03734	-3.60739

H	6.916	-1.67688	-2.42325
H	5.22995	1.64506	-4.5582
H	6.99673	-0.0813	-4.32142
C	1.77897	3.33609	1.06722
C	1.4037	4.19656	0.02825
C	1.88893	3.85996	2.36045
C	1.14356	5.54035	0.27248
H	1.31089	3.79576	-0.97811
C	1.65095	5.20847	2.60915
H	2.16923	3.19555	3.17366
C	1.27618	6.04842	1.5632
H	0.82762	6.19043	-0.5376
H	1.74676	5.60381	3.61643
H	1.07502	7.0987	1.75569
C	2.89884	-1.29884	2.83164
C	2.54786	-0.91551	4.13148
C	3.44175	-2.57476	2.63607
C	2.73085	-1.78131	5.2067
H	2.11851	0.07029	4.28855
C	3.63557	-3.44344	3.70572
H	3.7027	-2.88136	1.6263
C	3.27743	-3.04574	4.99328
H	2.44413	-1.47602	6.20844
H	4.05482	-4.43127	3.5394
H	3.41935	-3.72363	5.83002
O	1.48992	-0.53677	-1.64076
C	1.53463	-1.78204	-2.39053
H	0.50207	-1.95168	-2.70502
C	2.34294	-1.57703	-3.67245
H	3.41735	-1.66527	-3.52782
H	2.10291	-0.6138	-4.12222
C	2.00949	-2.93441	-1.52535
H	3.05434	-2.79565	-1.24031
H	1.40843	-2.99723	-0.6141
H	1.90861	-3.86672	-2.08607
Cl	1.8751	-2.85651	-4.85368
B	-2.6249	-1.27544	0.8467
O	-3.88115	-1.54817	0.32203
B	-4.5579	-0.51031	-0.31689
O	-3.99863	0.68022	-0.54103
B	-2.56949	0.93307	-0.26309
O	-2.03221	-0.08289	0.70346
C	-2.35966	2.42294	0.33972
C	-1.75913	2.67746	1.57686

C	-2.78384	3.53302	-0.40542
C	-1.60573	3.97568	2.06491
H	-1.4087	1.83356	2.16797
C	-2.63658	4.83385	0.0669
H	-3.24587	3.35964	-1.37573
C	-2.04796	5.05834	1.31141
H	-1.12655	4.14508	3.0256
H	-2.97914	5.67577	-0.53065
H	-1.91893	6.07172	1.68361
C	-6.04969	-0.78772	-0.75903
C	-6.78536	0.20689	-1.41452
C	-6.67357	-2.01613	-0.51439
C	-8.10019	-0.01521	-1.81401
H	-6.30181	1.1614	-1.60437
C	-7.98848	-2.24902	-0.91038
H	-6.10968	-2.7929	-0.00429
C	-8.70371	-1.2463	-1.56185
H	-8.65724	0.76749	-2.32176
H	-8.45786	-3.20893	-0.71251
H	-9.72989	-1.42365	-1.87258
C	-1.89312	-2.44449	1.61763
C	-2.42902	-3.73814	1.63702
C	-0.68769	-2.22084	2.2965
C	-1.78497	-4.7767	2.3041
H	-3.36645	-3.91814	1.11726
C	-0.04181	-3.24901	2.97995
H	-0.26698	-1.2159	2.30271
C	-0.59076	-4.53023	2.97841
H	-2.2133	-5.77549	2.30412
H	0.88123	-3.05376	3.51638
H	-0.08607	-5.33466	3.50688
O	-1.88758	0.76003	-1.55694
C	-0.51206	0.96674	-1.59323
C	0.1893	-0.27527	-1.00246
H	-0.2277	1.84446	-0.99149
H	0.35618	-0.1999	0.07211
H	-0.44303	-1.1459	-1.18299
C	-0.10214	1.21231	-3.04077
H	0.96112	1.45308	-3.12542
H	-0.3248	0.33173	-3.65626
H	-0.6944	2.04592	-3.42376

Path B:

I



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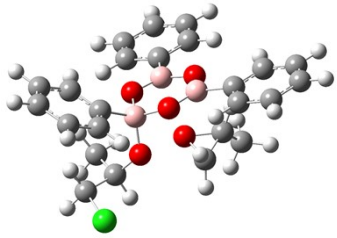
B	1.20143	1.37809	-0.01489
O	-0.12455	1.26947	0.04994
O	2.05024	0.27227	-0.04769
B	-0.83883	-0.02793	-0.00149
B	1.4625	-0.98381	0.02935
O	0.14098	-1.16192	0.09546
C	-1.88869	-0.13565	1.23775
C	-2.93187	0.79554	1.34553
C	-1.81428	-1.12344	2.22562
C	-3.85148	0.75041	2.38947
H	-3.01961	1.56455	0.58125
C	-2.72904	-1.18264	3.27806
H	-1.01601	-1.8597	2.1616
C	-3.75209	-0.24283	3.36386
H	-4.65071	1.48581	2.44534
H	-2.64479	-1.96263	4.03164
H	-4.46849	-0.28368	4.18068
C	2.43062	-2.23647	0.04759
C	1.91121	-3.52973	0.1809
C	3.81798	-2.0939	-0.06759
C	2.74493	-4.64481	0.19663
H	0.83416	-3.64439	0.27682
C	4.66143	-3.20223	-0.05434
H	4.22942	-1.09295	-0.16874
C	4.12404	-4.48111	0.07784
H	2.32421	-5.64115	0.30186
H	5.73653	-3.07282	-0.14604
H	4.77862	-5.34858	0.08918
C	1.88122	2.80644	-0.04257
C	3.27089	2.96262	-0.0912
C	1.08854	3.96027	-0.0198
C	3.85486	4.22709	-0.11637
H	3.8934	2.07162	-0.10885
C	1.66172	5.22864	-0.04451

H	0.00924	3.83914	0.01736
C	3.04847	5.36322	-0.09297
H	4.93613	4.33023	-0.15398
H	1.03166	6.11383	-0.02649
H	3.49972	6.3518	-0.11243
O	-1.50956	-0.04648	-1.30404
C	-2.3184	-1.12688	-1.62744
H	-2.84159	-1.52008	-0.73931
C	-3.3619	-0.65975	-2.63497
H	-3.93931	-1.49588	-3.03367
H	-2.86148	-0.12807	-3.4464
C	-1.5152	-2.26114	-2.27941
H	-1.02398	-1.89015	-3.18556
H	-0.74109	-2.59047	-1.58577
H	-2.1535	-3.11174	-2.54403
Cl	-4.55839	0.49087	-1.93419

II

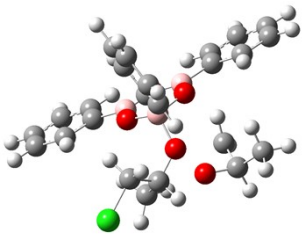


Charge = −1 Multiplicity = 1

B	0.75833	1.54145	-0.58554
O	-0.55878	1.36823	-0.47046
O	1.65361	0.48106	-0.69556
B	-1.15193	0.01458	-0.28533
B	1.12106	-0.80701	-0.77381
O	-0.19562	-1.03259	-0.74291
C	-2.52855	-0.10686	-1.14072
C	-3.53267	0.86172	-0.99183
C	-2.8	-1.18012	-1.9966
C	-4.75445	0.75804	-1.65092
H	-3.34667	1.70207	-0.32645
C	-4.02062	-1.29815	-2.66355
H	-2.02914	-1.9355	-2.13558
C	-5.00472	-0.32901	-2.4895
H	-5.51761	1.51951	-1.50923
H	-4.20512	-2.14611	-3.31935
H	-5.95889	-0.41702	-3.00289
C	2.14111	-1.99498	-0.99289

C	1.67957	-3.31453	-1.05855
C	3.51974	-1.7756	-1.08854
C	2.56116	-4.38065	-1.21389
H	0.60903	-3.48831	-0.97923
C	4.41181	-2.835	-1.24112
H	3.8884	-0.75317	-1.04408
C	3.93153	-4.14146	-1.30425
H	2.18489	-5.39909	-1.26111
H	5.4797	-2.64569	-1.31306
H	4.62325	-4.97117	-1.42375
C	1.37864	2.99733	-0.5845
C	2.75501	3.20874	-0.72369
C	0.55234	4.11662	-0.42858
C	3.29364	4.49334	-0.70954
H	3.4031	2.34433	-0.8475
C	1.07991	5.40485	-0.41384
H	-0.51623	3.95302	-0.31704
C	2.45398	5.59434	-0.55443
H	4.36495	4.63934	-0.81941
H	0.42441	6.26282	-0.29148
H	2.86944	6.59856	-0.54266
O	1.60016	-1.12896	1.8673
C	2.67217	-0.2242	2.09953
C	1.31187	0.07604	2.56704
H	3.00748	0.28611	1.19736
H	0.66402	0.76646	2.03318
H	1.08346	-0.06142	3.62452
C	3.74234	-0.72632	3.02999
H	3.28938	-1.21401	3.89738
H	4.37348	-1.45664	2.51488
H	4.37678	0.09503	3.37657
O	-1.36446	-0.07318	1.16915
C	-1.93297	-1.15794	1.82283
H	-1.63378	-1.07686	2.88104
C	-3.46449	-1.1295	1.80117
H	-3.84776	-1.1449	0.78057
Cl	-4.12803	0.3622	2.57094
H	-3.87281	-1.96933	2.36764
C	-1.47608	-2.53393	1.32083
H	-1.85499	-3.32151	1.98242
H	-1.83586	-2.7186	0.30414
H	-0.38485	-2.56365	1.30365

TS1



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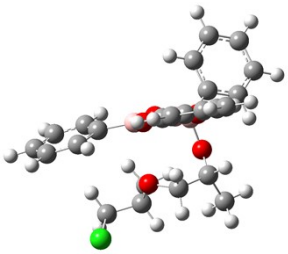
B	-1.68715	1.281	0.04951
O	-0.36354	1.33959	0.23168
O	-2.38121	0.07582	0.00901
B	0.49374	0.13136	0.3259
B	-1.65364	-1.09591	0.17067
O	-0.32689	-1.09492	0.3644
C	1.40444	0.22331	1.66851
C	2.75663	0.59597	1.69331
C	0.7925	-0.04322	2.90195
C	3.45601	0.69918	2.89756
H	3.27603	0.79785	0.75497
C	1.48108	0.0578	4.1072
H	-0.25303	-0.34755	2.91344
C	2.8235	0.43299	4.10811
H	4.50484	0.98573	2.88606
H	0.97548	-0.15884	5.04518
H	3.37021	0.51191	5.04441
C	-2.44026	-2.46203	0.11934
C	-1.7584	-3.67628	0.26653
C	-3.82509	-2.50163	-0.07978
C	-2.43455	-4.89217	0.21446
H	-0.68276	-3.65069	0.42373
C	-4.51077	-3.71228	-0.1313
H	-4.36129	-1.5632	-0.19493
C	-3.81378	-4.91019	0.01541
H	-1.88978	-5.825	0.32801
H	-5.58602	-3.72596	-0.28692
H	-4.34508	-5.85715	-0.02606
C	-2.52165	2.60846	-0.13348
C	-3.90522	2.58304	-0.34217
C	-1.88201	3.85335	-0.09853
C	-4.63024	3.76004	-0.51096
H	-4.40933	1.62054	-0.37137
C	-2.59723	5.0357	-0.26582
H	-0.80775	3.87677	0.06564
C	-3.9749	4.98914	-0.47275

H	-5.70408	3.72277	-0.67233
H	-2.08544	5.9935	-0.23505
H	-4.53697	5.90981	-0.6039
O	1.28154	0.14862	-0.95797
C	1.81295	-0.98681	-1.62192
H	2.53994	-0.58412	-2.33206
C	2.60585	-1.8205	-0.62248
H	3.42293	-1.21935	-0.22897
Cl	3.35516	-3.26266	-1.42652
H	1.97028	-2.2011	0.17843
C	0.72269	-1.76138	-2.36001
H	1.17026	-2.43613	-3.09382
H	0.10655	-2.34744	-1.67506
H	0.07836	-1.05075	-2.88565
H	1.11934	2.0024	-1.92175
C	2.03726	1.97133	-1.34453
C	3.37531	2.10087	-1.93144
O	3.81759	0.94025	-1.352
H	1.93505	2.24249	-0.29892
H	3.33907	2.07949	-3.04351
C	4.15058	3.34387	-1.49199
H	3.77758	4.27055	-1.94425
H	4.10655	3.42796	-0.40146
H	5.19855	3.20236	-1.7757

III



Charge = −1 Multiplicity = 1

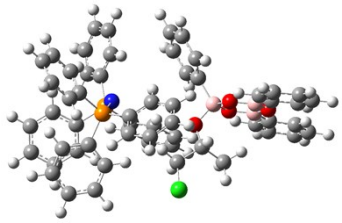
B	1.25466	1.38118	-0.46357
O	0.00911	1.22033	-1.05451
O	1.93603	0.36792	0.08057
B	-0.47642	-0.08261	-1.17207
B	1.38841	-1.02122	0.14011
O	0.24055	-1.14854	-0.80526
C	-1.90998	-0.25975	-1.81841
C	-2.79721	0.81911	-1.9079
C	-2.36739	-1.52307	-2.21131
C	-4.10415	0.6434	-2.3577

H	-2.45471	1.79972	-1.58877
C	-3.66948	-1.70914	-2.67148
H	-1.68365	-2.36511	-2.13109
C	-4.54264	-0.62413	-2.73902
H	-4.78587	1.48834	-2.39915
H	-4.00894	-2.69784	-2.96859
H	-5.56297	-0.76632	-3.08488
C	2.54069	-2.08606	-0.28203
C	2.79018	-2.39402	-1.62509
C	3.35662	-2.70511	0.67147
C	3.807	-3.26769	-2.00489
H	2.15786	-1.94071	-2.3858
C	4.37841	-3.5818	0.30966
H	3.16579	-2.49546	1.72153
C	4.60918	-3.8656	-1.03461
H	3.97457	-3.48773	-3.05691
H	4.99459	-4.04909	1.07484
H	5.40313	-4.54987	-1.32364
C	1.84325	2.8489	-0.4049
C	3.09138	3.08611	0.18362
C	1.13633	3.94302	-0.91658
C	3.62047	4.37172	0.25674
H	3.63976	2.23676	0.5827
C	1.65617	5.23344	-0.84729
H	0.1654	3.76578	-1.3719
C	2.90122	5.44854	-0.25972
H	4.59136	4.53865	0.71547
H	1.09376	6.07221	-1.2487
H	3.31033	6.45387	-0.20368
O	0.94794	-1.31743	1.51218
C	0.64986	-0.3344	2.45212
C	-0.5497	0.58189	2.07948
H	1.50219	0.35685	2.57478
H	-0.19278	1.45694	1.5299
H	-1.02582	0.95272	3.00294
C	0.43199	-1.046	3.78816
H	-0.41805	-1.73357	3.73055
H	1.31964	-1.6355	4.03179
H	0.24758	-0.33198	4.59771
O	-1.52763	0.01968	1.23326
C	-2.39162	-0.9477	1.78587
H	-2.40606	-0.84361	2.88252
C	-3.78645	-0.66229	1.25101
H	-3.76916	-0.61976	0.16

Cl	-4.41545	0.92762	1.82316
H	-4.49559	-1.42021	1.58713
C	-1.98458	-2.36402	1.38656
H	-2.59975	-3.10384	1.91049
H	-2.11164	-2.48829	0.30753
H	-0.92669	-2.51715	1.60473

Path C:

I



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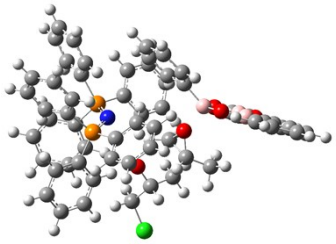
P	-2.79839	-1.48096	0.09378
C	-3.99356	-2.24866	1.22042
C	-4.40317	-3.57323	1.03062
C	-4.49673	-1.5066	2.28955
C	-5.32442	-4.14344	1.90046
H	-4.00217	-4.1583	0.20713
C	-5.41804	-2.0845	3.16049
H	-4.14961	-0.48863	2.4447
C	-5.83277	-3.39783	2.96419
H	-5.64217	-5.17016	1.75382
H	-5.8045	-1.50954	3.99535
H	-6.54859	-3.84742	3.64461
C	-1.31406	-2.49066	0.01955
C	-1.28052	-3.62917	-0.80128
C	-0.18382	-2.09515	0.73809
C	-0.1111	-4.36999	-0.89501
H	-2.14478	-3.90599	-1.39916
C	0.98869	-2.84223	0.62804
H	-0.1898	-1.18384	1.33187
C	1.02194	-3.97188	-0.18207
H	-0.06936	-5.23371	-1.54957
H	1.89139	-2.49327	1.11879
H	1.94765	-4.52922	-0.28671
C	-3.53334	-1.52668	-1.56517
C	-2.69202	-1.28832	-2.65976

C	-4.90464	-1.70587	-1.76209
C	-3.22082	-1.24692	-3.94484
H	-1.62502	-1.14555	-2.50881
C	-5.42739	-1.66248	-3.05202
H	-5.56181	-1.87527	-0.91432
C	-4.58772	-1.43878	-4.14011
H	-2.5617	-1.07891	-4.78997
H	-6.49278	-1.801	-3.2046
H	-4.99876	-1.41446	-5.14441
C	-3.17653	2.35868	1.77374
C	-3.93264	3.53605	1.78793
C	-2.60043	1.87547	2.95088
C	-4.11451	4.22437	2.98159
H	-4.39262	3.9048	0.87489
C	-2.78764	2.57224	4.14247
H	-1.99618	0.97298	2.92665
C	-3.54175	3.74169	4.15797
H	-4.70414	5.1348	2.99574
H	-2.33401	2.20039	5.05527
H	-3.684	4.28203	5.08825
C	-4.3965	1.57712	-0.73467
C	-5.61771	1.35876	-0.08515
C	-4.36567	1.74898	-2.12156
C	-6.79938	1.32875	-0.81776
H	-5.64347	1.22149	0.99302
C	-5.55213	1.71983	-2.84884
H	-3.41834	1.90098	-2.62998
C	-6.76608	1.51397	-2.19859
H	-7.74511	1.16744	-0.31119
H	-5.52495	1.85079	-3.92554
H	-7.68919	1.49473	-2.76914
C	-1.56819	2.31726	-0.68546
C	-1.78731	3.60723	-1.19292
C	-0.31678	1.71195	-0.80186
C	-0.75053	4.27899	-1.82422
H	-2.76245	4.07973	-1.10074
C	0.72709	2.40323	-1.42162
H	-0.11868	0.72417	-0.39177
C	0.50706	3.67801	-1.93101
H	-0.91587	5.27457	-2.2226
H	1.708	1.93545	-1.44559
H	1.32199	4.2153	-2.40628
O	1.96766	-0.28346	-0.57313
C	2.4003	-1.03999	-1.6717

H	2.77374	-2.0231	-1.34262
C	1.11186	-1.25996	-2.46278
H	0.35562	-1.66893	-1.79403
H	0.76554	-0.31472	-2.89083
C	3.47822	-0.36797	-2.51897
H	4.42745	-0.32088	-1.98213
H	3.64114	-0.93292	-3.44115
H	3.17987	0.65376	-2.77583
Cl	1.27817	-2.43127	-3.82133
B	2.928	0.08972	0.4888
O	3.86062	-1.03669	0.7172
O	3.65193	1.31239	0.05734
B	4.98554	1.37171	-0.06018
B	5.19545	-0.91879	0.59788
O	5.79528	0.27343	0.21594
C	6.1228	-2.16142	0.87001
C	7.51412	-2.07485	0.74596
C	5.56832	-3.39209	1.24168
C	8.32772	-3.17916	0.98504
H	7.95374	-1.1237	0.45801
C	6.37202	-4.50212	1.48286
H	4.48766	-3.4653	1.34157
C	7.75574	-4.39487	1.35392
H	9.4059	-3.09556	0.8851
H	5.92633	-5.44963	1.77168
H	8.38759	-5.25825	1.5414
C	5.67402	2.69481	-0.56385
C	4.89866	3.8298	-0.83183
C	7.05588	2.77471	-0.76874
C	5.48084	5.00788	-1.28944
H	3.82499	3.77258	-0.66666
C	7.6481	3.9483	-1.22807
H	7.66567	1.89897	-0.56299
C	6.85929	5.06673	-1.48897
H	4.86699	5.88171	-1.48921
H	8.72211	3.99462	-1.38272
H	7.31833	5.98411	-1.84616
C	2.09312	0.41646	1.84855
C	2.03142	-0.4767	2.92618
C	1.41305	1.63447	2.00016
C	1.29234	-0.1989	4.07698
H	2.60183	-1.40175	2.87187
C	0.67976	1.93358	3.14617
H	1.49243	2.37774	1.21086

C	0.60678	1.00793	4.18782
H	1.26909	-0.91387	4.89511
H	0.17537	2.89291	3.23574
H	0.04803	1.23925	5.09176

II



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C	-3.84255	-2.3379	-0.78938
C	-3.50507	-3.69145	-0.72206
C	-5.10466	-1.91249	-0.35623
C	-4.41957	-4.60924	-0.20941
H	-2.52575	-4.02435	-1.05383
C	-6.01337	-2.83164	0.15407
H	-5.37094	-0.85946	-0.41682
C	-5.66779	-4.18005	0.23302
H	-4.1545	-5.66006	-0.15614
H	-6.98799	-2.49704	0.4939
H	-6.37534	-4.89712	0.63669
C	-1.2409	-1.9474	-2.04874
C	-1.32537	-2.20691	-3.42256
C	-0.1342	-2.37285	-1.31098
C	-0.2962	-2.89182	-4.05554
H	-2.18056	-1.85768	-3.99402
C	0.90085	-3.04459	-1.96015
H	-0.06293	-2.14981	-0.24764
C	0.81787	-3.30495	-3.32423
H	-0.35371	-3.08765	-5.12105
H	1.77863	-3.33404	-1.39256
H	1.63006	-3.82245	-3.82488
C	-3.33239	0.00833	-2.4478
C	-2.63515	1.17851	-2.77826
C	-4.47746	-0.36949	-3.16041
C	-3.10921	1.96121	-3.82932
H	-1.74452	1.51165	-2.21854

C	-4.94102	0.43243	-4.19849
H	-5.0019	-1.28796	-2.91694
C	-4.25432	1.59666	-4.53336
H	-2.56953	2.86207	-4.10454
H	-5.83121	0.14325	-4.74725
H	-4.60986	2.21781	-5.34966
C	-3.49795	-0.8119	2.4463
C	-4.38198	-0.38354	3.44465
C	-3.16974	-2.16641	2.34925
C	-4.96458	-1.30991	4.30368
H	-4.60873	0.67341	3.55707
C	-3.75787	-3.09056	3.20826
H	-2.44458	-2.49162	1.61017
C	-4.66089	-2.66459	4.17819
H	-5.65154	-0.97362	5.07307
H	-3.50704	-4.1424	3.11575
H	-5.12027	-3.38532	4.84701
C	-3.88152	1.58006	0.75877
C	-5.25968	1.42639	0.95548
C	-3.39768	2.6391	-0.02355
C	-6.14893	2.33986	0.39686
H	-5.64736	0.59056	1.52854
C	-4.30033	3.54367	-0.57573
H	-2.33265	2.73566	-0.27149
C	-5.669	3.40316	-0.36294
H	-7.21554	2.21682	0.55401
H	-3.92308	4.35621	-1.18949
H	-6.3637	4.11371	-0.79952
C	-1.39025	1.16399	2.33979
C	-1.28215	0.88196	3.70793
C	-0.49531	2.05131	1.72867
C	-0.26933	1.46765	4.4608
H	-1.96596	0.19139	4.18969
C	0.50384	2.63965	2.50169
H	-0.53419	2.2754	0.64799
C	0.62711	2.34603	3.85764
H	-0.17853	1.22954	5.51522
H	1.19915	3.3252	2.02428
H	1.42492	2.79487	4.4423
O	-0.52171	2.55404	-1.1593
C	0.13159	3.61507	-1.71641
H	0.63813	3.36391	-2.67821
C	-0.92756	4.6791	-2.05028
H	-1.72809	4.22448	-2.63538

H	-1.34347	5.08987	-1.12553
C	1.19328	4.21924	-0.7863
H	1.91615	3.44733	-0.49954
H	1.73636	5.05253	-1.24238
H	0.70338	4.58094	0.12694
Cl	-0.31415	6.08582	-3.01792
H	0.24245	0.33437	-0.76742
C	1.28919	0.56528	-0.61974
C	2.26758	0.47865	-1.70798
O	2.17561	-0.58964	-0.71817
H	1.53998	1.20419	0.22163
H	1.90789	0.10265	-2.66358
C	3.50682	1.32506	-1.75248
H	4.37924	0.73707	-2.0513
H	3.35315	2.11147	-2.49662
H	3.70106	1.8057	-0.79236
B	3.17502	-1.06932	0.52824
O	4.21094	-1.78394	-0.15653
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B	4.86769	0.58398	1.10753
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O	5.83964	-0.15037	0.45112
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C	7.91454	-1.67113	-1.00806
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C	7.24809	-4.04034	-2.30788
H	5.25199	-3.68564	-1.57948
C	8.55846	-3.56701	-2.34847
H	9.91394	-2.01367	-1.73039
H	6.98972	-4.96528	-2.81456
H	9.3197	-4.12331	-2.88735
C	5.22517	1.97792	1.71882
C	4.22745	2.72346	2.36013
C	6.50647	2.53026	1.61147
C	4.49603	3.98663	2.87697
H	3.2347	2.28915	2.44825
C	6.78476	3.79198	2.12945
H	7.28576	1.95994	1.11305
C	5.77828	4.52098	2.76029
H	3.71231	4.55771	3.36703
H	7.78213	4.21135	2.04006
H	5.99325	5.50746	3.15999

C	2.15085	-1.97276	1.35962
C	2.15796	-3.3675	1.24553
C	1.15864	-1.38603	2.15827
C	1.19116	-4.15511	1.86878
H	2.941	-3.83778	0.6545
C	0.19276	-2.16518	2.79153
H	1.14446	-0.30437	2.29026
C	0.19859	-3.55124	2.63683
H	1.21508	-5.23576	1.76135
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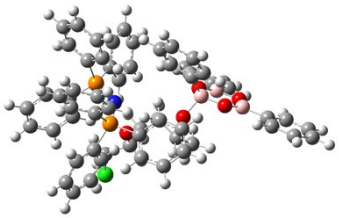
TS1



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C	-3.78334	-3.57284	-0.72151
C	-5.21333	-1.64197	-0.42856
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H	-2.83141	-4.00343	-1.01845
C	-6.21981	-2.46074	0.06907
H	-5.37507	-0.56924	-0.50774
C	-6.0082	-3.8345	0.17776
H	-4.63471	-5.45951	-0.1454
H	-7.16602	-2.02798	0.37687
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C	-1.30009	-2.09178	-1.95398
C	-1.40361	-2.45945	-3.30351
C	-0.22013	-2.51551	-1.17893
C	-0.41896	-3.25357	-3.87292
H	-2.23894	-2.1101	-3.90437
C	0.77537	-3.29458	-1.76944
H	-0.12907	-2.20997	-0.13835
C	0.67304	-3.66453	-3.10508
H	-0.48966	-3.53603	-4.91801

H	1.6378	-3.5787	-1.17665
H	1.45437	-4.26565	-3.55917
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C	-2.26896	1.07198	-2.88393
C	-4.34011	-0.15667	-3.22322
C	-2.59553	1.88402	-3.966
H	-1.35037	1.28018	-2.32202
C	-4.66034	0.67705	-4.29181
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H	-1.909	2.66825	-4.26947
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C	-1.3652	0.87111	3.71043
C	-0.51745	2.09258	1.79267
C	-0.37248	1.4319	4.50814
H	-2.06459	0.16986	4.15229
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H	-0.31164	1.16161	5.55684

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H	1.32564	2.75244	4.57576
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H	1.17262	3.24232	-2.58618
C	-0.48118	4.48438	-2.04459
H	-1.22432	4.00022	-2.67946
H	-0.969	4.86684	-1.14309
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O	2.03594	-0.73008	-0.68491
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H	1.62148	-0.08314	-2.60428
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H	4.12892	0.4077	-2.21689
H	3.16935	1.82746	-2.67453
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B	4.74636	0.57453	1.07295
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C	7.85984	-1.75589	-0.85293
C	6.23179	-3.40004	-1.505
C	8.85986	-2.48914	-1.48527
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H	5.20169	-3.74722	-1.50798
C	8.54135	-3.68285	-2.12948
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C	4.10972	2.7113	2.33841
C	6.36924	2.5529	1.53203
C	4.36897	3.98112	2.84396

H	3.12954	2.25625	2.45518
C	6.63888	3.82287	2.03564
H	7.1453	1.9924	1.01763
C	5.63761	4.53831	2.68964
H	3.58965	4.53945	3.35615
H	7.62627	4.25881	1.91771
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C	2.10044	-1.99497	1.41028
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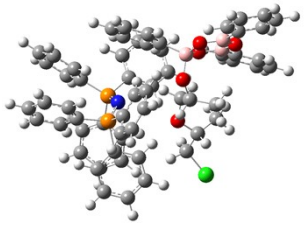
III



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C	-3.72735	-3.47085	-1.28833
C	-5.13491	-1.6424	-0.56423
C	-4.72916	-4.37161	-0.93301
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C	-6.13295	-2.54415	-0.21625
H	-5.2921	-0.57941	-0.4013
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H	-4.56831	-5.43513	-1.07448
H	-7.06486	-2.182	0.20527
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C	-1.25792	-1.82729	-2.2364
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C	-0.09658	-2.23035	-1.58357
C	-0.51156	-2.83895	-4.28826
H	-2.37713	-1.78822	-4.09398
C	0.87532	-2.9297	-2.30376
H	0.07432	-1.97839	-0.53979
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H	-0.66343	-3.07198	-5.33701
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C	-4.38809	0.52745	-2.91509
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H	-1.06797	1.1891	-2.48818
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C	-4.48981	-0.72056	3.28973
C	-3.29124	-2.40545	2.02849
C	-5.14916	-1.72116	3.99631
H	-4.66853	0.32173	3.54026
C	-3.95368	-3.40177	2.73936
H	-2.53438	-2.66784	1.29535
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H	-5.85616	-1.45514	4.7749
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C	-1.39971	0.46458	3.81816

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8. References.

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Wallingford CT, 2016.